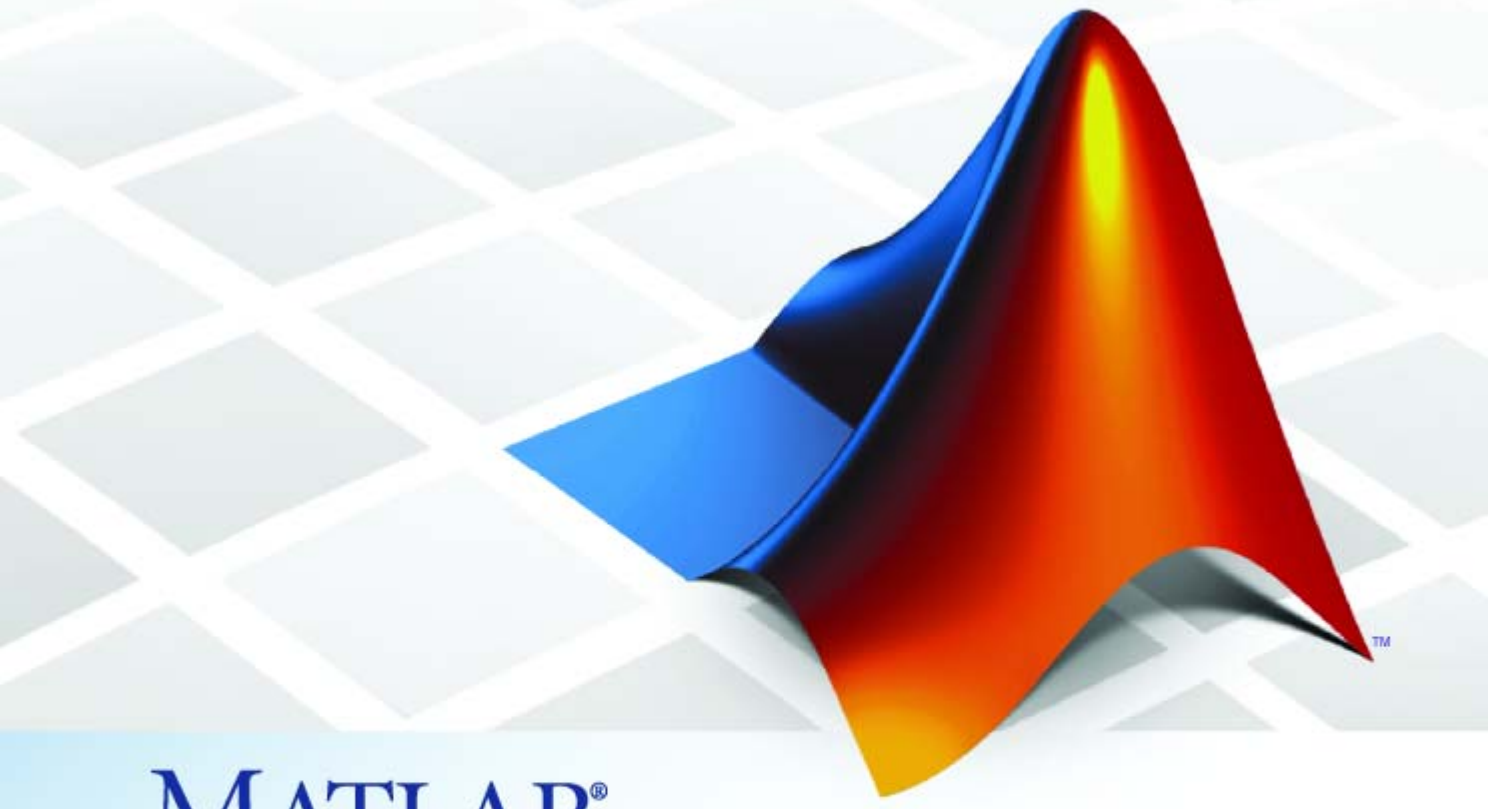
Bioinformatics Toolbox™ 3
Reference



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508-647-7000 (Phone)

508-647-7001 (Fax)

The MathWorks, Inc.
3 Apple Hill Drive
Natick, MA 01760-2098

For contact information about worldwide offices, see the MathWorks Web site.

Bioinformatics Toolbox™ Reference

Revision History

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September 2009	Online only	Revised for Version 3.4 (Release 2009b)

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Function Reference

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Phylogenetic Tree Tools (p. 1-15)	Read phylogenetic tree files, calculate pairwise distances between sequences, and build a phylogenetic tree
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Statistical Learning (p. 1-33)	Classify and identify features in data sets, set up cross-validation experiments, and compare different classification methods
Mass Spectrometry (p. 1-34)	Read data from common mass spectrometry file formats, preprocess raw mass spectrometry data from instruments, and analyze spectra to identify patterns and compounds
Bioanalytics (p. 1-36)	Read, process, and analyze data from any separation technique that produces signal data, such as spectroscopy, NMR, electrophoresis, or chromatography

Constructor

biograph	Create
clustergram	Compute hierarchical clustering, display dendrogram and heat map, and create
DataMatrix	Create
geneont	Create geneont object and term objects
HeatMap	Display heat map of matrix data and create
phytree	Create

Data Formats and Databases

affyprobeseqread	Read data file containing probe sequence information for Affymetrix GeneChip array
affyread	Read microarray data from Affymetrix GeneChip file
affysnpannotread	Read Affymetrix Mapping DNA array data from CSV-format annotation file
agferead	Read Agilent® Feature Extraction Software file
blastformat	Create local BLAST database
blastread	Read data from NCBI BLAST report file
blastreadlocal	Read data from local BLAST report
celintensityread	Read probe intensities from Affymetrix CEL files
cytobandread	Read cytogenetic banding information
emblread	Read data from EMBL file
fastainfo	Return information about FASTA file
fastaread	Read data from FASTA file
fastawrite	Write to file using FASTA format
fastqinfo	Return information about FASTQ file
fastqread	Read data from FASTQ file
fastqwrite	Write to file using FASTQ format
galread	Read microarray data from GenePix array list file
genbankread	Read data from GenBank® file

genpeptread	Read data from GenPept file
geoseriesread	Read Gene Expression Omnibus (GEO) Series (GSE) format data
geosoftread	Read Gene Expression Omnibus (GEO) SOFT format data
getblast	Retrieve BLAST report from NCBI Web site
getembl	Retrieve sequence information from EMBL database
getgenbank	Retrieve sequence information from GenBank database
getgenpept	Retrieve sequence information from GenPept database
getgeodata	Retrieve Gene Expression Omnibus (GEO) format data
gethmmalignment	Retrieve multiple sequence alignment associated with hidden Markov model (HMM) profile from PFAM database
gethmmprof	Retrieve hidden Markov model (HMM) profile from PFAM database
gethmmtree	Retrieve phylogenetic tree data from PFAM database
getpdb	Retrieve protein structure data from Protein Data Bank (PDB) database
goannotread	Read annotations from Gene Ontology annotated file
gprread	Read microarray data from GenePix Results (GPR) file
ilmnbsread	Read gene expression data exported from Illumina® BeadStudio™ software

imageneread	Read microarray data from ImaGene Results file
jcampread	Read JCAMP-DX-formatted files
multialignread	Read multiple sequence alignment file
multialignwrite	Write multiple alignment to file
mzcdfinfo	Return information about netCDF file containing mass spectrometry data
mzcdfread	Read mass spectrometry data from netCDF file
mzxmlinfo	Return information about mzXML file
mzxmlread	Read data from mzXML file
pdbread	Read data from Protein Data Bank (PDB) file
pdbwrite	Write to file using Protein Data Bank (PDB) format
pfamhmmread	Read data from PFAM HMM-formatted file
phytreeread	Read phylogenetic tree file
phytreewrite	Write phylogenetic tree object to Newick-formatted file
scfread	Read trace data from SCF file
sffinfo	Return information about SFF file
sffread	Read data from SFF file
sptread	Read data from SPOT file
tgspcinfo	Return information about SPC file
tgspcread	Read data from SPC file

Data Visualization

cghfreqplot	Display frequency of DNA copy number alterations across multiple samples
clustergram	Compute hierarchical clustering, display dendrogram and heat map, and create
featuresmap	Draw linear or circular map of features from GenBank structure
HeatMap	Display heat map of matrix data and create
maboxplot	Create box plot for microarray data
maimage	Spatial image for microarray data
mairplot	Create intensity versus ratio scatter plot of microarray data
maloglog	Create loglog plot of microarray data
mapcaplot	Create Principal Component Analysis (PCA) plot of microarray data
mavolcanoplot	Create significance versus gene expression ratio (fold change) scatter plot of microarray data
microplateplot	Display visualization of microtiter plate
molviewer	Display and manipulate 3-D molecule structure
msdotplot	Plot set of peak lists from LC/MS or GC/MS data set
msheatmap	Create pseudocolor image of set of mass spectra
msviewer	Explore mass spectrum or set of mass spectra

multialignviewer	Display and interactively adjust multiple sequence alignment
ntdensity	Plot density of nucleotides along sequence
pdbdistplot	Visualize intermolecular distances in Protein Data Bank (PDB) file
probesetplot	Plot Affymetrix probe set intensity values
proteinplot	Open Protein Plot window to investigate properties of amino acid sequence
proteinpropplot	Plot properties of amino acid sequence
ramachandran	Draw Ramachandran plot for Protein Data Bank (PDB) data
rnaplot	Draw secondary structure of RNA sequence
seqdotplot	Create dot plot of two sequences
seqtool	Open Sequence Tool window to interactively explore biological sequences
showalignment	Display color-coded sequence alignment
showhmmprof	Plot hidden Markov model (HMM) profile
traceplot	Draw nucleotide trace plots

Trace Tools

scfread	Read trace data from SCF file
traceplot	Draw nucleotide trace plots

Sequence Conversion

aa2int	Convert amino acid sequence from letter to integer representation
aa2nt	Convert amino acid sequence to nucleotide sequence
aminolookup	Find amino acid codes, integers, abbreviations, names, and codons
baselookup	Find nucleotide codes, integers, names, and complements
dna2rna	Convert DNA sequence to RNA sequence
int2aa	Convert amino acid sequence from integer to letter representation
int2nt	Convert nucleotide sequence from integer to letter representation
nt2aa	Convert nucleotide sequence to amino acid sequence
nt2int	Convert nucleotide sequence from letter to integer representation
rna2dna	Convert RNA sequence to DNA sequence
rnaconvert	Convert secondary structure of RNA sequence between bracket and matrix notations
seq2regexp	Convert sequence with ambiguous characters to regular expression
seqcomplement	Calculate complementary strand of nucleotide sequence
seqrcomplement	Calculate reverse complementary strand of nucleotide sequence
seqreverse	Calculate reverse strand of nucleotide sequence

Sequence Utilities

aminolookup	Find amino acid codes, integers, abbreviations, names, and codons
baselookup	Find nucleotide codes, integers, names, and complements
blastlocal	Perform search on local BLAST database to create BLAST report
blastncbi	Create remote NCBI BLAST report request ID or link to NCBI BLAST report
cleave	Cleave amino acid sequence with enzyme
cleavelookup	Find cleavage rule for enzyme or compound
featuresparse	Parse features from GenBank, GenPept, or EMBL data
geneticcode	Return nucleotide codon to amino acid mapping for genetic code
joinseq	Join two sequences to produce shortest supersequence
oligoprop	Calculate sequence properties of DNA oligonucleotide
palindromes	Find palindromes in sequence
pdbdistplot	Visualize intermolecular distances in Protein Data Bank (PDB) file
proteinplot	Open Protein Plot window to investigate properties of amino acid sequence
proteinpropplot	Plot properties of amino acid sequence
ramachandran	Draw Ramachandran plot for Protein Data Bank (PDB) data

randseq	Generate random sequence from finite alphabet
rebasecuts	Find restriction enzymes that cut nucleotide sequence
restrict	Split nucleotide sequence at restriction site
revgeneticcode	Return reverse mapping (amino acid to nucleotide codon) for genetic code
rnafold	Predict minimum free-energy secondary structure of RNA sequence
seqconsensus	Calculate consensus sequence
seqdisp	Format long sequence output for easy viewing
seqinsertgaps	Insert gaps into nucleotide or amino acid sequence
seqlogo	Display sequence logo for nucleotide or amino acid sequences
seqmatch	Find matches for every string in library
seqprofile	Calculate sequence profile from set of multiply aligned sequences
seqshoworfs	Display open reading frames in sequence

Sequence Statistics

aacount	Count amino acids in sequence
aminolookup	Find amino acid codes, integers, abbreviations, names, and codons
basecount	Count nucleotides in sequence

baselookup	Find nucleotide codes, integers, names, and complements
codonbias	Calculate codon frequency for each amino acid coded for in nucleotide sequence
codoncount	Count codons in nucleotide sequence
cpgisland	Locate CpG islands in DNA sequence
dimercount	Count dimers in nucleotide sequence
isoelectric	Estimate isoelectric point for amino acid sequence
molweight	Calculate molecular weight of amino acid sequence
nmercount	Count n-mers in nucleotide or amino acid sequence
ntdensity	Plot density of nucleotides along sequence
seqshowwords	Graphically display words in sequence
seqwordcount	Count number of occurrences of word in sequence

Sequence Visualization

featuresmap	Draw linear or circular map of features from GenBank structure
multialignviewer	Display and interactively adjust multiple sequence alignment
rnaplot	Draw secondary structure of RNA sequence
seqdotplot	Create dot plot of two sequences

seqtool	Open Sequence Tool window to interactively explore biological sequences
showalignment	Display color-coded sequence alignment

Pairwise Sequence Alignment

fastaread	Read data from FASTA file
localalign	Return local optimal and suboptimal alignments between two sequences
multialignviewer	Display and interactively adjust multiple sequence alignment
nwalign	Globally align two sequences using Needleman-Wunsch algorithm
seqdotplot	Create dot plot of two sequences
showalignment	Display color-coded sequence alignment
swalign	Locally align two sequences using Smith-Waterman algorithm

Multiple Sequence Alignment

fastaread	Read data from FASTA file
multialign	Align multiple sequences using progressive method
multialignread	Read multiple sequence alignment file

multialignviewer	Display and interactively adjust multiple sequence alignment
multialignwrite	Write multiple alignment to file
profalign	Align two profiles using Needleman-Wunsch global alignment
seqpdist	Calculate pairwise distance between sequences
showalignment	Display color-coded sequence alignment

Scoring Matrices

blosum	Return BLOSUM scoring matrix
dayhoff	Return Dayhoff scoring matrix
gonnet	Return Gonnet scoring matrix
nuc44	Return NUC44 scoring matrix for nucleotide sequences
pam	Return Point Accepted Mutation (PAM) scoring matrix

Phylogenetic Tree Tools

dnds	Estimate synonymous and nonsynonymous substitution rates
dndsml	Estimate synonymous and nonsynonymous substitution rates using maximum likelihood method

gethmmtree	Retrieve phylogenetic tree data from PFAM database
phytreeread	Read phylogenetic tree file
phytreetool	View, edit, and explore phylogenetic tree data
phytreewrite	Write phylogenetic tree object to Newick-formatted file
seqinsertgaps	Insert gaps into nucleotide or amino acid sequence
seqlinkage	Construct phylogenetic tree from pairwise distances
seqneighjoin	Neighbor-joining method for phylogenetic tree reconstruction
seqpdist	Calculate pairwise distance between sequences

Phylogenetic Tree Methods

Following are methods to use with a phytree object.

cluster (phytree)	Validate clusters in phylogenetic tree
get (phytree)	Retrieve information about phylogenetic tree object
getbyname (phytree)	Branches and leaves from phytree object
getcanonical (phytree)	Calculate canonical form of phylogenetic tree
getmatrix (phytree)	Convert phytree object into relationship matrix
getnewickstr (phytree)	Create Newick-formatted string

pdist (phytree)	Calculate pairwise patristic distances in phytree object
plot (phytree)	Draw phylogenetic tree
prune (phytree)	Remove branch nodes from phylogenetic tree
reorder (phytree)	Reorder leaves of phylogenetic tree
reroot (phytree)	Change root of phylogenetic tree
select (phytree)	Select tree branches and leaves in phytree object
subtree (phytree)	Extract phylogenetic subtree
view (phytree)	View phylogenetic tree
weights (phytree)	Calculate weights for phylogenetic tree

Graph Theory

graphallshortestpaths	Find all shortest paths in graph
graphconncomp	Find strongly or weakly connected components in graph
graphisdag	Test for cycles in directed graph
graphisomorphism	Find isomorphism between two graphs
graphisspantree	Determine if tree is spanning tree
graphmaxflow	Calculate maximum flow in directed graph
graphminspantree	Find minimal spanning tree in graph
graphpred2path	Convert predecessor indices to paths
graphshortestpath	Solve shortest path problem in graph

graphtopoorder	Perform topological sort of directed acyclic graph
graphtraverse	Traverse graph by following adjacent nodes

Graph Visualization Methods

Following are methods to use with a biograph object.

allshortestpaths (biograph)	Find all shortest paths in biograph object
conncomp (biograph)	Find strongly or weakly connected components in biograph object
dolayout (biograph)	Calculate node positions and edge trajectories
get (biograph)	Retrieve information about biograph object
getancestors (biograph)	Find ancestors in biograph object
getdescendants (biograph)	Find descendants in biograph object
getedgesbynodeid (biograph)	Get handles to edges in biograph object
getmatrix (biograph)	Get connection matrix from biograph object
getnodesbyid (biograph)	Get handles to nodes
getrelatives (biograph)	Find relatives in biograph object
isdag (biograph)	Test for cycles in biograph object
isomorphism (biograph)	Find isomorphism between two biograph objects
isspantree (biograph)	Determine if tree created from biograph object is spanning tree

maxflow (biograph)	Calculate maximum flow in biograph object
minspantree (biograph)	Find minimal spanning tree in biograph object
set (biograph)	Set property of biograph object
shortestpath (biograph)	Solve shortest path problem in biograph object
topoorder (biograph)	Perform topological sort of directed acyclic graph extracted from biograph object
traverse (biograph)	Traverse biograph object by following adjacent nodes
view (biograph)	Draw figure from biograph object

Gene Ontology

goannotread	Read annotations from Gene Ontology annotated file
num2goid	Convert numbers to Gene Ontology IDs

Gene Ontology Methods

Following are methods to use with a geneont object.

getancestors (geneont)	Find terms that are ancestors of specified Gene Ontology (GO) term
getdescendants (geneont)	Find terms that are descendants of specified Gene Ontology (GO) term

getmatrix (geneont)	Convert geneont object into relationship matrix
getrelatives (geneont)	Find terms that are relatives of specified Gene Ontology (GO) term

Protein Analysis

aacount	Count amino acids in sequence
aminolookup	Find amino acid codes, integers, abbreviations, names, and codons
atomiccomp	Calculate atomic composition of protein
cleave	Cleave amino acid sequence with enzyme
cleavelookup	Find cleavage rule for enzyme or compound
evalrasmolscript	Send RasMol script commands to Molecule Viewer window
isoelectric	Estimate isoelectric point for amino acid sequence
isotopicdist	Calculate high-resolution isotope mass distribution and density function
molviewer	Display and manipulate 3-D molecule structure
molweight	Calculate molecular weight of amino acid sequence
pdbdistplot	Visualize intermolecular distances in Protein Data Bank (PDB) file
pdbsuperpose	Superpose 3-D structures of two proteins

pdbtransform	Apply linear transformation to 3-D structure of molecule
proteinplot	Open Protein Plot window to investigate properties of amino acid sequence
proteinpropplot	Plot properties of amino acid sequence
ramachandran	Draw Ramachandran plot for Protein Data Bank (PDB) data

Profile Hidden Markov Models

gethmmalignment	Retrieve multiple sequence alignment associated with hidden Markov model (HMM) profile from PFAM database
gethmmprof	Retrieve hidden Markov model (HMM) profile from PFAM database
gethmmtree	Retrieve phylogenetic tree data from PFAM database
hmmprofalign	Align query sequence to profile using hidden Markov model alignment
hmmprofestimate	Estimate profile hidden Markov model (HMM) parameters using pseudocounts
hmmprofgenerate	Generate random sequence drawn from profile hidden Markov model (HMM)
hmmprofmerge	Concatenate prealigned strings of several sequences to profile hidden Markov model (HMM)

hmmprofstruct	Create or edit hidden Markov model (HMM) profile structure
pfamhmmread	Read data from PFAM HMM-formatted file
showhmmprof	Plot hidden Markov model (HMM) profile

Microarray File Formats

affyprobeseqread	Read data file containing probe sequence information for Affymetrix GeneChip array
affyread	Read microarray data from Affymetrix GeneChip file
affysnpannotread	Read Affymetrix Mapping DNA array data from CSV-format annotation file
agferead	Read Agilent Feature Extraction Software file
celintensityread	Read probe intensities from Affymetrix CEL files
galread	Read microarray data from GenePix array list file
geoseriesread	Read Gene Expression Omnibus (GEO) Series (GSE) format data
geosoftread	Read Gene Expression Omnibus (GEO) SOFT format data
getgeodata	Retrieve Gene Expression Omnibus (GEO) format data
gprread	Read microarray data from GenePix Results (GPR) file

ilmnbsread	Read gene expression data exported from Illumina BeadStudio software
imageneread	Read microarray data from ImaGene Results file
sptread	Read data from SPOT file

Microarray Utilities

affysnpintensitysplit	Split Affymetrix SNP probe intensity information for alleles A and B
affysnpquartets	Create table of SNP probe quartet results for Affymetrix probe set
ilmnbslookup	Look up Illumina BeadStudio target (probe) sequence and annotation information
magetfield	Extract data from microarray structure
probelibraryinfo	Create table of probe set library information
probesetlink	Display probe set information on NetAffx Web site
probesetlookup	Look up information for Affymetrix probe set
probesetplot	Plot Affymetrix probe set intensity values
probesetvalues	Create table of Affymetrix probe set intensity values

Microarray Data Analysis and Visualization

cghcbs	Perform circular binary segmentation (CBS) on array-based comparative genomic hybridization (aCGH) data
cghfreqplot	Display frequency of DNA copy number alterations across multiple samples
chromosomeplot	Plot chromosome ideogram with G-banding pattern
clustergram	Compute hierarchical clustering, display dendrogram and heat map, and create
HeatMap	Display heat map of matrix data and create
maboxplot	Create box plot for microarray data
mafdr	Estimate false discovery rate (FDR) of differentially expressed genes from two experimental conditions or phenotypes
maimage	Spatial image for microarray data
mairplot	Create intensity versus ratio scatter plot of microarray data
maloglog	Create loglog plot of microarray data
mapcaplot	Create Principal Component Analysis (PCA) plot of microarray data
mattest	Perform two-sample t-test to evaluate differential expression of genes from two experimental conditions or phenotypes

mavolcanoplot	Create significance versus gene expression ratio (fold change) scatter plot of microarray data
microplateplot	Display visualization of microtiter plate
probesetplot	Plot Affymetrix probe set intensity values
redbluecmap	Create red and blue colormap
redgreencmap	Create red and green colormap

Microarray Normalization and Filtering

affygcrma	Perform GC Robust Multi-array Average (GCRMA) procedure on Affymetrix microarray probe-level data
affyinvarsetnorm	Perform rank invariant set normalization on probe intensities from multiple Affymetrix CEL or DAT files
affyprobeaffinities	Compute Affymetrix probe affinities from their sequences and MM probe intensities
affyrma	Perform Robust Multi-array Average (RMA) procedure on Affymetrix microarray probe-level data
exprprofrange	Calculate range of gene expression profiles
exprprofvar	Calculate variance of gene expression profiles

gcrma	Perform GC Robust Multi-array Average (GCRMA) background adjustment, quantile normalization, and median-polish summarization on Affymetrix microarray probe-level data
gcrmabackadj	Perform GC Robust Multi-array Average (GCRMA) background adjustment on Affymetrix microarray probe-level data using sequence information
geneentropyfilter	Remove genes with low entropy expression values
genelowvalfilter	Remove gene profiles with low absolute values
generangefilter	Remove gene profiles with small profile ranges
genevarfilter	Filter genes with small profile variance
mainvarsetnorm	Perform rank invariant set normalization on gene expression values from two experimental conditions or phenotypes
malowess	Smooth microarray data using Lowess method
manorm	Normalize microarray data
quantilenorm	Quantile normalization over multiple arrays
rmabackadj	Perform background adjustment on Affymetrix microarray probe-level data using Robust Multi-array Average (RMA) procedure

rmasummary	Calculate gene expression values from Affymetrix microarray probe-level data using Robust Multi-array Average (RMA) procedure
zonebackadj	Perform background adjustment on Affymetrix microarray probe-level data using zone-based method

HeatMap Methods

Following are methods to use with a HeatMap object.

addTitle (HeatMap)	Add title to heat map
addXLabel (HeatMap)	Label *x*-axis of heat map
addYLabel (HeatMap)	Label *y*-axis of heat map
plot (HeatMap)	Render heat map for HeatMap object
view (HeatMap)	View heat map of HeatMap object

Clustergram Methods

Following are methods to use with a clustergram object.

addTitle (clustergram)	Add title to clustergram
addXLabel (clustergram)	Label *x*-axis of clustergram
addYLabel (clustergram)	Label *y*-axis of clustergram
clusterGroup (clustergram)	Select cluster group
get (clustergram)	Retrieve information about clustergram object

plot (clustergram)	Render clustergram and dendrograms for clustergram object
set (clustergram)	Set property of clustergram object
view (clustergram)	View clustergram and dendrograms of clustergram object

ExpressionSet Methods

Following are methods to use with an ExpressionSet object.

abstract (bioma.ExpressionSet)	Retrieve or set abstract describing experiment in ExpressionSet object
elementData (bioma.ExpressionSet)	Retrieve or set data element (DataMatrix object) in ExpressionSet object
elementNames (bioma.ExpressionSet)	Retrieve or set element names of DataMatrix objects in ExpressionSet object
expressions (bioma.ExpressionSet)	Retrieve or set `Expressions` DataMatrix object from ExpressionSet object
exprWrite (bioma.ExpressionSet)	Write expression values in ExpressionSet object to text file
exptData (bioma.ExpressionSet)	Retrieve or set experiment data in ExpressionSet object
exptInfo (bioma.ExpressionSet)	Retrieve or set experiment information in ExpressionSet object
featureData (bioma.ExpressionSet)	Retrieve or set feature metadata in ExpressionSet object

featureNames (bioma.ExpressionSet)	Retrieve or set feature names in ExpressionSet object
featureVarDesc (bioma.ExpressionSet)	Retrieve or set feature variable descriptions in ExpressionSet object
featureVarNames (bioma.ExpressionSet)	Retrieve or set feature variable names in ExpressionSet object
featureVarValues (bioma.ExpressionSet)	Retrieve or set feature variable data values in ExpressionSet object
pubMedID (bioma.ExpressionSet)	Retrieve or set PubMed IDs in ExpressionSet object
sampleData (bioma.ExpressionSet)	Retrieve or set sample metadata in ExpressionSet object
sampleNames (bioma.ExpressionSet)	Retrieve or set sample names in ExpressionSet object
sampleVarDesc (bioma.ExpressionSet)	Retrieve or set sample variable descriptions in ExpressionSet object
sampleVarNames (bioma.ExpressionSet)	Retrieve or set sample variable names in ExpressionSet object
sampleVarValues (bioma.ExpressionSet)	Retrieve or set sample variable values in ExpressionSet object
size (bioma.ExpressionSet)	Return size of ExpressionSet object

ExptData Methods

Following are methods to use with an ExptData object.

combine (bioma.data.ExptData)	Combine two ExptData objects
dmNames (bioma.data.ExptData)	Retrieve or set `Name` properties of DataMatrix objects in ExptData object

elementData (bioma.data.ExptData)	Retrieve or set data element (DataMatrix object) in ExptData object
elementNames (bioma.data.ExptData)	Retrieve or set element names of DataMatrix objects in ExptData object
featureNames (bioma.data.ExptData)	Retrieve or set feature names in ExptData object
isempty (bioma.data.ExptData)	Determine whether ExptData object is empty
sampleNames (bioma.data.ExptData)	Retrieve or set sample names in ExptData object
size (bioma.data.ExptData)	Return size of ExptData object

DataMatrix Methods

Following are methods to use with a DataMatrix object.

colnames (DataMatrix)	Retrieve or set column names of DataMatrix object
disp (DataMatrix)	Display DataMatrix object
dmarrayfun (DataMatrix)	Apply function to each element in DataMatrix object
dmbsxfun (DataMatrix)	Apply element-by-element binary operation to two DataMatrix objects with singleton expansion enabled
dmwrite (DataMatrix)	Write DataMatrix object to text file
double (DataMatrix)	Convert DataMatrix object to double-precision array
eq (DataMatrix)	Test DataMatrix objects for equality

ge (DataMatrix)	Test DataMatrix objects for greater than or equal to
get (DataMatrix)	Retrieve information about DataMatrix object
gt (DataMatrix)	Test DataMatrix objects for greater than
horzcat (DataMatrix)	Concatenate DataMatrix objects horizontally
isequal (DataMatrix)	Test DataMatrix objects for equality
isequalwithequalnans (DataMatrix)	Test DataMatrix objects for equality, treating NaNs as equal
ldivide (DataMatrix)	Left array divide DataMatrix objects
le (DataMatrix)	Test DataMatrix objects for less than or equal to
lt (DataMatrix)	Test DataMatrix objects for less than
max (DataMatrix)	Return maximum values in DataMatrix object
mean (DataMatrix)	Return average or mean values in DataMatrix object
median (DataMatrix)	Return median values in DataMatrix object
min (DataMatrix)	Return minimum values in DataMatrix object
minus (DataMatrix)	Subtract DataMatrix objects
ndims (DataMatrix)	Return number of dimensions in DataMatrix object
ne (DataMatrix)	Test DataMatrix objects for inequality
numel (DataMatrix)	Return number of elements in DataMatrix object
plot (DataMatrix)	Draw 2-D line plot of DataMatrix object

plus (DataMatrix)	Add DataMatrix objects
power (DataMatrix)	Array power DataMatrix objects
rdivide (DataMatrix)	Right array divide DataMatrix objects
rownames (DataMatrix)	Retrieve or set row names of DataMatrix object
set (DataMatrix)	Set property of DataMatrix object
single (DataMatrix)	Convert DataMatrix object to single-precision array
sortcols (DataMatrix)	Sort columns of DataMatrix object in ascending or descending order
sortrows (DataMatrix)	Sort rows of DataMatrix object in ascending or descending order
std (DataMatrix)	Return standard deviation values in DataMatrix object
sum (DataMatrix)	Return sum of elements in DataMatrix object
times (DataMatrix)	Multiply DataMatrix objects
var (DataMatrix)	Return variance values in DataMatrix object
vertcat (DataMatrix)	Concatenate DataMatrix objects vertically

MetaData Methods

Following are methods to use with a MetaData object.

combine (bioma.data.MetaData)	Combine two MetaData objects
isempty (bioma.data.MetaData)	Determine whether MetaData object is empty

sampleNames (bioma.data.MetaData)	Retrieve or set sample names in MetaData object
size (bioma.data.MetaData)	Return size of MetaData object
variableDesc (bioma.data.MetaData)	Retrieve or set variable descriptions for samples in MetaData object
variableNames (bioma.data.MetaData)	Retrieve or set variable names for samples in MetaData object
variableValues (bioma.data.MetaData)	Retrieve or set variable values for samples in MetaData object
varValuesTable (bioma.data.MetaData)	Create 2-D graphic table GUI of variable values in MetaData object

MIAME Methods

Following are methods to use with a MIAME object.

combine (bioma.data.MIAME)	Combine two MIAME objects
isempty (bioma.data.MIAME)	Determine whether MIAME object is empty

Statistical Learning

classperf	Evaluate performance of classifier
crossvalind	Generate cross-validation indices
knnclassify	Classify data using nearest neighbor method
knnimpute	Impute missing data using nearest-neighbor method

optimalleaforder	Determine optimal leaf ordering for hierarchical binary cluster tree
randfeatures	Generate randomized subset of features
rankfeatures	Rank key features by class separability criteria
svmclassify	Classify data using support vector machine
svmsmoset	Create or edit Sequential Minimal Optimization (SMO) options structure
svmtrain	Train support vector machine classifier

Mass Spectrometry

isotopicdist	Calculate high-resolution isotope mass distribution and density function
jcampread	Read JCAMP-DX-formatted files
msalign	Align peaks in signal to reference peaks
msbackadj	Correct baseline of signal with peaks
msdotplot	Plot set of peak lists from LC/MS or GC/MS data set
msheatmap	Create pseudocolor image of set of mass spectra
mslowess	Smooth signal with peaks using nonparametric method
msnorm	Normalize set of signals with peaks

mspalign	Align mass spectra from multiple peak lists from LC/MS or GC/MS data set
mspeaks	Convert raw peak data to peak list (centroided data)
msppresample	Resample signal with peaks while preserving peaks
msresample	Resample signal with peaks
mssgolay	Smooth signal with peaks using least-squares polynomial
msviewer	Explore mass spectrum or set of mass spectra
mzcdf2peaks	Convert mzCDF structure to peak list
mzcdfinfo	Return information about netCDF file containing mass spectrometry data
mzcdfread	Read mass spectrometry data from netCDF file
mzxml2peaks	Convert mzXML structure to peak list
mzxmlinfo	Return information about mzXML file
mzxmlread	Read data from mzXML file
samplealign	Align two data sets containing sequential observations by introducing gaps
tgspcinfo	Return information about SPC file
tgspcread	Read data from SPC file

Bioanalytics

jcampread	Read JCAMP-DX-formatted files
msalign	Align peaks in signal to reference peaks
msbackadj	Correct baseline of signal with peaks
mslowess	Smooth signal with peaks using nonparametric method
msnorm	Normalize set of signals with peaks
mspeaks	Convert raw peak data to peak list (centroided data)
msppresample	Resample signal with peaks while preserving peaks
msresample	Resample signal with peaks
mssgolay	Smooth signal with peaks using least-squares polynomial
tgspcinfo	Return information about SPC file
tgspcread	Read data from SPC file

2

Class Reference

bioma.data.ExptData	Contain data values from microarray experiment
bioma.data.MetaData	Contain metadata from microarray experiment
bioma.data.MIAME	Contain experiment information from microarray gene expression experiment
bioma.ExpressionSet	Contain data from microarray gene expression experiment

3

Alphabetical List

Purpose

Convert amino acid sequence from letter to integer representation

Syntax

```
SeqInt = aa2int(SeqChar)
```

Arguments

SeqChar One of the following:

- String of single-letter codes specifying an amino acid sequence. For valid letter codes, see the table Mapping Amino Acid Letter Codes to Integers on page 3-2. Unknown characters are mapped to `0`. Integers are arbitrarily assigned to IUB/IUPAC letters.
- MATLAB structure containing a `Sequence` field that contains an amino acid sequence, such as returned by `fastaread`, `getgenpept`, `genpeptread`, `getpdb`, or `pdbread`.

Return Values

SeqInt Amino acid sequence specified by a row vector of integers.

Description

SeqInt = `aa2int(`*SeqChar*`)` converts *SeqChar*, a character string of single-letter codes specifying an amino acid sequence, to *SeqInt*, a row vector of integers specifying the same amino acid sequence. For valid letter codes, see the table Mapping Amino Acid Letter Codes to Integers on page 3-2.

Mapping Amino Acid Letter Codes to Integers

Amino Acid	Code	Integer
Alanine	A	1
Arginine	R	2
Asparagine	N	3

Mapping Amino Acid Letter Codes to Integers (Continued)

Amino Acid	Code	Integer
Aspartic acid (Aspartate)	D	4
Cysteine	C	5
Glutamine	Q	6
Glutamic acid (Glutamate)	E	7
Glycine	G	8
Histidine	H	9
Isoleucine	I	10
Leucine	L	11
Lysine	K	12
Methionine	M	13
Phenylalanine	F	14
Proline	P	15
Serine	S	16
Threonine	T	17
Tryptophan	W	18
Tyrosine	Y	19
Valine	V	20
Asparagine or Aspartic acid (Aspartate)	B	21
Glutamine or Glutamic acid (Glutamate)	Z	22
Unknown amino acid (any amino acid)	X	23
Translation stop	*	24

Mapping Amino Acid Letter Codes to Integers (Continued)

Amino Acid	Code	Integer
Gap of indeterminate length	-	25
Unknown character (any character or symbol not in table)	?	0

Examples

Converting a Simple Sequence

Convert the sequence of letters MATLAB to integers.

```
SeqInt = aa2int('MATLAB')

SeqInt =

   13    1   17   11    1   21
```

Converting a Random Sequence

1 Create a random string to represent an amino acid sequence.

```
SeqChar = randseq(20, 'alphabet', 'amino')

SeqChar =

   dwcztecakfuecvifchds
```

2 Convert the amino acid sequence from letter to integer representation.

```
SeqInt = aa2int(SeqChar)

SeqInt =

  Columns 1 through 13
     4  18   5  22  17   7   5   1  12  14   0   7   5

  Columns 14 through 20
```

```
    20   10   14    5    9    4   16
```

See Also

Bioinformatics Toolbox™ functions: `aminolookup`, `int2aa`, `int2nt`, `nt2int`

Purpose

Convert amino acid sequence to nucleotide sequence

Syntax

```
SeqNT = aa2nt(SeqAA)
SeqNT = aa2nt(SeqAA, ...'GeneticCode',
GeneticCodeValue, ...)
SeqNT = aa2nt(SeqAA, ...'Alphabet' AlphabetValue, ...)
```

Arguments

SeqAA

One of the following:

- String of single-letter codes specifying an amino acid sequence. For valid letter codes, see the table Mapping Amino Acid Letter Codes to Integers on page 3-2. Unknown characters are mapped to `0`.
- Row vector of integers specifying an amino acid sequence. For valid integers, see the table Mapping Amino Acid Integers to Letter Codes on page 3-805.
- MATLAB structure containing a `Sequence` field that contains an amino acid sequence, such as returned by `fastaread`, `getgenpept`, `genpeptread`, `getpdb`, or `pdbread`.

Examples: `'ARN'` or `[1 2 3]`

GeneticCodeValue

Integer or string specifying a genetic code number or code name from the table Genetic Code on page 3-8. Default is `1` or `'Standard'`.

Tip If you use a code name, you can truncate the name to the first two letters of the name.

AlphabetValue

String specifying a nucleotide alphabet. Choices are:

- `'DNA'` (default) — Uses the symbols `A`, `C`, `G`, and `T`.
- `'RNA'` — Uses the symbols `A`, `C`, `G`, and `U`.

Return Values

SeqNT	Nucleotide sequence specified by a character string of letter codes.

Description

SeqNT = aa2nt(*SeqAA*) converts an amino acid sequence, specified by *SeqAA*, to a nucleotide sequence, returned in *SeqNT*, using the standard genetic code.

In general, the mapping from an amino acid to a nucleotide codon is not a one-to-one mapping. For amino acids with multiple possible nucleotide codons, this function randomly selects a codon corresponding to that particular amino acid. For the ambiguous characters `B` and `Z`, one of the amino acids corresponding to the letter is selected randomly, and then a codon sequence is selected randomly. For the ambiguous character `X`, a codon sequence is selected randomly from all possibilities.

SeqNT = aa2nt(*SeqAA*, ...'*PropertyName*', *PropertyValue*, ...) calls `aa2nt` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

SeqNT = aa2nt(*SeqAA*, ...'GeneticCode', *GeneticCodeValue*, ...) specifies a genetic code to use when converting an amino acid sequence to a nucleotide sequence. *GeneticCodeValue* can be an integer or string specifying a code number or code name from the table Genetic Code on page 3-8. Default is `1` or `'Standard'`. The amino acid to nucleotide codon mapping for the Standard genetic code is shown in the table Standard Genetic Code on page 3-9.

Tip If you use a code name, you can truncate the name to the first two letters of the name.

SeqNT = aa2nt(*SeqAA*, ...'Alphabet' *AlphabetValue*, ...) specifies a nucleotide alphabet. *AlphabetValue* can be 'DNA', which uses the symbols A, C, G, and T, or 'RNA', which uses the symbols A, C, G, and U. Default is 'DNA'.

Genetic Code

Code Number	Code Name
1	Standard
2	Vertebrate Mitochondrial
3	Yeast Mitochondrial
4	Mold, Protozoan, Coelenterate Mitochondrial, and Mycoplasma/Spiroplasma
5	Invertebrate Mitochondrial
6	Ciliate, Dasycladacean, and Hexamita Nuclear
9	Echinoderm Mitochondrial
10	Euplotid Nuclear
11	Bacterial and Plant Plastid
12	Alternative Yeast Nuclear
13	Ascidian Mitochondrial
14	Flatworm Mitochondrial
15	Blepharisma Nuclear
16	Chlorophycean Mitochondrial
21	Trematode Mitochondrial

Genetic Code (Continued)

Code Number	Code Name
22	Scenedesmus Obliquus Mitochondrial
23	Thraustochytrium Mitochondrial

Standard Genetic Code

Amino Acid Name	Amino Acid Code	Nucleotide Codon
Alanine	A	GCT GCC GCA GCG
Arginine	R	CGT CGC CGA CGG AGA AGG
Asparagine	N	ATT AAC
Aspartic acid (Aspartate)	D	GAT GAC
Cysteine	C	TGT TGC
Glutamine	Q	CAA CAG
Glutamic acid (Glutamate)	E	GAA GAG
Glycine	G	GGT GGC GGA GGG
Histidine	H	CAT CAC
Isoleucine	I	ATT ATC ATA
Leucine	L	TTA TTG CTT CTC CTA CTG
Lysine	K	AAA AAG
Methionine	M	ATG
Phenylalanine	F	TTT TTC
Proline	P	CCT CCC CCA CCG

Standard Genetic Code (Continued)

Amino Acid Name	Amino Acid Code	Nucleotide Codon
Serine	S	TCT TCC TCA TCG AGT AGC
Threonine	T	ACT ACC ACA ACG
Tryptophan	W	TGG
Tyrosine	Y	TAT, TAC
Valine	V	GTT GTC GTA GTG
Asparagine or Aspartic acid (Aspartate)	B	Random codon from D and N
Glutamine or Glutamic acid (Glutamate)	Z	Random codon from E and Q
Unknown amino acid (any amino acid)	X	Random codon
Translation stop	*	TAA TAG TGA
Gap of indeterminate length	-	---
Unknown character (any character or symbol not in table)	?	???

Examples

- Convert an amino acid sequence to a nucleotide sequence using the standard genetic code.

```
aa2nt('MATLAP')

ans =

ATGGCGACGTTAGCGCCG
```

- Convert an amino acid sequence to a nucleotide sequence using the Vertebrate Mitochondrial genetic code.

```
aa2nt('MATLAP', 'GeneticCode', 2)

ans =

ATGGCAACTCTAGCGCCT
```

- Convert an amino acid sequence to a nucleotide sequence using the Echinoderm Mitochondrial genetic code and the RNA alphabet.

```
aa2nt('MATLAP','GeneticCode','ec','Alphabet','RNA')

ans =

AUGGCCACAUUGGCACCU
```

- Convert an amino acid sequence with the ambiguous character `B`.

```
aa2nt('abcd')

Warning: The sequence contains ambiguous characters.

ans =

GCCACATGCGAC
```

See Also

Bioinformatics Toolbox functions: `aminolookup`, `baselookup`, `geneticcode`, `nt2aa`, `revgeneticcode`, `seqtool`

MATLAB function: `rand`

Purpose

Count amino acids in sequence

Syntax

```
AAStruct = aacount(SeqAA)
AAStruct = aacount(SeqAA, ...'Chart', ChartValue, ...)
AAStruct = aacount(SeqAA, ...'Others', OthersValue, ...)
AAStruct = aacount(SeqAA, ...'Structure', StructureValue,
   ...)
```

Arguments

SeqAA

One of the following:

- String of single-letter codes specifying an amino acid sequence. For valid letter codes, see the table Mapping Amino Acid Letter Codes to Integers on page 3-2. Unknown characters are mapped to `0`.
- Row vector of integers specifying an amino acid sequence. For valid integers, see the table Mapping Amino Acid Integers to Letter Codes on page 3-805.
- MATLAB structure containing a `Sequence` field that contains an amino acid sequence, such as returned by `fastaread`, `getgenpept`, `genpeptread`, `getpdb`, or `pdbread`.

Examples: `'ARN'` or `[1 2 3]`

ChartValue

String specifying a chart type. Choices are `'pie'` or `'bar'`.

OthersValue	String specifying how to count ambiguous characters (B, Z, X), the stop character (*), and gaps indicated by a hyphen (-). Choices are 'full' (lists the ambiguous characters in separate fields) or 'bundle' (lists the ambiguous characters together in the field Others). Default is 'bundle'.
StructureValue	Suppresses the unknown characters warning when set to 'full' .

Return Values

AAStruct	1-by-1 MATLAB structure containing fields for the standard 20 amino acids (A, R, N, D, C, Q, E, G, H, I, L, K, M, F, P, S, T, W, Y, and V).

Description

AAStruct = aacount(*SeqAA*) counts the number of each type of amino acid in *SeqAA*, an amino acid sequence, and returns the counts in *AAStruct*, a 1-by-1 MATLAB structure containing fields for the standard 20 amino acids (A, R, N, D, C, Q, E, G, H, I, L, K, M, F, P, S, T, W, Y, and V).

- If a sequence contains ambiguous characters (B, Z, or X), the stop character (*), or gaps indicated with a hyphen (-), then these characters are counted in the field Others and the following warning message appears:

```
Warning: Ambiguous symbols appear in the sequence. These will be in Others.
```

- If a sequence contains characters other than the 20 standard amino acids, ambiguous, stop, and gap characters, then these characters are counted in the field Others, and the following warning message appears:

```
Warning: Unknown symbols appear in the sequence. These will be in Others.
```

- If the property 'Others' is set to 'full', ambiguous characters are listed separately in the fields B, Z, X, Stop, and Gap.

AAStruct = aacount(*SeqAA*, ...'*PropertyName*', *PropertyValue*, ...) calls aacount with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

AAStruct = aacount(*SeqAA*, ...'Chart', *ChartValue*, ...) creates a chart showing the relative proportions of the amino acids. *ChartValue* can be 'pie' or 'bar'.

AAStruct = aacount(*SeqAA*, ...'Others', *OthersValue*, ...) specifies how to count ambiguous characters (B, Z, or X), the stop character (*), and gaps indicated by a hyphen (-). Choices are 'full' (lists the ambiguous characters in separate fields) or 'bundle' (lists the ambiguous characters together in the field Others). Default is 'bundle'.

AAStruct = aacount(*SeqAA*, ...'Structure', *StructureValue*, ...) suppresses the unknown characters warning when *StructureValue* is set to 'full'.

- aacount(*SeqAA*) — Displays fields for 20 amino acids, and, if there are ambiguous or unknown characters, adds an Others field with the ambiguous and unknown character counts.
- aacount(*SeqAA*, 'Others', 'full') — Displays fields for 20 amino acids, 3 ambiguous amino acids, stops, gaps, and, if there are unknown characters, adds an Others field with the unknown counts.
- aacount(*SeqAA*, 'Structure', 'full') — Displays fields for 20 amino acids and an Others field. If there are ambiguous or unknown characters, adds the counts to the Others field; otherwise displays 0 in the Others field.
- aacount(*SeqAA*, 'Others', 'full', 'Structure', 'full') — Displays fields for 20 amino acids, 3 ambiguous amino acids, stops,

gaps, and an `Others` field. If there are unknown characters, add the counts to the `Others` field; otherwise displays `0` in the `Others` field.

Examples

1 Create an amino acid sequence.

```
Seq = 'MATLAB';
```

2 Count the amino acids in the sequence and return the results in a structure.

```
AA =  aacount(Seq)

Warning: Ambiguous symbols 'B' appear in the sequence. These will be in Others.

AA =

     A: 2
     R: 0
     N: 0
     D: 0
     C: 0
     Q: 0
     E: 0
     G: 0
     H: 0
     I: 0
     L: 1
     K: 0
     M: 1
     F: 0
     P: 0
     S: 0
     T: 1
     W: 0
     Y: 0
     V: 0
Others: 1
```

3 Get the count for alanine (A) residues.

```
AA.A

ans =

       2
```

4 Create a random character string to represent an amino acid sequence.

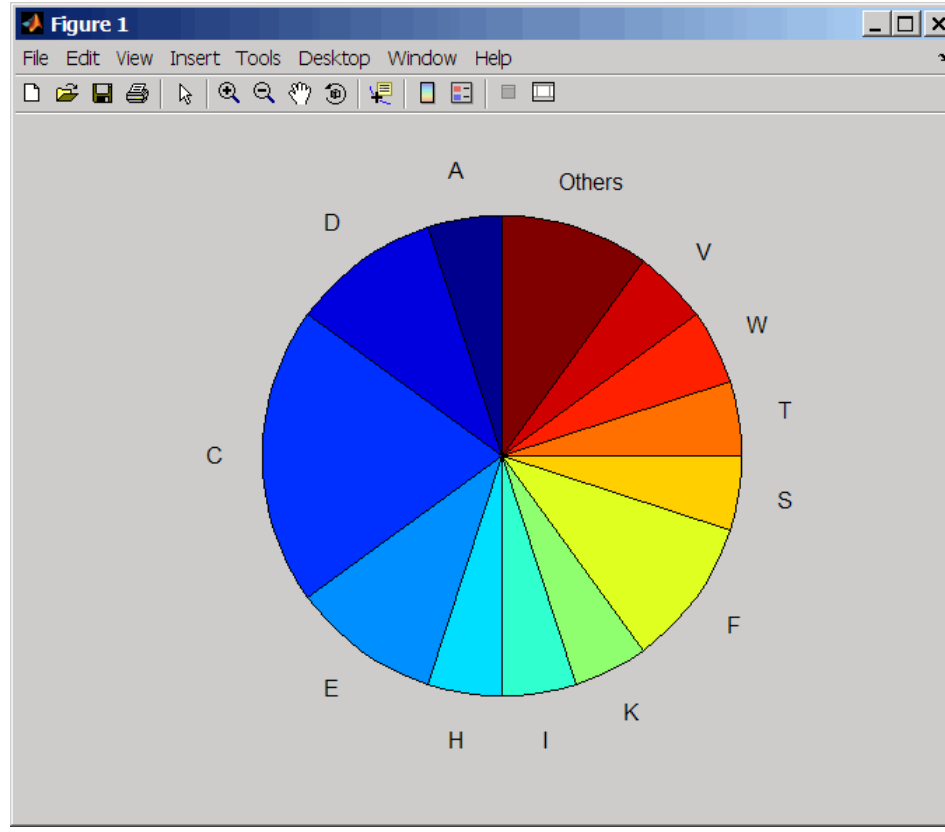
```
Seq = randseq(20, 'alphabet', 'amino')

Seq =

   dwcztecakfuecvifchds
```

5 Count the amino acids in the sequence, return the results in a structure, and display the results in a pie chart.

```
AA =  aacount(Seq, 'chart', 'pie');
```



See Also

Bioinformatics Toolbox functions: `aminolookup`, `atomiccomp`, `basecount`, `codoncount`, `dimercount`, `isoelectric`, `molweight`, `proteinplot`, `proteinpropplot`, `seqtool`

bioma.ExpressionSet.abstract

Purpose

Retrieve or set abstract describing experiment in ExpressionSet object

Syntax

```
Abstract = abstract(ESObj)
NewESObj = abstract(ESObj, NewAbstract)
```

Description

`Abstract = abstract(ESObj)` returns a string containing the abstract information describing the experiment from a MIAME object in an ExpressionSet object.

`NewESObj = abstract(ESObj, NewAbstract)` replaces the abstract information in the MIAME object in `ESObj`, an ExpressionSet object, with `NewAbstract`, a string containing new abstract information, and returns `NewESObj`, a new ExpressionSet object.

Inputs

ESObj

Object of the `bioma.ExpressionSet` class.

NewAbstract

String containing new abstract information.

Outputs

Abstract

String containing the abstract information describing the experiment from a MIAME object in an ExpressionSet object.

NewESObj

Object of the `bioma.ExpressionSet` class, returned after replacing the abstract information.

Examples

Construct an ExpressionSet object from `EDObj`, an ExptData object, `MDObj2`, a MetaData object containing sample variable information, and `MIAMEObj`, a MIAME object. Retrieve the abstract information stored in the MIAME object stored in the ExpressionSet object:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
```

```
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Construct MIAME object
MIAMEObj = MIAME(geoStruct);
% Import bioma package to make constructor function
% available
import bioma.*
% Construct ExpressionSet object
ESObj = ExpressionSet(EDObj, 'SData', MDObj2, 'EInfo', MIAMEObj);
% Retrieve abstract text from the MIAME object
Abstract = abstract(ESObj)
```

See Also

`bioma.ExpressionSet` | `bioma.data.MIAME`

How To

- "Working with ExpressionSet Objects"

addTitle (clustergram)

Purpose

Add title to clustergram

Syntax

```
addTitle(CGObject, Title)
addTitle(CGObject, Title, 'Property1Name', Property1Value,
   'Property2Name', Property2Value, ...)
H = addTitle(CGObject)
```

Arguments

CGObject	Clustergram object created with the function `clustergram`.
Title	String used as the title in the Clustergram window.

Return Values

H	Handle to a MATLAB text object used as the title for the clustergram.

Description

`addTitle(`*CGObject*`, `*Title*`)` adds a title above the clustergram displayed in the Clustergram window.

`addTitle(`*CGObject*`, `*Title*`, 'Property1Name', `*Property1Value*`, 'Property2Name', `*Property2Value*`, ...)` specifies text object properties for the title. For more information on the property name/property value pairs you can use to modify the text, see Text Properties.

H `= addTitle(`*CGObject*`)` returns the handle to the text object used as the title for the clustergram.

Examples

Supply a title for the clustergram object created in the Examples section of the `clustergram` function. Use 14-point, italic text for the title.

```
addTitle(cgo, 'Expression Levels During Diauxic Shift', ...
           'FontSize', 14, 'FontAngle', 'Italic')
```

Return a handle to the title text object, then use the `set` function to change the font size to 16 points.

```
h = addTitle(cgo)
set(h, 'FontSize', 16)
```

See Also

Bioinformatics Toolbox function: `clustergram` (object constructor)

Bioinformatics Toolbox object: clustergram object

Bioinformatics Toolbox methods of a clustergram object: `addXLabel`, `addYLabel`, `get`, `plot`, `set`, `view`

addTitle (HeatMap)

Purpose

Add title to heat map

Syntax

```
addTitle(HMObject, Title)
addTitle(HMObject, Title, 'Property1Name', Property1Value,
   'Property2Name', Property2Value, ...)
H = addTitle(HMObject)
```

Arguments

HMObject	HeatMap object created with the function `HeatMap`.
Title	String used as the title in the HeatMap window.

Return Values

H	Handle to a MATLAB text object used as the title for the heat map.

Description

`addTitle(`*HMObject*`, `*Title*`)` adds a title above the heat map displayed in the HeatMap window.

`addTitle(`*HMObject*`, `*Title*`, 'Property1Name', `*Property1Value*`, 'Property2Name', `*Property2Value*`, ...)` specifies text object properties for the title. For more information on the property name/property value pairs you can use to modify the text, see Text Properties.

H `= addTitle(`*HMObject*`)` returns the handle to the text object used as the title for the heat map.

Examples

Supply a title for the HeatMap object created in the Examples section of the `HeatMap` function. Use 14-point, italic text for the title.

```
addTitle(hmo, 'Example Heat Map', 'FontSize', 14, ...
              'FontAngle','Italic')
```

Return a handle to the title text object, then use the `set` function to change the font size to 16 points.

```
h = addTitle(hmo)
set(h, 'FontSize', 16)
```

See Also

Bioinformatics Toolbox function: `HeatMap` (object constructor)

Bioinformatics Toolbox object: HeatMap object

Bioinformatics Toolbox methods of a HeatMap object: `addXLabel`, `addYLabel`, `plot`, `view`

addXLabel (clustergram)

Purpose

Label *x*-axis of clustergram

Syntax

```
addXLabel(CGObject, Label)
addXLabel(CGObject, Label, 'Property1Name', Property1Value,
   'Property2Name', Property2Value, ...)
H = addXLabel(CGObject)
```

Arguments

CGObject	Clustergram object created with the function `clustergram`.
Label	String used as the *x*-axis label in the Clustergram window.

Return Values

H	Handle to a MATLAB text object used as the *x*-axis label for the clustergram.

Description

`addXLabel(`*CGObject*`, `*Label*`)` adds a label below the *x*-axis of a clustergram displayed in the Clustergram window.

`addXLabel(`*CGObject*`, `*Label*`, 'Property1Name', `*Property1Value*`, 'Property2Name', `*Property2Value*`, ...)` specifies text object properties for the *x*-axis label. For more information on the property name/property value pairs you can use to modify the text, see Text Properties.

H `= addXLabel(`*CGObject*`)` returns the handle to the text object used as the *x*-axis label for the clustergram.

Examples

Supply an *x*-axis label for the clustergram object created in the Examples section of the `clustergram` function. Use 12-point, italic text for the label.

```
addXLabel(cgo, 'Diauxic Shift Times', 'FontSize', 12, ...
          'FontAngle', 'Italic')
```

Return a handle to the *x*-axis label text object, then use the `set` function to change the font size to 14 points.

```
h = addXLabel(cgo)
set(h, 'FontSize', 14)
```

See Also

Bioinformatics Toolbox function: `clustergram` (object constructor)

Bioinformatics Toolbox object: clustergram object

Bioinformatics Toolbox methods of a clustergram object: `addTitle`, `addYLabel`, `get`, `plot`, `set`, `view`

addXLabel (HeatMap)

Purpose

Label *x*-axis of heat map

Syntax

```
addXLabel(HMObject, Label)
addXLabel(HMObject, Label, 'Property1Name', Property1Value,
   'Property2Name', Property2Value, ...)
H = addXLabel(HMObject)
```

Arguments

HMObject	HeatMap object created with the function `HeatMap`.
Label	String used as the *x*-axis label in the HeatMap window.

Return Values

H	Handle to a MATLAB text object used as the *x*-axis label for the heat map.

Description

`addXLabel(`*HMObject*`, `*Label*`)` adds a label below the *x*-axis of a heat map displayed in the HeatMap window.

`addXLabel(`*HMObject*`, `*Label*`, 'Property1Name', `*Property1Value*`, 'Property2Name', `*Property2Value*`, ...)` specifies text object properties for the *x*-axis label. For more information on the property name/property value pairs you can use to modify the text, see Text Properties.

H `= addXLabel(`*HMObject*`)` returns the handle to the text object used as the *x*-axis label for the heat map.

Examples

Supply an *x*-axis label for the HeatMap object created in the Examples section of the `HeatMap` function. Use 12-point, italic text for the label.

```
addXLabel(hmo, 'Times', 'FontSize', 12, 'FontAngle', 'Italic')
```

Return a handle to the *x*-axis label text object, then use the `set` function to change the font size to 14 points.

```
h = addXLabel(hmo)
```

```
set(h, 'FontSize', 14)
```

See Also

Bioinformatics Toolbox function: `HeatMap` (object constructor)

Bioinformatics Toolbox object: HeatMap object

Bioinformatics Toolbox methods of a HeatMap object: `addTitle`, `addYLabel`, `plot`, `view`

addYLabel (clustergram)

Purpose

Label *y*-axis of clustergram

Syntax

```
addYLabel(CGObject, Label)
addYLabel(CGObject, Label, 'Property1Name', Property1Value,
   'Property2Name', Property2Value, ...)
H = addYLabel(CGObject)
```

Arguments

CGObject	Clustergram object created with the function `clustergram`.
Label	String used as the *y*-axis label in the Clustergram window.

Return Values

H	Handle to a MATLAB text object used as the *y*-axis label for the clustergram.

Description

`addYLabel(`*CGObject*`, `*Label*`)` adds a label to the left of the *y*-axis of a clustergram displayed in the Clustergram window.

`addYLabel(`*CGObject*`, `*Label*`, 'Property1Name', `*Property1Value*`, 'Property2Name', `*Property2Value*`, ...)` specifies text object properties for the *y*-axis label. For more information on the property name/property value pairs you can use to modify the text, see Text Properties.

H `= addYLabel(`*CGObject*`)` returns the handle to the text object used as the *y*-axis label for the clustergram.

Examples

Supply a *y*-axis label for the clustergram object created in the Examples section of the `clustergram` function. Use 12-point, italic text for the label.

```
addYLabel(cgo, 'Genes', "FontSize', 12, 'FontAngle', 'Italic')
```

Return a handle to the *y*-axis label text object, then use the `set` function to change the font size to 14 points.

```
h = addYLabel(cgo)
set(h, 'FontSize', 14)
```

See Also

Bioinformatics Toolbox function: `clustergram` (object constructor)

Bioinformatics Toolbox object: clustergram object

Bioinformatics Toolbox methods of a clustergram object: `addTitle`, `addXLabel`, `get`, `plot`, `set`, `view`

addYLabel (HeatMap)

Purpose

Label *y*-axis of heat map

Syntax

```
addYLabel(HMObject, Label)
addYLabel(HMObject, Label, 'Property1Name', Property1Value,
   'Property2Name', Property2Value, ...)
H = addYLabel(HMObject)
```

Arguments

HMObject	HeatMap object created with the function `HeatMap`.
Label	String used as the *y*-axis label in the HeatMap window.

Return Values

H	Handle to a MATLAB text object used as the *y*-axis label for the heat map.

Description

`addYLabel(`*HMObject*`, `*Label*`)` adds a label to the left of the *y*-axis of a heat map displayed in the HeatMap window.

`addYLabel(`*HMObject*`, `*Label*`, 'Property1Name', `*Property1Value*`, 'Property2Name', `*Property2Value*`, ...)` specifies text object properties for the *y*-axis label. For more information on the property name/property value pairs you can use to modify the text, see Text Properties.

H `= addYLabel(`*HMObject*`)` returns the handle to the text object used as the *y*-axis label for the heat map.

Examples

Supply a *y*-axis label for the HeatMap object created in the Examples section of the `HeatMap` function. Use 12-point, italic text for the label.

```
addYLabel(hmo, 'Samples', "FontSize', 12, 'FontAngle', 'Italic')
```

Return a handle to the *y*-axis label text object, then use the `set` function to change the font size to 14 points.

```
h = addYLabel(hmo)
```

```
set(h, 'FontSize', 14)
```

See Also

Bioinformatics Toolbox function: `HeatMap` (object constructor)

Bioinformatics Toolbox object: HeatMap object

Bioinformatics Toolbox methods of a HeatMap object: `addTitle`, `addXLabel`, `plot`, `view`

Purpose

Perform GC Robust Multi-array Average (GCRMA) procedure on Affymetrix microarray probe-level data

Syntax

```
Expression = affygcrma(CELFiles, CDFFile, SeqFile)
Expression = affygcrma(ProbeStructure, Seq)
Expression = affygcrma(CELFiles, CDFFile, SeqFile,
...'CELPath', CELPathValue, ...)
Expression = affygcrma(CELFiles, CDFFile, SeqFile,
   ...'CDFPath', CDFPathValue, ...)
Expression = affygcrma(CELFiles, CDFFile, SeqFile,
   ...'SeqPath', SeqPathValue, ...)
Expression = affygcrma(..., 'ChipIndex',
ChipIndexValue, ...)
Expression = affygcrma(..., 'OpticalCorr',
OpticalCorrValue,
   ...)
Expression = affygcrma(..., 'CorrConst',
CorrConstValue, ...)
Expression = affygcrma(..., 'Method', MethodValue, ...)
Expression = affygcrma(..., 'TuningParam',
TuningParamValue,
   ...)
Expression = affygcrma(..., 'GSBCorr', GSBCorrValue, ...)
Expression = affygcrma(..., 'Median', MedianValue, ...)
Expression = affygcrma(..., 'Output', OutputValue, ...)
Expression = affygcrma(..., 'Showplot', ShowplotValue, ...)
Expression = affygcrma(..., 'Verbose', VerboseValue, ...)
```

Arguments

CELFiles

Any of the following:

- String specifying a single CEL file name.
- `'*'`, which reads all CEL files in the current directory.
- `' '`, which opens the Select CEL Files dialog box from which you select the CEL files. From this dialog box, you can press and hold **Ctrl** or **Shift** while clicking to select multiple CEL files.
- Cell array of CEL file names.

CDFFile

Either of the following:

- String specifying a CDF file name.
- `' '`, which opens the Select CDF File dialog box from which you select the CDF file.

SeqFile

Either of the following:

- String specifying a file name of a sequence file (tab-separated or FASTA) that contains the following information for a specific type of Affymetrix GeneChip array:
  - Probe set IDs
  - Probe *x*-coordinates
  - Probe *y*-coordinates
  - Probe sequences in each probe set
  - Affymetrix GeneChip array type (FASTA file only)

  The sequence file (tab-separated or FASTA) must be on the MATLAB search path or in

	the Current Directory (unless you use the `SeqPath` property). In a tab-separated file, each row represents a probe; in a FASTA file, each header represents a probe. • An *N*-by-25 matrix of sequence information, such as returned by `affyprobeseqread`.
`Seq`	An *N*-by-25 matrix of sequence information, such as returned by `affyprobeseqread`.
`ProbeStructure`	MATLAB structure containing information from the CEL files, including probe intensities, probe indices, and probe set IDs, returned by the `celintensityread` function.
`CELPathValue`	String specifying the path and directory where the files specified in *`CELFiles`* are stored.
`CDFPathValue`	String specifying the path and directory where the file specified in *`CDFFile`* is stored.
`SeqPathValue`	String specifying a directory or path and directory where *`SeqFile`* is stored.
`ChipIndexValue`	Positive integer specifying a chip. This chip's sequence information and mismatch probe intensity data is used to compute probe affinities. Default is `1`.
`OpticalCorrValue`	Controls the use of optical background correction on the input probe intensity values. Choices are `true` (default) or `false`.
`CorrConstValue`	Value that specifies the correlation constant, rho, for log background intensity for each PM/MM probe pair. Choices are any value ≥ `0` and ≤ `1`. Default is `0.7`.

MethodValue	String that specifies the method to estimate the signal. Choices are `'MLE'`, a faster, ad hoc Maximum Likelihood Estimate method, or `'EB'`, a slower, more formal, empirical Bayes method. Default is `'MLE'`.
TuningParamValue	Value that specifies the tuning parameter used by the estimate method. This tuning parameter sets the lower bound of signal values with positive probability. Choices are a positive value. Default is `5` (MLE) or `0.5` (EB). **Tip** For information on determining a setting for this parameter, see Wu et al., 2004.
GSBCorrValue	Specifies whether to perform gene-specific binding (GSB) correction using probe affinity data. Choices are `true` (default) or `false`. If there is no probe affinity information, this property is ignored.
MedianValue	Specifies the use of the median of the ranked values instead of the mean for normalization. Choices are `true` or `false` (default).

OutputValue — Specifies the scale of the returned gene expression values. Choices are:

- `'log'`
- `'log2'`
- `'log10'`
- `'natural'`
- `@`*`functionname`*

In the last instance, the data is transformed as defined by the function *`functionname`*. Default is `'log2'`.

ShowplotValue — Controls the display of a plot showing the $\log_2$ of mismatch (MM) probe intensity values from a specified chip (CEL file), versus that chip's MM probe affinities. The plot also shows the LOWESS fit for computing NSB data of the specified chip. Choices are `true`, `false`, or *`I`*, an integer specifying a chip. If set to `true`, the first chip is plotted. Default is:

- `false` — When return values are specified.
- `true` — When return values are not specified.

VerboseValue — Controls the display of the status of the reading of files and GCRMA processing. Choices are `true` (default) or `false`.

Return Values

Expression	DataMatrix object containing the $\log_2$ gene expression values that have been background adjusted, normalized, and summarized using the GC Robust Multi-array Average (GCRMA) procedure. Each row in *Expression* corresponds to a gene (probe set), and each column corresponds to an Affymetrix CEL file.

Description

Note This function does not work on the Solaris™ platform.

Expression = affygcrma(*CELFiles*, *CDFFile*, *SeqFile*) reads the specified Affymetrix CEL files, the associated CDF library file (created from Affymetrix GeneChip arrays for expression or genotyping assays), and the associated sequence file or matrix. It then processes the probe intensity values using GCRMA background adjustment, quantile normalization, and median-polish summarization procedures, then returns *Expression*, a DataMatrix object containing the $\log_2$ based gene expression values in a matrix, the probe set IDs as row names, and the CEL file names as column names. Note that each row in *Expression* corresponds to a gene (probe set), and each column corresponds to an Affymetrix CEL file. (Each CEL file is generated from a separate chip. All chips should be of the same type.)

CELFiles is a string or cell array of CEL file names. *CDFFile* is a string specifying a CDF file name. If you set *CELFiles* to '*', then it reads all CEL files in the current directory. If you set *CELFiles* or *CDFFile* to ' ', then it opens the Select Files dialog box from which you select the CEL files or CDF file. From this dialog box, you can press and hold **Ctrl** or **Shift** while clicking to select multiple CEL files. *SeqFile* is a file or matrix containing sequence information for probes on a specific type of Affymetrix GeneChip array.

Note For details on the reading of files and GCRMA processing, see `celintensityread`, `affyprobeseqread`, `affyprobeaffinities`, `gcrma`, `gcrmabackadj`, `quantilenorm`, and `rmasummary`.

`Expression` = `affygcrma(`*`ProbeStructure`*`, `*`Seq`*`)` uses GCRMA background adjustment, quantile normalization, and median-polish summarization procedures to process the probe intensity values in *`ProbeStructure`*. *`ProbeStructure`* is a MATLAB structure containing information from the CEL files, including probe intensities, probe indices, and probe set IDs, returned by the `celintensityread` function. *`Seq`* is a matrix containing sequence information for probes on a specific type of Affymetrix GeneChip array.

`Expression` = `affygcrma(..., '`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `affygcrma` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`Expression` = `affygcrma(`*`CELFiles`*`, `*`CDFFile`*`, `*`SeqFile`*`, ...'CELPath', `*`CELPathValue`*`, ...)` specifies a path and directory where the files specified by *`CELFiles`* are stored.

`Expression` = `affygcrma(`*`CELFiles`*`, `*`CDFFile`*`, `*`SeqFile`*`, ...'CDFPath', `*`CDFPathValue`*`, ...)` specifies a path and directory where the file specified by *`CDFFile`* is stored.

`Expression` = `affygcrma(`*`CELFiles`*`, `*`CDFFile`*`, `*`SeqFile`*`, ...'SeqPath', `*`SeqPathValue`*`, ...)` specifies a path and directory where the file specified by *`SeqFile`* is stored.

`Expression` = `affygcrma(..., 'ChipIndex', `*`ChipIndexValue`*`, ...)` computes probe affinities from MM probe intensity data using sequence information and mismatch probe intensity values from the chip specified by *`ChipIndexValue`*. Default *`ChipIndexValue`* is `1`.

Expression = affygcrma(..., 'OpticalCorr', *OpticalCorrValue*, ...) controls the use of optical background correction on the input probe intensity values. Choices are `true` (default) or `false`.

Expression = affygcrma(..., 'CorrConst', *CorrConstValue*, ...) specifies the correlation constant, rho, for background intensity for each PM/MM probe pair. Choices are any value ≥ `0` and ≤ `1`. Default is `0.7`.

Expression = affygcrma(..., 'Method', *MethodValue*, ...) specifies the method to estimate the signal. Choices are `'MLE'`, a faster, ad hoc Maximum Likelihood Estimate method, or `'EB'`, a slower, more formal, empirical Bayes method. Default is `'MLE'`.

Expression = affygcrma(..., 'TuningParam', *TuningParamValue*, ...) specifies the tuning parameter used by the estimate method. This tuning parameter sets the lower bound of signal values with positive probability. Choices are a positive value. Default is `5` (MLE) or `0.5` (EB).

Tip For information on determining a setting for this parameter, see Wu et al., 2004.

Expression = affygcrma(..., 'GSBCorr', *GSBCorrValue*, ...) specifies whether to perform gene-specific binding (GSB) correction using probe affinity data. Choices are `true` (default) or `false`. If there is no probe affinity information, this property is ignored.

Expression = affygcrma(..., 'Median', *MedianValue*, ...) specifies the use of the median of the ranked values instead of the mean for normalization. Choices are `true` or `false` (default).

Expression = affygcrma(..., 'Output', *OutputValue*, ...) specifies the scale of the returned gene expression values. *OutputValue* can be:

- 'log'
- 'log2'
- 'log10'
- 'natural'
- @*functionname*

In the last instance, the data is transformed as defined by the function *functionname*. Default is 'log2'.

Expression = affygcrma(..., 'Showplot', *ShowplotValue*, ...) controls the display of a plot showing the $\log_2$ of mismatch (MM) probe intensity values from a specified chip (CEL file), versus that chip's MM probe affinities. The plot also shows the LOWESS fit for computing NSB data of the specified chip. Choices are true, false, or *I*, an integer specifying a chip. If set to true, the first chip is plotted. Default is:

- false — When return values are specified.
- true — When return values are not specified.

Expression = affygcrma(..., 'Verbose', *VerboseValue*, ...) controls the display of the status of the reading of files and GCRMA processing. Choices are true (default) or false.

Examples

The following example assumes that you have the HG_U95Av2.CDF library file stored at D:\Affymetrix\LibFiles\HGGenome, and that your current directory points to a location containing CEL files and a sequence file associated with this CDF library file. In this example, the affygcrma function reads all the CEL files and the sequence file in the current directory and a CDF file in a specified directory. It also performs GCRMA background adjustment, quantile normalization, and summarization procedures on the PM probe intensity values, and returns a DataMatrix object, containing the metadata and processed data.

```
Expression = affygcrma('*', 'HG_U95Av2.CDF','HG-U95Av2_probe_tab',...
```

```
'CDFPath', 'D:\Affymetrix\LibFiles\HGGenome');
```

References

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[3] Wu, Z., and Irizarry, R.A. (2005). Stochastic Models Inspired by Hybridization Theory for Short Oligonucleotide Arrays. Proceedings of RECOMB 2004. J Comput Biol. *12(6)*, 882–93.

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[6] Speed, T. (2006). Background models and GCRMA. Lecture 10, Statistics 246, University of California Berkeley. `http://www.stat.berkeley.edu/users/terry/Classes/s246.2006/-Week10/Week10L1.pdf`.

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and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823–6834.

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[10] Mosteller, F., and Tukey, J. (1977). Data Analysis and Regression (Reading, Massachusetts: Addison-Wesley Publishing Company), pp. 165–202.

See Also

Bioinformatics Toolbox functions: `affyprobeaffinities`, `affyprobeseqread`, `affyrma`, `celintensityread`, `gcrma`, `gcrmabackadj`, `mafdr`, `mattest`, `quantilenorm`, `rmasummary`

Purpose

Perform rank invariant set normalization on probe intensities from multiple Affymetrix CEL or DAT files

Syntax

```
NormData = affyinvarsetnorm(Data)
[NormData, MedStructure] = affyinvarsetnorm(Data)
... affyinvarsetnorm(..., 'Baseline', BaselineValue, ...)
... affyinvarsetnorm(..., 'Thresholds',
ThresholdsValue, ...)
... affyinvarsetnorm(..., 'StopPercentile',
   StopPercentileValue, ...)
... affyinvarsetnorm(..., 'RayPercentile',
   RayPercentileValue, ...)
... affyinvarsetnorm(..., 'Method', MethodValue, ...)
... affyinvarsetnorm(..., 'Showplot', ShowplotValue, ...)
```

Arguments

Data	Matrix of intensity values where each row corresponds to a perfect match (PM) probe and each column corresponds to an Affymetrix CEL or DAT file. (Each CEL or DAT file is generated from a separate chip. All chips should be of the same type.)
MedStructure	Structure of each column's intensity median before and after normalization, and the index of the column chosen as the baseline.
BaselineValue	Property to control the selection of the column index *N* from *Data* to be used as the baseline column. Default is the column index whose median intensity is the median of all the columns.

ThresholdsValue Property to set the thresholds for the lowest average rank and the highest average rank, which are used to determine the invariant set. The rank invariant set is a set of data points whose proportional rank difference is smaller than a given threshold. The threshold for each data point is determined by interpolating between the threshold for the lowest average rank and the threshold for the highest average rank. Select these two thresholds empirically to limit the spread of the invariant set, but allow enough data points to determine the normalization relationship.

ThresholdsValue is a 1-by-2 vector [*LT, HT*] where *LT* is the threshold for the lowest average rank and *HT* is threshold for the highest average rank. Values must be between `0` and `1`. Default is [`0.05, 0.005`].

StopPercentileValue Property to stop the iteration process when the number of data points in the invariant set reaches *N* percent of the total number of data points. Default is `1`.

Note If you do not use this property, the iteration process continues until no more data points are eliminated.

RayPercentileValue Property to select the *N* percentage of the highest ranked invariant set of data points to fit a straight line through, while the remaining data points are fitted to a running median curve. The final running median curve is a piecewise linear curve. Default is `1.5`.

MethodValue — Property to select the smoothing method used to normalize the data. Enter `'lowess'` or `'runmedian'`. Default is `'lowess'`.

ShowplotValue — Property to control the plotting of two pairs of scatter plots (before and after normalization). The first pair plots baseline data versus data from a specified column (chip) from the matrix *Data*. The second is a pair of M-A scatter plots, which plots M (ratio between baseline and sample) versus A (the average of the baseline and sample). Enter either `'all'` (plot a pair of scatter plots for each column or chip) or specify a subset of columns (chips) by entering the column number(s) or a range of numbers.

For example:

- `..., 'Showplot', 3, ...)` plots data from column 3.
- `..., 'Showplot', [3,5,7], ...)` plots data from columns 3, 5, and 7.
- `..., 'Showplot', 3:9, ...)` plots data from columns 3 to 9.

Description

NormData = `affyinvarsetnorm(`*Data*`)` normalizes the values in each column (chip) of probe intensities in *Data* to a baseline reference, using the invariant set method. *NormData* is a matrix of normalized probe intensities from *Data*.

Specifically, `affyinvarsetnorm`:

- Selects a baseline index, typically the column whose median intensity is the median of all the columns.

- For each column, determines the proportional rank difference (*prd*) for each pair of ranks, *RankX* and *RankY*, from the sample column and the baseline reference.

  prd = abs(*RankX* - *RankY*)

- For each column, determines the invariant set of data points by selecting data points whose proportional rank differences (*prd*) are below *threshold*, which is a predetermined threshold for a given data point (defined by the *ThresholdsValue* property). It repeats the process until either no more data points are eliminated, or a predetermined percentage of data points is reached.

  The invariant set is data points with a *prd* < *threshold*.

- For each column, uses the invariant set of data points to calculate the lowess or running median smoothing curve, which is used to normalize the data in that column.

`[NormData, MedStructure] = affyinvarsetnorm(Data)` also returns a structure of the index of the column chosen as the baseline and each column's intensity median before and after normalization.

Note If *Data* contains NaN values, then *NormData* will also contain NaN values at the corresponding positions.

`... affyinvarsetnorm(..., 'PropertyName', PropertyValue, ...)` calls `affyinvarsetnorm` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... affyinvarsetnorm(..., 'Baseline', BaselineValue, ...)` lets you select the column index *N* from *Data* to be the baseline column.

Default is the index of the column whose median intensity is the median of all the columns.

`... affyinvarsetnorm(..., 'Thresholds', ThresholdsValue, ...)` sets the thresholds for the lowest average rank and the highest average rank, which are used to determine the invariant set. The rank invariant set is a set of data points whose proportional rank difference is smaller than a given threshold. The threshold for each data point is determined by interpolating between the threshold for the lowest average rank and the threshold for the highest average rank. Select these two thresholds empirically to limit the spread of the invariant set, but allow enough data points to determine the normalization relationship.

ThresholdsValue is a 1-by-2 vector [*LT, HT*], where *LT* is the threshold for the lowest average rank and *HT* is threshold for the highest average rank. Values must be between `0` and `1`. Default is [`0.05, 0.005`].

`... affyinvarsetnorm(..., 'StopPercentile', StopPercentileValue, ...)` stops the iteration process when the number of data points in the invariant set reaches *N* percent of the total number of data points. Default is `1`.

Note If you do not use this property, the iteration process continues until no more data points are eliminated.

`... affyinvarsetnorm(..., 'RayPercentile', RayPercentileValue, ...)` selects the *N* percentage of the highest ranked invariant set of data points to fit a straight line through, while the remaining data points are fitted to a running median curve. The final running median curve is a piecewise linear curve. Default is `1.5`.

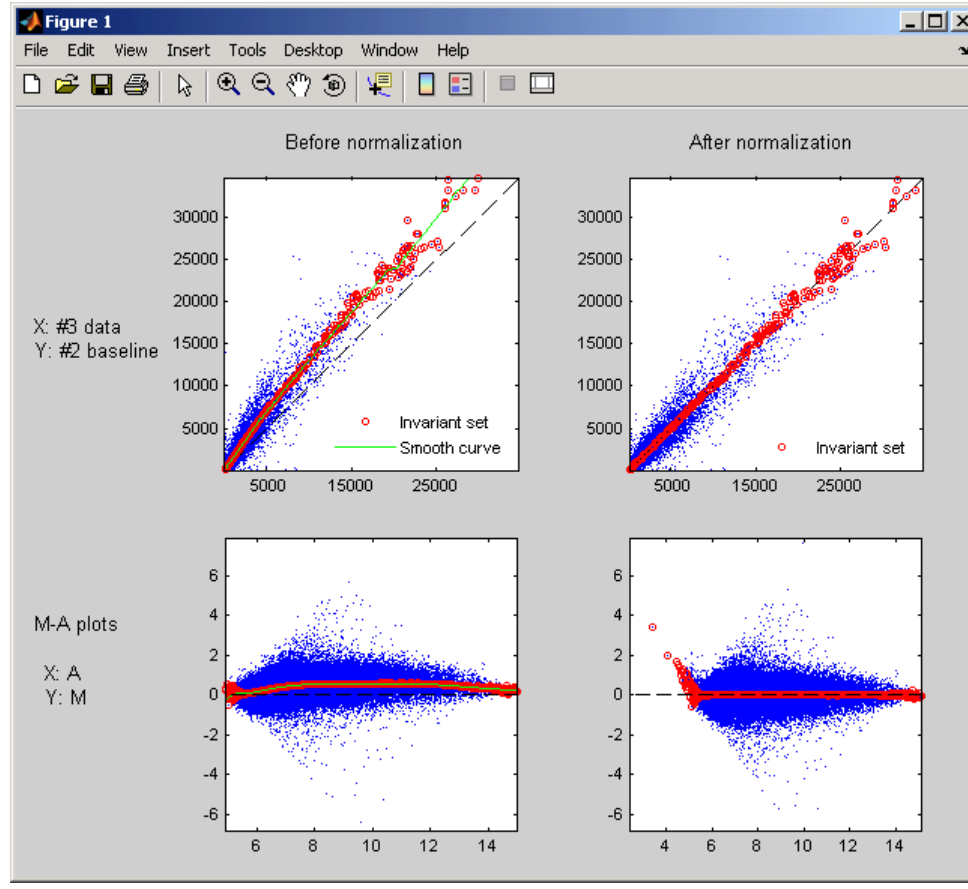
`... affyinvarsetnorm(..., 'Method', MethodValue, ...)` selects the smoothing method for normalizing the data. When *MethodValue* is `'lowess'`, `affyinvarsetnorm` uses the lowess method.

When *MethodValue* is 'runmedian', affyinvarsetnorm uses the running median method. Default is 'lowess'.

... affyinvarsetnorm(..., 'Showplot', *ShowplotValue*, ...) plots two pairs of scatter plots (before and after normalization). The first pair plots baseline data versus data from a specified column (chip) from the matrix *Data*. The second is a pair of M-A scatter plots, which plots M (ratio between baseline and sample) versus A (the average of the baseline and sample). When *ShowplotValue* is 'all', affyinvarsetnorm plots a pair of scatter plots for each column or chip. When *ShowplotValue* is a number(s) or range of numbers, affyinvarsetnorm plots a pair of scatter plots for the indicated column numbers (chips).

For example:

- ..., 'Showplot', 3) plots the data from column 3 of *Data*.
- ..., 'Showplot', [3,5,7]) plots the data from columns 3, 5, and 7 of *Data*.
- ..., 'Showplot', 3:9) plots the data from columns 3 to 9 of *Data*.



Examples

1 Load a MAT-file, included with the Bioinformatics Toolbox software, which contains Affymetrix data variables, including `pmMatrix`, a matrix of PM probe intensity values from multiple CEL files.

```
load prostatecancerrawdata
```

2 Normalize the data in `pmMatrix`, using the `affyinvarsetnorm` function.

```
NormMatrix = affyinvarsetnorm(pmMatrix);
```

The `prostatecancerrawdata.mat` file used in the previous example contains data from Best et al., 2005.

References

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See Also

Bioinformatics Toolbox functions: `affyread`, `celintensityread`, `mainvarsetnorm`, `malowess`, `manorm`, `quantilenorm`, `rmabackadj`, `rmasummary`

Purpose

Compute Affymetrix probe affinities from their sequences and MM probe intensities

Syntax

```
[AffinPM, AffinMM] = affyprobeaffinities(SequenceMatrix,
   MMIntensity)
[AffinPM, AffinMM,
   BaseProf] = affyprobeaffinities(SequenceMatrix,
   MMIntensity)
[AffinPM, AffinMM, BaseProf,
   Stats] = affyprobeaffinities(SequenceMatrix,
MMIntensity)
... = affyprobeaffinities(SequenceMatrix, MMIntensity,
...'ProbeIndices', ProbeIndicesValue, ...)
... = affyprobeaffinities(SequenceMatrix, MMIntensity,
   ...'Showplot', ShowplotValue, ...)
```

Arguments

SequenceMatrix

An *N*-by-25 matrix of sequence information for the perfect match (PM) probes on an Affymetrix GeneChip array, where *N* is the number of probes on the array. Each row corresponds to a probe, and each column corresponds to one of the 25 sequence positions. Nucleotides in the sequences are represented by one of the following integers:

- `0` — None
- `1` — A
- `2` — C
- `3` — G
- `4` — T

Tip You can use the `affyprobeseqread` function to generate this matrix. If you have this sequence information in letter representation, you can convert it to integer representation using the `nt2int` function.

`MMIntensity`

Column vector containing mismatch (MM) probe intensities from a CEL file, generated from a single Affymetrix GeneChip array. Each row corresponds to a probe.

Tip You can extract this column vector from the `MMIntensities` matrix returned by the `celintensityread` function.

`ProbeIndicesValue`

Column vector containing probe indexing information. Probes within a probe set are numbered 0 through *N* - 1, where *N* is the number of probes in the probe set.

Tip You can use the `affyprobeseqread` function to generate this column vector.

`ShowplotValue`

Controls the display of a plot showing the affinity values of each of the four bases (A, C, G, and T) for each of the 25 sequence positions, for all probes on the Affymetrix GeneChip array. Choices are `true` or `false` (default).

Return Values

AffinPM	Column vector of PM probe affinities, computed from their probe sequences and MM probe intensities.
AffinMM	Column vector of MM probe affinities, computed from their probe sequences and MM probe intensities.
BaseProf	4-by-4 matrix containing the four parameters for a polynomial of degree 3, for each base, A, C, G, and T. Each row corresponds to a base, and each column corresponds to a parameter. These values are estimated from the probe sequences and intensities, and represent all probes on an Affymetrix GeneChip array.
Stats	Row vector containing four statistics in the following order: • R-square statistic • F statistic • p-value • Error variance

Description

`[`*AffinPM*`, `*AffinMM*`] = affyprobeaffinities(`*SequenceMatrix*`, `*MMIntensity*`)` returns a column vector of PM probe affinities and a column vector of MM probe affinities, computed from their probe sequences and MM probe intensities. Each row in *AffinPM* and *AffinMM* corresponds to a probe. NaN is returned for probes with no sequence information. Each probe affinity is the sum of position-dependent base affinities. For a given base type, the positional effect is modeled as a polynomial of degree 3.

`[`*AffinPM*`, `*AffinMM*`, `*BaseProf*`] = affyprobeaffinities(`*SequenceMatrix*`, `*MMIntensity*`)` also estimates affinity coefficients using multiple linear regression. It returns *BaseProf*, a 4-by-4 matrix containing the four parameters

for a polynomial of degree 3, for each base, A, C, G, and T. Each row corresponds to a base, and each column corresponds to a parameter. These values are estimated from the probe sequences and intensities, and represent all probes on an Affymetrix GeneChip array.

`[AffinPM, AffinMM, BaseProf, Stats] = affyprobeaffinities(SequenceMatrix, MMIntensity)` also returns `Stats`, a row vector containing four statistics in the following order:

- R-square statistic
- F statistic
- p-value
- Error variance

`... = affyprobeaffinities(SequenceMatrix, MMIntensity, ...'PropertyName', PropertyValue, ...)` calls `affyprobeaffinities` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = affyprobeaffinities(SequenceMatrix, MMIntensity, ...'ProbeIndices', ProbeIndicesValue, ...)` uses probe indices to normalize the probe intensities with the median of their probe set intensities.

Tip Use of the `ProbeIndices` property is recommended only if your `MMIntensity` data are not from a nonspecific binding experiment.

`... = affyprobeaffinities(SequenceMatrix, MMIntensity, ...'Showplot', ShowplotValue, ...)` controls the display of a plot of the probe affinity base profile. Choices are `true` or `false` (default).

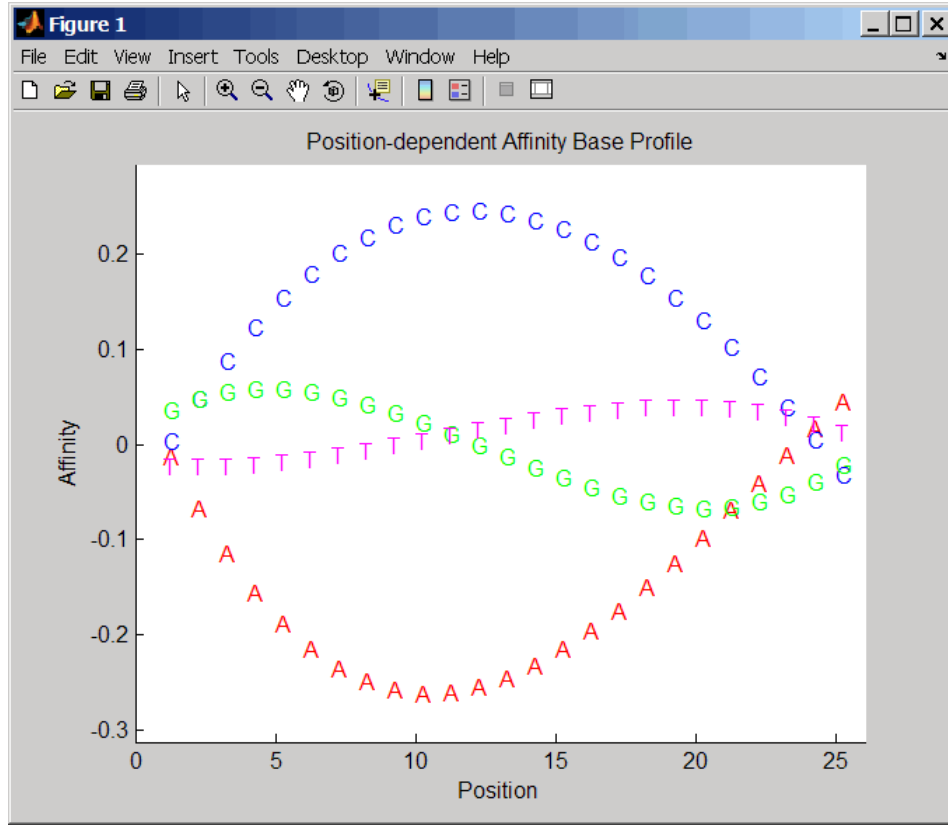
Examples

1. Load the MAT-file, included with the Bioinformatics Toolbox software, that contains Affymetrix data from a prostate cancer study. The variables in the MAT-file include `seqMatrix`, a matrix containing sequence information for PM probes, `mmMatrix`, a matrix containing MM probe intensity values, and `probeIndices`, a column vector containing probe indexing information.

   ```
   load prostatecancerrawdata
   ```

2. Compute the Affymetrix PM and MM probe affinities from their sequences and MM probe intensities, and also plot the affinity values of each of the four bases (A, C, G, and T) for each of the 25 sequence positions, for all probes on the Affymetrix GeneChip array.

   ```
   [apm, amm] = affyprobeaffinities(seqMatrix, mmMatrix(:,1),...
                'ProbeIndices', probeIndices, 'showplot', true);
   ```



The `prostatecancerrawdata.mat` file used in this example contains data from Best et al., 2005.

References

[1] Naef, F., and Magnasco, M.O. (2003). Solving the Riddle of the Bright Mismatches: Labeling and Effective Binding in Oligonucleotide Arrays. Physical Review E *68*, 011906.

[2] Wu, Z., Irizarry, R.A., Gentleman, R., Murillo, F.M. and Spencer, F. (2004). A Model Based Background Adjustment for Oligonucleotide

Expression Arrays. Journal of the American Statistical Association *99(468)*, 909–917.

[3] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L., Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan, W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823–6834.

See Also

Bioinformatics Toolbox functions: `affygcrma`, `affyprobeseqread`, `affyread`, `celintensityread`, `probelibraryinfo`

affyprobeseqread

Purpose

Read data file containing probe sequence information for Affymetrix GeneChip array

Syntax

```
Struct = affyprobeseqread(SeqFile, CDFFile)
Struct = affyprobeseqread(SeqFile, CDFFile, ...'SeqPath',
SeqPathValue, ...)
Struct = affyprobeseqread(SeqFile, CDFFile, ...'CDFPath',
   CDFPathValue, ...)
Struct = affyprobeseqread(SeqFile, CDFFile, ...'SeqOnly',
   SeqOnlyValue, ...)
```

Arguments

SeqFile

String specifying a file name of a sequence file (tab-separated or FASTA) that contains the following information for a specific type of Affymetrix GeneChip array:

- Probe set IDs
- Probe *x*-coordinates
- Probe *y*-coordinates
- Probe sequences in each probe set
- Affymetrix GeneChip array type (FASTA file only)

The sequence file (tab-separated or FASTA) must be on the MATLAB search path or in the Current Directory (unless you use the `SeqPath` property). In a tab-separated file, each row represents a probe; in a FASTA file, each header represents a probe.

CDFFile

Either of the following:

- String specifying a file name of an Affymetrix CDF library file, which contains information that specifies which probe set each probe belongs to on a specific type of Affymetrix GeneChip array. The

CDF library file must be on the MATLAB search path or in the MATLAB Current Directory (unless you use the `CDFPath` property).

- CDF structure, such as returned by the `affyread` function, which contains information that specifies which probe set each probe belongs to on a specific type of Affymetrix GeneChip array.

Caution Make sure that *`SeqFile`* and *`CDFFile`* contain information for the same type of Affymetrix GeneChip array.

`SeqPathValue` String specifying a directory or path and directory where *`SeqFile`* is stored.

`CDFPathValue` String specifying a directory or path and directory where *`CDFFile`* is stored.

`SeqOnlyValue` Controls the return of a structure, *`Struct`*, with only one field, `SequenceMatrix`. Choices are `true` or `false` (default).

Return Values

`Struct` MATLAB structure containing the following fields:

- `ProbeSetIDs`
- `ProbeIndices`
- `SequenceMatrix`

Description

`Struct` = `affyprobeseqread(`*`SeqFile`*`, `*`CDFFile`*`)` reads the data from files *`SeqFile`* and *`CDFFile`*, and stores the data in the MATLAB structure *`Struct`*, which contains the following fields.

Field	Description
`ProbeSetIDs`	Cell array containing the probe set IDs from the Affymetrix CDF library file.
`ProbeIndices`	Column vector containing probe indexing information. Probes within a probe set are numbered 0 through *N* - 1, where *N* is the number of probes in the probe set.
`SequenceMatrix`	An *N*-by-25 matrix of sequence information for the perfect match (PM) probes on the Affymetrix GeneChip array, where *N* is the number of probes on the array. Each row corresponds to a probe, and each column corresponds to one of the 25 sequence positions. Nucleotides in the sequences are represented by one of the following integers: • `0` — None • `1` — A • `2` — C • `3` — G • `4` — T **Note** Probes without sequence information are represented in `SequenceMatrix` as a row containing all `0`s. **Tip** You can use the `int2nt` function to convert the nucleotide sequences in `SequenceMatrix` to letter representation.

Struct = affyprobeseqread(*SeqFile*, *CDFFile*, ...'*PropertyName*', *PropertyValue*, ...) calls affyprobeseqread with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

Struct = affyprobeseqread(*SeqFile*, *CDFFile*, ...'SeqPath', *SeqPathValue*, ...) lets you specify a path and directory where *SeqFile* is stored.

Struct = affyprobeseqread(*SeqFile*, *CDFFile*, ...'CDFPath', *CDFPathValue*, ...) lets you specify a path directory where *CDFFile* is stored.

Struct = affyprobeseqread(*SeqFile*, *CDFFile*, ...'SeqOnly', *SeqOnlyValue*, ...) controls the return of a structure, *Struct*, with only one field, SequenceMatrix. Choices are true or false (default).

Examples

1. Read the data from a FASTA file and associated CDF library file, assuming both are located on the MATLAB search path or in the Current Directory.

```
S1 = affyprobeseqread('HG-U95A_probe_fasta', 'HG_U95A.CDF');
```

2. Read the data from a tab-separated file and associated CDF structure, assuming the tab-separated file is located in the specified directory and the CDF structure is in your MATLAB Workspace.

```
S2 = affyprobeseqread('HG-U95A_probe_tab',hgu95aCDFStruct,...
     'seqpath','C:\Affymetrix\SequenceFiles\HGGenome');
```

3. Access the nucleotide sequences of the first probe set (rows 1 through 20) in the SequenceMatrix field of the S2 structure.

```
seq = int2nt(S2.SequenceMatrix(1:20,:))
```

See Also

Bioinformatics Toolbox functions: `affygcrma`, `affyinvarsetnorm`, `affyread`, `celintensityread`, `int2nt`, `probelibraryinfo`, `probesetlink`, `probesetlookup`, `probesetplot`, `probesetvalues`

Purpose

Read microarray data from Affymetrix GeneChip file

Syntax

```
AffyStruct = affyread(File)
AffyStruct = affyread(File, LibraryPath)
```

Description

Note This function does not work on the Solaris platform.

AffyStruct = affyread(*File*) reads an Affymetrix file and creates a MATLAB structure. The affyread function can read Affymetrix EXP, DAT, CEL, CLF, BGP, CDF, and GIN files associated with Affymetrix GeneChip arrays for expression, genotyping (SNP), or resequencing assays. It can read Affymetrix CHP files associated with Affymetrix GeneChip arrays for expression assays only.

AffyStruct = affyread(*File*, *LibraryPath*) specifies the path and directory of a CDF or GIN library file.

Reading many CEL files and/or a large CEL file can require extended amounts of memory from the operating system. If you receive any errors related to memory or have trouble reading CEL files, try the following:

- Increase the virtual memory (swap space) for your operating system (with a recommended initial size of 3,069 and a maximum size of 16,368) as described at:

  http://www.mathworks.com/support/tech-notes/1100/1106.html#6

- Set the 3-GB switch (32-bit Windows® XP only) as described at:

  http://www.mathworks.com/support/tech-notes/1100/1107.html

For help resolving errors related to memory, see "Resolving "Out of Memory" Errors".

Inputs

File

String specifying a file name or a path and file name of one of the following Affymetrix file types associated with Affymetrix GeneChip arrays for expression, genotyping (SNP), or resequencing assays. However, if the file name is for a CHP file, it must be associated with an Affymetrix GeneChip array for an expression assay.

- **EXP** — Data file containing information about experimental conditions and protocols.
- **DAT** — Data file containing raw image data (pixel intensity values).
- **CEL** — Data file containing information about the intensity values of the individual probes.
- **CHP** — Data file containing summary information of the probe sets, including intensity values.
- **CLF** — Cell layout file that maps probe IDs to a location (*x*- and *y*-coordinates) in the CEL file.
- **BGP** — Background probe file that lists the probes to use for background correction.
- **CDF** — Library file containing information about which probes belong to which probe set.
- **GIN** — Library file containing information about the probe sets, such as the gene name associated with the probe set.

If you specify only a file name, put that file on the MATLAB search path or in the current directory. If you specify only a file name of a CDF or GIN library file, you can specify the path and directory in the *LibraryPath* input argument.

Tip You can learn more about the Affymetrix GeneChip files and download sample files from:

```
http://www.affymetrix.com/support/technical/sample_data/demo_data.affx
```

Note Some Affymetrix sample data files (DAT, EXP, CEL, and CHP) are combined in a DTT or CAB file. Download and use the Affymetrix Data Transfer Tool to extract these files from the DTT or CAB file. You can download the Data Transfer Tool from:

```
http://www.affymetrix.com/products/software/specific/dtt.affx
```

You will have to register and log in at the Affymetrix Web site to download the Data Transfer Tool.

`LibraryPath`

String specifying the path and directory of a:

- CDF library file associated with *`File`* when *`File`* is a CHP file
- CDF library file when *`File`* is a CDF file
- GIN library file when *`File`* is a GIN file

Note If you do not specify *`LibraryPath`* when reading a CHP file, `affyread` looks in the current directory for the CDF file. If it does not find the CDF file, it still reads the CHP file. However, it omits the probe set names and types from the return value, *`AffyStruct`*.

Outputs

AffyStruct

MATLAB structure containing information from an Affymetrix data or library file, for expression, genotyping (SNP), or resequencing assay types.

The following tables describe the fields in *AffyStruct* for the different Affymetrix file types.

EXP, DAT, CEL, CHP, CLF, BGP, CDF, and GIN Files

Field	Description
Name	File name.
DataPath	Path and directory of the file.
LibPath	Path and directory of the CDF and GIN library files associated with the file you are reading.
FullPathName	Path and directory of the file.
ChipType	Name of the Affymetrix GeneChip array (for example, DrosGenome1 or HG-Focus).
Date or CreateDate	File creation date.

EXP File

Field	Description
ChipLot Operator SampleType SampleDesc Project Comments Reagents ReagentLot	Information about experimental conditions and protocols captured by the Affymetrix software.

EXP File (Continued)

Field	Description
Protocol	
Station	
Module	
HybridizeDate	
ScanPixelSize	
ScanFilter	
ScanDate	
ScannerID	
NumberOfScans	
ScannerType	
NumProtocolSteps	
ProtocolSteps	

DAT File

Field	Description
NumPixelsPerRow	Number of pixels per row in the image created from the GeneChip array (number of columns).
NumRows	Number of rows in the image created from the GeneChip array.
MinData	Minimum intensity value in the image created from the GeneChip array.
MaxData	Maximum intensity value in the image created from the GeneChip array.
PixelSize	Size of one pixel in the image created from the GeneChip array.
CellMargin	Size of gaps between cells in the image created from the GeneChip array.

DAT File (Continued)

Field	Description
`ScanSpeed`	Speed of the scanner used to create the image.
`ScanDate`	Date the scan was performed.
`ScannerID`	Name of the scanning device used.

`UpperLeftX`
`UpperLeftY`
`UpperRightX`
`UpperRightY`
`LowerLeftX`
`LowerLeftY`
`LowerRightX`
`LowerRightY`
	Pixel coordinates of the scanned image.

`ServerName`	Not used.
`Image`	A `NumRows`-by-`NumPixelsPerRow` image of the scanned GeneChip array.

CEL File

Field	Description
`FileVersion`	Version of the CEL file format.
`Algorithm`	Algorithm used in the image-processing step that converts from DAT format to CEL format.
`AlgParams`	String containing parameters used by the algorithm in the image-processing step.
`NumAlgParams`	Number of parameters in `AlgParams`.

CEL File (Continued)

Field	Description
`CellMargin`	Size of gaps between cells in the image created from the GeneChip array, used for computing the intensity values of the cells.
`Rows`	Number of rows of probes.
`Cols`	Number of columns of probes.
`NumMasked`	Number of masked probes, which are not used in subsequent processing.
`NumOutliers`	Number of cells identified as outliers (extremely high or extremely low intensity) by the image-processing step.
`NumProbes`	Number of probes (`Rows * Cols`) on the GeneChip array.

`UpperLeftX`
`UpperLeftY`
`UpperRightX`
`UpperRightY`
`LowerLeftX`
`LowerLeftY`
`LowerRightX`
`LowerRightY`
	Pixel coordinates of the scanned image.

CEL File (Continued)

Field	Description
`ProbeColumnNames`	Cell array containing the eight column names in the `Probes` field: • `PosX` — *x*-coordinate of the cell • `PosY` — *y*-coordinate of the cell • `Intensity` — Intensity value of the cell • `StdDev` — Standard deviation of intensity value • `Pixels` — Number of pixels in the cell • `Outlier` — True/false flag indicating if the cell was marked as an outlier • `Masked` — True/false flag indicating if the cell was masked • `ProbeType` — Integer indicating the probe type (for example, `1` = expression)
`Probes`	`NumProbes`-by-8 array of information about the individual probes, including intensity values. The `ProbeColumnNames` field contains the column names of this array.

CHP File

Field	Description
`AssayType`	Type of assay associated with the GeneChip array (for example, Expression, Genotyping, or Resequencing).
`CellFile`	File name of the CEL file from which the CHP file was created.
`Algorithm`	Algorithm used to convert from CEL format to CHP format.

CHP File (Continued)

Field	Description
`AlgVersion`	Version of the algorithm used to create the CHP file.
`NumAlgParams`	Number of parameters in `AlgParams`.
`AlgParams`	String containing parameters used in steps required to create the CHP file (for example, background correction).
`NumChipSummary`	Number of entries in `ChipSummary`.
`ChipSummary`	Summary information for the GeneChip array, including background average, standard deviation, max, and min.
`BackgroundZones`	Structure containing information about the zones used in the background adjustment step.
`Rows`	Number of rows of probes.
`Cols`	Number of columns of probes.
`NumProbeSets`	Number of probe sets on the GeneChip array.
`NumQCProbeSets`	Number of QC probe sets on the GeneChip array.
`ProbeSets` (Expression GeneChip array)	`NumProbeSets`-by-1 structure array containing information for each expression probe set, including the following fields: • `Name` — Name of the probe set. • `ProbeSetType` — Type of the probe set. • `CompDataExists` — True/false flag indicating if the probe set has additional computed information. • `NumPairs` — Number of probe pairs in the probe set. • `NumPairsUsed` — Number of probe pairs in the probe set used for calculating the probe set signal (not masked). • `Signal` — Summary intensity value for the probe set. • `Detection` — Indicator of statistically significant difference between the intensity value of the PM probes and the

CHP File (Continued)

Field	Description
	intensity value of the MM probes in a single probe set (`Present`, `Absent`, or `Marginal`). • `DetectionPValue` — P-value for the `Detection` indicator. • `CommonPairs` — When `CompDataExists` is `true`, contains the number of common pairs between the experiment and the baseline after the removal of outliers and masked probes. • `SignalLogRatio` — When `CompDataExists` is `true`, contains the change in signal between the experiment and baseline. • `SignalLogRatioLow` — When `CompDataExists` is `true`, contains the lowest ratios of probes between the experiment and the baseline. • `SignalLogRatioHigh` — When `CompDataExists` is `true`, contains the highest ratios of probes between the experiment and the baseline. • `Change` — When `CompDataExists` is `true`, describes how the probe changes versus a baseline experiment. Choices are `Increase`, `Marginal Increase`, `No Change`, `Decrease`, or `Marginal Decrease`. • `ChangePValue` — When `CompDataExists` is `true`, contains the p-value associated with `Change`.

CHP File (Continued)

Field	Description
`ProbeSets` (Genotyping GeneChip array)	`NumProbeSets`-by-1 structure array containing information for each genotyping probe set, including the following fields: • `Name` — Name of the probe set. • `AlleleCall` — Allele that is present for the probe set. Possibilities are `AA` (homozygous for the major allele), `AB` (heterozygous for the major and minor allele), `BB` (homozygous for the minor allele), or `NoCall` (unable to determine allele). • `Confidence` — Measure of the accuracy of the allele call. • `RAS1` — Relative Allele Signal 1 for the SNP site, which is calculated using sense probes. • `RAS2`— Relative Allele Signal 2 for the SNP site, which is calculated using antisense probes. • `PValueAA` — p-value for an `AA` call. • `PValueAB` — p-value for an `AB` call. • `PValueBB` — p-value for a `BB` call. • `PValueNoCall` — p-value for a `NoCall` call.
`ProbeSets` (Resequencing GeneChip array)	`NumProbeSets`-by-1 structure array containing information for each resequencing probe set, including the following fields: • `CalledBases` — 1-by-`NumProbeSets` character array containing the bases called by the resequencing algorithm. Possible values are `a`, `c`, `g`, `t`, and `n`. • `Scores` — 1-by-`NumProbeSets` array containing the score associated with each base call.

CLF File

Field	Description
`LibSetName`	Name of a collection of related library files for a given chip. There is only one `LibSetName` for a CLF file. For example, PGF and CLF files intended for use together must have the same `LibSetName`.
`LibSetVersion`	Version of a collection of related library files for a given chip. There is only one `LibSetVersion` for a CLF file. For example, PGF and CLF files intended for use together must have the same `LibSetVersion`.
`GUID`	Unique identifier for the CLF file.
`CLFFormatVersion`	Version of the CLF file format.
`Rows`	Number of rows in the CEL file. **Note** The CLF file is 1 base, which means the first row and column are designated 1,1, not 0,0.
`Cols`	Number of columns in the CEL file. **Note** The CLF file is 1 base, which means the first row and column are designated 1,1, not 0,0.

CLF File (Continued)

Field	Description
`StartID`	Starting number for the numbering of elements in the CLF file. **Tip** This information is useful when numbering does not start with 1.
`EndID`	Ending number for the numbering of elements in the CLF file. **Tip** This information is useful when numbering does not start with 1 and/or there are gaps in the numbering.
`Order`	Order in which the probe IDs are numbered in the CEL file, either `'row_major'` or `'col_major'`.
`DataColNames`	Names of the columns in the CEL file that contain data.
`Data`	If the numbering of elements in the CLF file is sequential, this field contains a function handle that calculates the *x*- and *y*-coordinates of each element in the file from the probe ID. If the numbering of elements in the CLF file is not sequential, this field contains a matrix indicating the number value of each element in the file.

BGP File

Field	Description
`LibSetName`	Name of a collection of related library files for a given chip. There is only one `LibSetName` for a BGP file.
`LibSetVersion`	Version of a collection of related library files for a given chip. There is only one `LibSetVersion` for a BGP file.
`GUID`	Unique identifier for a BGP file.
`ExecGUID`	Information about the algorithm used to generate the BGP file.
`ExecVersion`	
`Cmd`	
`Data`	Structure containing the following fields: • `probe_id` — ID of the probe to use for background correction. • `probeset_id` — ID of the probe set in the PGF file to which the probe belongs. • `type` — Classification information for the probe. • `gc_count` — Combined number of G and C bases in the probe. • `probe_length`— Length of the probe in base pairs. • `interrogation_position` — Interrogation position of the probe. It is typically 13 for 25-mer PM/MM probes. • `probe_sequence` — Sequence of the probe on the array, going in the direction from array surface to solution. For most standard Affymetrix arrays, this direction is from 3’

BGP File (Continued)

Field	Description
	to 5'. For example, for a sense target (st) probe (see the `probe_type` field), complement the sequence in this field before looking for matches to transcript sequences. For an antisense target (at), reverse this sequence. • `atom_id` — ID of the atom to which the probe belongs. • `x` — Column coordinate of the probe in the CEL file. • `y` — Row coordinate of the probe in the CEL file. • `probeset_type` — Classification information for the probe set, such as control, affx, or spike. This type information can include multiple classifications and can also be nested. • `probe_type` — Classification information for the probe, such as pm (perfect match), mm (mismatch), st (sense target), or at (antisense target). This type information can include multiple classifications and can also be nested.

CDF File

Field	Description
`Rows`	Number of rows of probes.
`Cols`	Number of columns of probes.

CDF File (Continued)

Field	Description
`NumProbeSets`	Number of probe sets on the GeneChip array.
`NumQCProbeSets`	Number of QC probe sets on the GeneChip array.
`ProbeSetColumnNames`	Cell array containing the six column names in the `ProbePairs` field in the `ProbeSets` array: • `GroupNumber` — Number identifying the group to which the probe pair belongs. For expression arrays, this value is always `1`. For genotyping arrays, this value is typically `1` (allele A, sense), `2` (allele B, sense), `3` (allele A, antisense), or `4` (allele B, antisense). • `Direction` — Number identifying the direction of the probe pair. `1` = sense and `2` = antisense. • `PMPosX` — *x*-coordinate of the perfect match probe. • `PMPosY` — *y*-coordinate of the perfect match probe. • `MMPosX` — *x*-coordinate of the mismatch probe. • `MMPosY` — *y*-coordinate of the mismatch probe.
`ProbeSets`	`NumProbeSets`-by-1 structure array containing information for each probe set, including the following fields: • `Name` — Name of the probe set. • `ProbeSetType` — Type of the probe set. • `CompDataExists` — True/false flag indicating if the probe set has additional computed information. • `NumPairs` — Number of probe pairs in the probe set. • `NumQCProbes` — Number of QC probes in the probe set. • `QCType` — Type of QC probes.

CDF File (Continued)

Field	Description
	• `GroupNames` — Name of the group to which the probe set belongs. For expression arrays, this field contains the name of the probe set. For genotyping arrays, this field contains the name of the alleles, for example `{'A' 'C' 'A' 'C'}'`. • `ProbePairs` — `NumPairs`-by-6 array of information about the probe pairs. The column names of this array are contained in the `ProbeSetColumnNames` field.

GIN File

Field	Description
`Version`	GIN file format version.
`ProbeSetName`	Probe set ID/name.
`ID`	Identifier for the probe set (gene ID).
`Description`	Description of the probe set.
`SourceNames`	Source or sources of the probe sets.
`SourceURL`	Source URL or URLs for the probe sets.
`SourceID`	Vector of numbers specifying which `SourceNames` or `SourceURL` each probe set is associated with.

Examples

The following example uses the demo data and CDF library file from the *E. coli* Antisense Genome array, which you can download from:

```
http://www.affymetrix.com/support/technical/sample_data/demo_data.affx
```

After downloading the demo data, you need the Affymetrix Data Transfer Tool to extract the CEL, DAT, and CHP files from a DTT file. You can download the Data Transfer Tool from:

```
http://www.affymetrix.com/products/software/specific/dtt.affx
```

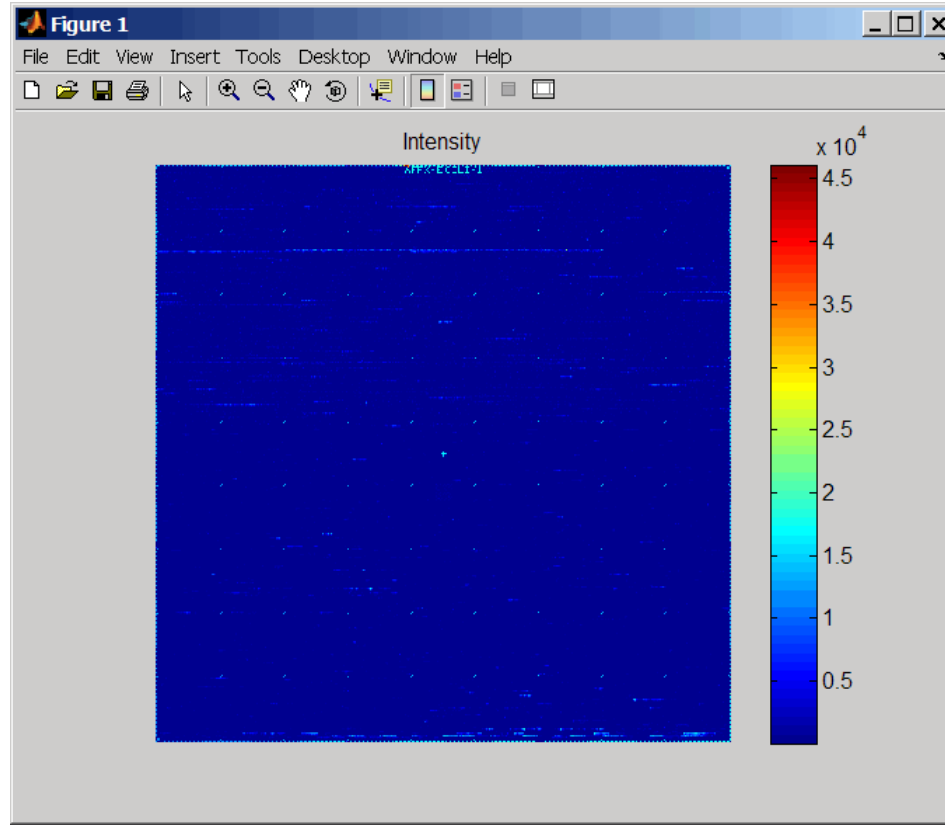
The following example assumes that you have stored the files `Ecoli-antisense-121502.CEL`, `Ecoli-antisense-121502.dat`, and `Ecoli-antisense-121502.chp` on the MATLAB search path or in the current directory. It also assumes that you have stored the associated CDF library file, `Ecoli_ASv2.CDF`, at `D:\Affymetrix\LibFiles\Ecoli`.

1 Read the contents of a CEL file into a MATLAB structure.

```
celStruct = affyread('Ecoli-antisense-121502.CEL');
```

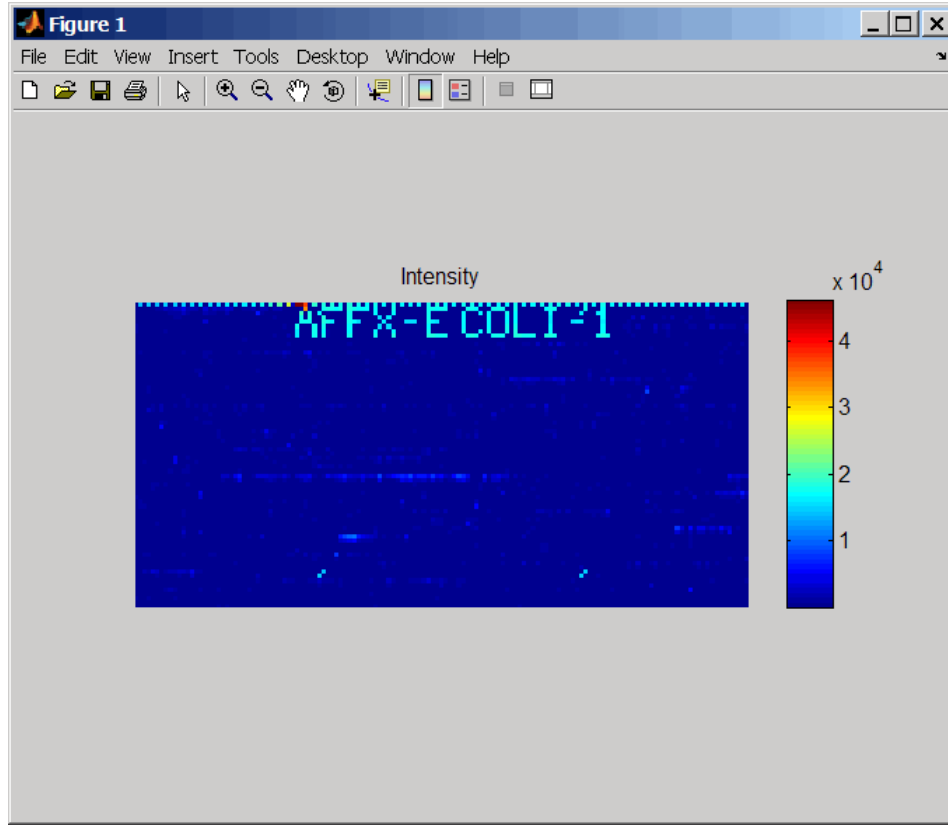
2 Display a spatial plot of the probe intensities.

```
maimage(celStruct, 'Intensity')
```



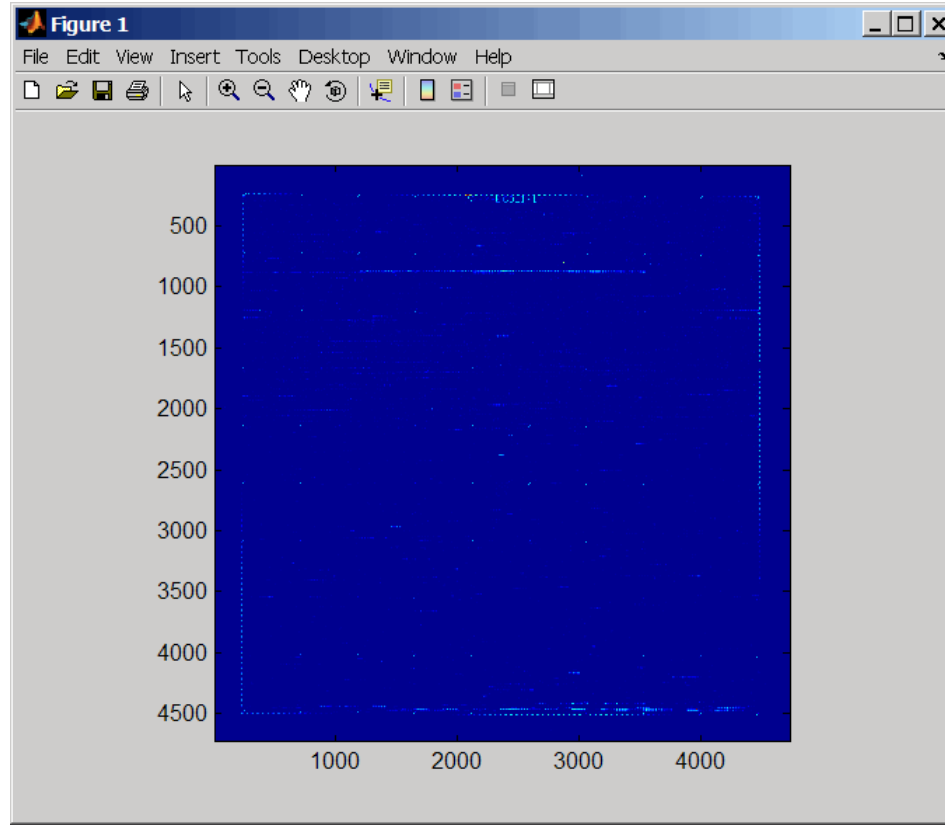
3 Zoom in on a specific region of the plot.

```
axis([200 340 0 70])
```



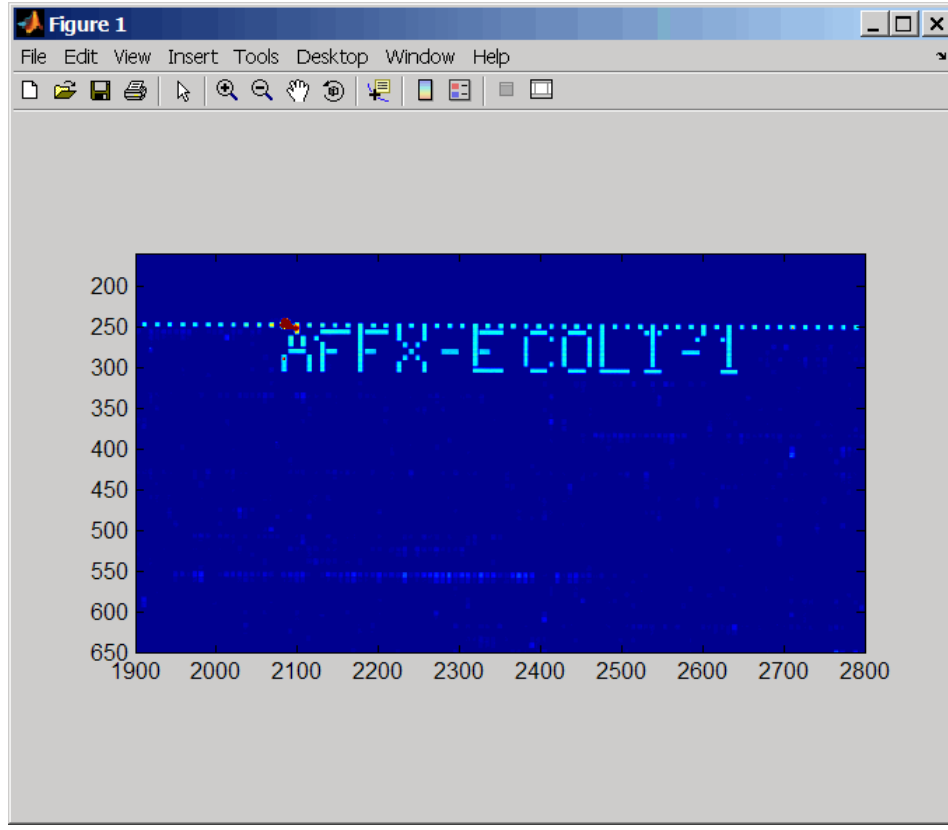
4 Read the contents of a DAT file into a MATLAB structure. Display the raw image data, and then use the `axis image` function to set the correct aspect ratio.

```
datStruct = affyread('Ecoli-antisense-121502.dat');
imagesc(datStruct.Image)
axis image
```



5 Zoom in on a specific region of the plot.

```
axis([1900 2800 160 650])
```



6 Read the contents of a CHP file into a MATLAB structure, specifying the location of the associated CDF library file. Then extract information for probe set `3315278`.

```
chpStruct = affyread('Ecoli-antisense-121502.chp',...
            'D:\Affymetrix\LibFiles\Ecoli');
geneName = probesetlookup(chpStruct,'3315278')

geneName =
```

```
          Identifier: '3315278'
        ProbeSetName: 'argG_b3172_at'
           CDFIndex: 5213
           GINIndex: 3074
         Description: [1x82 char]
              Source: 'NCBI EColi Genome'
           SourceURL: [1x74 char]
```

See Also

affyrma | affygcrma | affysnpannotread | affysnpintensitysplit | agferead | celintensityread | geoseriesread | gprread | ilmnbsread | probelibraryinfo | probesetlink | probesetlookup | probesetplot | probesetvalues | sptread

Tutorials

- Working with AffymetrixData
- Preprocessing AffymetrixMicroarray Data at the Probe Level

How To

- "Resolving "Out of Memory" Errors"

Related Links

-
-
-
-

Purpose

Perform Robust Multi-array Average (RMA) procedure on Affymetrix microarray probe-level data

Syntax

```
Expression = affyrma(CELFiles, CDFFile)
Expression = affyrma(ProbeStructure)
Expression = affyrma(CELFiles, CDFFile, ...'CELPath',
CELPathValue, ...)
Expression = affyrma(CELFiles, CDFFile, ...'CDFPath',
   CDFPathValue, ...)
Expression = affyrma(..., 'Method', MethodValue, ...)
Expression = affyrma(..., 'Truncate', TruncateValue, ...)
Expression = affyrma(..., 'Median', MedianValue, ...)
Expression = affyrma(..., 'Output', OutputValue, ...)
Expression = affyrma(..., 'Showplot', ShowplotValue, ...)
Expression = affyrma(..., 'Verbose', VerboseValue, ...)
```

Arguments

CELFiles — Any of the following:

- String specifying a single CEL file name.
- `'*'`, which reads all CEL files in the current directory.
- `' '`, which opens the Select CEL Files dialog box from which you select the CEL files. From this dialog box, you can press and hold **Ctrl** or **Shift** while clicking to select multiple CEL files.
- Cell array of CEL file names.

CDFFile — Either of the following:

- String specifying a CDF file name.
- `' '`, which opens the Select CDF File dialog box from which you select the CDF file.

ProbeStructure	MATLAB structure containing information from the CEL files, including probe intensities, probe indices, and probe set IDs, returned by the `celintensityread` function.
CELPathValue	String specifying the path and directory where the files specified in *CELFiles* are stored.
CDFPathValue	String specifying the path and directory where the file specified in *CDFFile* is stored.
MethodValue	Specifies the estimation method for the background adjustment model parameters. Choices are `'RMA'` (to use estimation method described by Bolstad, 2005) or `'MLE'` (to estimate the parameters using maximum likelihood). Default is `'RMA'`.
TruncateValue	Specifies the background noise model. Choices are `true` (use a truncated Gaussian distribution) or `false` (use a nontruncated Gaussian distribution). Default is `true`.
MedianValue	Specifies the use of the median of the ranked values instead of the mean for normalization. Choices are `true` or `false` (default).

OutputValue Specifies the scale of the returned gene expression values. Choices are:

- `'log'`
- `'log2'`
- `'log10'`
- `'natural'`
- `@`*`functionname`*

In the last instance, the data is transformed as defined by the function *`functionname`*. Default is `'log2'`.

ShowplotValue Controls the plotting of a histogram showing the distribution of PM probe intensity values (blue) and the convoluted probability distribution function (red), with estimated parameters mu, sigma and alpha. Enter either `'all'` (plot a histogram for each column or chip) or specify a subset of columns (chips) by entering the column number, list of numbers, or range of numbers.

For example:

- `(..., 'Showplot', 3, ...)` plots the intensity values in column 3.
- `(..., 'Showplot', [3,5,7], ...)` plots the intensity values in columns 3, 5, and 7.
- `(..., 'Showplot', 3:9, ...)` plots the intensity values in columns 3 to 9.

VerboseValue Controls the display of the status of the reading of files and RMA processing. Choices are `true` (default) or `false`.

Return Values

Expression	DataMatrix object containing the $\log_2$ based gene expression values that have been background adjusted, normalized, and summarized using the Robust Multi-array Average (RMA) procedure. Each row in *Expression* corresponds to a gene (probe set), and each column corresponds to an Affymetrix CEL file.

Description

Note This function does not work on the Solaris platform.

Expression = affyrma(*CELFiles*, *CDFFile*) reads the specified Affymetrix CEL files and the associated CDF library file (created from Affymetrix GeneChip arrays for expression or genotyping assays), processes the probe intensity values using RMA background adjustment, quantile normalization, and summarization procedures, then returns *Expression*, a DataMatrix object containing the $\log_2$ based gene expression values in a matrix, the probe set IDs as row names, and the CEL file names as column names. Note that each row in *Expression* corresponds to a gene (probe set), and each column corresponds to an Affymetrix CEL file. (Each CEL file is generated from a separate chip. All chips should be of the same type.)

CELFiles is a string or cell array of CEL file names. *CDFFile* is a string specifying a CDF file name. If you set *CELFiles* to '*', then it reads all CEL files in the current directory. If you set *CELFiles* to ' ', then it opens the Select CEL Files dialog box from which you select the CEL files.

Note For details on the reading of files and RMA processing, see celintensityread, rmabackadj, quantilenorm, and rmasummary.

Expression = affyrma(*ProbeStructure*) uses RMA background adjustment, quantile normalization, and summarization procedures to process the probe intensity values in *ProbeStructure*, a MATLAB structure containing information from the CEL files, including probe intensities, probe indices, and probe set IDs, returned by the celintensityread function, and returns *Expression*.

Expression = affyrma(..., '*PropertyName*', *PropertyValue*, ...) calls affyrma with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

Expression = affyrma(*CELFiles*, *CDFFile*, ...'CELPath', *CELPathValue*, ...) specifies a path and directory where the files specified by *CELFiles* are stored.

Expression = affyrma(*CELFiles*, *CDFFile*, ...'CDFPath', *CDFPathValue*, ...) specifies a path and directory where the file specified by *CDFFile* is stored.

Expression = affyrma(..., 'Method', *MethodValue*, ...) specifies the estimation method for the background adjustment model parameters. When *MethodValue* is 'RMA', affyrma implements the estimation method described by Bolstad, 2005. When *MethodValue* is 'MLE', affyrma estimates the parameters using maximum likelihood. Default is 'RMA'.

Expression = affyrma(..., 'Truncate', *TruncateValue*, ...) specifies the background noise model used. When *TruncateValue* is false, affyrma uses nontruncated Gaussian as the background noise model. Default is true.

Expression = affyrma(..., 'Median', *MedianValue*, ...) specifies the use of the median of the ranked values instead of the mean for normalization. Choices are true or false (default).

Expression = affyrma(..., 'Output', *OutputValue*, ...) specifies the scale of the returned gene expression values. *OutputValue* can be:

- 'log'
- 'log2'
- 'log10'
- 'natural'
- @*functionname*

In the last instance, the data is transformed as defined by the function *functionname*. Default is 'log2'.

Expression = affyrma(..., 'Showplot', *ShowplotValue*, ...) lets you plot a histogram showing the distribution of PM probe intensity values (blue) and the convoluted probability distribution function (red), with estimated parameters mu, sigma and alpha. When *ShowplotValue* is 'all', rmabackadj plots a histogram for each column or chip. When *ShowplotValue* is a number, list of numbers, or range of numbers, rmabackadj plots a histogram for the indicated column number (chip).

For example:

- (..., 'Showplot', 3,...) plots the intensity values in column 3.
- (..., 'Showplot', [3,5,7],...) plots the intensity values in columns 3, 5, and 7.
- (..., 'Showplot', 3:9,...) plots the intensity values in columns 3 to 9.

Expression = affyrma(..., 'Verbose', *VerboseValue*, ...) controls the display of the status of the reading of files and RMA processing. Choices are true (default) or false.

Examples

The following example assumes that you have the HG_U95Av2.CDF library file stored at D:\Affymetrix\LibFiles\HGGenome, and that

your current directory points to a location containing CEL files associated with this CDF library file. In this example, the `affyrma` function reads all the CEL files in the current directory and a CDF file in a specified directory. It also performs RMA background adjustment, quantile normalization, and summarization procedures on the PM probe intensity values, and returns a DataMatrix object, containing the metadata and processed data.

```
Expression = affyrma('*', 'HG_U95Av2.CDF',...
                     'CDFPath', 'D:\Affymetrix\LibFiles\HGGenome');
```

References

[1] Irizarry, R.A., Hobbs, B., Collin, F., Beazer-Barclay, Y.D., Antonellis, K.J., Scherf, U., Speed, T.P. (2003). Exploration, Normalization, and Summaries of High Density Oligonucleotide Array Probe Level Data. Biostatistics. *4*, 249–264.

[2] Mosteller, F., and Tukey, J. (1977). Data Analysis and Regression (Reading, Massachusetts: Addison-Wesley Publishing Company), pp. 165–202.

[3] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L., Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan, W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823–6834.

[4] Bolstad, B. (2005). "affy: Built-in Processing Methods" `http://www.bioconductor.org/packages/2.1/bioc/vignettes/affy/inst/doc/builtinMethods.pdf`

See Also

`affygcrma`, `celintensityread`, `gcrma`, `mafdr`, `mattest`, `quantilenorm`, `rmabackadj`, `rmasummary`

Purpose

Read Affymetrix Mapping DNA array data from CSV-format annotation file

Syntax

```
AnnotStruct = affysnpannotread(File, PID)
AnnotStruct = affysnpannotread(File, PID, 'LookUpField',
   LookUpFieldValue)
```

Arguments

File	String specifying a file name or a path and file name of an Affymetrix CSV annotation file for a Mapping 10K array set, Mapping 100K array set, or Mapping 500K array set. If you specify only a file name, that file must be on the MATLAB search path or in the current directory.
PID	String or cell array of strings specifying one or more probe set IDs on an Affymetrix mapping array.
LookUpFieldValue	String or cell array of strings specifying one or more column headers in an Affymetrix CSV annotation file. Default are the fields shown in the following table.

Return Values

AnnotStruct	MATLAB structure containing information for one or more probe sets from *File*, an Affymetrix CSV annotation file. *AnnotStruct* contains a subset of the fields in *File*. The fields are described in the table below.

Description

AnnotStruct = affysnpannotread(*File*, *PID*) reads *File*, an Affymetrix CSV annotation file for a Mapping 10K array set, Mapping 100K array set, or Mapping 500K array set, and returns *AnnotStruct*,

a MATLAB structure containing annotation information for one or more probe sets specified by *PID*, a string or cell array of strings specifying one or more probe set IDs. *AnnotStruct* contains a subset of the fields in *File*. The fields are described in the following table.

Structure Created from an Affymetrix CSV Annotation File

Field	Description
ProbeSetIDs	Cell array containing the unique probe set IDs specified by the *PID* input.
Chromosome	Cell array containing the chromosome number on which each probe set is located.
ChromPosition	Cell array containing the SNP genomic position on the chromosome for each probe set.
Cytoband	Cell array containing the cytogenetic banding region of the chromosome on which each probe set is located.
Sequence	Cell array containing the sequence of each probe set.
AlleleA	Cell array containing the base that is allele A for each probe set.
AlleleB	Cell array containing the base that is allele B for each probe set.
Accession	Cell array containing the GenBank accession number for each probe set.
FragmentLength	Cell array containing the length of each probe set.

AnnotStruct = affysnpannotread(*File*, *PID*, 'LookUpField', *LookUpFieldValue*) returns annotation information from only the field (column) specified by *LookUpFieldValue*, a string or cell array of strings specifying one or more column headers in an Affymetrix CSV annotation file. Default are the fields shown in the previous table.

Note You can download Affymetrix CSV annotation files such as `Mapping50K_Xba240.na25.annot.csv` from:

```
http://www.affymetrix.com/support/technical/annotationfilesmain.affx
```

Examples

The following example assumes that you have the `Mapping50K_Xba240.CDF` file stored at `C:\AffyLibFiles\`, and that your current directory points to a location containing the `Mapping50K_Xba240.na25.annot.csv` annotation file.

1. Use the `affyread` function to create a structure containing information from the `Mapping50K_Xba240.CDF` library file.

```
cdf = affyread('C:\AffyLibFiles\Mapping50K_Xba240.CDF');
```

2. Create a variable containing a cell array of the names of the probe sets, which are stored in the `Name` field of the `ProbeSets` field of the `cdf` structure.

```
probesetIDs = {cdf.ProbeSets.Name}';
```

3. Return a structure containing annotation information for all the probe sets in the `Mapping50K_Xba240.na25.annot.csv` annotation file.

```
snpInfo = affysnpannotread('Mapping50K_Xba240.na25.annot.csv',probesetIDs)

snpInfo =

       ProbeSetIDs: {59024x1 cell}
        Chromosome: [59024x1 int8]
     ChromPosition: [59024x1 double]
          Cytoband: {59024x1 cell}
          Sequence: {59024x1 cell}
           AlleleA: {59024x1 cell}
```

```
          AlleleB: {59024x1 cell}
        Accession: {59024x1 cell}
    FragmentLength: [59024x1 double]
```

See Also

Bioinformatics Toolbox functions: `affysnpintensitysplit`, `affyread`

Purpose

Split Affymetrix SNP probe intensity information for alleles A and B

Syntax

```
ProbeStructSplit = affysnpintensitysplit(ProbeStruct)
ProbeStructSplit = affysnpintensitysplit(ProbeStruct,
   'Controls', ControlsValue)
```

Arguments

ProbeStruct	MATLAB structure containing probe intensity information from an Affymetrix Mapping DNA array, such as returned by `celintensityread`.
ControlsValue	Controls the inclusion of control probes in *ProbeStructSplit*. Choices are `true` or `false` (default).

Return Values

ProbeStructSplit	MATLAB structure containing probe intensity information from an Affymetrix Mapping DNA array, split into information for alleles A and B.

Description

ProbeStructSplit = `affysnpintensitysplit(`*ProbeStruct*`)` splits *ProbeStruct*, a structure containing probe intensity information from an Affymetrix Mapping DNA array, into *ProbeStructSplit*, a structure containing probe intensity information from an Affymetrix Mapping DNA array, split into information for alleles A and B.

ProbeStructSplit contains the following fields.

Field	Description
`CDFName`	File name of the Affymetrix CDF library file.
`CELNames`	Cell array of names of the Affymetrix CEL files.
`NumChips`	Number of CEL files read into the input structure.

Field	Description
`NumProbeSets`	Number of probe sets in each CEL file.
`NumProbes`	Maximum number of probes for just one allele in each CEL file. **Note** If the number of probes for allele A is not the same as for allele B, the larger number is used.
`ProbeSetIDs`	Cell array of the probe set IDs from the Affymetrix CDF library file.
`ProbeIndices`	Column vector containing probe indexing information for just one allele in each cell file. Probes within a probe set are numbered `0` through `N - 1`, where `N` is the number of probes for one allele in the probe set. **Note** `ProbeIndices` has the same number of elements as `NumProbes`.
`PMAIntensities`	Matrix containing perfect match (PM) probe intensity values for allele A. Each row corresponds to an allele A probe, and each column corresponds to a CEL file. The rows are ordered the same way as in `ProbeIndices`, and the columns are ordered the same way as in the *`CELFiles`* input argument to the `celintensityread` function.

Field	Description
`PMBIntensities`	Matrix containing perfect match (PM) probe intensity values for allele B. Each row corresponds to an allele B probe, and each column corresponds to a CEL file. The rows are ordered the same way as in `ProbeIndices`, and the columns are ordered the same way as in the *`CELFiles`* input argument to the `celintensityread` function.
`MMAIntensities` (optional)	Matrix containing mismatch (MM) probe intensity values for allele A. Each row corresponds to an allele A probe, and each column corresponds to a CEL file. The rows are ordered the same way as in `ProbeIndices`, and the columns are ordered the same way as in the *`CELFiles`* input argument to the `celintensityread` function.
`MMBIntensities` (optional)	Matrix containing mismatch (MM) probe intensity values for allele B. Each row corresponds to an allele B probe, and each column corresponds to a CEL file. The rows are ordered the same way as in `ProbeIndices`, and the columns are ordered the same way as in the *`CELFiles`* input argument to the `celintensityread` function.

`ProbeStructSplit` `= affysnpintensitysplit(`*`ProbeStruct`*`, 'Controls', `*`ControlsValue`*`)` controls the return of control probe intensities. Choices are `true` or `false` (default).

Note Control probes sometimes contain information for only one allele. In this case, the value for the corresponding allele (A or B) that is not present is set to NaN.

Examples

The following example assumes that your current directory points to a location containing the `Mapping50K_Hind240.CDF` library file and 18 CEL files associated with this CDF library file. These files are associated with an Affymetrix Mapping DNA array.

1. Use the `celintensityread` function to read the `Mapping50K_Hind240.CDF` library file and 18 CEL files associated with it into a MATLAB structure.

```
ps = celintensityread('*','Mapping50K_Hind240.CDF')

ps =

          CDFName: 'Mapping50K_Hind240.CDF'
         CELNames: {18x1 cell}
         NumChips: 18
     NumProbeSets: 57299
        NumProbes: 1145780
      ProbeSetIDs: {57299x1 cell}
     ProbeIndices: [1145780x1 uint8]
     GroupNumbers: [1145780x1 uint8]
    PMIntensities: [1145780x18 single]
```

2. Extract the PM probe intensities for allele A and allele B into another MATLAB structure, without including intensity information for the control probes.

```
ps_split = affysnpintensitysplit(ps)

ps_split =

           CDFName: 'Mapping50K_Hind240.CDF'
          CELNames: {18x1 cell}
          NumChips: 18
      NumProbeSets: 57275
         NumProbes: 572750
       ProbeSetIDs: {57275x1 cell}
      ProbeIndices: [572750x1 uint8]
```

```
        PMAIntensities: [572750x18 single]
        PMBIntensities: [572750x18 single]
```

See Also

Bioinformatics Toolbox functions: `affysnpannotread`, `affyread`, `celintensityread`

affysnpquartets

Purpose

Create table of SNP probe quartet results for Affymetrix probe set

Syntax

```
SNPQStruct = affysnpquartets(CELStruct, CDFStruct, PS)
```

Arguments

CELStruct	Structure created by the `affyread` function from an Affymetrix CEL file, which contains information about the intensity values of the individual probes.
CDFStruct	Structure created by the `affyread` function from an Affymetrix CDF library file associated with the CEL file. The CDF library file contains information about which probes belong to which probe set.
PS	Probe set index or the probe set ID/name.

Return Values

SNPQStruct	Structure containing probe quartet results for a specific SNP probe set from the data in a CEL file and associated CDF library file.

Description

SNPQStruct = affysnpquartets(*CELStruct*, *CDFStruct*, *PS*) creates *SNPQStruct*, a structure containing probe quartet results for a specific SNP probe set, specified by *PS*, from the probe-level data in a CEL file and associated CDF library file. *CELStruct* is a structure created by the `affyread` function from an Affymetrix CEL file. *PS* is a probe set index or probe set ID/name from *CDFStruct*, a structure created by the `affyread` function from an Affymetrix CDF library file associated with the CEL file. *SNPQStruct* is a structure containing the following fields.

Field	Description
`'ProbeSet'`	Identifier for the probe set.
`'AlleleA'`	String specifying the base that is allele A for the probe set.

Field	Description
'AlleleB'	String specifying the base that is allele B for the probe set.
'Quartet'	Structure array containing intensity values for PM (perfect match) and MM (mismatch) probe pairs, including the sense and antisense probes for alleles A and B. Each structure in the array corresponds to a probe pair in the probe set.

Examples

The following example uses the NA06985_Hind_B5_3005533.CEL file. You can download this and other sample CEL files from:

```
http://www.affymetrix.com/support/technical/sample_data/hapmap_trio_data.affx
```

The NA06985_Hind_B5_3005533.CEL file is included in the 100K_trios.hind.1.zip file.

The following example uses the CDF library file for the Mapping 50K Hind 240 array, which you can download from:

```
http://www.affymetrix.com/support/technical/byproduct.affx?product=100k
```

The following example assumes that the NA06985_Hind_B5_3005533.CEL file is stored on the MATLAB search path or in the current directory. It also assumes that the associated CDF library file, Mapping50K_Hind240.cdf, is stored at D:\Affymetrix\LibFiles\.

1 Read the contents of a CEL file into a MATLAB structure.

```
celStruct = affyread('NA06985_Hind_B5_3005533.CEL');
```

2 Read the contents of a CDF file into a MATLAB structure.

```
cdfStruct = affyread('D:\Affymetrix\LibFiles\Mapping50K_Hind240.cdf');
```

3 Create a structure containing SNP probe quartet results for the `SNP_A-1684395` probe set.

```
SNPQStruct = affysnpquartets(celStruct,cdfStruct,'SNP_A-1684395')

SNPQStruct =

    ProbeSet: 'SNP_A-1684395'
     AlleleA: 'A'
     AlleleB: 'G'
     Quartet: [1x5 struct]
```

4 View the intensity values of the first probe pair in the probe set.

```
SNPQStruct.Quartet(1)

ans =

        A_Sense_PM: 5013
        B_Sense_PM: 1290
        A_Sense_MM: 1485
        B_Sense_MM: 686
    A_Antisense_PM: 3746
    B_Antisense_PM: 1406
    A_Antisense_MM: 1527
    B_Antisense_MM: 958
```

See Also

Bioinformatics Toolbox functions: `affyread`, `probesetvalues`

Purpose

Read Agilent Feature Extraction Software file

Syntax

```
AGFEData = agferead(File)
```

Arguments

File	Microarray data file generated with the Agilent Feature Extraction Software.

Description

AGFEData = agferead(*File*) reads files generated with the Feature Extraction Software from Agilent microarray scanners and creates a structure (*AGFEData*) containing the following fields:

- Header
- Stats
- Columns
- Rows
- Names
- IDs
- Data
- ColumnNames
- TextData
- TextColumnNames

The Feature Extraction Software takes an image from an Agilent microarray scanner and generates raw intensity data for each spot on the plate. For more information about this software, see:

```
http://www.chem.agilent.com/scripts/pds.asp?lpage=2547
```

Examples

1. Read in a sample Agilent Feature Extraction Software file. Note that the file `fe_sample.txt` is not provided with the Bioinformatics Toolbox software.

```
agfeStruct = agferead('fe_sample.txt')
```

2 Plot the median foreground.

```
maimage(agfeStruct,'gMedianSignal');
maboxplot(agfeStruct,'gMedianSignal');
```

See Also

Bioinformatics Toolbox functions: `affyread`, `celintensityread`, `galread`, `geoseriesread`, `geosoftread`, `gprread`, `ilmnbsread`, `imageneread`, `magetfield`, `sptread`

Purpose

Find all shortest paths in biograph object

Syntax

```
[dist] = allshortestpaths(BGObj)
[dist] = allshortestpaths(BGObj, ...'Directed',
DirectedValue, ...)
[dist] = allshortestpaths(BGObj, ...'Weights', WeightsValue,
   ...)
```

Arguments

BGObj	Biograph object created by `biograph` (object constructor).
DirectedValue	Property that indicates whether the graph is directed or undirected. Enter `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.
WeightsValue	Column vector that specifies custom weights for the edges in the N-by-N adjacency matrix extracted from a biograph object, *BGObj*. It must have one entry for every nonzero value (edge) in the matrix. The order of the custom weights in the vector must match the order of the nonzero values in the matrix when it is traversed column-wise. This property lets you use zero-valued weights. By default, `allshortestpaths` gets weight information from the nonzero entries in the matrix.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

`[dist] = allshortestpaths(BGObj)` finds the shortest paths between every pair of nodes in a graph represented by an N-by-N adjacency matrix extracted from a biograph object, *BGObj*, using Johnson's

algorithm. Nonzero entries in the matrix represent the weights of the edges.

Output *dist* is an N-by-N matrix where *dist*(S,T) is the distance of the shortest path from source node S to target node T. Elements in the diagonal of this matrix are always 0, indicating the source node and target node are the same. A 0 not in the diagonal indicates that the distance between the source node and target node is 0. An Inf indicates there is no path between the source node and the target node.

Johnson's algorithm has a time complexity of O(N*log(N)+N*E), where N and E are the number of nodes and edges respectively.

[...] = allshortestpaths (*BGObj*, '*PropertyName*', *PropertyValue*, ...) calls allshortestpaths with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

[*dist*] = allshortestpaths(*BGObj*, ...'Directed', *DirectedValue*, ...) indicates whether the graph is directed or undirected. Set *DirectedValue* to false for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is true.

[*dist*] = allshortestpaths(*BGObj*, ...'Weights', *WeightsValue*, ...) lets you specify custom weights for the edges. *WeightsValue* is a column vector having one entry for every nonzero value (edge) in the N-by-N adjacency matrix extracted from a biograph object, *BGObj*. The order of the custom weights in the vector must match the order of the nonzero values in the N-by-N adjacency matrix when it is traversed column-wise. This property lets you use zero-valued weights. By default, allshortestpaths gets weight information from the nonzero entries in the N-by-N adjacency matrix.

References

[1] Johnson, D.B. (1977). Efficient algorithms for shortest paths in sparse networks. Journal of the ACM *24(1)*, 1-13.

[2] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphallshortestpaths`

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: `conncomp`, `isdag`, `isomorphism`, `isspantree`, `maxflow`, `minspantree`, `shortestpath`, `topoorder`, `traverse`

aminolookup

Purpose

Find amino acid codes, integers, abbreviations, names, and codons

Syntax

```
aminolookup
aminolookup(SeqAA)
aminolookup('Code', CodeValue)
aminolookup('Integer', IntegerValue)
aminolookup('Abbreviation', AbbreviationValue)
aminolookup('Name', NameValue)
```

Arguments

SeqAA	String of single-letter codes or three-letter abbreviations representing an amino acid sequence. For valid codes and abbreviations, see the table Amino Acid Lookup on page 3-111.
CodeValue	String specifying a single-letter code representing an amino acid. For valid single-letter codes, see the table Amino Acid Lookup on page 3-111.
IntegerValue	Single integer representing an amino acid. For valid integers, see the table Amino Acid Lookup on page 3-111.
AbbreviationValue	String specifying a three-letter abbreviation representing an amino acid. For valid three-letter abbreviations, see the table Amino Acid Lookup on page 3-111.
NameValue	String specifying an amino acid name. For valid amino acid names, see the table Amino Acid Lookup on page 3-111.

Description

`aminolookup` displays a table of amino acid codes, integers, abbreviations, names, and codons.

Amino Acid Lookup

Code	Integer	Abbreviation	Amino Acid Name	Codons
A	1	Ala	Alanine	GCU GCC GCA GCG
R	2	Arg	Arginine	CGU CGC CGA CGG AGA AGG
N	3	Asn	Asparagine	AAU AAC
D	4	Asp	Aspartic acid (Aspartate)	GAU GAC
C	5	Cys	Cysteine	UGU UGC
Q	6	Gln	Glutamine	CAA CAG
E	7	Glu	Glutamic acid (Glutamate)	GAA GAG
G	8	Gly	Glycine	GGU GGC GGA GGG
H	9	His	Histidine	CAU CAC
I	10	Ile	Isoleucine	AUU AUC AUA
L	11	Leu	Leucine	UUA UUG CUU CUC CUA CUG
K	12	Lys	Lysine	AAA AAG
M	13	Met	Methionine	AUG
F	14	Phe	Phenylalanine	UUU UUC
P	15	Pro	Proline	CCU CCC CCA CCG
S	16	Ser	Serine	UCU UCC UCA UCG AGU AGC

Amino Acid Lookup (Continued)

Code	Integer	Abbreviation	Amino Acid Name	Codons
T	17	Thr	Threonine	ACU ACC ACA ACG
W	18	Trp	Tryptophan	UGG
Y	19	Tyr	Tyrosine	UAU UAC
V	20	Val	Valine	GUU GUC GUA GUG
B	21	Asx	Asparagine or Aspartic acid (Aspartate)	AAU AAC GAU GAC
Z	22	Glx	Glutamine or Glutamic acid (Glutamate)	CAA CAG GAA GAG
X	23	Xaa	Any amino acid	All codons
*	24	END	Termination codon (translation stop)	UAA UAG UGA
-	25	GAP	Gap of unknown length	NA

`aminolookup(`*`SeqAA`*`)` converts between single-letter codes and three-letter abbreviations for an amino acid sequence. If the input is a string of single-letter codes, then the output is a character string of three-letter abbreviations. If the input is a string of three-letter abbreviations, then the output is a string of the corresponding single-letter codes.

If you enter one of the ambiguous single-letter codes `B`, `Z`, or `X`, this function displays the corresponding abbreviation for the ambiguous amino acid character.

```
aminolookup('abc')

ans =

AlaAsxCys
```

`aminolookup('Code', CodeValue)` displays the corresponding amino acid three-letter abbreviation and name.

`aminolookup('Integer', IntegerValue)` displays the corresponding amino acid single-letter code, three-letter abbreviation, and name.

`aminolookup('Abbreviation', AbbreviationValue)` displays the corresponding amino acid single-letter code and name.

`aminolookup('Name', NameValue)` displays the corresponding amino acid single-letter code and three-letter abbreviation.

Examples

- Convert an amino acid sequence in single-letter codes to the corresponding three-letter abbreviations.

  ```
  aminolookup('MWKQAEDIRDIYDF')

  ans =

  MetTrpLysGlnAlaGluAspIleArgAspIleTyrAspPhe
  ```

- Convert an amino acid sequence in three-letter abbreviations to the corresponding single-letter codes.

  ```
  aminolookup('MetTrpLysGlnAlaGluAspIleArgAspIleTyrAspPhe')

  ans =

  MWKQAEDIRDIYDF
  ```

- Display the three-letter abbreviation and name for the amino acid corresponding to the single-letter code `R`.

```
aminolookup('Code', 'R')

ans =

Arg Arginine
```

- Display the single-letter code, three-letter abbreviation, and name for the amino acid corresponding to the integer `1`.

```
aminolookup('Integer', 1)

ans =

A Ala Alanine
```

- Display the single-letter code and name for the amino acid corresponding to the three-letter abbreviation `asn`.

```
aminolookup('Abbreviation', 'asn')

ans =

N Asparagine
```

- Display the single-letter code and three-letter abbreviation for the amino acid proline.

```
aminolookup('Name','proline')

ans =

P Pro
```

See Also

Bioinformatics Toolbox functions: `aa2int`, `aa2nt`, `aacount`, `geneticcode`, `int2aa`, `isotopicdist`, `nt2aa`, `revgeneticcode`

Purpose

Calculate atomic composition of protein

Syntax

```
NumberAtoms = atomiccomp(SeqAA)
```

Arguments

SeqAA	Amino acid sequence. Enter a character string or vector of integers from the table Mapping Amino Acid Letter Codes to Integers on page 3-2. You can also enter a structure with the field `Sequence`.

Description

NumberAtoms = `atomiccomp(`*SeqAA*`)` counts the type and number of atoms in an amino acid sequence (*SeqAA*) and returns the counts in a 1-by-1 structure (*NumberAtoms*) with fields `C`, `H`, `N`, `O`, and `S`.

Examples

1 Retrieve an amino acid sequence from the NCBI GenPept database.

```
rhodopsin = getgenpept('NP_000530');
```

2 Count the atoms in the sequence.

```
rhodopsinAC = atomiccomp(rhodopsin)

rhodopsinAC =

    C: 1814
    H: 2725
    N: 423
    O: 477
    S: 25
```

3 Count the number of carbon atoms in the sequence.

```
rhodopsinAC.C

ans =

        1814
```

See Also

Bioinformatics Toolbox functions: `aacount`, `molweight`, `proteinplot`

Purpose

Count nucleotides in sequence

Syntax

```
NTStruct = basecount(SeqNT)
NTStruct = basecount(SeqNT, ...'Chart', ChartValue, ...)
NTStruct = basecount(SeqNT, ...'Others', OthersValue, ...)
NTStruct = basecount(SeqNT, ...'Structure', StructureValue,
   ...)
```

Arguments

SeqNT	One of the following: • String of codes specifying a nucleotide sequence. For valid letter codes, see the table Mapping Nucleotide Letter Codes to Integers on page 3-1121 • Row vector of integers specifying a nucleotide sequence. For valid integers, see the table Mapping Nucleotide Integers to Letter Codes on page 3-809 • MATLAB structure containing a `Sequence` field that contains a nucleotide sequence, such as returned by `fastaread`, `fastqread`, `emblread`, `getembl`, `genbankread`, or `getgenbank`.
ChartValue	String specifying a chart type. Choices are `'pie'` or `'bar'`.
OthersValue	String specifying how to count ambiguous characters, including gaps indicated by a hyphen (-). Choices are `'full'` (lists the ambiguous characters in separate fields) or `'bundle'` (lists the ambiguous characters together in the field `Others`). Default is `'bundle'`.
StructureValue	Suppresses the unknown characters warning when set to `'full'` .

Return Values

NTStruct	1-by-1 MATLAB structure containing the fields A, C, G, and T.

Description

NTStruct = basecount(*SeqNT*) counts the number of each type of base in a SeqNT, a nucleotide sequence, and returns the counts in *NTStruct*, a 1-by-1 MATLAB structure containing the fields A, C, G, and T.

- For sequences with the character U, the number of U characters is added to the T field.
- If a sequence contains ambiguous nucleotide characters (R, Y, K, M, S, W, B, D, H, V, or N), or gaps indicated by a hyphen (-), then these characters are counted in the field Others, and the following warning message appears:

```
Warning: Ambiguous symbols appear in the sequence. These will be in Others.
```

- If a sequence contains undefined nucleotide characters (E, F, H, I, J, L, O, P, Q, X, or Z), then these characters are counted in the field Others, and the following warning message appears.

```
Warning: Unknown symbols appear in the sequence. These will be in Others.
```

- If the property 'Others' is set to 'full', ambiguous characters are listed separately in the fields R, Y, K, M, S, W, B, D, H, V, N, and Gap.

NTStruct = basecount(*SeqNT*, ...'*PropertyName*', *PropertyValue*, ...) calls basecount with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

NTStruct = basecount(*SeqNT*, ...'Chart', *ChartValue*, ...) creates a chart showing the relative proportions of the nucleotides. *ChartValue* can be 'pie' or 'bar'.

NTStruct = basecount(*SeqNT*, ...'Others', *OthersValue*, ...) specifies how to count ambiguous characters (R, Y, K, M, S, W, B, D, H, V, and N), or gaps indicated by a hyphen (-). Choices are 'full' (lists the ambiguous characters in separate fields) or 'bundle' (lists the ambiguous characters together in the field Others). Default is 'bundle'.

NTStruct = basecount(*SeqNT*, ...'Structure', *StructureValue*, ...) suppresses the unknown characters warning when set to 'full'.

- basecount(SeqNT) — Displays fields for four nucleotides, and, if there are ambiguous and unknown characters, add an Others field with the ambiguous and unknown character counts.
- basecount(SeqNT, 'Others', 'full') — Displays fields for 4 nucleotides, 11 ambiguous nucleotides, gaps, and, if there are unknown characters, adds an Others field with the unknown counts.
- basecount(SeqNT, 'Structure', 'full') — Displays fields for four nucleotides and an Others field. If there are ambiguous or unknown characters, adds the counts to the Others field; otherwise displays 0 in the Others field.
- basecount(SeqNT, 'Others', 'full', 'Structure', 'full') — Displays fields for 4 nucleotides, 11 ambiguous nucleotides, gaps, and an Others field. If there are unknown characters, adds the counts to the Others field; otherwise displays 0 in the Others field.

Examples

1 Count the bases in a DNA sequence and return the results in a structure.

```
Bases = basecount('TAGCTGGCCAAGCGAGCTTG')

Bases =

    A: 4
    C: 5
    G: 7
    T: 4
```

2 Get the count for adenosine (A) bases.

```
Bases.A

ans =

    4
```

3 Count the bases in a DNA sequence containing ambiguous characters, listing the ambiguous characters in separate fields.

```
basecount('ABCDGGCCAAGCGAGCTTG','Others','full')

ans =

    A: 4
    C: 5
    G: 6
    T: 2
    R: 0
    Y: 0
    K: 0
    M: 0
    S: 0
    W: 0
    B: 1
    D: 1
    H: 0
    V: 0
    N: 0
  Gap: 0
```

See Also

Bioinformatics Toolbox functions: `aacount`, `baselookup`, `codoncount`, `cpgisland`, `dimercount`, `nmercount`, `ntdensity`, `seqtool`

Purpose

Find nucleotide codes, integers, names, and complements

Syntax

```
baselookup
baselookup('Complement', SeqNT)
baselookup('Code', CodeValue)
baselookup('Integer', IntegerValue)
baselookup('Name', NameValue)
```

Arguments

SeqNT

Nucleotide sequence(s) represented by one of the following:

- String of single-letter codes from the table Nucleotide Lookup on page 3-122
- Cell array of sequences
- Two-dimensional character array of sequences

Note If the input is multiple sequences, the complement for each sequence is determined independently.

CodeValue

Nucleotide letter code represented by one of the following:

- String specifying a single-letter code representing a nucleotide. For valid single-letter codes, see the table Nucleotide Lookup on page 3-122.
- Cell array of letter codes.
- Two-dimensional character array of letter codes.

IntegerValue	Single integer representing a nucleotide. For valid integers, see the table Nucleotide Lookup on page 3-122.
NameValue	Nucleotide name represented by one of the following: • String specifying a nucleotide name. For valid nucleotide names, see the table Nucleotide Lookup on page 3-122. • Cell array of names. • Two-dimensional character array of names.

Description

`baselookup` displays a table of nucleotide codes, integers, names, and complements.

Nucleotide Lookup

Code	Integer	Nucleotide Name	Meaning	Complement
A	1	Adenine	A	T
C	2	Cytosine	C	G
G	3	Guanine	G	C
T	4	Thymine	T	A
U	4	Uracil	U	A
R	5	Purine	A or G	Y
Y	6	Pyrimidine	C or T	R
K	7	Keto	G or T	M
M	8	Amino	A or C	K

Nucleotide Lookup (Continued)

Code	Integer	Nucleotide Name	Meaning	Complement
S	9	Strong interaction (3 H bonds)	C or G	S
W	10	Weak interaction (2 H bonds)	A or T	W
B	11	Not A	C or G or T	V
D	12	Not C	A or G or T	H
H	13	Not G	A or C or T	D
V	14	Not T or U	A or C or G	B
N, X	15	Any nucleotide	A or C or G or T or U	N
-	16	Gap of indeterminate length	Gap	-

`baselookup('Complement', SeqNT)` displays the complementary nucleotide sequence.

`baselookup('Code', CodeValue)` displays the corresponding meaning and nucleotide name. For ambiguous nucleotide codes (`R`, `Y`, `K`, `M`, `S`, `W`, `B`, `D`, `H`, `V`, `N`, and `X`), the nucleotide name is a descriptive name.

`baselookup('Integer', IntegerValue)` displays the corresponding letter code, meaning, and nucleotide name.

`baselookup('Name', NameValue)` displays the corresponding letter code, meaning, and nucleotide name or descriptive name.

Examples

- Convert a nucleotide sequence to its complementary sequence.

```
baselookup('Complement', 'TAGCTGRCCAAGGCCAAGCGAGCTTN')

ans =

ATCGACYGGTTCCGGTTCGCTCGAAN
```

- Display the meaning and nucleotide name or descriptive name for the nucleotide codes `G` and `Y`.

```
baselookup('Code', 'G')

ans =

G  Guanine


baselookup('Code', 'Y')

ans =

T|C  pYrimidine
```

- Display the nucleotide letter code, meaning, and nucleotide name or descriptive name for the integers `1` and `7`.

```
baselookup('Integer', 1)

ans =

A  A - Adenine


baselookup('Integer', 7)

ans =
```

```
K  G|T - Keto
```

- Display the corresponding nucleotide letter code, meaning, and name for `cytosine` and `purine`.

```
baselookup('Name','cytosine')

ans =

C C - Cytosine


baselookup('Name','purine')

ans =

R G|A - puRine
```

See Also

Bioinformatics Toolbox functions: `aa2nt`, `basecount`, `codoncount`, `dimercount`, `geneticcode`, `int2nt`, `nt2aa`, `nt2int`, `revgeneticcode`, `seqtool`

biograph object

Purpose

Data structure containing generic interconnected data used to implement directed graph

Description

A biograph object is a data structure containing generic interconnected data used to implement a directed graph. Nodes represent proteins, genes, or any other biological entity, and edges represent interactions, dependences, or any other relationship between the nodes. A biograph object also stores information, such as color properties and text label characteristics, used to create a 2-D visualization of the graph.

You create a biograph object using the object constructor function `biograph`. You can view a graphical representation of a biograph object using the `view` method.

Method Summary

Following are methods of a biograph object:

allshortestpaths (biograph)	Find all shortest paths in biograph object
conncomp (biograph)	Find strongly or weakly connected components in biograph object
dolayout (biograph)	Calculate node positions and edge trajectories
get (biograph)	Retrieve information about biograph object
getancestors (biograph)	Find ancestors in biograph object
getdescendants (biograph)	Find descendants in biograph object
getedgesbynodeid (biograph)	Get handles to edges in biograph object
getmatrix (biograph)	Get connection matrix from biograph object
getnodesbyid (biograph)	Get handles to nodes
getrelatives (biograph)	Find relatives in biograph object

isdag (biograph)	Test for cycles in biograph object
isomorphism (biograph)	Find isomorphism between two biograph objects
isspantree (biograph)	Determine if tree created from biograph object is spanning tree
maxflow (biograph)	Calculate maximum flow in biograph object
minspantree (biograph)	Find minimal spanning tree in biograph object
set (biograph)	Set property of biograph object
shortestpath (biograph)	Solve shortest path problem in biograph object
topoorder (biograph)	Perform topological sort of directed acyclic graph extracted from biograph object
traverse (biograph)	Traverse biograph object by following adjacent nodes
view (biograph)	Draw figure from biograph object

Following are methods of a node object:

getancestors (biograph)	Find ancestors in biograph object
getdescendants (biograph)	Find descendants in biograph object
getrelatives (biograph)	Find relatives in biograph object

Property Summary

A biograph object contains two kinds of objects, node objects and edge objects, that have their own properties. For a list of the properties of node objects and edge objects, see the following tables.

Properties of a Biograph Object

Property	Description
`ID`	String to identify the biograph object. Default is `''`.
`Label`	String to label the biograph object. Default is `''`.
`Description`	String that describes the biograph object. Default is `''`.
`LayoutType`	String that specifies the algorithm for the layout engine. Choices are: • `'hierarchical'` (default) — Uses a topological order of the graph to assign levels, and then arranges the nodes from top to bottom, while minimizing crossing edges. • `'radial'` — Uses a topological order of the graph to assign levels, and then arranges the nodes from inside to outside of the circle, while minimizing crossing edges. • `'equilibrium'` — Calculates layout by minimizing the energy in a dynamic spring system.

Properties of a Biograph Object (Continued)

Property	Description
`EdgeType`	String that specifies how edges display. Choices are: • `'straight'` • `'curved'` (default) • `'segmented'` **Note** Curved or segmented edges occur only when necessary to avoid obstruction by nodes. Biograph objects with `LayoutType` equal to `'equilibrium'` or `'radial'` cannot produce curved or segmented edges.
`Scale`	Positive number that post-scales the node coordinates. Default is `1`.
`LayoutScale`	Positive number that scales the size of the nodes before calling the layout engine. Default is `1`.
`EdgeTextColor`	Three-element numeric vector of RGB values. Default is `[0, 0, 0]`, which defines black.
`EdgeFontSize`	Positive number that sets the size of the edge font in points. Default is `8`.
`ShowArrows`	Controls the display of arrows with the edges. Choices are `'on'` (default) or `'off'`.
`ArrowSize`	Positive number that sets the size of the arrows in points. Default is `8`.
`ShowWeights`	Controls the display of text indicating the weight of the edges. Choices are `'on'` (default) or `'off'`.

Properties of a Biograph Object (Continued)

Property	Description
`ShowTextInNodes`	String that specifies the node property used to label nodes when you display a biograph object using the `view` method. Choices are: • `'Label'` — Uses the `Label` property of the node object (default). • `'ID'` — Uses the `ID` property of the node object. • `'None'`
`NodeAutoSize`	Controls precalculating the node size before calling the layout engine. Choices are `'on'` (default) or `'off'`.
`NodeCallback`	User-defined callback for all nodes. Enter the name of a function, a function handle, or a cell array with multiple function handles. After using the `view` function to display the biograph object in the Biograph Viewer, you can double-click a node to activate the first callback, or right-click and select a callback to activate. Default is the anonymous function, `@(node) inspect(node)`, which displays the Property Inspector dialog box.

Properties of a Biograph Object (Continued)

Property	Description
`EdgeCallback`	User-defined callback for all edges. Enter the name of a function, a function handle, or a cell array with multiple function handles. After using the `view` function to display the biograph object in the Biograph Viewer, you can double-click an edge to activate the first callback, or right-click and select a callback to activate. Default is the anonymous function, `@(edge) inspect(edge)`, which displays the Property Inspector dialog box.
`CustomNodeDrawFcn`	Function handle to a customized function to draw nodes. Default is `[]`.
`Nodes`	Read-only column vector with handles to node objects of a biograph object. The size of the vector is the number of nodes. For properties of node objects, see Properties of a Node Object on page 3-131.
`Edges`	Read-only column vector with handles to edge objects of a biograph object. The size of the vector is the number of edges. For properties of edge objects, see Properties of an Edge Object on page 3-133.

Properties of a Node Object

Property	Description
`ID`	Character string defined when the biograph object is created, either by the *`NodeIDs`* input argument or internally by the `biograph` constructor function. You can modify this property using the `set` method, but each node object's `ID` must be unique.

Properties of a Node Object (Continued)

Property	Description
`Label`	String for labeling a node when you display a biograph object using the `view` method. Default is `''`.
`Description`	String that describes the node. Default is `''`.
`Position`	Two-element numeric vector of *x*- and *y*-coordinates, for example, `[150, 150]`. If you do not specify this property, default is initially `[]`, then when the layout algorithms are executed, it becomes a two-element numeric vector of *x*- and *y*-coordinates computed by the layout engine.
`Shape`	String that specifies the shape of the nodes. Choices are: • `'box'`(default) • `'ellipse'` • `'circle'` • `'rectangle'` • `'diamond'` • `'trapezium'` • `'invtrapezium'` • `'house'` • `'inverse'` • `'parallelogram'`

Properties of a Node Object (Continued)

Property	Description
`Size`	Two-element numeric vector calculated before calling the layout engine using the actual font size and shape of the node. Default is `[10, 10]`.
`Color`	Three-element numeric vector of RGB values that specifies the fill color of the node. Default is `[1, 1, 0.7]`, which defines yellow.
`LineWidth`	Positive number. Default is `1`.
`LineColor`	Three-element numeric vector of RGB values that specifies the outline color of the node. Default is `[0.3, 0.3, 1]`, which defines blue.
`FontSize`	Positive number that sets the size of the node font in points. Default is `8`.
`TextColor`	Three-element numeric vector of RGB values that specifies the color of the node labels. Default is `[0, 0, 0]`, which defines black.
`UserData`	Miscellaneous, user-defined data that you want to associate with the node. The node does not use this property, but you can access and specify it using the `get` and `set` functions. Default is `[]`.

Properties of an Edge Object

Property	Description
`ID`	Character string automatically generated from the node `ID`s when the biograph object is created by the `biograph` constructor function. You can modify this property using the `set` method, but each edge object's `ID` must be unique.

Properties of an Edge Object (Continued)

Property	Description
`Label`	String for labeling an edge when you display a biograph object using the `view` method. Default is `''`.
`Description`	String that describes the edge. Default is `''`.
`Weight`	Value that represents the weight (cost, distance, length, or capacity) associated with the edge. Default is `1`.
`LineWidth`	Positive number. Default is `1`.
`LineColor`	Three-element numeric vector of RGB values that specifies the color of the edge. Default is `[0.5, 0.5, 0.5]`, which defines gray.
`UserData`	Miscellaneous, user-defined data that you want to associate with the edge. The edge does not use this property, but you can access and specify it using the `get` and `set` functions. Default is `[]`.

Examples

Determining Properties and Property Values of a Biograph Object

You can display all properties and their current values of a biograph object, *`BGobj`*, by using the following syntax:

```
get(BGobj)
```

You can return all properties and their current values of *`BGobj`*, a biograph object, to *`BGstruct`*, a scalar structure in which each field name is a property of a biograph object, and each field contains the value of that property, by using the following syntax:

```
BGstruct = get(BGobj)
```

You can return the value of a specific property of a biograph object, *BGobj*, by using either of the following syntaxes:

```
PropertyValue = get(BGobj, 'PropertyName')

PropertyValue = BGobj.PropertyName
```

You can return the value of specific properties of a biograph object, *BGobj*, by using the following syntax:

```
[Property1Value, Property2Value, ...] = get(BGobj, ...
 'Property1Name', 'Property2Name', ...)
```

Determining Properties and Property Values of a Node or Edge of a Biograph Object

You can display all properties and their current values of the *n*th node or *n*th edge of a biograph object, *BGobj*, by using the following syntaxes:

```
get(BGobj.nodes(n))

get(BGobj.edges(n))
```

Determining Possible Values of Biograph Object Properties

You can display possible values for all properties that have a fixed set of property values in a biograph object, *BGobj*, by using the following syntax:

```
set(BGobj)
```

You can display possible values for a specific property that has a fixed set of property values in a biograph object, *BGobj*, by using the following syntax:

```
set(BGobj,  'PropertyName')
```

Specifying Properties of a Biograph Object

You can set a specific property of a biograph object, *BGobj*, by using either of the following syntaxes:

```
set(BGobj, 'PropertyName', PropertyValue)

BGobj.PropertyName = PropertyValue
```

You can set multiple properties of a biograph object, *BGobj*, by using the following syntax:

```
set(BGobj,  'Property1Name', Property1Value, ...
'Property2Name', Property2Value, ...)
```

Specifying Properties of a Node of a Biograph Object

You can set a specific property of the *n*th node of a biograph object, *BGobj*, by using either of the following syntaxes:

```
set(BGobj.nodes(n), 'PropertyName', PropertyValue)

BGobj.nodes(n).PropertyName = PropertyValue
```

Tip To specify properties of a node using the node's `ID`, use the `getnodesbyid` function to create a handle for the node:

```
nodehandle = getnodesbyid(BGobj, NodeID)
```

Then use the handle for the node in either of the following syntaxes:

```
set(nodehandle, 'PropertyName', PropertyValue)

nodehandle.PropertyName = PropertyValue
```

Specifying Properties of an Edge of a Biograph Object

You can set a specific property of the *n*th edge of a biograph object, *BGobj*, by using either of the following syntaxes:

```
set(BGobj.edges(n), 'PropertyName', PropertyValue)

BGobj.edges(n).PropertyName = PropertyValue
```

Tip To specify properties of an edge using the source and sink node's `ID`'s, use the `getedgesbynodeid` function to create a handle for the edge:

```
edgehandle = getedgesbynodeid(BGobj, SourceNodeID, ...
                                     SinkNodeID)
```

Then use the handle for the edge in either of the following syntaxes:

```
set(edgehandle, 'PropertyName', PropertyValue)
```

```
edgehandle.PropertyName = PropertyValue
```

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor),

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `dolayout`, `get`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getmatrix`, `getnodesbyid`, `getrelatives`, `isdag`, `isomorphism`, `isspantree`, `maxflow`, `minspantree`, `set`, `shortestpath`, `topoorder`, `traverse`, `view`

biograph

Purpose

Create biograph object

Syntax

```
BGobj = biograph(CMatrix)
BGobj = biograph(CMatrix, NodeIDs)
BGobj = biograph(CMatrix, NodeIDs, ...'ID', IDValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'Label', LabelValue,
   ...)
BGobj = biograph(CMatrix, NodeIDs, ...'Description',
   DescriptionValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'LayoutType',
   LayoutTypeValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'EdgeType',
   EdgeTypeValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'Scale', ScaleValue,
   ...)
BGobj = biograph(CMatrix, NodeIDs, ...'LayoutScale',
   LayoutScaleValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'EdgeTextColor',
   EdgeTextColorValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'EdgeFontSize',
   EdgeFontSizeValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'ShowArrows',
   ShowArrowsValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'ArrowSize',
   ArrowSizeValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'ShowWeights',
   ShowWeightsValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'ShowTextInNodes',
   ShowTextInNodesValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'NodeAutoSize',
   NodeAutoSizeValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'NodeCallback',
   NodeCallbackValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'EdgeCallback',
   EdgeCallbackValue, ...)
BGobj = biograph(CMatrix, NodeIDs, ...'CustomNodeDrawFcn',
   CustomNodeDrawFcnValue, ...)
```

Arguments

CMatrix

Full or sparse square matrix that acts as a connection matrix. That is, a value of `1` indicates a connection between nodes while a `0` indicates no connection. The number of rows/columns is equal to the number of nodes.

NodeIDs

Node identification strings. Enter any of the following:

- Cell array of strings with the number of strings equal to the number of rows or columns in the connection matrix *CMatrix*. Each string must be unique.
- Character array with the number of rows equal to the number of nodes. Each row in the array must be unique.
- String with the number of characters equal to the number of nodes. Each character must be unique.

Default values are the row or column numbers.

Note You must specify *NodeIDs* if you want to specify property name/value pairs. Set *NodeIDs* to `[ ]` to use the default values of the row/column numbers.

IDValue

String to identify the biograph object. Default is `''`.

LabelValue

String to label the biograph object. Default is `''`.

DescriptionValue

String that describes the biograph object. Default is `''`.

LayoutTypeValue

String that specifies the algorithm for the layout engine. Choices are:

- `'hierarchical'` (default) — Uses a topological order of the graph to assign levels, and then arranges the nodes from top to bottom, while minimizing crossing edges.
- `'radial'` — Uses a topological order of the graph to assign levels, and then arranges the nodes from inside to outside of the circle, while minimizing crossing edges.
- `'equilibrium'` — Calculates layout by minimizing the energy in a dynamic spring system.

EdgeTypeValue

String that specifies how edges display. Choices are:

- `'straight'`
- `'curved'` (default)
- `'segmented'`

Note Curved or segmented edges occur only when necessary to avoid obstruction by nodes. Biograph objects with `LayoutType` equal to `'equilibrium'` or `'radial'` cannot produce curved or segmented edges.

ScaleValue	Positive number that post-scales the node coordinates. Default is `1`.
LayoutScaleValue	Positive number that scales the size of the nodes before calling the layout engine. Default is `1`.
EdgeTextColorValue	Three-element numeric vector of RGB values. Default is `[0, 0, 0]`, which defines black.
EdgeFontSizeValue	Positive number that sets the size of the edge font in points. Default is `8`.
ShowArrowsValue	Controls the display of arrows for the edges. Choices are `'on'` (default) or `'off'`.
ArrowSizeValue	Positive number that sets the size of the arrows in points. Default is `8`.
ShowWeightsValue	Controls the display of text indicating the weight of the edges. Choices are `'on'` (default) or `'off'`.
ShowTextInNodesValue	String that specifies the node property used to label nodes when you display a biograph object using the `view` method. Choices are: • `'Label'` — Uses the `Label` property of the node object (default). • `'ID'` — Uses the `ID` property of the node object. • `'None'`
NodeAutoSizeValue	Controls precalculating the node size before calling the layout engine. Choices are `'on'` (default) or `'off'`.

NodeCallbackValue	User callback for all nodes. Enter the name of a function, a function handle, or a cell array with multiple function handles. After using the `view` function to display the biograph in the Biograph Viewer, you can double-click a node to activate the first callback, or right-click and select a callback to activate. Default is `@(node) inspect(node)`, which displays the Property Inspector dialog box.
EdgeCallbackValue	User callback for all edges. Enter the name of a function, a function handle, or a cell array with multiple function handles. After using the `view` function to display the biograph in the Biograph Viewer, you can double-click an edge to activate the first callback, or right-click and select a callback to activate. Default is `@(edge) inspect(edge)`, which displays the Property Inspector dialog box.
CustomNodeDrawFcnValue	Function handle to a customized function to draw nodes. Default is `[]`.

Description

BGobj = biograph(*CMatrix*) creates a biograph object, *BGobj*, using a connection matrix, *CMatrix*. All nondiagonal and positive entries in the connection matrix, *CMatrix*, indicate connected nodes, rows represent the source nodes, and columns represent the sink nodes.

BGobj = biograph(*CMatrix*, *NodeIDs*) specifies the node identification strings. *NodeIDs* can be:

- Cell array of strings with the number of strings equal to the number of rows or columns in the connection matrix *CMatrix*. Each string must be unique.

- Character array with the number of rows equal to the number of nodes. Each row in the array must be unique.
- String with the number of characters equal to the number of nodes. Each character must be unique.

Default values are the row or column numbers.

Note If you want to specify property name/value pairs, you must specify *NodeIDs*. Set *NodeIDs* to `[]` to use the default values of the row/column numbers.

BGobj = biograph(..., '*PropertyName*', *PropertyValue*, ...) calls `biograph` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'ID', *IDValue*, ...) specifies an ID for the biograph object. Default is `''`.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'Label', *LabelValue*, ...) specifies a label for the biograph object. Default is `''`.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'Description', *DescriptionValue*, ...) specifies a description of the biograph object. Default is `''`.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'LayoutType', *LayoutTypeValue*, ...) specifies the algorithm for the layout engine.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'EdgeType', *EdgeTypeValue*, ...) specifies how edges display.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'Scale', *ScaleValue*, ...) post-scales the node coordinates. Default is `1`.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'LayoutScale', *LayoutScaleValue*, ...) scales the size of the nodes before calling the layout engine. Default is 1.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'EdgeTextColor', *EdgeTextColorValue*, ...) specifies a three-element numeric vector of RGB values. Default is [0, 0, 0], which defines black.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'EdgeFontSize', *EdgeFontSizeValue*, ...) sets the size of the edge font in points. Default is 8.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'ShowArrows', *ShowArrowsValue*, ...) controls the display of arrows for the edges. Choices are 'on' (default) or 'off'.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'ArrowSize', *ArrowSizeValue*, ...) sets the size of the arrows in points. Default is 8.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'ShowWeights', *ShowWeightsValue*, ...) controls the display of text indicating the weight of the edges. Choices are 'on' (default) or 'off'.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'ShowTextInNodes', *ShowTextInNodesValue*, ...) specifies the node property used to label nodes when you display a biograph object using the view method.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'NodeAutoSize', *NodeAutoSizeValue*, ...) controls precalculating the node size before calling the layout engine. Choices are 'on' (default) or 'off'.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'NodeCallback', *NodeCallbackValue*, ...) specifies user callback for all nodes.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'EdgeCallback', *EdgeCallbackValue*, ...) specifies user callback for all edges.

BGobj = biograph(*CMatrix*, *NodeIDs*, ...'CustomNodeDrawFcn', *CustomNodeDrawFcnValue*, ...) specifies function handle to customized function to draw nodes. Default is [].

Examples

1 Create a biograph object with default node IDs, and then use the `get` function to display the node IDs.

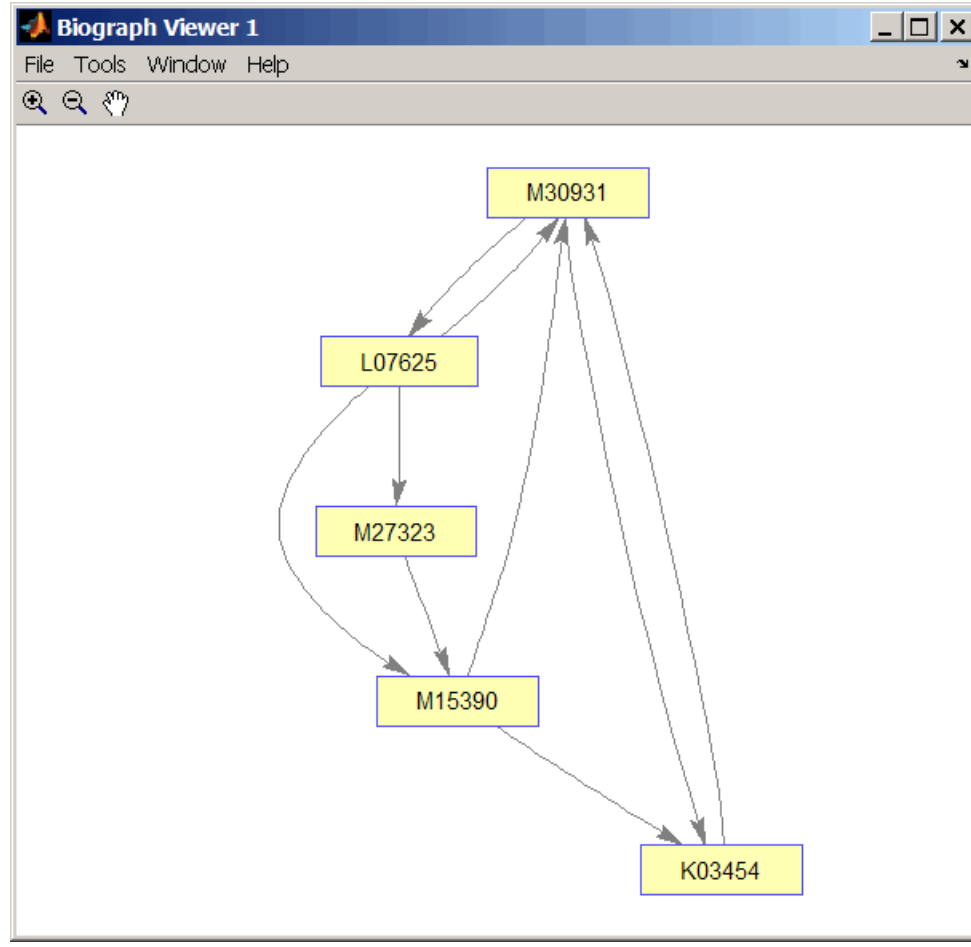
```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];
bg1 = biograph(cm)
Biograph object with 5 nodes and 9 edges.
get(bg1.nodes,'ID')

ans =

    'Node 1'
    'Node 2'
    'Node 3'
    'Node 4'
    'Node 5'
```

2 Create a biograph object, assign the node IDs, and then use the `get` function to display the node IDs.

```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];
ids = {'M30931','L07625','K03454','M27323','M15390'};
bg2 = biograph(cm,ids);
get(bg2.nodes,'ID')

ans =

    'M30931'
    'L07625'
    'K03454'
    'M27323'
    'M15390'
```

3 Use the `view` method to display the biograph object.

```
view(bg2)
```



See Also

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `dolayout`, `get`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getmatrix`, `getnodesbyid`, `getrelatives`, `isdag`, `isomorphism`, `isspantree`, `maxflow`, `minspantree`, `set`, `shortestpath`, `topoorder`, `traverse`, `view`

Purpose

Contain data values from microarray experiment

Description

The ExptData class is designed to contain data values, such as gene expression values, from a microarray experiment. It stores the data values in one or more DataMatrix objects, each having the same row names (feature names) and column names (sample names). It provides a convenient way to store related experiment data in a single data structure (object). It also lets you manage and subset the data.

The ExptData class includes properties and methods that let you access, retrieve, and change data values from a microarray experiment. These properties and methods are useful to view and analyze the data.

Construction

`EDobj = bioma.data.ExptData(Data1, Data2, ...)` creates an ExptData object, from one or more matrices of data. Each matrix can be a logical matrix, a numeric matrix, or a DataMatrix object.

`EDobj = bioma.data.ExptData(..., {DMobj1, Name1}, {DMobj2, Name2}, ...)` specifies an element name for each DataMatrix object. `Name#` is a string specifying a unique name. Default names are `Elmt1`, `Elmt2`, etc.

`EDobj = bioma.data.ExptData({Data1, Data2, ...})` creates an ExptData object, from a cell array of matrices of data. Each matrix can be a logical matrix, a numeric matrix, or a DataMatrix object.

`EDobj = bioma.data.ExptData(..., 'PropertyName', PropertyValue)` constructs the object using options, specified as property name/property value pairs.

`EDobj = bioma.data.ExptData(..., 'ElementNames', ElementNamesValue)` specifies element names for the matrix inputs. `ElementNamesValue` is a cell array of strings. Default names are `Elmt1`, `Elmt2`, etc.

`EDobj = bioma.data.ExptData(..., 'FeatureNames', FeatureNamesValue)` specifies feature names (row names) for the ExptData object. .

EDobj = bioma.data.ExptData(..., 'SampleNames', *SampleNamesValue*) specifies sample names (column names) for the ExptData object.

Inputs

Data#

Matrix of experimental data values specified by any of the following:

- Logical matrix
- Numeric matrix
- DataMatrix object

All inputs must have the same dimensions. All DataMatrix objects must also have the same row names and columns names. If you provide logical or numeric matrices, bioma.data.ExptData converts them to DataMatrix objects with either default row and column names, or the row and column names of DataMatrix inputs, if provided.

The rows must correspond to features and the columns must correspond to samples.

DMobj#

Variable name of a DataMatrix object in the MATLAB Workspace.

Name#

String specifying an element name for the corresponding DataMatrix object

ElementNamesValue

Cell array of strings that specifies unique element names for the matrix inputs. The number of elements in *ElementNamesValue* must equal the number input matrices.

Default: {`Elmt1`, `Elmt2`, ...}

`FeatureNamesValue`

Feature names (row names) for the ExptData object, specified by one of the following:

- Cell array of strings
- Character array
- Numeric or logical vector
- Single string, which is used as a prefix for the feature names, with feature numbers appended to the prefix
- Logical `true` or `false` (default). If `true`, `bioma.data.ExptData` assigns unique feature names using the format `Feature1`, `Feature2`, etc.

If you use a cell array of strings, character array, or vector, then the number of elements must be equal in number to the number of rows in *`Data1`*.

`SampleNamesValue`

Sample names (column names) for the ExptData object, specified by one of the following:

- Cell array of strings
- Character array
- Numeric or logical vector
- Single string, which is used as a prefix for the sample names, with sample numbers appended to the prefix
- Logical `true` or `false` (default). If `true`, `bioma.data.ExptData` assigns unique sample names using the format `Sample1`, `Sample2`, etc.

If you use a cell array of strings, character array, or vector, then the number of elements must be equal in number to the number of columns in *Data1*. If the ExptData object is part of an ExpressionSet object that contains a MetaData object, the sample names (column names) in the ExptData object must match the sample names (row names) in a MetaData object.

Properties

`ElementClass`

Class type of the DataMatrix objects in the experiment

Cell array of strings specifying the class type of each DataMatrix object in the ExptData object. Possible values are MATLAB classes, such as `single`, `double`, and `logical`. This information is read-only.

Attributes:

`SetAccess`	`private`

`Name`

Name of the ExptData object.

String specifying the name of the ExptData object. Default is `[]`.

`NElements`

Number of elements in the experiment

Positive integer specifying the number of elements (DataMatrix objects) in the experiment data. This value is equivalent to the number of DataMatrix objects in the ExptData object. This information is read-only.

Attributes:

`SetAccess`	`private`

`NFeatures`

Number of features in the experiment

Positive integer specifying the number of features in the experiment. This value is equivalent to the number of rows in each DataMatrix object in the ExptData object. This information is read-only.

Attributes:

`SetAccess`	`private`

`NSamples`

Number of samples in the experiment

Positive integer specifying the number of samples in the experiment. This value is equivalent to the number of columns in each DataMatrix object in the ExptData object. This information is read-only.

Attributes:

`SetAccess`	`private`

Methods

combine	Combine two ExptData objects
dmNames	Retrieve or set `Name` properties of DataMatrix objects in ExptData object
elementData	Retrieve or set data element (DataMatrix object) in ExptData object
elementNames	Retrieve or set element names of DataMatrix objects in ExptData object
featureNames	Retrieve or set feature names in ExptData object

isempty	Determine whether ExptData object is empty
sampleNames	Retrieve or set sample names in ExptData object
size	Return size of ExptData object

Instance Hierarchy

An ExpressionSet object contains an ExptData object. An ExptData object contains one or more DataMatrix objects.

Attributes

To learn about attributes of classes, see Class Attributes in the MATLAB Object-Oriented Programming documentation.

Copy Semantics

Value. To learn how this affects your use of the class, see Copying Objects in the MATLAB Programming Fundamentals documentation.

Indexing

ExptData objects support 1-D parenthesis ( ) indexing to extract, assign, and delete data.

ExptData objects do not support:

- Dot . indexing
- Curly brace { } indexing

Examples

The `mouseExprsData.txt` file used in this example contains data from Hovatta et al., 2005.

Construct an ExptData object containing one DataMatrix object:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
```

```
EDObj = ExptData(dmObj);
% Display information about the ExptData object
EDObj
% Name the ExptData object
EDObj.Name = 'My ExptData Object'
```

References

[1] Hovatta, I., Tennant, R S., Helton, R., et al. (2005). Glyoxalase 1 and glutathione reductase 1 regulate anxiety in mice. Nature *438*, 662–666.

See Also

`bioma.ExpressionSet` | `bioma.data.MetaData` | `bioma.data.MIAME`

Tutorials

- Working with Data Objects for Microarray Experiment Data
- Analyzing Illumina Bead Summary Gene Expression Data

How To

- Class Attributes
- Property Attributes
- “Working with ExptData Objects”

bioma.data.MetaData class

Purpose

Contain metadata from microarray experiment

Description

The MetaData class is designed to contain metadata (variable values and descriptions) from a microarray experiment. It provides a convenient way to store related metadata in a single data structure (object). It also lets you manage and subset the data.

The metadata is a collection of variable names, for example related to samples or microarray features, along with descriptions and values for the variables. A MetaData object stores the metadata in two dataset arrays.

- **Values dataset array** — A dataset array containing the measured value of each variable per sample or feature. In this dataset array, the columns correspond to variables and rows correspond to either samples or features. The number and names of the columns in this dataset array must match the number and names of the rows in the Descriptions dataset array. If this dataset array contains *sample* metadata, then the number and names of the rows (samples) must match the number and names of the columns in the DataMatrix objects in the same ExpressionSet object. If this dataset array contains *feature* metadata, then the number and names of the rows (features) must match the number and names of the rows in the DataMatrix objects in the same ExpressionSet object.
- **Descriptions dataset array** — A dataset array containing a list of the variable names and their descriptions. In this dataset array, each row corresponds to a variable. The row names are the variable names, and a column, named `VariableDescription`, contains a description of the variable. The number and names of the rows in the Descriptions dataset array must match the number and names of the columns in the Values dataset array.

The MetaData class includes properties and methods that let you access, retrieve, and change metadata variables, and their values and descriptions. These properties and methods are useful to view and analyze the metadata.

Construction

MDobj = bioma.data.MetaData(*VarValues*) creates a MetaData object from one dataset array whose rows correspond to sample (observation) names and whose columns correspond to variables. The dataset array contains the measured value of each variable per sample.

MDobj = bioma.data.MetaData(*VarValues*, *VarDescriptions*) creates a MetaData object from two dataset arrays. *VarDescriptions* is a dataset array whose rows correspond to variables. The row names are the variable names, and another column, named VariableDescription, contains a description of each variable.

MDobj = bioma.data.MetaData(*VarValues*, *VarDesc*) creates a MetaData object from a dataset array and *VarDesc* a cell array of strings containing descriptions of the variables.

MDobj = bioma.data.MetaData(..., '*PropertyName*', *PropertyValue*) constructs the object using options, specified as property name/property value pairs.

MDobj = bioma.data.MetaData('File', *FileValue*) creates a MetaData object from a text file containing a table of metadata. The table row labels must be sample names, and its column headers must be variable names.

MDobj = bioma.data.MetaData('File', *FileValue*, ...'Path', *PathValue*) specifies a directory or path and directory where *FileValue* is stored.

MDobj = bioma.data.MetaData('File', *FileValue*, ...'Delimiter', *DelimiterValue*) specifies a delimiter symbol to use as a column separator for *FileValue*. Default is '\t'.

MDobj = bioma.data.MetaData('File', *FileValue*, ...'RowNames', *RowNamesValue*) specifies the row names (sample names) for the MetaData object. Default is the information in the first column of the table.

MDobj = bioma.data.MetaData('File', *FileValue*, ...'ColumnNames', *ColumnNamesValue*) specifies the columns of data to read from the table. *ColumnNamesValue* is a cell array of strings

specifying the column header names. Default is to read all columns of data from the table, assuming the first row contains column headers.

MDobj = bioma.data.MetaData('File', *FileValue*, ...'VarDescChar', *VarDescCharValue*) specifies that lines in the table prefixed by *VarDescCharValue* to be read as descriptions and used to create the *VarDescriptions* dataset array. By default, bioma.data.MetaData does not read variable description information, and does not create a Descriptions dataset array. These prefixed lines must appear at the top of the file, before the table of metadata values.

MDobj = bioma.data.MetaData(...'Name', *NameValue*) specifies a name for the MetaData object.

MDobj = bioma.data.MetaData('File', *FileValue*, ...'Description', *DescriptionValue*) specifies a description for the MetaData object.

MDobj = bioma.data.MetaData('File', *FileValue*, ...'SampleNames', *SampleNamesValue*) specifies sample names (row names) for the MetaData object.

MDobj = bioma.data.MetaData('File', *FileValue*, ...'VariableNames', *VariableNamesValue*) specifies variable names (column names) for the MetaData object.

Inputs

VarValues

Dataset array whose rows correspond to sample (observation) names and whose columns correspond to variables. The dataset array contains the measured value of each variable per sample or feature.

The number and names of the columns in the *VarValues* dataset array must match the number and names of the rows in the *VarDescriptions* dataset array. If *VarValues* contains *sample* metadata, then the number and names of the rows (samples) must match the number and names of the columns in the DataMatrix objects in the same ExpressionSet object. If *VarValues* contains

feature metadata, then the number and names of the rows (features) must match the number and names of the rows in the DataMatrix objects in the same ExpressionSet object.

VarDescriptions

Dataset array whose rows correspond to variables. The row names are the variable names, and a column, named `VariableDescription`, contains a description of the variable. The number and names of the rows in the *VarDescriptions* dataset array must match the number and names of the columns in the *VarValues* dataset array.

VarDesc

Cell array of strings containing descriptions of the variables. The number of elements in *VarDesc* must equal the number of columns (variable names) in *VarValues*.

FileValue

String specifying a text file containing a table of metadata. The table row labels must be sample or feature names, and its column headers must be variable names. The text file must be on the MATLAB search path or in the Current Folder (unless you use the `Path` property).

PathValue

String specifying a directory or path and directory where *FileValue* is stored.

DelimiterValue

String specifying a delimiter symbol to use as a column separator for *FileValue*. Typical choices are:

- `' '`
- `'\t'` (default)
- `','`

- `';'`
- `'|'`

`RowNamesValue`

Row names (sample or feature names) for the MetaData object, specified by one of the following:

- Cell array of strings
- Single number indicating the column of the table containing the row names
- Character string indicating the column header of the table containing the row names

If you specify `[]` for *`RowNamesValue`*, then `bioma.data.MetaData` provides numbered row names, starting with `1`.

Default: `1`, which specifies the information in the first column of the table

`ColumnNamesValue`

Cell array of strings specifying the column header names to indicate which columns of data to read from the table. Default is to read all columns of data from the table, assuming the first row contains column headers. If the table does not have column headers, specify `[]` for *`ColumnNamesValue`* to read all columns of data and provide numbered column names, starting with `1`.

`VarDescCharValue`

String specifying a character to prefix lines in the table that are to be read as descriptions and used to create the *`VarDescriptions`* dataset array. By default, `bioma.data.MetaData` does not read variable description information, and does not create a *`VarDescriptions`* dataset array. These prefixed lines must appear at the top of the file, before the table of metadata values.

NameValue

String specifying a name for the MetaData object.

DescriptionValue

String specifying a description for the MetaData object.

SampleNamesValue

Cell array of strings specifying sample names for the MetaData object. The number of elements in the cell array must equal the number of samples in the MetaData object. This input overwrites sample names from the input file. Default are the sample names (row names) from the input file.

VariableNamesValue

Cell array of strings specifying variable names for the MetaData object. The number of elements in the cell array must equal the number of variables in the MetaData object. This input overwrites variable names from the input file. Default are the variable names (column names) from the input file.

Properties

`Description`

Description of the MetaData object.

String specifying a description of the MetaData object. Default is `[]`.

`DimensionLabels`

Row and column labels for the MetaData object.

Two-element cell array containing strings specifying labels of the rows and columns respectively in the MetaData object. Default is `{'Samples', 'Variables'}`.

`Name`

Name of the MetaData object.

String specifying the name of the MetaData object. Default is `[]`.

`NSamples`

Number of samples (observations) in the experiment

Positive integer specifying the number of samples in the experiment. This value is equivalent to the number of rows in the *`VarValues`* dataset array. This information is read-only

Attributes:

`SetAccess`	`private`

`NVariables`

Number of variables in the experiment

Positive integer specifying the number of variables in the experiment. This value is equivalent to the number of columns in the *`VarValues`* dataset array. This information is read-only

Attributes:

`SetAccess`	`private`

Methods

combine	Combine two MetaData objects
isempty	Determine whether MetaData object is empty
sampleNames	Retrieve or set sample names in MetaData object
size	Return size of MetaData object
variableDesc	Retrieve or set variable descriptions for samples in MetaData object
variableNames	Retrieve or set variable names for samples in MetaData object

variableValues	Retrieve or set variable values for samples in MetaData object
varValuesTable	Create 2-D graphic table GUI of variable values in MetaData object

Instance Hierarchy

An ExpressionSet object contains two MetaData objects, one for sample information and one for microarray feature information. A MetaData object contains two dataset arrays. One dataset array contains the measured value of each variable per sample or feature. The other dataset array contains a list of the variable names and their descriptions.

Attributes

To learn about attributes of classes, see Class Attributes in the MATLAB Object-Oriented Programming documentation.

Copy Semantics

Value. To learn how this affects your use of the class, see Copying Objects in the MATLAB Programming Fundamentals documentation.

Indexing

MetaData objects support 2-D parenthesis ( ) indexing and dot . indexing to extract, assign, and delete data.

MetaData objects do not support:

- Curly brace { } indexing
- Linear indexing

Examples

Construct a MetaData object containing sample variable information from a text file:

```
% Import bioma.data package to make constructor function
% available
import bioma.data.*
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
```

```
% Display information about the MetaData object
MDObj2
% Supply a description for the MetaData object
MDObj2.Description = 'This MetaData Object contains sample variable info.'
```

See Also

`bioma.ExpressionSet` | `bioma.data.ExptData` | `bioma.data.MIAME`

Tutorials

- Working with Data Objects for Microarray Experiment Data
- Analyzing Illumina Bead Summary Gene Expression Data

How To

- Class Attributes
- Property Attributes
- “Working with MetaData Objects”

Purpose

Contain experiment information from microarray gene expression experiment

Description

The MIAME class is designed to contain information about experimental methods and conditions from a microarray gene expression experiment. It loosely follows the Minimum Information About a Microarray Experiment (MIAME) specification. It can include information about:

- Experiment design
- Microarrays used in the experiment
- Samples used
- Sample preparation and labeling
- Hybridization procedures and parameters
- Normalization controls
- Preprocessing information
- Data processing specifications

It provides a convenient way to store related information about a microarray experiment in a single data structure (object).

The MIAME class includes properties and methods that let you access, retrieve, and change experiment information related to a microarray experiment. These properties and methods are useful to view and analyze the information.

Construction

`MIAMEobj` `= bioma.data.MIAME()` creates an empty MIAME object for storing experiment information from a microarray gene expression experiment.

`MIAMEobj` `= bioma.data.MIAME(`*`GeoSeriesStruct`*`)` creates a MIAME object from a structure containing Gene Expression Omnibus (GEO) Series data.

MIAMEobj = bioma.data.MIAME(..., '*PropertyName*', *PropertyValue*) constructs the object using options, specified as property name/property value pairs.

MIAMEobj = bioma.data.MIAME(...,'Investigator', *InvestigatorValue*) specifies the name of the experiment investigator.

MIAMEobj = bioma.data.MIAME(...,'Lab', *LabValue*) specifies the laboratory that conducted the experiment.

MIAMEobj = bioma.data.MIAME(...,'Contact', *ContactValue*) specifies the contact information for the experiment investigator or laboratory.

MIAMEobj = bioma.data.MIAME(...,'URL', *URLValue*) specifies the experiment URL.

Inputs

GeoSeriesStruct

Gene Expression Omnibus (GEO) Series data specified by either:

- MATLAB structure returned by the `getgeodata` function
- `Structure.Header.Series` substructure returned by the `getgeodata` function

InvestigatorValue

String specifying the name of the experiment investigator.

LabValue

String specifying the laboratory that conducted the experiment.

ContactValue

String specifying the contact information for the experiment investigator or laboratory

URLValue

String specifying the experiment URL.

Properties

`Abstract`

Abstract describing the experiment

String containing an abstract describing the experiment.

`Arrays`

Information about the microarray chips used in the experiment

Cell array containing information about the microarray chips used in the experiment. Information can include array name, array platform, number of features on the array, and so on.

`Contact`

Contact information for the experiment investigator or laboratory

Character array containing contact information for the experiment investigator or laboratory.

`ExptDesign`

Brief description of the experiment design

Character array containing description of the experiment design.

`Hybridization`

Information about the experiment hybridization

Cell array containing information about the hybridization protocol used in the experiment. Information can include hybridization time, concentration, volume, temperature, and so on.

`Investigator`

Name of the experiment investigator

Character array containing the name of the experiment investigator.

`Laboratory`

Name of the laboratory where the experiment was conducted

Character array containing the name of laboratory.

`Other`

Other information about the experiment

Cell array containing other information about the experiment, not covered by the other properties.

`Preprocessing`

Information about the experiment preprocessing steps

Cell array containing information about the preprocessing steps used on the data from the experiment.

`PubMedID`

PubMed identifiers for relevant publications.

Character array containing PubMed identifiers for papers relevant to the data set used in the experiment.

`QualityControl`

Information about the experiment quality controls

Cell array containing information about the experiment quality control steps. Information can include replicates, dye swap, and so on.

`Samples`

Information about samples used in the experiment

Cell array containing information about the samples used in the experiment. Information can include sample source, sample organism, treatment type, compound, labeling protocol, external control, and so on.

`Title`

Experiment title

Character array containing a single sentence experiment title.

`URL`

URL for the experiment

Character array containing URL for the experiment.

Methods

combine	Combine two MIAME objects
isempty	Determine whether MIAME object is empty

Instance Hierarchy

An ExpressionSet object contains a MIAME object.

Attributes

To learn about attributes of classes, see Class Attributes in the MATLAB Object-Oriented Programming documentation.

Copy Semantics

Value. To learn how this affects your use of the class, see Copying Objects in the MATLAB Programming Fundamentals documentation.

Examples

Construct a MIAME object from a structure containing information from a Gene Expression Omnibus (GEO) Series record:

```
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Import bioma.data package to make constructor function
% available
import bioma.data.*
% Construct MIAME object
MIAMEObj1 = MIAME(geoStruct);
% Display information about the MIAME object
MIAMEObj1
% Supply a URL for the MIAME object
MIAMEObj1.URL = 'www.nonexistinglab.com'
```

Construct a MIAME object using properties:

```
% Import bioma.data package to make constructor function
% available
import bioma.data.*
% Construct MIAME object
MIAMEObj2 = MIAME('investigator', 'Jane Researcher',...
                  'lab', 'One Bioinformatics Laboratory',...
                  'contact', 'jresearcher@lab.not.exist',...
                  'url', 'www.lab.not.exist',...
                  'title', 'Normal vs. Diseased Experiment',...
                  'abstract', 'Example of using expression data',...
                  'other', {'Notes:Created from a text file.'});
% Display information about the MIAME object
MIAMEObj2
% Replace the URL for the MIAME object
MIAMEObj2.URL = 'www.nonexistinglab.com'
```

See Also

`bioma.ExpressionSet` | `bioma.data.ExptData` | `bioma.data.MetaData` | `getgeodata`

Tutorials

- Working with Data Objects for Microarray Experiment Data
- Analyzing Illumina Bead Summary Gene Expression Data

How To

- Class Attributes
- Property Attributes
- “Working with MIAME Objects”

Superclasses

AExperiment

Purpose

Contain data from microarray gene expression experiment

Description

The ExpressionSet class is designed to contain data from a microarray gene expression experiment, including expression values, sample and feature metadata, and information about experimental methods and conditions. It provides a convenient way to store related information about a microarray gene expression experiment in a single data structure (object). It also lets you manage and subset the data.

The ExpressionSet class includes properties and methods that let you access, retrieve, and change data, metadata, and other information about the microarray gene expression experiment. These properties and methods are useful for viewing and analyzing the data.

Construction

`ExprSetobj = bioma.ExpressionSet(Data)` creates an ExpressionSet object, from *`Data`*, a numeric matrix, a DataMatrix object, or an ExptData object, which contains one or more DataMatrix objects with the same dimensions, row names and column names.

`ExprSetobj = bioma.ExpressionSet(Data, {DMobj1, Name1}, {DMobj2, Name2}, ...)` creates an ExpressionSet object, from *`Data`*, and additional DataMatrix objects with specified element names. All DataMatrix objects must have the same dimensions, row names, and column names.

`ExprSetobj = bioma.ExpressionSet(..., 'PropertyName', PropertyValue)` constructs the object using options, specified as property name/property value pairs.

`ExprSetobj = bioma.ExpressionSet(..., 'SData', SDataValue)` includes a MetaData object containing sample metadata in the ExpressionSet object.

`ExprSetobj = bioma.ExpressionSet(..., 'FData', FDataValue)` includes a MetaData object containing microarray feature metadata in the ExpressionSet object.

ExprSetobj = bioma.ExpressionSet(..., 'EInfo', *EInfoValue*) includes a MIAME object, which contains experiment information, in the ExpressionSet object.

Inputs

Data

Any of the following:

- Numeric matrix
- DataMatrix object
- ExptData object, which contains one or more DataMatrix objects having the same dimensions

If you provide a DataMatrix object, bioma.ExpressionSet creates an ExptData object from it and names the DataMatrix object Expressions. If you provide an ExptData object, bioma.ExpressionSet renames the first DataMatrix object in the ExptData object to Expressions, unless another DataMatrix object in the ExptData object is already named Expressions.

DMobj#

Variable name of a DataMatrix object. Each DataMatrix object must have the same dimensions as *Data*.

Name#

String specifying an element name for the corresponding DataMatrix object. Each DataMatrix object in an ExpressionSet object has an element name. At least one DataMatrix object in an ExpressionSet object has an element name of Expressions. By default, it is the first DataMatrix object.

SDataValue

Variable name of a MetaData object containing sample metadata for the experiment. The variable name must exist in the MATLAB Workspace.

FDataValue

Variable name of a MetaData object containing microarray feature metadata for the experiment. The variable name must exist in the MATLAB Workspace.

EInfoValue

Variable name of a MIAME object, which contains information about the experiment methods and conditions. The variable name must exist in the MATLAB Workspace.

Properties

`NElements`

Number of elements in the experiment

Positive integer specifying the number of elements (DataMatrix objects) in the experiment data. This value is equivalent to the number of DataMatrix objects in the ExperimentSet object. This information is read-only.

Attributes:

`SetAccess`	`private`

`NFeatures`

Number of features in the experiment

Positive integer specifying the number of features in the experiment. This value is equivalent to the number of rows in each DataMatrix object in the ExperimentSet object. This information is read-only.

Attributes:

```
SetAccess                    private
```

`NSamples`

Number of samples in the experiment

Positive integer specifying the number of samples in the experiment. This value is equivalent to the number of columns in each DataMatrix object in the ExperimentSet object. This information is read-only.

Attributes:

```
SetAccess                    private
```

Methods

abstract	Retrieve or set abstract describing experiment in ExpressionSet object
elementData	Retrieve or set data element (DataMatrix object) in ExpressionSet object
elementNames	Retrieve or set element names of DataMatrix objects in ExpressionSet object
expressions	Retrieve or set `Expressions` DataMatrix object from ExpressionSet object
exprWrite	Write expression values in ExpressionSet object to text file
exptData	Retrieve or set experiment data in ExpressionSet object
exptInfo	Retrieve or set experiment information in ExpressionSet object

featureData	Retrieve or set feature metadata in ExpressionSet object
featureNames	Retrieve or set feature names in ExpressionSet object
featureVarDesc	Retrieve or set feature variable descriptions in ExpressionSet object
featureVarNames	Retrieve or set feature variable names in ExpressionSet object
featureVarValues	Retrieve or set feature variable data values in ExpressionSet object
pubMedID	Retrieve or set PubMed IDs in ExpressionSet object
sampleData	Retrieve or set sample metadata in ExpressionSet object
sampleNames	Retrieve or set sample names in ExpressionSet object
sampleVarDesc	Retrieve or set sample variable descriptions in ExpressionSet object
sampleVarNames	Retrieve or set sample variable names in ExpressionSet object
sampleVarValues	Retrieve or set sample variable values in ExpressionSet object
size	Return size of ExpressionSet object

Instance Hierarchy

An ExpressionSet object contains an ExptData object, two MetaData objects, and a MIAME object. These objects can be empty.

Attributes

To learn about attributes of classes, see Class Attributes in the MATLAB Object-Oriented Programming documentation.

Copy Semantics

Value. To learn how this affects your use of the class, see Copying Objects in the MATLAB Programming Fundamentals documentation.

Indexing

ExpressionSet objects support 2-D parenthesis ( ) indexing to extract, assign, and delete data.

ExpressionSet objects do not support:

- Dot . indexing
- Curly brace { } indexing
- Linear indexing

Examples

The `mouseExprsData.txt` file used in this example contains data from Hovatta et al., 2005.

Construct an ExpressionSet object from `EDObj`, an ExptData object, `MDObj2`, a MetaData object containing sample variable information, and `MIAMEObj`, a MIAME object:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Construct MIAME object
MIAMEObj = MIAME(geoStruct);
```

```
% Import bioma package to make constructor function
% available
import bioma.*
% Construct ExpressionSet object
ESObj = ExpressionSet(EDObj, 'SData', MDObj2, 'EInfo', MIAMEObj);
% Display information about the ExpressionSet object
ESObj
```

References

[1] Hovatta, I., Tennant, R S., Helton, R., et al. (2005). Glyoxalase 1 and glutathione reductase 1 regulate anxiety in mice. Nature *438*, 662–666.

See Also

`bioma.data.ExptData` | `bioma.data.MetaData` | `bioma.data.MIAME`

Tutorials

- Working with Data Objects for Microarray Experiment Data
- Analyzing Illumina Bead Summary Gene Expression Data

How To

- Class Attributes
- Property Attributes
- “Working with ExpressionSet Objects”

blastformat

Purpose

Create local BLAST database

Syntax

```
blastformat('Inputdb', InputdbValue)
blastformat(..., 'FormatPath', FormatPathValue, ...)
blastformat(..., 'Title', TitleValue, ...)
blastformat(..., 'Log', LogValue, ...)
blastformat(..., 'Protein', ProteinValue, ...)
blastformat(..., 'FormatArgs', FormatArgsValue, ...)
```

Arguments

InputdbValue	String specifying a file name or path and file name of a FASTA file containing a set of sequences to be formatted as a blastable database. If you specify only a file name, that file must be on the MATLAB search path or in the current directory. (This corresponds to the `formatdb` option `-i`.)
FormatPathValue	String specifying the full path to the `formatdb` executable file, including the name and extension of the executable file. Default is the system path.
TitleValue	String specifying the title for the local database. Default is the input FASTA file name. (This corresponds to the `formatdb` option `-t`.)
LogValue	String specifying the file name or path and file name for the log file associated with the local database. Default is `formatdb.log`. (This corresponds to the `formatdb` option `-l`.)

ProteinValue	Specifies whether the sequences formatted as a local BLAST database are protein or not. Choices are `true` (default) or `false`. (This corresponds to the `formatdb` option `-p`.)
FormatArgsValue	NCBI `formatdb` command string, that is, a string containing one or more instances of `-x` and the option associated with it, used to specify input arguments. For an example, see Using blastformat with formatdb Syntax and Input Arguments on page 3-180.

Description

Note To use the `blastformat` function, you must have a local copy of the NCBI `formatdb` executable file available from your system. You can download the `formatdb` executable file by accessing

```
http://blast.ncbi.nlm.nih.gov/download.shtml
```

then clicking the **download** link under the **blast** column for your platform. Run the downloaded executable and configure it for your system. For more information, see the readme file on the NCBI ftp site at:

```
ftp://ftp.ncbi.nih.gov/blast/documents/blast.html
```

For convenience, consider placing the NCBI `formatdb` executable file on your system path.

`blastformat('Inputdb', InputdbValue)` calls a local version of the NCBI `formatdb` executable file with *`InputdbValue`*, a file name or path and file name of a FASTA file containing a set of sequences. If you specify only a file name, that file must be on the MATLAB search path or in the current directory. (This corresponds to the `formatdb` option `-i`.)

It then formats the sequences as a local, blastable database, by creating multiple files, each with the same name as the *`InputdbValue`* FASTA

file, but with different extensions. The database files are placed in the same location as the FASTA file.

Note If you rename the database files, make sure they all have the same name.

`blastformat(..., '`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `blastformat` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows.

`blastformat(..., 'FormatPath', `*`FormatPathValue`*`, ...)` specifies the full path to the `formatdb` executable file, including the name and extension of the executable file. Default is the system path.

`blastformat(..., 'Title', `*`TitleValue`*`, ...)` specifies the title for the local database. Default is the input FASTA file name. (This corresponds to the `formatdb` option `-t`.)

Note The `'Title'` property does not change the file name of the database files. This title is used internally only, and appears in the report structure returned by the `blastlocal` function.

`blastformat(..., 'Log', `*`LogValue`*`, ...)` specifies the file name or path and file name for the log file associated with the local database. Default is `formatdb.log`. The log file captures the progress of the database creation and formatting. (This corresponds to the `formatdb` option `-l`.)

`blastformat(..., 'Protein', `*`ProteinValue`*`, ...)` specifies whether the sequences formatted as a local BLAST database are protein or not. Choices are `true` (default) or `false`. (This corresponds to the `formatdb` option `-p`.)

`blastformat(..., 'FormatArgs', FormatArgsValue, ...)` specifies options using the input arguments for the NCBI `formatdb` function. *`FormatArgsValue`* is a string containing one or more instances of *`-x`* and the option associated with it. For example, to specify that the input is a database in ASN.1 format, instead of a FASTA file, you would use the following syntax:

```
blastformat('Inputdb', 'ecoli.asn', 'FormatArgs', '-a T')
```

Tip Use the `'FormatArgs'` property to specify `formatdb` options for which there are no corresponding property name/property value pairs.

Note For a complete list of valid input arguments for the NCBI `formatdb` function, make sure that the `formatdb` executable file is located on your system path or current directory, then type the following at your system's command prompt.

```
formatdb -
```

Using formatdb Syntax

You can also use the syntax and input arguments accepted by the NCBI `formatdb` function, instead of the property name/property value pairs listed previously. To do so, supply a single string containing multiple options using the *`-x option`* syntax. For example, you can specify the `ecoli.nt` FASTA file, a title of `myecoli`, and that the sequences are not protein by using

```
blastformat('-i ecoli.nt -t myecoli -p F')
```

Note For a complete list of valid input arguments for the NCBI `formatdb` function, make sure that the `formatdb` executable file is located on your system path or current directory, then type the following at your system's command prompt.

```
formatdb -
```

Examples

Using blastformat with Property Name/Value Pairs

The following example assumes you have a FASTA nucleotide file, such as the *E. coli* file `NC_004431.fna`, which you can download from , saved to your MATLAB current directory.

Create a local blastable database from the `NC_004431.fna` FASTA file and give it a title using the `'title'` property.

```
blastformat('inputdb', 'NC_004431.fna', 'protein', 'false',...
            'title', 'myecoli_nt');
```

Using blastformat with formatdb Syntax and Input Arguments

The following example assumes you have a FASTA amino acid file, such as the *E. coli* file `NC_004431.faa`, which you can download from , saved to your MATLAB current directory.

Create a local blastable database from the `NC_004431.faa` FASTA file and rename the title and log file using `formatdb` syntax and input arguments.

```
blastformat('inputdb', 'NC_004431.faa',...
            'formatargs', '-t myecoli_aa -l ecoli_aa.log');
```

References

[1] Altschul, S.F., Gish, W., Miller, W., Myers, E.W., and Lipman, D.J. (1990). Basic local alignment search tool. J. Mol. Biol. *215*, 403–410.

[2] Altschul, S.F., Madden, T.L., Schäffer, A.A., Zhang, J., Zhang, Z., Miller, W., and Lipman, D.J. (1997). Gapped BLAST and PSI-BLAST:

a new generation of protein database search programs. Nucleic Acids Res. *25*, 3389–3402.

For more information on the NCBI `formatdb` function, see:

```
http://blast.ncbi.nlm.nih.gov/docs/formatdb.html
```

See Also

Bioinformatics Toolbox functions: `blastlocal`, `blastncbi`, `blastread`, `blastreadlocal`, `getblast`

blastlocal

Purpose

Perform search on local BLAST database to create BLAST report

Syntax

```
blastlocal('InputQuery', InputQueryValue)
Data = blastlocal('InputQuery', InputQueryValue)
... blastlocal(..., 'Program', ProgramValue, ...)
... blastlocal(..., 'Database', DatabaseValue, ...)
... blastlocal(..., 'BlastPath', BlastPathValue, ...)
... blastlocal(..., 'Expect', ExpectValue, ...)
... blastlocal(..., 'Format', FormatValue, ...)
... blastlocal(..., 'ToFile', ToFileValue, ...)
... blastlocal(..., 'Filter', FilterValue, ...)
... blastlocal(..., 'GapOpen', GapOpenValue, ...)
... blastlocal(..., 'GapExtend', GapExtendValue, ...)
... blastlocal(..., 'BLASTArgs', BLASTArgsValue, ...)
```

Arguments

InputQueryValue — String specifying the file name or path and file name of a FASTA file containing query nucleotide or amino acid sequence(s). (This corresponds to the `blastall` option `-i`.)

ProgramValue — String specifying a BLAST program. Choices are:

- `'blastp'` (default) — Search protein query versus protein database.
- `'blastn'` — Search nucleotide query versus nucleotide database.
- `'blastx'` — Search translated nucleotide query versus protein database.
- `'tblastn'` — Search protein query versus translated nucleotide database.
- `'tblastx'` — Search translated nucleotide query versus translated nucleotide database.

(The *ProgramValue* argument corresponds to the `blastall` option `-p`.)

DatabaseValue — String specifying a file name or path and file name of a local BLAST database (formatted using the NCBI `formatdb` function) to search. Default is a local version of the `nr` database in the MATLAB current directory. (This corresponds to the `blastall` option `-d`.)

BlastPathValue — String specifying the full path to the `blastall` executable file, including the name and extension of the executable file. Default is the system path.

ExpectValue — Value specifying the statistical significance threshold for matches against database sequences. Choices are any real number. Default is `10`. (This corresponds to the `blastall` option `-e`.)

FormatValue — Integer specifying the alignment format of the BLAST search results. Choices are:

- `0` (default) — Pairwise
- `1` — Query-anchored, showing identities
- `2` — Query-anchored, no identities
- `3` — Flat query-anchored, showing identities
- `4` — Flat query-anchored, no identities
- `5` — Query-anchored, no identities and blunt ends
- `6` — Flat query-anchored, no identities and blunt ends
- `8` — Tabular
- `9` — Tabular with comment lines

	(This corresponds to the `blastall` option `-m`.)
`ToFileValue`	String specifying a file name or path and file name in which to save the contents of the BLAST report. (This corresponds to the `blastall` option `-o`.)
`FilterValue`	Controls the application of a filter (DUST filter for the blastn program or SEG filter for other programs) to the query sequence(s). Choices are `true` (default) or `false`. (This corresponds to the `blastall` option `-F`.)
`GapOpenValue`	Integer that specifies the penalty for opening a gap in the alignment of sequences. Default is `-1`. (This corresponds to the `blastall` option `-G`.)
`GapExtendValue`	Integer that specifies the penalty for extending a gap in the alignment of sequences. Default is `-1`. (This corresponds to the `blastall` option `-E`.)
`BLASTArgsValue`	NCBI `blastall` command string, that is a string containing one or more instances of `-x` and the option associated with it, used to specify input arguments. For an example, see step 2 in "Examples" on page 3-191.

Return Values

`Data`	MATLAB structure or array of structures (if multiple query sequences) containing fields corresponding to BLAST keywords and data from a local BLAST report.

Description

This function assumes that

The Basic Local Alignment Search Tool (BLAST) offers a fast and powerful comparative analysis of protein and nucleotide sequences against known sequences in online or local databases.

Note To use the `blastlocal` function, you must have a local copy of the NCBI `blastall` executable file (version 2.2.17) available from your system. You can download the `blastall` executable file by accessing

```
http://blast.ncbi.nlm.nih.gov/download.shtml
```

then clicking the **download** link under the **blast** column for your platform. Run the downloaded executable and configure it for your system. For more information, see the readme file on the NCBI ftp site at:

```
ftp://ftp.ncbi.nih.gov/blast/documents/blast.html
```

For convenience, consider placing the NCBI `blastall` executable file on your system path.

`blastlocal('InputQuery', InputQueryValue)` submits query sequence(s) specified by *`InputQueryValue`*, a FASTA file containing nucleotide or amino acid sequence(s), for a BLAST search of a local BLAST database, by calling a local version of the NCBI `blastall` executable file. The BLAST search results are displayed in the MATLAB Command Window. (This corresponds to the `blastall` option `-i`.)

`Data` `= blastlocal('InputQuery', InputQueryValue)` returns the BLAST search results in *`Data`*, a MATLAB structure or array of structures (if multiple query sequences) containing fields corresponding to BLAST keywords and data from a local BLAST report.

`Data` contains a subset of the following fields, based on the specified alignment format.

Field	Description
`Algorithm`	NCBI algorithm used to do a BLAST search.

Field	Description
`Query`	Identifier of the query sequence submitted to a BLAST search.
`Length`	Length of the query sequence.
`Database`	All databases searched.
`Hits.Name`	Name of a database sequence (subject sequence) that matched the query sequence.
`Hits.Score`	Alignment score between the query sequence and the subject sequence.
`Hits.Expect`	Expectation value for the alignment between the query sequence and the subject sequence.
`Hits.Length`	Length of a subject sequence.
`Hits.HSPs.Score`	Pairwise alignment score for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.Expect`	Expectation value for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.Identities`	Identities (match, possible, and percent) for a high-scoring sequence pair between the query sequence and a subject sequence.

Field	Description
`Hits.HSPs.Positives`	Identical or similar residues (match, possible, and percent) for a high-scoring sequence pair between the query sequence and a subject amino acid sequence. **Note** This field applies only to translated nucleotide or amino acid query sequences and/or databases.
`Hits.HSPs.Gaps`	Nonaligned residues (match, possible, and percent) for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.Mismatches`	Residues that are not similar to each other (match, possible, and percent) for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.Frame`	Reading frame of the translated nucleotide sequence for a high-scoring sequence pair between the query sequence and a subject sequence. **Note** This field applies only when performing translated searches, that is, when using `tblastx`, `tblastn`, and `blastx`.

Field	Description
`Hits.HSPs.Strand`	Sense (`Plus` = 5' to 3' and `Minus` = 3' to 5') of the DNA strands for a high-scoring sequence pair between the query sequence and a subject sequence. **Note** This field applies only when using a nucleotide query sequence and database.
`Hits.HSPs.Alignment`	Three-row matrix showing the alignment for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.QueryIndices`	Indices of the query sequence residue positions for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.SubjectIndices`	Indices of the subject sequence residue positions for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.AlignmentLength`	Length of the pairwise alignment for a high-scoring sequence pair between the query sequence and a subject sequence.
`Alignment`	Entire alignment for the query sequence and the subject sequence(s).
`Statistics`	Summary of statistical details about the performed search, such as lambda values, gap penalties, number of sequences searched, and number of hits.

`... blastlocal(..., '`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `blastlocal` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows.

`... blastlocal(..., 'Program', `*`ProgramValue`*`, ...)` specifies the BLAST program. Choices are `'blastp'` (default), `'blastn'`, `'blastx'`, `'tblastn'`, and `'tblastx'`. (This corresponds to the `blastall` option `-p`.) For help in selecting an appropriate BLAST program, visit:

```
http://blast.ncbi.nlm.nih.gov/producttable.shtml
```

`... blastlocal(..., 'Database', `*`DatabaseValue`*`, ...)` specifies the local BLAST database (formatted using the NCBI `formatdb` function) to search. Default is a local version of the `nr` database in the MATLAB current directory. (This corresponds to the `blastall` option `-d`.)

`... blastlocal(..., 'BlastPath', `*`BlastPathValue`*`, ...)` specifies the full path to the `blastall` executable file, including the name and extension of the executable file. Default is the system path.

`... blastlocal(..., 'Expect', `*`ExpectValue`*`, ...)` specifies a statistical significance threshold for matches against database sequences. Choices are any real number. Default is `10`. (This corresponds to the `blastall` option `-e`.) You can learn more about the statistics of local sequence comparison at:

```
http://blast.ncbi.nlm.nih.gov/tutorial/Altschul-1.html#head2
```

`... blastlocal(..., 'Format', `*`FormatValue`*`, ...)` specifies the alignment format of the BLAST search results. Choices are:

- `0` (default) — Pairwise
- `1` — Query-anchored, showing identities

- 2 — Query-anchored, no identities
- 3 — Flat query-anchored, showing identities
- 4 — Flat query-anchored, no identities
- 5 — Query-anchored, no identities and blunt ends
- 6 — Flat query-anchored, no identities and blunt ends
- 7 — Not used
- 8 — Tabular
- 9 — Tabular with comment lines

(This corresponds to the `blastall` option `-m`.)

`... blastlocal(..., 'ToFile', ToFileValue, ...)` saves the contents of the BLAST report to the specified file. (This corresponds to the `blastall` option `-o`.)

`... blastlocal(..., 'Filter', FilterValue, ...)` specifies whether a filter (DUST filter for the blastn program or SEG filter for other programs) is applied to the query sequence(s). Choices are `true` (default) or `false`. (This corresponds to the `blastall` option `-F`.)

`... blastlocal(..., 'GapOpen', GapOpenValue, ...)` specifies the penalty for opening a gap in the alignment of sequences. Default is `-1`. (This corresponds to the `blastall` option `-G`.)

`... blastlocal(..., 'GapExtend', GapExtendValue, ...)` specifies the penalty for extending a gap in the alignment of sequences. Default is `-1`. (This corresponds to the `blastall` option `-E`.)

`... blastlocal(..., 'BLASTArgs', BLASTArgsValue, ...)` specifies options using the input arguments for the NCBI `blastall` function. *`BLASTArgsValue`* is a string containing one or more instances or `-x` and the option associated with it. For example, to specify the `BLOSUM 45` matrix, you would use the following syntax:

```
blastlocal('InputQuery', ecoliquery.txt, 'BLASTArgs', '-M BLOSUM45')
```

Tip Use the `'BlastArgs'` property to specify `blastall` options for which there are no corresponding property name/property value pairs.

Note For a complete list of valid input arguments for the NCBI `blastall` function, make sure that the `blastall` executable file is located on your system path or current directory, then type the following at your system's command prompt.

```
blastall -
```

Using blastall Syntax

You can also use the syntax and input arguments accepted by the NCBI `blastall` function, instead of the property name/property value pairs listed previously. To do so, supply a single string containing multiple options using the *`-x option`* syntax. For example, you can specify the `ecoliquery.txt` FASTA file as your query sequences, the `blastp` program, and the `ecoli` local database, by using

```
blastlocal('-i ecoliquery.txt -p blastp -d ecoli')
```

Note For a complete list of valid input arguments for the NCBI `blastall` function, make sure that the `blastall` executable file is located on your system path or current directory, then type the following at your system's command prompt.

```
blastall -
```

Examples

The following examples assume you have a FASTA nucleotide file and a FASTA amino acid file for *E. coli*, such as the files `NC_004431.fna` and

NC_004431.faa, which you can download from , saved to your MATLAB current directory.

Performing a Nucleotide Translated Search

1. Create local blastable databases from the NC_004431.fna and NC_004431.faa FASTA files by using the blastformat function.

```
blastformat('inputdb', 'NC_004431.fna',
'protein', 'false');
blastformat('inputdb', 'NC_004431.faa');
```

2. Use the getgenbank function to retrieve sequence information for the *E. coli* threonine operon from the GenBank database.

```
S = getgenbank('M28570');
```

3. Create a query file by using the fastawrite function to create a FASTA file named query_nt.fa from this sequence information, using only the accession number as the header.

```
S.Header = S.Accession;
fastawrite('query_nt.fa', S);
```

4. Use MATLAB syntax to submit the query sequence in the query_nt.fa FASTA file for a BLAST search of the local amino acid database NC_004431.faa. Specify the BLAST program blastx. Return the BLAST search results in results, a MATLAB structure.

```
results = blastlocal('inputquery', 'query_nt.fa',...
                     'database', 'NC_004431.faa',...
                     'program',  'blastx');
```

Performing a Nucleotide Search Using blastall Syntax

1. If you have not already done so, create local blastable databases and a query file as described in steps 1 through 3 in Performing a Nucleotide Translated Search on page 3-192.

2 Use `blastall` syntax to submit the query sequence in the `query_nt.fa` FASTA file for a BLAST search of the local nucleotide database `NC_004431.fna`. Specify the BLAST program `blastn` and an expectation value of `0.0001`. Return the BLAST search results in `results`, a MATLAB structure.

```
results = blastlocal('-i query_nt.fa -d NC_004431.fna ...
                      -p blastn -e 0.0001');
```

Performing a Nucleotide Search and Creating a Formatted Report

1 If you have not already done so, create local blastable databases and a query file as described in steps 1 through 3 in Performing a Nucleotide Translated Search on page 3-192.

2 Submit the query sequence in the `query_nt.fa` FASTA file for a BLAST search of the local nucleotide database `NC_004431.fna`. Specify the BLAST program `blastn` and a tabular alignment format. Save the contents of the BLAST report to a file named `myecoli_nt.txt`.

```
blastlocal('inputquery', 'query_nt.fa',...
           'database', 'NC_004431.fna', 'tofile',...
           'myecoli_nt.txt', 'blastargs', '-p blastn -m 8');
```

References

[1] Altschul, S.F., Gish, W., Miller, W., Myers, E.W., and Lipman, D.J. (1990). Basic local alignment search tool. J. Mol. Biol. *215*, 403–410.

[2] Altschul, S.F., Madden, T.L., Schäffer, A.A., Zhang, J., Zhang, Z., Miller, W., and Lipman, D.J. (1997). Gapped BLAST and PSI-BLAST: a new generation of protein database search programs. Nucleic Acids Res. *25*, 3389–3402.

For more information on the NCBI `blastall` function, see:

```
http://blast.ncbi.nlm.nih.gov/docs/blastall.html
```

See Also

Bioinformatics Toolbox functions: `blastformat`, `blastncbi`, `blastread`, `blastreadlocal`, `getblast`

Purpose

Create remote NCBI BLAST report request ID or link to NCBI BLAST report

Syntax

```
blastncbi(Seq, Program)
RID = blastncbi(Seq, Program)
[RID, RTOE] = blastncbi(Seq, Program)
... blastncbi(Seq, Program, ...'Database',
DatabaseValue, ...)
... blastncbi(Seq, Program, ...'Descriptions',
   DescriptionsValue, ...)
... blastncbi(Seq, Program, ...'Alignments',
AlignmentsValue,
   ...)
... blastncbi(Seq, Program, ...'Filter', FilterValue, ...)
... blastncbi(Seq, Program, ...'Expect', ExpectValue, ...)
... blastncbi(Seq, Program, ...'Word', WordValue, ...)
... blastncbi(Seq, Program, ...'Matrix', MatrixValue, ...)
... blastncbi(Seq, Program, ...'GapOpen',
GapOpenValue, ...)
... blastncbi(Seq, Program, ...'ExtendGap', ExtendGapValue,
   ...)
... blastncbi(Seq, Program, ...'GapCosts', GapCostsValue,
   ...)
... blastncbi(Seq, Program, ...'Inclusion', InclusionValue,
   ...)
... blastncbi(Seq, Program, ...'Pct', PctValue, ...)
... blastncbi(Seq, Program, ...'Entrez', EntrezValue, ...)
```

Arguments

Seq

Nucleotide or amino acid sequence specified by any of the following:

- GenBank, GenPept, or RefSeq accession number
- GI sequence identifier
- FASTA file
- URL pointing to a sequence file
- String
- Character array
- MATLAB structure containing a `Sequence` field

Program

String specifying a BLAST program. Choices are:

- `'blastn'` — Search nucleotide query versus nucleotide database.
- `'blastp'` — Search protein query versus protein database.
- `'blastx'` — Search translated nucleotide query versus protein database.
- `'megablast'` — Quickly search for highly similar nucleotide sequences.
- `'psiblast'` — Search protein query using position-specific iterative BLAST.
- `'tblastn'` — Search protein query versus translated nucleotide database.
- `'tblastx'` — Search translated nucleotide query versus translated nucleotide database.

DatabaseValue	String specifying a database. Compatible databases depend on the type of sequence specified by *Seq*, and the program specified by *Program*. For a list of database choices for nucleotide sequences and amino acid sequences, see the lists in the section "Description" on page 3-201.
DescriptionsValue	Value specifying the number of short descriptions to include in the report. Default is `100`, unless *Program* = `'psiblast'`, then default is `500`.
AlignmentsValue	Value specifying the number of sequences for which high-scoring segment pairs (HSPs) are reported. Default is `100`, unless *Program* = `'psiblast'`, then default is `500`.
FilterValue	String specifying a filter. Possible choices are: • `'L'` (default) — Low complexity. • `'R'` — Human repeats. • `'m'` — Mask for lookup table. • `'lcase'` — Turn on the lowercase mask. Choices vary depending on the selected *Program*. For more information, see the table Choices for Optional Properties by BLAST Program on page 3-207.
ExpectValue	Value specifying the statistical significance threshold for matches against database sequences. Choices are any real number. Default is `10`.

WordValue

Value specifying a word length for the query sequence.

Choices for amino acid sequences are:

- 2
- 3 (default)

Choices for nucleotide sequences are:

- 7
- 11 (default)
- 15

Choices when *Program* = 'megablast' are:

- 11
- 12
- 16
- 20
- 24
- 28 (default)
- 32
- 48
- 64

MatrixValue

String specifying the substitution matrix for amino acid sequences only. The matrix assigns the score for a possible alignment of any two amino acid residues. Choices are:

- `'PAM30'`
- `'PAM70'`
- `'BLOSUM45'`
- `'BLOSUM62'` (default)
- `'BLOSUM80'`

GapOpenValue

Integer that specifies the penalty for opening a gap in the alignment of amino acid sequences.

Choices and default depend on the substitution matrix specified by the `'Matrix'` property. For more information, see the table Choices for the GapCosts Property by Matrix on page 3-208.

ExtendGapValue

Integer that specifies the penalty for extending a gap in the alignment of amino acid sequences.

Choices and default depend on the substitution matrix specified by the `'Matrix'` property. For more information, see the table Choices for the GapCosts Property by Matrix on page 3-208.

GapCostsValue

Vector containing two integers: the first is the penalty for opening a gap, and the second is the penalty for extending the gap, in the alignment of amino acid sequences.

Choices and default depend on the substitution matrix specified by the `'Matrix'` property. For more information, see the table Choices for the GapCosts Property by Matrix on page 3-208.

InclusionValue — Value specifying the statistical significance threshold for including a sequence in the Position-Specific Scoring Matrix (PSSM) created by PSI-BLAST for the subsequent iteration. Default is `0.005`.

Note Specify an *InclusionValue* only when *Program* = `'psiblast'`.

PctValue — Value specifying the percent identity and the corresponding match and mismatch score for matching existing sequences in a public database. Choices are:

- `None`
- `99` (default) — `99`, `1`, `-3`
- `98` — `98`, `1`, `-3`
- `95` — `95`, `1`, `-3`
- `90` — `90`, `1`, `-2`
- `85` — `85`, `1`, `-2`
- `80` — `80`, `2`, `-3`
- `75` — `75`, `4`, `-5`
- `60` — `60`, `1`, `-1`

Note Specify a *PctValue* only when *Program* = `'megablast'`.

EntrezValue — String specifying Entrez query syntax to search a subset of the selected database.

Tip Use this property to limit searches based on molecule types, sequence lengths, organisms, and so on.

Return Values

RID	Request ID for the NCBI BLAST report.
RTOE	Request Time Of Execution, which is an estimate of the time (in minutes) until completion.

Tip Use this time estimate with the `'WaitTime'` property when using the `getblast` function.

Description

The Basic Local Alignment Search Tool (BLAST) offers a fast and powerful comparative analysis of protein and nucleotide sequences against known sequences in online databases.

`blastncbi(`*`Seq`*`, `*`Program`*`)` sends a BLAST request to NCBI against a *`Seq`*, a nucleotide or amino acid sequence, using *`Program`*, a specified BLAST program, and then returns a command window link to the NCBI BLAST report. For help in selecting an appropriate BLAST program, visit:

```
http://blast.ncbi.nlm.nih.gov/producttable.shtml
```

`RID` `= blastncbi(`*`Seq`*`, `*`Program`*`)` returns *`RID`*, the Request ID for the report.

`[`*`RID`*`, `*`RTOE`*`] = blastncbi(`*`Seq`*`, `*`Program`*`)` returns both *`RID`*, the Request ID for the NCBI BLAST report, and *`RTOE`*, the Request Time Of Execution, which is an estimate of the time until completion.

Tip Use *RTOE* with the 'WaitTime' property when using the getblast function.

... blastncbi(..., '*PropertyName*', *PropertyValue*,...) calls blastncbi with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are explained below. Additional information on these optional properties can be found at:

```
http://www.ncbi.nlm.nih.gov/staff/tao/URLAPI/blastcgihelp_new.html
```

... blastncbi(*Seq*, *Program*, ...'Database', *DatabaseValue*, ...) specifies a database for the alignment search. Compatible databases depend on the type of sequence specified by *Seq*, and the program specified by *Program*.

Database choices for nucleotide sequences are:

- 'nr' (default)
- 'refseq_rna'
- 'refseq_genomic'
- 'est'
- 'est_human'
- 'est_mouse'
- 'est_others'
- 'gss'
- 'htgs'
- 'pat'
- 'pdb'

- 'month'
- 'alu_repeats'
- 'dbsts'
- 'chromosome'
- 'wgs'
- 'env_nt'

Database choices for amino acid sequences are:

- 'nr' (default)
- 'refseq_protein'
- 'swissprot'
- 'pat'
- 'month'
- 'pdb'
- 'env_nr'

For help in selecting an appropriate database, visit:

```
http://blast.ncbi.nlm.nih.gov/producttable.shtml
```

`... blastncbi(`*`Seq`*`, `*`Program`*`, ...'Descriptions', `*`DescriptionsValue`*`, ...)` specifies the number of short descriptions to include in the report, when you do not specify return values.

`... blastncbi(`*`Seq`*`, `*`Program`*`, ...'Alignments', `*`AlignmentsValue`*`, ...)` specifies the number of sequences for which high-scoring segment pairs (HSPs) are reported, when you do not specify return values.

`... blastncbi(`*`Seq`*`, `*`Program`*`, ...'Filter', `*`FilterValue`*`, ...)` specifies the filter to apply to the query sequence.

... blastncbi(*Seq*, *Program*, ...'Expect', *ExpectValue*, ...) specifies a statistical significance threshold for matches against database sequences. Choices are any real number. Default is 10. You can learn more about the statistics of local sequence comparison at:

```
http://blast.ncbi.nlm.nih.gov/tutorial/Altschul-1.html#head2
```

... blastncbi(*Seq*, *Program*, ...'Word', *WordValue*, ...) specifies a word size for the query sequence.

... blastncbi(*Seq*, *Program*, ...'Matrix', *MatrixValue*, ...) specifies the substitution matrix for amino acid sequences only. This matrix assigns the score for a possible alignment of two amino acid residues.

... blastncbi(*Seq*, *Program*, ...'GapOpen', *GapOpenValue*, ...) specifies the penalty for opening a gap in the alignment of amino acid sequences. Choices and default depend on the substitution matrix specified by the 'Matrix' property. For more information, see the table Choices for the GapCosts Property by Matrix on page 3-208.

For more information about allowed gap penalties for various matrices, see:

```
http://blast.ncbi.nlm.nih.gov/html/sub_matrix.html
```

... blastncbi(*Seq*, *Program*, ...'ExtendGap', *ExtendGapValue*, ...) specifies the penalty for extending a gap greater than one space in the alignment of amino acid sequences. Choices and default depend on the substitution matrix specified by the 'Matrix' property. For more information, see the table Choices for the GapCosts Property by Matrix on page 3-208.

... blastncbi(*Seq*, *Program*, ...'GapCosts', *GapCostsValue*, ...) specifies the penalty for opening and extending a gap in the alignment of amino acid sequences. *GapCostsValue* is a vector containing two integers: the first is the penalty for opening a gap, and the second is the penalty for extending the gap. Choices and default depend on the substitution matrix specified by the 'Matrix' property.

For more information, see the table Choices for the GapCosts Property by Matrix on page 3-208.

`... blastncbi(`*`Seq`*`, `*`Program`*`, ...'Inclusion', `*`InclusionValue`*`, ...)` specifies the statistical significance threshold for including a sequence in the Position-Specific Scoring Matrix (PSSM) created by PSI-BLAST for the subsequent iteration. Default is `0.005`.

Note Specify an *`InclusionValue`* only when *`Program`* `= 'psiblast'`.

`... blastncbi(`*`Seq`*`, `*`Program`*`, ...'Pct', `*`PctValue`*`, ...)` specifies the percent identity and the corresponding match and mismatch score for matching existing sequences in a public database. Default is `99`.

Note Specify a *`PctValue`* only when *`Program`* `= 'megablast'`.

`... blastncbi(`*`Seq`*`, `*`Program`*`, ...'Entrez', `*`EntrezValue`*`, ...)` specifies Entrez query syntax to search a subset of the selected database.

Note For more information about Entrez query syntax, see:

```
http://www.ncbi.nlm.nih.gov/books/bv.fcgi?rid=helpentrez.chapter.EntrezHelp
```

Tip Use this property to limit searches based on molecule types, sequence lengths, organisms, and so on. For more information on limiting searches, see:

```
http://blast.ncbi.nlm.nih.gov/blastcgihelp.shtml#entrez_query
```

Choices for Optional Properties by BLAST Program

When BLAST program is...	Then choices for the following properties are...					
	Database	**Filter**	**Word**	**Matrix**	**GapCosts**	**Pct**

`'blastn'`	`'nr'` (default)
	`'est'`
	`'est_human'`
	`'est_mouse'`
	`'est_others'`
	`'gss'`
	`'htgs'`
	`'pat'`
	`'pdb'`
	`'month'`
	`'alu_repeats'`
	`'dbsts'`
	`'chromosome'`
	`'wgs'`
	`'refseq_rna'`
	`'refseq_genomic'`
	`'env_nt'`
		`'L'` (default)
		`'R'`
		`'m'`
		`'lcase'`
			7
			11
			(default)
			15
				—	—	—

`'megablast'`		`'L'`	11 12 16 20 24 28 (default) 32 48 64			None 99 (default) 98 95 90 85 80 75 60

`'tblastn'`		`'L'` (default)
		`'m'`
		`'lcase'`
			2
			3 (default)
				`'PAM30'`
				`'PAM70'`
				`'BLOSUM45'`
				`'BLOSUM62'` (default)
				`'BLOSUM80'`
					See the next table.	—

`'tblastx'`		`'L'` (default)
		`'R'`
		`'m'`
		`'lcase'`				

`'blastp'`
`'blastx'`
`'psiblast'`
	`'nr'` (default)
	`'swissprot'`
	`'pat'`
	`'pdb'`
	`'month'`
	`'refseq_protein'`
	`'env_nr'`
		`'L'` (default)
		`'m'`
		`'lcase'`				

Choices for the GapCosts Property by Matrix

When substitution matrix is...	Then choices for GapCosts are...
'PAM30'	[7 2] [6 2] [5 2] [10 1] [9 1] (default) [8 1]
'PAM70' 'BLOSUM80'	[8 2] [7 2] [6 2] [11 1] [10 1] (default) [9 1]
'BLOSUM45'	[13 3] [12 3] [11 3] [10 3] [15 2] (default) [14 2] [13 2] [12 2] [19 1] [18 1] [17 1] [16 1]
'BLOSUM62'	[9 2] [8 2] [7 2] [12 1] [11 1] (default) [10 1]

Examples

```
% Get a sequence from the Protein Data Bank and create
% a MATLAB structure.
S = getpdb('1CIV')

% Use the structure as input for a BLAST search with an
% expectation of 1e-10.
blastncbi(S,'blastp','expect',1e-10)

% Click the URL link (Link to NCBI BLAST Request) to go
% directly to the NCBI request.

% You can also perform a typical BLAST protein search directly
% with an accession number and an alternative scoring matrix.
RID = blastncbi('AAA59174','blastp','matrix','PAM70',...
                              'expect',1e-10)

% You can pass the RID to GETBLAST to parse the report and
% load it into a MATLAB structure.
Struct = getblast(RID)
```

References

[1] Altschul, S.F., Gish, W., Miller, W., Myers, E.W. and Lipman, D.J. (1990). Basic local alignment search tool. J. Mol. Biol. *215*, 403–410.

[2] Altschul, S.F., Madden, T.L., Schäffer, A.A., Zhang, J., Zhang, Z., Miller, W. and Lipman, D.J. (1997). Gapped BLAST and PSI-BLAST: a new generation of protein database search programs. Nucleic Acids Res. *25*, 3389–3402.

See Also

Bioinformatics Toolbox functions: `blastformat`, `blastlocal`, `blastread`, `blastreadlocal`, `getblast`

blastread

Purpose

Read data from NCBI BLAST report file

Syntax

```
Data = blastread(BLASTReport)
```

Arguments

BLASTReport	NCBI BLAST-formatted report specified by any of the following: • File name or path and file name, such as returned by the `getblast` function with the `'ToFile'` property. • URL pointing to an NCBI BLAST report. • MATLAB character array that contains the text for an NCBI BLAST report. If you specify only a file name, that file must be on the MATLAB search path or in the current directory.

Return Values

Data	MATLAB structure or array of structures (if multiple query sequences) containing fields corresponding to BLAST keywords and data from an NCBI BLAST report.

Description

The Basic Local Alignment Search Tool (BLAST) offers a fast and powerful comparative analysis of protein and nucleotide sequences against known sequences in online databases. BLAST reports can be lengthy, and parsing the data from the various formats can be cumbersome.

`Data = blastread(BLASTReport)` reads a BLAST report from *BLASTReport*, an NCBI-formatted report, and returns *Data*, a MATLAB structure or array of structures (if multiple query sequences) containing

fields corresponding to the BLAST keywords. `blastread` parses the basic BLAST reports `BLASTN`, `BLASTP`, `BLASTX`, `TBLASTN`, and `TBLASTX`.

`Data` contains the following fields.

Field	Description
`RID`	Request ID for retrieving results for a specific NCBI BLAST search.
`Algorithm`	NCBI algorithm used to do a BLAST search.
`Query`	Identifier of the query sequence submitted to a BLAST search.
`Database`	All databases searched.
`Hits.Name`	Name of a database sequence (subject sequence) that matched the query sequence.
`Hits.Length`	Length of a subject sequence.
`Hits.HSPs.Score`	Pairwise alignment score for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.Expect`	Expectation value for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.Identities`	Identities (match, possible, and percent) for a high-scoring sequence pair between the query sequence and a subject sequence.

Field	Description
`Hits.HSPs.Positives`	Identical or similar residues (match, possible, and percent) for a high-scoring sequence pair between the query sequence and a subject amino acid sequence. **Note** This field applies only to translated nucleotide or amino acid query sequences and/or databases.
`Hits.HSPs.Gaps`	Nonaligned residues (match, possible, and percent) for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.Frame`	Reading frame of the translated nucleotide sequence for a high-scoring sequence pair between the query sequence and a subject sequence. **Note** This field applies only when performing translated searches, that is, when using `tblastx`, `tblastn`, and `blastx`.

Field	Description
`Hits.HSPs.Strand`	Sense (`Plus` = 5' to 3' and `Minus` = 3' to 5') of the DNA strands for a high-scoring sequence pair between the query sequence and a subject sequence. **Note** This field applies only when using a nucleotide query sequence and database.
`Hits.HSPs.Alignment`	Three-row matrix showing the alignment for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.QueryIndices`	Indices of the query sequence residue positions for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.SubjectIndices`	Indices of the subject sequence residue positions for a high-scoring sequence pair between the query sequence and a subject sequence.
`Statistics`	Summary of statistical details about the performed search, such as lambda values, gap penalties, number of sequences searched, and number of hits.

Examples

1 Create an NCBI BLAST report request using a GenPept accession number.

```
RID = blastncbi('AAA59174', 'blastp', 'expect', 1e-10)
```

```
RID =

    '1175088155-31624-126008617054.BLASTQ3'
```

2 Pass the Request ID for the report to the `getblast` function, and save the report data to a text file.

```
getblast(RID, 'ToFile' ,'AAA59174_BLAST.rpt');
```

Note You may need to wait for the report to become available on the NCBI Web site before you can run the preceding command.

---

3 Using the saved file, read the results into a MATLAB structure.

```
resultsStruct = blastread('AAA59174_BLAST.rpt')

resultsStruct =

           RID: '1175093446-29831-201366571074.BLASTQ2'
     Algorithm: 'BLASTP 2.2.16 [Mar-11-2007]'
         Query: [1x63 char]
      Database: [1x96 char]
          Hits: [1x50 struct]
    Statistics: [1x1034 char]
```

References

[1] Altschul, S.F., Gish, W., Miller, W., Myers, E.W. and Lipman, D.J. (1990). Basic local alignment search tool. J. Mol. Biol. *215*, 403–410.

[2] Altschul, S.F., Madden, T.L., Schäffer, A.A., Zhang, J., Zhang, Z., Miller, W. and Lipman, D.J. (1997). Gapped BLAST and PSI-BLAST: a new generation of protein database search programs. Nucleic Acids Res. *25*, 3389–3402.

For more information about reading and interpreting NCBI BLAST reports, see:

http://www.ncbi.nlm.nih.gov/Education/BLASTinfo/Blast_output.html

See Also

Bioinformatics Toolbox functions: `blastformat`, `blastlocal`, `blastncbi`, `blastreadlocal`, `getblast`

blastreadlocal

Purpose

Read data from local BLAST report

Syntax

```
Data = blastreadlocal(BLASTReport, Format)
```

Arguments

BLASTReport

BLAST report specified by any of the following:

- File name or path and file name of a locally created BLAST report file, such as returned by the `blastlocal` function with the `'ToFile'` property.
- MATLAB character array that contains the text for a local BLAST report.

If you specify only a file name, that file must be on the MATLAB search path or in the current directory.

Format

Integer specifying the alignment format used to create *BLASTReport*. Choices are:

- `0` — Pairwise
- `1` — Query-anchored, showing identities
- `2` — Query-anchored, no identities
- `3` — Flat query-anchored, showing identities
- `4` — Flat query-anchored, no identities
- `5` — Query-anchored, no identities and blunt ends
- `6` — Flat query-anchored, no identities and blunt ends
- `7` — Not used
- `8` — Tabular
- `9` — Tabular with comment lines

Return Values

Data	MATLAB structure or array of structures (if multiple query sequences) containing fields corresponding to BLAST keywords and data from a local BLAST report.

Description

The Basic Local Alignment Search Tool (BLAST) offers a fast and powerful comparative analysis of protein and nucleotide sequences against known sequences in online and local databases. BLAST reports can be lengthy, and parsing the data from the various formats can be cumbersome.

Data = blastreadlocal(*BLASTReport*, *Format*) reads *BLASTReport*, a locally created BLAST report file, and returns *Data*, a MATLAB structure or array of structures (if multiple query sequences) containing fields corresponding to BLAST keywords and data from a local BLAST report. *Format* is an integer specifying the alignment format used to create *BLASTReport*.

Note The function assumes the BLAST report was produced using version 2.2.17 of the `blastall` executable.

Data contains a subset of the following fields, based on the specified alignment format.

Field	Description
Algorithm	NCBI algorithm used to do a BLAST search.
Query	Identifier of the query sequence submitted to a BLAST search.
Length	Length of the query sequence.
Database	All databases searched.

Field	Description
`Hits.Name`	Name of a database sequence (subject sequence) that matched the query sequence.
`Hits.Score`	Alignment score between the query sequence and the subject sequence.
`Hits.Expect`	Expectation value for the alignment between the query sequence and the subject sequence.
`Hits.Length`	Length of a subject sequence.
`Hits.HSPs.Score`	Pairwise alignment score for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.Expect`	Expectation value for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.Identities`	Identities (match, possible, and percent) for a high-scoring sequence pair between the query sequence and a subject sequence.

Field	Description
`Hits.HSPs.Positives`	Identical or similar residues (match, possible, and percent) for a high-scoring sequence pair between the query sequence and a subject amino acid sequence. **Note** This field applies only to translated nucleotide or amino acid query sequences and/or databases.
`Hits.HSPs.Gaps`	Nonaligned residues (match, possible, and percent) for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.Mismatches`	Residues that are not similar to each other (match, possible, and percent) for a high-scoring sequence pair between the query sequence and a subject sequence.

Field	Description
`Hits.HSPs.Frame`	Reading frame of the translated nucleotide sequence for a high-scoring sequence pair between the query sequence and a subject sequence. **Note** This field applies only when performing translated searches, that is, when using `tblastx`, `tblastn`, and `blastx`.
`Hits.HSPs.Strand`	Sense (`Plus` = 5' to 3' and `Minus` = 3' to 5') of the DNA strands for a high-scoring sequence pair between the query sequence and a subject sequence. **Note** This field applies only when using a nucleotide query sequence and database.
`Hits.HSPs.Alignment`	Three-row matrix showing the alignment for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.QueryIndices`	Indices of the query sequence residue positions for a high-scoring sequence pair between the query sequence and a subject sequence.

Field	Description
`Hits.HSPs.SubjectIndices`	Indices of the subject sequence residue positions for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.AlignmentLength`	Length of the pairwise alignment for a high-scoring sequence pair between the query sequence and a subject sequence.
`Alignment`	Entire alignment for the query sequence and the subject sequence(s).
`Statistics`	Summary of statistical details about the performed search, such as lambda values, gap penalties, number of sequences searched, and number of hits.

Examples

The following examples assume you have a FASTA nucleotide file for *E. coli*, such as the file `NC_004431.fna`, which you can download from , saved to your MATLAB current directory.

Reading Data Using a Tabular Alignment Format

1. Create a local blastable database from the `NC_004431.fna` FASTA file.

```
blastformat('inputdb', 'NC_004431.fna', 'protein', 'false');
```

2. Use the `getgenbank` function to retrieve two sequences from the GenBank database.

```
S1 = getgenbank('M28570.1');
```

```
S2 = getgenbank('M12565');
```

3 Create a query file by using the `fastawrite` function to create a FASTA file named `query_multi_nt.fa` from these two sequences, using the only accession number as the header.

```
Seqs(1).Header = S1.Accession;
Seqs(1).Sequence = S1.Sequence;
Seqs(2).Header = S2.Accession;
Seqs(2).Sequence = S2.Sequence;
fastawrite('query_multi_nt.fa', Seqs);
```

4 Submit the query sequences in the `query_multi_nt.fa` FASTA file for a BLAST search of the local nucleotide database `NC_004431.fna`. Specify the BLAST program `blastn` and a tabular alignment format. Save the contents of the BLAST report to a file named `myecoli_nt8.txt`, and then read the local BLAST report.

```
blastlocal('inputquery', 'query_multi_nt.fa',...
           'database', 'NC_004431.fna',...
           'tofile', 'myecoli_nt8.txt', 'program', 'blastn',...
           'format', 8);
blastreadlocal('myecoli_nt8.txt', 8);
```

Reading Data Using a Query Anchored Format

1 If you have not already done so, create a local blastable database and a query file as described in steps 1 through 3 in Reading Data Using a Tabular Alignment Format on page 3-221.

2 Submit the query sequences in the `query_multi_nt.fa` FASTA file for a BLAST search of the local nucleotide database `NC_004431.fna`. Specify the BLAST program `blastn` and a query-anchored format. Save the contents of the BLAST report to a file named `myecoli_nt1.txt`, and then read the local BLAST report, saving the results in `results`, an array of structures.

```
blastlocal('inputquery', 'query_multi_nt.fa',...
```

```
                'database', 'NC_004431.fna',...
                'tofile', 'myecoli_nt1.txt', 'program', 'blastn',...
                'format', 1);
    results = blastreadlocal('myecoli_nt1.txt', 1);
```

References

[1] Altschul, S.F., Gish, W., Miller, W., Myers, E.W., and Lipman, D.J. (1990). Basic local alignment search tool. J. Mol. Biol. *215*, 403–410.

[2] Altschul, S.F., Madden, T.L., Schäffer, A.A., Zhang, J., Zhang, Z., Miller, W., and Lipman, D.J. (1997). Gapped BLAST and PSI-BLAST: a new generation of protein database search programs. Nucleic Acids Res. *25*, 3389–3402.

For more information about reading and interpreting BLAST reports, see:

```
http://www.ncbi.nlm.nih.gov/Education/BLASTinfo/information3.html
```

See Also

Bioinformatics Toolbox functions: `blastformat`, `blastlocal`, `blastncbi`, `blastread`, `getblast`

blosum

Purpose

Return BLOSUM scoring matrix

Syntax

```
Matrix = blosum(Identity)
[Matrix, MatrixInfo] = blosum(Identity)
... = blosum(Identity, ...'Extended', ExtendedValue, ...)
... = blosum(Identity, ...'Order', OrderValue, ...)
```

Arguments

Identity	Scalar specifying a percent identity level. Choices are: • Values from 30 to 90 in increments of 5 • 62 • 100
ExtendedValue	Controls the listing of extended amino acid codes. Choices are `true` (default) or `false`.
OrderValue	Character string of legal amino acid characters that specifies the order amino acids are listed in the matrix. The length of the character string must be 20 or 24.

Return Values

Matrix	BLOSUM (Blocks Substitution Matrix) scoring matrix with a specified percent identity.
MatrixInfo	Structure of information about *Matrix* containing the following fields: • `Name` • `Scale` • `Entropy` • `ExpectedScore` • `HighestScore`

- LowestScore
- Order

Description

Matrix = blosum(*Identity*) returns a BLOSUM (Blocks Substitution Matrix) scoring matrix with a specified percent identity. The default ordering of the output includes the extended characters B, Z, X, and *.

```
A R N D C Q E G H I L K M F P S T W Y V B Z X *
```

[*Matrix*, *MatrixInfo*] = blosum(*Identity*) returns *MatrixInfo*, a structure of information about *Matrix*, a BLOSUM matrix. *MatrixInfo* contains the following fields:

- Name
- Scale
- Entropy
- ExpectedScore
- HighestScore
- LowestScore
- Order

... = blosum(*Identity*, ...'*PropertyName*', *PropertyValue*, ...) calls blosum with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

... = blosum(*Identity*, ...'Extended', *ExtendedValue*, ...) controls the listing of extended amino acid codes. Choices are true (default) or false. If *ExtendedValue* is false, returns the scoring matrix for the standard 20 amino acids. Ordering of the output when *ExtendedValue* is false is

```
A R N D C Q E G H I L K M F P S T W Y V
```

`... = blosum(`*`Identity`*`, ...'Order', `*`OrderValue`*`, ...)` returns a BLOSUM matrix ordered by *`OrderValue`*, a character string of legal amino acid characters that specifies the order amino acids are listed in the matrix. The length of the character string must be `20` or `24`.

Examples

Return a BLOSUM matrix with a percent identity level of 50.

```
B50 = blosum(50)
```

Return a BLOSUM matrix with the amino acids in a specific order.

```
B75 = blosum(75,'Order','CSTPAGNDEQHRKMILVFYW')
```

See Also

Bioinformatics Toolbox functions: `dayhoff`, `gonnet`, `localalign`, `nuc44`, `nwalign`, `pam`, `swalign`

Purpose

Read probe intensities from Affymetrix CEL files

Syntax

```
ProbeStructure = celintensityread(CELFiles, CDFFile)
ProbeStructure = celintensityread(..., 'CELPath',
CELPathValue, ...)
ProbeStructure = celintensityread(..., 'CDFPath',
   CDFPathValue, ...)
ProbeStructure = celintensityread(..., 'PMOnly',
PMOnlyValue,
   ...)
ProbeStructure = celintensityread(..., 'Verbose',
   VerboseValue, ...)
```

Arguments

CELFiles

Any of the following:

- String specifying a single CEL file name.
- `'*'`, which reads all CEL files in the current directory.
- `' '`, which opens the Select CEL Files dialog box from which you select the CEL files. From this dialog box, you can press and hold **Ctrl** or **Shift** while clicking to select multiple CEL files.
- Cell array of CEL file names.

CDFFile

Either of the following:

- String specifying a CDF file name.
- `' '`, which opens the Select CDF File dialog box from which you select the CDF file.

CELPathValue

String specifying the path and directory where the files specified in *CELFiles* are stored.

CDFPathValue	String specifying the path and directory where the file specified in *CDFFile* is stored.
PMOnlyValue	Property to include or exclude the mismatch (MM) probe intensity values in the returned structure. Enter `true` to return only perfect match (PM) probe intensities. Enter `false` to return both PM and MM probe intensities. Default is `true`.
VerboseValue	Controls the display of a progress report showing the name of each CEL file as it is read. When *VerboseValue* is `false`, no progress report is displayed. Default is `true`.

Return Values

ProbeStructure	MATLAB structure containing information from the CEL files, including probe intensities, probe indices, and probe set IDs.

Description

Note This function does not work on the Solaris platform.

ProbeStructure = `celintensityread(`*CELFiles, CDFFile*`)` reads the specified Affymetrix CEL files and the associated CDF library file (created from Affymetrix GeneChip arrays for expression or genotyping assays), and then creates *ProbeStructure*, a structure containing information from the CEL files, including probe intensities, probe indices, and probe set IDs. *CELFiles* is a string or cell array of CEL file names. *CDFFile* is a string specifying a CDF file name.

If you set *CELFiles* to `'*'`, then it reads all CEL files in the current directory. If you set *CELFiles* to `' '`, then it opens the Select CEL Files dialog box from which you select the CEL files. From this dialog box, you can press and hold **Ctrl** or **Shift** while clicking to select multiple CEL files.

If you set *CDFFile* to `' '`, then it opens the Select CDF File dialog box from which you select the CDF file.

ProbeStructure = `celintensityread(...,` '*PropertyName*', *PropertyValue*, `...)` calls `celintensityread` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

ProbeStructure = `celintensityread(..., 'CELPath',` *CELPathValue*, `...)` specifies a path and directory where the files specified by *CELFiles* are stored.

ProbeStructure = `celintensityread(..., 'CDFPath',` *CDFPathValue*, `...)` specifies a path and directory where the file specified by *CDFFile* is stored.

ProbeStructure = `celintensityread(..., 'PMOnly',` *PMOnlyValue*, `...)` includes or excludes the mismatch (MM) probe intensity values. When *PMOnlyValue* is `true`, `celintensityread` returns only perfect match (PM) probe intensities. When *PMOnlyValue* is `false`, `celintensityread` returns both PM and MM probe intensities. Default is `true`.

You can learn more about the Affymetrix CEL files and download sample files from:

```
http://www.affymetrix.com/support/technical/sample_data/demo_data.affx
```

Note Some Affymetrix CEL files are combined with other data files in a DTT or CAB file. You must download and use the Affymetrix Data Transfer Tool to extract these files from the DTT or CAB file. You can download the Affymetrix Data Transfer Tool from:

```
http://www.affymetrix.com/products/software/specific/dtt.affx
```

You will have to register and log in at the Affymetrix Web site to download the Affymetrix Data Transfer Tool.

Tip Reading a large number of CEL files and/or a large CEL file can require extended amounts of memory from the operating system. If you receive any errors related to memory or have trouble reading CEL files, try the following:

- Increase the virtual memory (swap space) for your operating system (with a recommended initial size of 3,069 and a maximum size of 16,368) as described at:

  ```
  http://www.mathworks.com/support/tech-notes/1100/1106.html#6
  ```

- Set the 3 GB switch (32-bit Windows XP only) as described at:

  ```
  http://www.mathworks.com/support/tech-notes/1100/1107.html
  ```

ProbeStructure contains the following fields.

Field	Description
CDFName	File name of the Affymetrix CDF library file.
CELNames	Cell array of names of the Affymetrix CEL files.

Field	Description
`NumChips`	Number of CEL files read into the structure.
`NumProbeSets`	Number of probe sets in each CEL file.
`NumProbes`	Number of probes in each CEL file.
`ProbeSetIDs`	Cell array of the probe set IDs from the Affymetrix CDF library file.
`ProbeIndices`	Column vector containing probe indexing information. Probes within a probe set are numbered `0` through `N - 1`, where `N` is the number of probes in the probe set.
`GroupNumbers`	Column vector containing group numbers for probes within the probe set. For gene expression data, the group number for all probes is `1`. For SNP (genotyping) data, the group numbers for probes are: • `1` — Allele A – (sense) • `2` — Allele B – (sense) • `3` — Allele A + (antisense) • `4` — Allele B + (antisense)
`PMIntensities`	Matrix containing perfect match (PM) probe intensity values. Each row corresponds to a probe, and each column corresponds to a CEL file. The rows are ordered the same way as in `ProbeIndices`, and the columns are ordered the same way as in the *`CELFiles`* input argument.
`MMIntensities` (optional)	Matrix containing mismatch (MM) probe intensity values. Each row corresponds to a probe, and each column corresponds to a CEL file. The rows are ordered the same way as in `ProbeIndices`, and the columns

Field	Description
	are ordered the same way as in the *CELFiles* input argument.

ProbeStructure = celintensityread(..., 'Verbose', *VerboseValue*, ...) controls the display of a progress report showing the name of each CEL file as it is read. When *VerboseValue* is false, no progress report is displayed. Default is true.

Examples

The following example assumes that you have the HG_U95Av2.CDF library file stored at D:\Affymetrix\LibFiles\HGGenome, and that your current directory points to a location containing CEL files associated with this CDF library file. In this example, the celintensityread function reads all the CEL files in the current directory and a CDF file in a specified directory. The next command line uses the rmabackadj function to perform background adjustment on the PM probe intensities in the PMIntensities field of PMProbeStructure.

```
PMProbeStructure = celintensityread('*', 'HG_U95Av2.CDF',...
                   'CDFPath', 'D:\Affymetrix\LibFiles\HGGenome');
BackAdjustedMatrix = rmabackadj(PMProbeStructure.PMIntensities);
```

The following example lets you select CEL files and a CDF file to read using Open File dialog boxes:

```
PMProbeStructure = celintensityread(' ', ' ');
```

See Also

Bioinformatics Toolbox functions: affygcrma, affyinvarsetnorm, affyprobeseqread, affyread, affyrma, affysnpintensitysplit, agferead, gcrma, gcrmabackadj, gprread, ilmnbsread, probelibraryinfo, probesetlink, probesetlookup, probesetplot, probesetvalues, rmabackadj, rmasummary, sptread

Purpose

Perform circular binary segmentation (CBS) on array-based comparative genomic hybridization (aCGH) data

Syntax

```
SegmentStruct = cghcbs(CGHData)
SegmentStruct = cghcbs(CGHData, ...'Alpha',
AlphaValue, ...)
SegmentStruct = cghcbs(CGHData, ...'Permutations',
   PermutationsValue, ...)
SegmentStruct = cghcbs(CGHData, ...'Method', MethodValue,
   ...)
SegmentStruct = cghcbs(CGHData, ...'StoppingRule',
   StoppingRuleValue, ...)
SegmentStruct = cghcbs(CGHData, ...'Smooth', SmoothValue,
   ...)
SegmentStruct = cghcbs(CGHData, ...'Prune',
PruneValue, ...)
SegmentStruct = cghcbs(CGHData, ...'Errsum', ErrsumValue,
   ...)
SegmentStruct = cghcbs(CGHData, ...'WindowSize',
   WindowSizeValue, ...)
SegmentStruct = cghcbs(CGHData, ...'SampleIndex',
   SampleIndexValue, ...)
SegmentStruct = cghcbs(CGHData, ...'Chromosome',
   ChromosomeValue, ...)
SegmentStruct = cghcbs(CGHData, ...'Showplot',
ShowplotValue,
   ...)
SegmentStruct = cghcbs(CGHData, ...'Verbose', VerboseValue,
   ...)
```

Arguments

CGHData

Array-based comparative genomic hybridization (aCGH) data in either of the following forms:

- Structure with the following fields:
  - `Sample` — Cell array of strings containing the sample names (optional).
  - `Chromosome` — Vector containing the chromosome numbers on which the clones are located.
  - `GenomicPosition` — Vector containing the genomic positions (in any unit) to which the clones are mapped.
  - `Log2Ratio` — Matrix containing $\log_2$ ratio of test to reference signal intensity for each clone. Each row corresponds to a clone, and each column corresponds to a sample.
- Matrix in which each row corresponds to a clone. The first column contains the chromosome number, the second column contains the genomic position, and the remaining columns each contain the $\log_2$ ratio of test to reference signal intensity for a sample.

AlphaValue

Scalar that specifies the significance level for the statistical tests to accept change points. Default is `0.01`.

PermutationsValue

Scalar that specifies the number of permutations used for p-value estimation. Default is `10,000`.

MethodValue String that specifies the method to estimate the p-values. Choices are `'Perm'` or `'Hybrid'` (default). `'Perm'` does a full permutation, while `'Hybrid'` uses a faster, tail probability-based permutation. When using the `'Hybrid'` method, the `'Perm'` method is applied automatically when segment data length becomes less than 200.

StoppingRuleValue Controls the use of a heuristic stopping rule, based on the method described by Venkatraman and Olshen (2007), to declare a change without performing the full number of permutations for the p-value estimation, whenever it becomes very likely that a change has been detected. Choices are `true` or `false` (default).

Tip Set this property to `true` to increase processing speed. Set this property to `false` to maximize accuracy.

SmoothValue Controls the smoothing of outliers before segmenting using the procedure explained by Olshen et al. (2004). Choices are `true` (default) or `false`.

PruneValue Controls the elimination of change points identified due to local trends in the data that are not indicative of real copy number change, using the procedure explained by Olshen et al. (2004). Choices are `true` or `false` (default).

ErrsumValue — Scalar that specifies the allowed proportional increase in the error sum of squares when eliminating change points using the `'Prune'` property. Commonly used values are `0.05` and `0.1`. Default is `0.05`.

WindowSizeValue — Scalar that specifies the size of the window (in data points) used to divide the data when using the `'Perm'` method on large data sets. Default is `200`.

SampleIndexValue — A single sample index or a vector of sample indices that specify the sample(s) to analyze. Default is all sample indices.

ChromosomeValue — A single chromosome number or a vector of chromosome numbers that specify the data to analyze. Default is all chromosome numbers.

ShowplotValue — Controls the display of plots of the segment means over the original data. Choices are either:

- `true` — All chromosomes in all samples are plotted. If there are multiple samples in *`CGHData`*, then each sample is plotted in a separate Figure window.
- `false` — No plot.
- `W` — The layout displays all chromosomes in the whole genome in one plot in the Figure window.
- `S` — The layout displays each chromosome in a subplot in the Figure window.
- *`I`* — An integer specifying only one of the chromosomes in *`CGHData`* to be plotted.

Default is:

- `false` — When return values are specified.
- `true` and `W` — When return values are not specified.

`VerboseValue` Controls the display of a progress report of the analysis. Choices are `true` (default) or `false`.

Return Values

`SegmentStruct` Structure containing segmentation information in the following fields:

- `Sample` — Sample name from *`CGHData`* input argument. If the input argument does not include sample names, then sample names are assigned as `Sample1`, `Sample2`, and so forth.
- `SegmentData` — Structure array containing segment data for the sample in the following fields:
  - `Chromosome` — Chromosome number on which the segment is located.
  - `Start` — Genomic position at the start of the segment (in the same units as used for the *`CGHData`* input).
  - `End` — Genomic position at the end of the segment (in the same units as used for the *`CGHData`* input).
  - `Mean` — Mean value of the $\log_2$ ratio of the test to reference signal intensity for the segment.

Description

SegmentStruct = cghcbs(*CGHData*) performs circular binary segmentation (CBS) on array-based comparative genomic hybridization (aCGH) data to determine the copy number alteration segments (neighboring regions of DNA that exhibit a statistical difference in copy number) and change points.

Note The CBS algorithm recursively splits chromosomes into segments based on a maximum t statistic estimated by permutation. This computation can be time consuming. If n = number of data points, then computation time ~ O(n^2).

SegmentStruct = cghcbs(*CGHData*, ...'*PropertyName*', *PropertyValue*, ...) calls cghcbs with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

SegmentStruct = cghcbs(*CGHData*, ...'Alpha', *AlphaValue*, ...) specifies the significance level for the statistical tests to accept change points. Default is 0.01.

SegmentStruct = cghcbs(*CGHData*, ...'Permutations', *PermutationsValue*, ...) specifies the number of permutations used for p-value estimation. Default is 10,000.

SegmentStruct = cghcbs(*CGHData*, ...'Method', *MethodValue*, ...) specifies the method to estimate the p-values. Choices are 'Perm' or 'Hybrid' (default). 'Perm' does a full permutation, while 'Hybrid' uses a faster, tail probability-based permutation. When using the 'Hybrid' method, the 'Perm' method is applied automatically when segment data length becomes less than 200.

SegmentStruct = cghcbs(*CGHData*, ...'StoppingRule', *StoppingRuleValue*, ...) controls the use of a heuristic stopping rule, based on the method described by Venkatraman and Olshen (2007), to declare a change without performing the full number of permutations

for the p-value estimation, whenever it becomes very likely that a change has been detected. Choices are `true` or `false` (default).

SegmentStruct = cghcbs(*CGHData*, ...'Smooth', *SmoothValue*, ...) controls the smoothing of outliers before segmenting, using the procedure explained by Olshen et al. (2004). Choices are `true` (default) or `false`.

SegmentStruct = cghcbs(*CGHData*, ...'Prune', *PruneValue*, ...) controls the elimination of change points identified due to local trends in the data that are not indicative of real copy number change, using the procedure explained by Olshen et al. (2004). Choices are `true` or `false` (default).

SegmentStruct = cghcbs(*CGHData*, ...'Errsum', *ErrsumValue*, ...) specifies the allowed proportional increase in the error sum of squares when eliminating change points using the `'Prune'` property. Commonly used values are `0.05` and `0.1`. Default is `0.05`.

SegmentStruct = cghcbs(*CGHData*, ...'WindowSize', *WindowSizeValue*, ...) specifies the size of the window (in data points) used to divide the data when using the `'Perm'` method on large data sets. Default is `200`.

SegmentStruct = cghcbs(*CGHData*, ...'SampleIndex', *SampleIndexValue*, ...) analyzes only the sample(s) specified by *SampleIndexValue*, which can be a single sample index or a vector of sample indices. Default is all sample indices.

SegmentStruct = cghcbs(*CGHData*, ...'Chromosome', *ChromosomeValue*, ...) analyzes only the data on the chromosomes specified by *ChromosomeValue*, which can be a single chromosome number or a vector of chromosome numbers. Default is all chromosome numbers.

SegmentStruct = cghcbs(*CGHData*, ...'Showplot', *ShowplotValue*, ...) controls the display of plots of the segment means over the original data. Choices are `true`, `false`, `W`, `S`, or *I*, an integer specifying one of the chromosomes in *CGHData*. When *ShowplotValue* is `true`, all chromosomes in all samples are plotted. If

there are multiple samples in *CGHData*, then each sample is plotted in a separate Figure window. When *ShowplotValue* is `W`, the layout displays all chromosomes in one plot in the Figure window. When *ShowplotValue* is `S`, the layout displays each chromosome in a subplot in the Figure window. When *ShowplotValue* is *I*, only the specified chromosome is plotted. Default is either:

- `false` — When return values are specified.
- `true` and `W` — When return values are not specified.

SegmentStruct = `cghcbs(`*CGHData*`, ...'Verbose', `*VerboseValue*`, ...)` controls the display of a progress report of the analysis. Choices are `true` (default) or `false`.

Examples

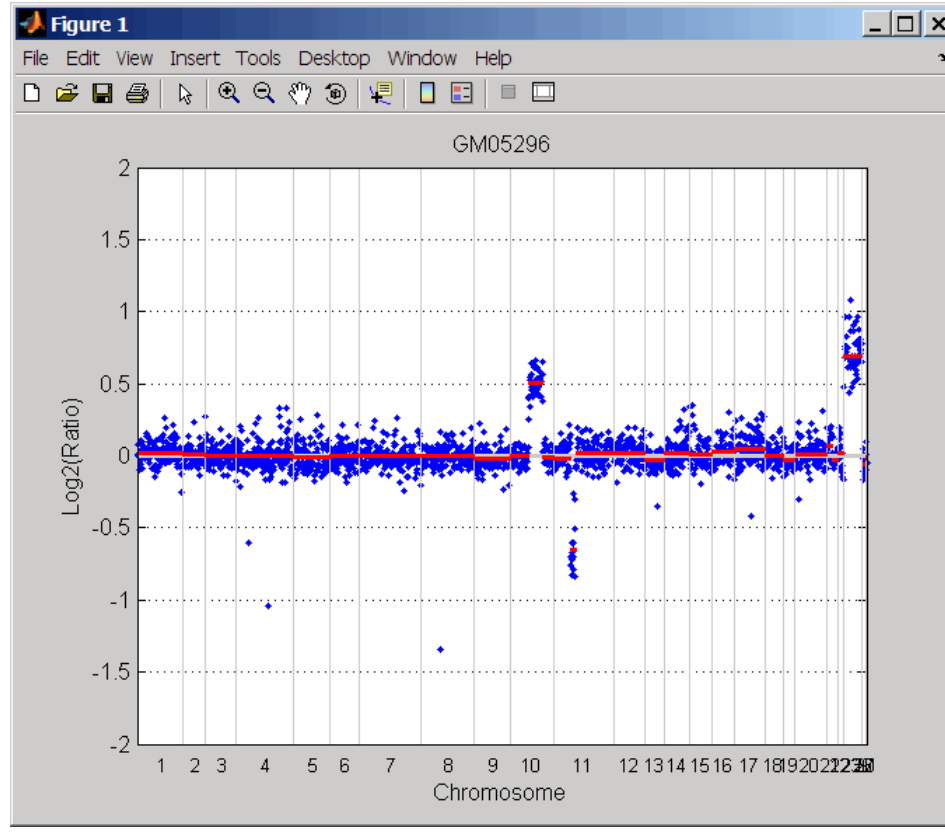
Analyzing Data from the Coriell Cell Line Study

1. Load a MAT-file, included with the Bioinformatics Toolbox software, which contains `coriell_data`, a structure of array-based CGH data.

   ```
   load coriell_baccgh
   ```

2. Analyze all chromosomes of sample 3 (GM05296) of the aCGH data and return segmentation data in a structure, `S`. Plot the segment means over the original data for all chromosomes of this sample.

   ```
   S = cghcbs(coriell_data,'sampleindex',3,'showplot',true);
   ```



Chromosome 10 shows a gain, while chromosome 11 shows a loss.

The `coriell_baccgh.mat` file used in this example contains data from Snijders et al., 2001.

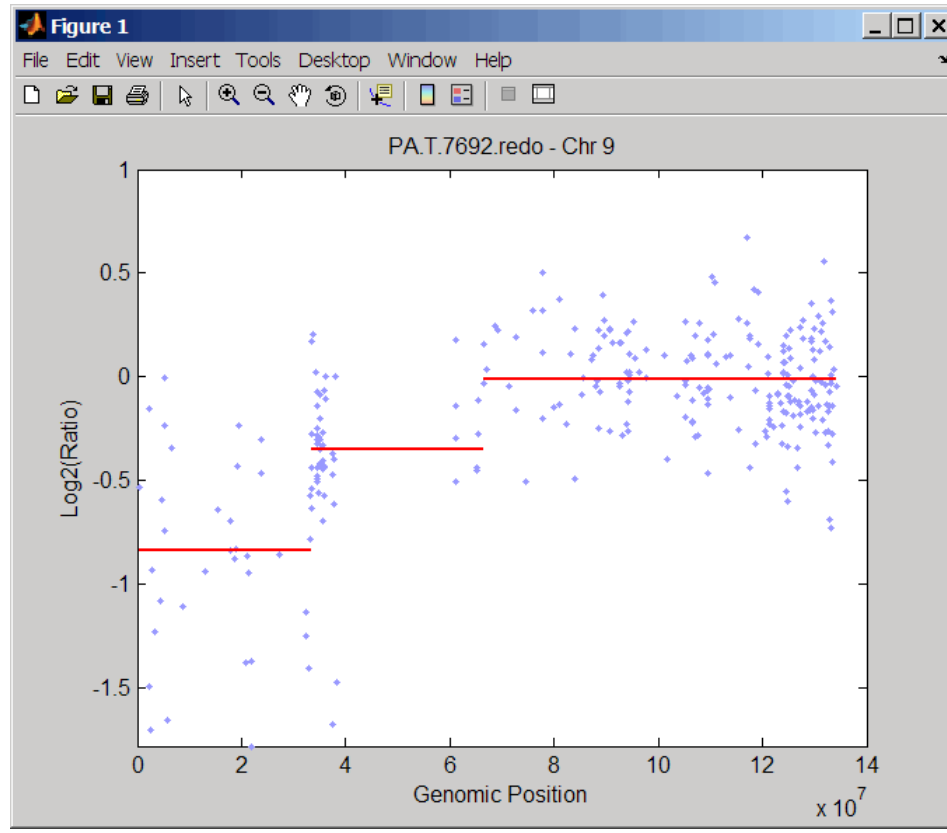
Analyzing Data from a Pancreatic Cancer Study

1. Load a MAT-file, included with the Bioinformatics Toolbox software, which contains `pancrea_data`, a structure of array-based CGH data from a pancreatic cancer study.

```
load pancrea_oligocgh
```

2 Analyze only chromosome 9 in sample 32 of the CGH data and return the segmentation data in a structure, `PS`. Plot the segment means over the original data for chromosome 9 in this sample.

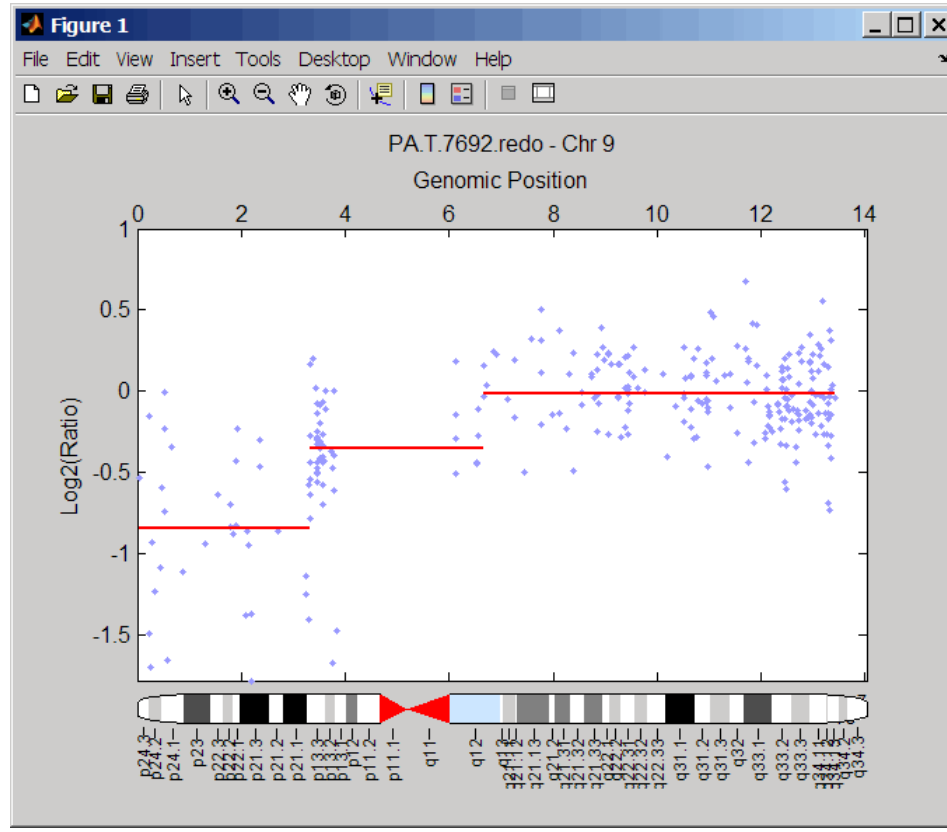
```
PS = cghcbs(pancrea_data,'sampleindex',32,'chromosome',9,...
            'showplot',9);
```



Chromosome 9 contains two segments that indicate losses. For more detailed information on interpreting the data, see Aguirre et al. (2004).

3 Use the `chromosomeplot` function with the `'addtoplot'` property to add the ideogram of chromosome 9 for *Homo sapiens* to the plot of the segmentation data.

```
chromosomeplot('hs_cytoBand.txt', 9, 'addtoplot', gca)
```



The pancrea_oligocgh.mat file used in this example contains data from Aguirre et al., 2004.

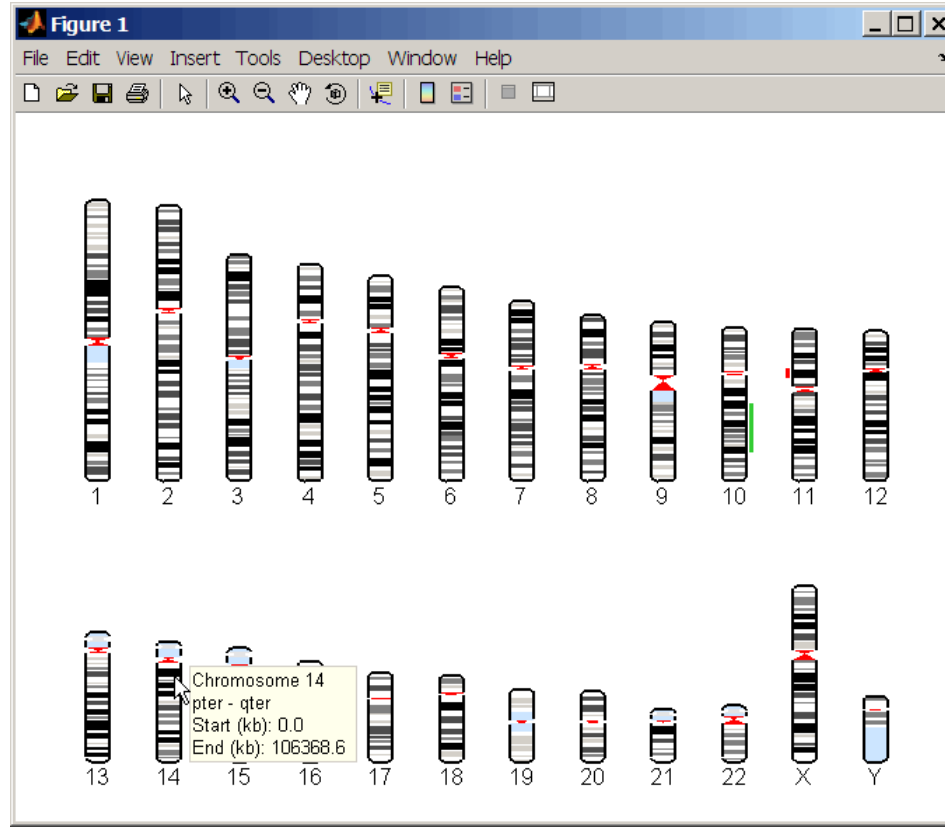
Displaying Copy Number Alteration Regions Aligned to a Chromosome Ideogram

1. Create a structure containing segment gain and loss information for chromosomes 10 and 11 from sample 3 from the Coriell cell line study, making sure the segment data is in bp units. (You can determine copy number variance (CNV) information by exploring S, the structure of segments returned by the cghcbs function in Analyzing Data from the Coriell Cell Line Study on page 3-240.) For the 'CNVType' field, use 1 to indicate a loss and 2 to indicate a gain.

```
cnvStruct = struct('Chromosome', [10 11],...
 'CNVType', [2 1],...
 'Start', [S.SegmentData(10).Start(2),...
  S.SegmentData(11).Start(2)]*1000,...
 'End',   [S.SegmentData(10).End(2),...
  S.SegmentData(11).End(2)]*1000)

cnvStruct =

    Chromosome: [10 11]
    CNVType: [2 1]
    Start: [66905000 35416000]
    End: [110412000 43357000]
```

2. Pass the structure to the chromosomeplot function using the 'CNV' property to display the copy number gains (green) and losses (red) aligned to the human chromosome ideogram. Specify kb units for the display of segment information in the data tip.

```
chromosomeplot('hs_cytoBand.txt', 'cnv', cnvStruct, 'unit', 2)
```



The `coriell_baccgh.mat` file used in this example contains data from Snijders et al., 2001.

References

[1] Olshen, A.B., Venkatraman, E.S., Lucito, R., and Wigler, M. (2004). Circular binary segmentation for the analysis of array-based DNA copy number data. Biostatistics *5, 4*, 557–572.

[2] Venkatraman, E.S., and Olshen, A.B. (2007). A Faster Circular Binary Segmentation Algorithm for the Analysis of Array CGH Data. Bioinformatics *23(6)*, 657–663.

[3] Venkatraman, E.S., and Olshen, A.B. (2006).
DNAcopy: A Package for Analyzing DNA Copy Data.
http://www.bioconductor.org/packages/2.1/bioc/html/DNAcopy.html

[4] Snijders, A.M., Nowak, N., Segraves, R., Blackwood, S., Brown, N., Conroy, J., Hamilton, G., Hindle, A.K., Huey, B., Kimura, K., Law, S., Myambo, K., Palmer, J., Ylstra, B., Yue, J.P., Gray, J.W., Jain, A.N., Pinkel, D., and Albertson, D.G. (2001). Assembly of microarrays for genome-wide measurement of DNA copy number. Nature Genetics *29*, 263–264.

[5] Aguirre, A.J., Brennan, C., Bailey, G., Sinha, R., Feng, B., Leo, C., Zhang, Y., Zhang, J., Gans, J.D., Bardeesy, N., Cauwels, C., Cordon-Cardo, C., Redston, M.S., DePinho, R.A., and Chin, L. (2004). High-resolution characterization of the pancreatic adenocarcinoma genome. PNAS *101, 24*, 9067–9072.

See Also

Bioinformatics Toolbox functions: `chromosomeplot`, `cytobandread`

Purpose

Display frequency of DNA copy number alterations across multiple samples

Syntax

```
FreqStruct = cghfreqplot(CGHData)
FreqStruct = cghfreqplot(CGHData, ...'Threshold',
ThresholdValue, ...)
FreqStruct = cghfreqplot(CGHData, ...'Group', GroupValue,
   ...)
FreqStruct = cghfreqplot(CGHData, ...'Subgrp', SubgrpValue,
   ...)
FreqStruct = cghfreqplot(CGHData, ...'Subplot',
SubplotValue,
   ...)
FreqStruct = cghfreqplot(CGHData, ...'Cutoff', CutoffValue,
   ...)
FreqStruct = cghfreqplot(CGHData, ...'Chromosome',
   ChromosomeValue, ...)
FreqStruct = cghfreqplot(CGHData, ...'IncludeX',
   IncludeXValue, ...)
FreqStruct = cghfreqplot(CGHData, ...'IncludeY',
   IncludeYValue, ...)
FreqStruct = cghfreqplot(CGHData, ...'Chrominfo',
   ChrominfoValue, ...)
FreqStruct = cghfreqplot(CGHData, ...'ShowCentr',
   ShowCentrValue, ...)
FreqStruct = cghfreqplot(CGHData, ...'Color', ColorValue,
   ...)
FreqStruct = cghfreqplot(CGHData, ...'YLim',
YLimValue, ...)
FreqStruct = cghfreqplot(CGHData, ...'Titles', TitlesValue,
   ...)
```

Arguments

CGHData

Array-based comparative genomic hybridization (aCGH) data in either of the following forms:

- Structure with the following fields:
  - `Sample` — Cell array of strings containing the sample names (optional).
  - `Chromosome` — Vector containing the chromosome numbers on which the clones are located.
  - `GenomicPosition` — Vector containing the genomic positions (in bp, kb, or mb units) to which the clones are mapped.
  - `Log2Ratio` — Matrix containing $\log_2$ ratio of test to reference signal intensity for each clone. Each row corresponds to a clone, and each column corresponds to a sample.
- Matrix in which each row corresponds to a clone. The first column contains the chromosome number, the second column contains the genomic position, and the remaining columns each contain the $\log_2$ ratio of test to reference signal intensity for a sample.

ThresholdValue

Positive scalar or vector that specifies the gain/loss threshold. A clone is considered to be a gain if its $\log_2$ ratio is above *`ThresholdValue`*, and a loss if its $\log_2$ ratio is below negative *`ThresholdValue`*.

The *`ThresholdValue`* is applied as follows:

- If a positive scalar, it is the gain and loss threshold for all the samples.

- If a two-element vector, the first element is the gain threshold for all samples, and the second element is the loss threshold for all samples.
- If a vector of the same length as the number of samples, each element in the vector is considered as a unique gain and loss threshold for each sample.

Default is `0.25`.

`GroupValue` Specifies the sample groups to calculate the frequency from. Choices are:

- A vector of sample column indices (for data with only one group). The samples specified in the vector are considered a group.
- A cell array of vectors of sample column indices (for data divided into multiple groups). Each element in the cell array is considered a group.

Default is a single group of all the samples in *`CGHData`*.

`SubgrpValue` Controls the analysis of samples by subgroups. Choices are `true` (default) or `false`.

`SubplotValue` Controls the display of all plots in one Figure window when more than one subgroup is analyzed. Choices are `true` (default) or `false` (displays plots in separate windows).

CutoffValue	Scalar or two-element numeric vector that specifies a cutoff, which controls the plotting of only the clones with frequency gains or losses greater than or equal to *CutoffValue*. If a two-element vector, the first element is the cutoff for gains, and the second element is for losses. Default is `0`.
ChromosomeValue	Single chromosome number or a vector of chromosome numbers that specify the chromosomes for which to display frequency plots. Default is all chromosomes in *CGHData*.
IncludeXValue	Controls the inclusion of the X chromosome in the analysis. Choices are `true` (default) or `false`.
IncludeYValue	Controls the inclusion of the Y chromosome in the analysis. Choices are `true` or `false` (default) .
ChrominfoValue	Cytogenetic banding information specified by either of the following: • Structure returned by the `cytobandread` function • String specifying the file name of an NCBI ideogram text file or a UCSC Genome Browser cytoband text file Default is *Homo sapiens* cytogenetic banding information from the UCSC Genome Browser, NCBI Build 36.1 (`http://genome.UCSC.edu`).

ShowCentrValue Controls the display of the centromere positions as vertical dashed lines in the frequency plot. Choices are `true` (default) or `false`.

Tip The centromere positions are obtained from *ChrominfoValue*.

ColorValue Color scheme for the vertical lines in the plot, indicating the frequency of the gains and losses, specified by either of the following:

- Name of or handle to a function that returns a colormap
- M-by-3 matrix containing RGB values. If M equals 1, then that single color is used for all gains and losses. If M equals 2 or more, then the first row is used for gains, the second row is used for losses, and remaining rows are ignored. For example, `[0 1 0;1 0 0]` specifies green for gain and red for loss.

The default color scheme is a range of colors from pure green (gain = 1) through yellow (0) to pure red (loss = –1).

YLimValue Two-element vector specifying the minimum and maximum values on the vertical axis. Default is `[1, -1]`.

TitlesValue Single string or a cell array of strings that specifies titles for the group(s), which are added to the tops of the plot(s).

Return Values

FreqStruct

Structure containing frequency data in the following fields:

- `Group` — Structure array, with each structure representing a group of samples. Each structure contains the following fields:
  - `Sample` — Cell array containing names of samples within the group.
  - `GainFrequency` — Column vector containing the average gain for each clone for a group of samples.
  - `LossFrequency` — Column vector containing the average loss for each clone for a group of samples.
- `Chromosome` — Column vector containing the chromosome numbers on which the clones are located.
- `GenomicPosition` — Column vector containing the genomic positions of the clones.

Tip You can use this output structure as input to the `cghfreqplot` function.

Description

FreqStruct = cghfreqplot(*CGHData*) displays the frequency of copy number gain or loss across multiple samples for each clone on an array against their genomic position along the chromosomes.

FreqStruct = cghfreqplot(*CGHData*, ...'*PropertyName*', *PropertyValue*, ...) calls `cghfreqplot` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single

quotation marks and is case insensitive. These property name/property value pairs are as follows:

FreqStruct = cghfreqplot(*CGHData*, ...'Threshold', *ThresholdValue*, ...) specifies the gain/loss threshold. A clone is considered to be a gain if its $\log_2$ ratio is above *ThresholdValue*, and a loss if its $\log_2$ ratio is below negative *ThresholdValue*.

The *ThresholdValue* is applied as follows:

- If a positive scalar, it is the gain and loss threshold for all the samples.
- If a two-element vector, the first element is the gain threshold for all samples, and the second element is the loss threshold for all samples.
- If a vector of the same length as the number of samples, each element in the vector is considered as a unique gain and loss threshold for each sample.

Default is 0.25.

FreqStruct = cghfreqplot(*CGHData*, ...'Group', *GroupValue*, ...) specifies the sample groups to calculate the frequency from. Choices are:

- A vector of sample column indices (for data with only one group). The samples specified in the vector are considered a group.
- A cell array of vectors of sample column indices (for data divided into multiple groups). Each element in the cell array is considered a group.

Default is a single group of all the samples in *CGHData*.

FreqStruct = cghfreqplot(*CGHData*, ...'Subgrp', *SubgrpValue*, ...) controls the analysis of samples by subgroups. Choices are true (default) or false.

FreqStruct = cghfreqplot(*CGHData*, ...'Subplot', *SubplotValue*, ...) controls the display of all plots in one Figure

window when more than one subgroup is analyzed. Choices are `true` (default) or `false` (displays plots in separate windows).

FreqStruct = cghfreqplot(*CGHData*, ...'Cutoff', *CutoffValue*, ...) specifies a cutoff value, which controls the plotting of only the clones with frequency gains or losses greater than or equal to *CutoffValue*. *CutoffValue* is a scalar or two-element numeric vector. If a two-element numeric vector, the first element is the cutoff for gains, and the second element is for losses. Default is `0`.

FreqStruct = cghfreqplot(*CGHData*, ...'Chromosome', *ChromosomeValue*, ...) displays the frequency plots only of chromosome(s) specified by *ChromosomeValue*, which can be a single chromosome number or a vector of chromosome numbers. Default is all chromosomes in *CGHData*.

FreqStruct = cghfreqplot(*CGHData*, ...'IncludeX', *IncludeXValue*, ...) controls the inclusion of the X chromosome in the analysis. Choices are `true` (default) or `false`.

FreqStruct = cghfreqplot(*CGHData*, ...'IncludeY', *IncludeYValue*, ...) controls the inclusion of the Y chromosome in the analysis. Choices are `true` or `false` (default).

FreqStruct = cghfreqplot(*CGHData*, ...'Chrominfo', *ChrominfoValue*, ...) specifies the cytogenetic banding information for the chromosomes. *ChrominfoValue* can be either of the following

- Structure returned by the `cytobandread` function
- String specifying the file name of an NCBI ideogram text file or a UCSC Genome Browser cytoband text file

Default is *Homo sapiens* cytogenetic banding information from the UCSC Genome Browser, NCBI Build 36.1 (`http://genome.UCSC.edu`).

Tip You can download files containing cytogenetic G-banding data from the NCBI or UCSC Genome Browser ftp site. For example, you can download the cytogenetic banding data for *Homo sapiens* from:

```
ftp://ftp.ncbi.nlm.nih.gov/genomes/H_sapiens/mapview/ideogram.gz
```

or

```
ftp://hgdownload.cse.ucsc.edu/goldenPath/hg18/database/cytoBandIdeo.txt.gz
```

FreqStruct = cghfreqplot(*CGHData*, ...'ShowCentr', *ShowCentrValue*, ...) controls the display of the centromere positions as vertical dashed lines in the frequency plot. Choices are `true` (default) or `false`.

Tip The centromere positions are obtained from *ChrominfoValue*.

FreqStruct = cghfreqplot(*CGHData*, ...'Color', *ColorValue*, ...) specifies a color scheme for the vertical lines in the plot, indicating the frequency of the gains and losses. Choices are:

- Name of or handle to a function that returns a colormap.
- M-by-3 matrix containing RGB values. If M equals 1, then that single color is used for all gains and losses. If M equals 2 or more, then the first row is used for gains, the second row is used for losses, and remaining rows are ignored. For example, `[0 1 0;1 0 0]` specifies green for gain and red for loss.

The default color scheme is a range of colors from pure green (gain = 1) through yellow (0) to pure red (loss = –1).

FreqStruct = cghfreqplot(*CGHData*, ...'YLim', *YLimValue*, ...) specifies the y vertical limits for the frequency plot. *YLimValue* is

a two-element vector specifying the minimum and maximum values on the vertical axis. Default is `[1, -1]`.

`FreqStruct` `= cghfreqplot(`*`CGHData`*`, ...'Titles', `*`TitlesValue`*`, ...)` specifies titles for the group(s), which are added to the tops of the plot(s). *`TitlesValue`* can be a single string or a cell array of strings.

Examples

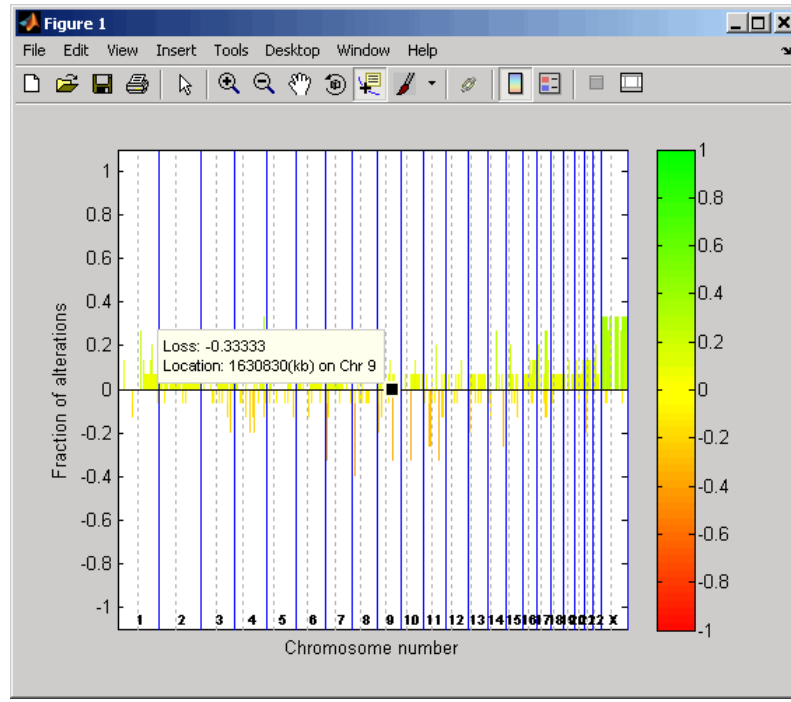
Plotting Data from the Coriell Cell Line Study

1. Load a MAT-file, included with the Bioinformatics Toolbox software, which contains `coriell_data`, a structure of array-based CGH data.

   ```
   load coriell_baccgh
   ```

2. Display a frequency plot of the copy number alterations across all samples in the Coriell aCGH data.

   ```
   Struct = cghfreqplot(coriell_data);
   ```



3 View data tips for the data, chromosomes, and centromeres by clicking the Data Cursor button on the toolbar, then clicking data, a blue chromosome boundary line, or a dotted centromere line in the plot. To delete this data tip, right-click it, then select **Delete Current Datatip**.

4 Display a color bar indicating the degree of gain or loss by clicking the Insert Colorbar button on the toolbar.

The `coriell_baccgh.mat` file used in this example contains data from Snijders et al., 2001.

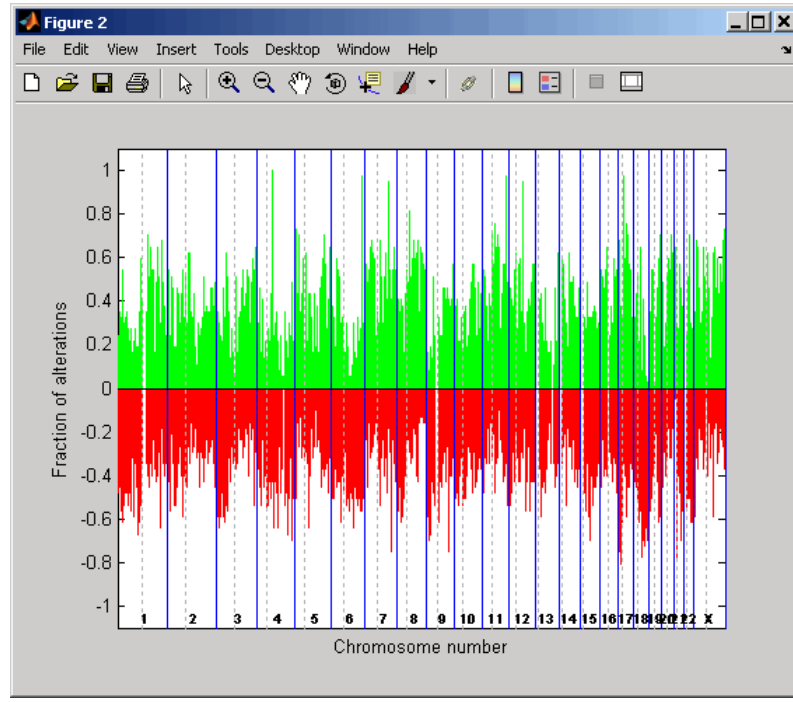
Plotting Pancreatic Cancer Study Data Using a Green and Red Color Scheme

1. Load a MAT-file, included with the Bioinformatics Toolbox software, which contains `pancrea_data`, a structure of array-based CGH data from a pancreatic cancer study.

```
load pancrea_oligocgh
```

2. Display a frequency plot of the copy number alterations across all samples in the pancreatic cancer data, using a green and red color scheme.

```
cghfreqplot(pancrea_data, 'Color', [0 1 0; 1 0 0])
```



The pancrea_oligocgh.mat file used in this example contains data from Aguirre et al., 2004.

Plotting Groups of aCGH Data, Specifying a Frequency Value Cutoff, and Adding a Chromosome Ideogram

1. Load a MAT-file, included with the Bioinformatics Toolbox software, which contains pancrea_data, a structure of array-based CGH data from a pancreatic cancer study.

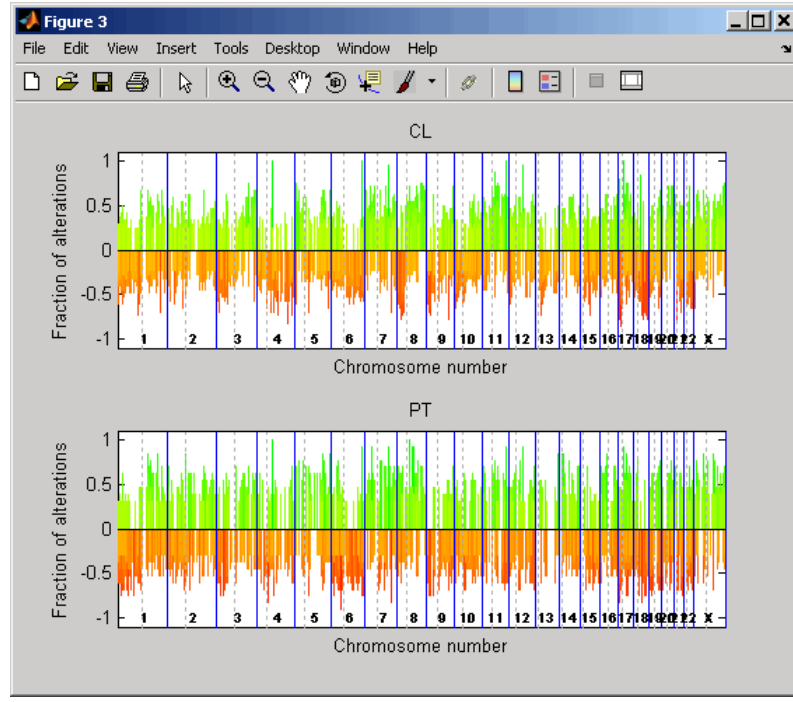
   ```
   load pancrea_oligocgh
   ```

2. Define two groups of data.

   ```
   grp1=strmatch('PA.C', pancrea_data.Sample);
   grp2=strmatch('PA.T', pancrea_data.Sample);
   ```

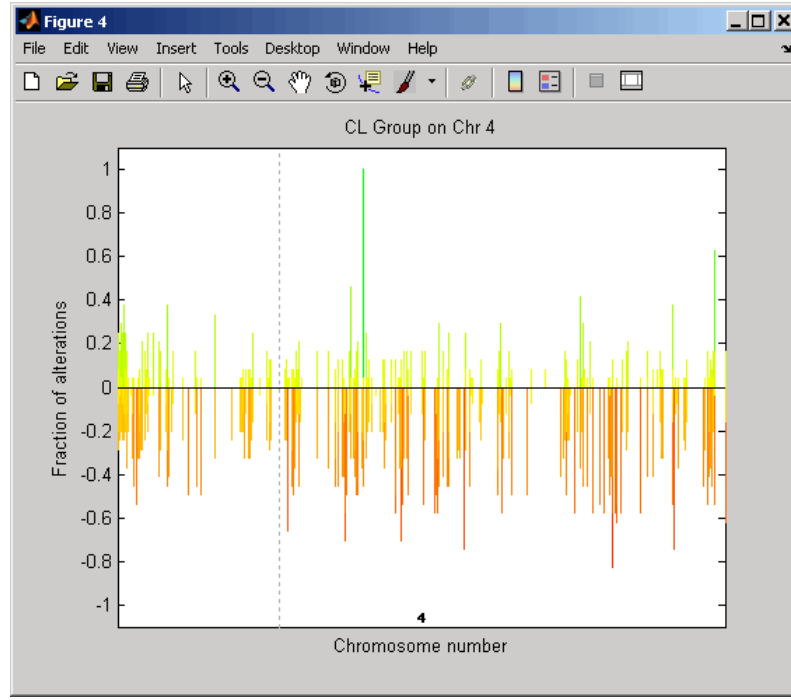
3. Display a frequency plot of the copy number alterations across all samples in the two groups and limit the plotting to only the clones with frequency gains or losses greater than or equal to 0.25.

   ```
   SP = cghfreqplot(pancrea_data, 'Group', {grp1, grp2},...
                    'Title', {'CL', 'PT'}, 'Cutoff', 0.25);
   ```



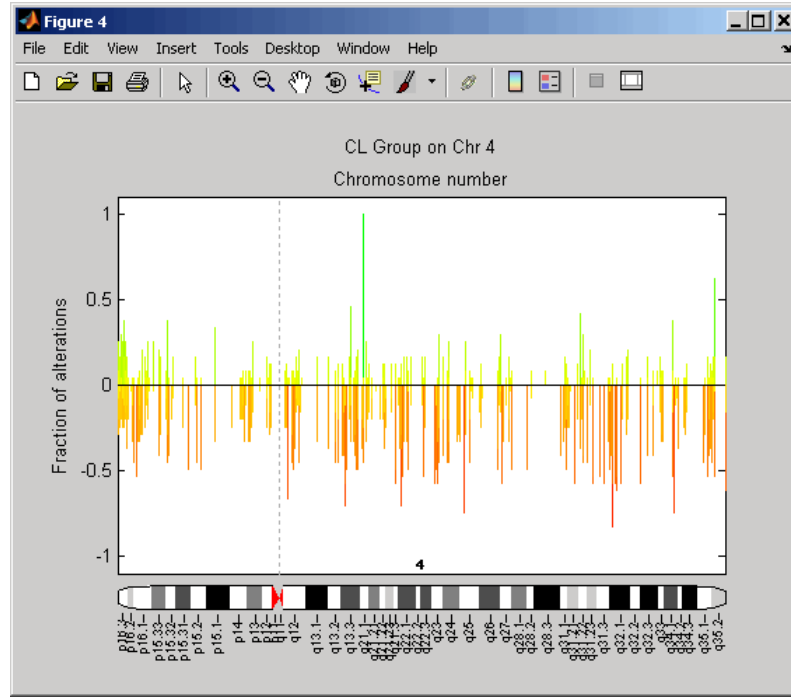
4 Display a frequency plot of the copy number alterations across all samples in the first group and limit the plot to chromosome 4 only.

```
SP = cghfreqplot(pancrea_data, 'Group', grp1, ...
                 'Title', 'CL Group on Chr 4', 'Chromosome', 4);
```



5 Use the `chromosomeplot` function with the `'addtoplot'` property to add the ideogram of chromosome 4 for *Homo sapiens* to this frequency plot. Because the plot of the frequency data from the pancreatic cancer study is in kb units, use the `'Unit'` property to convert the ideogram data to kb units.

```
chromosomeplot('hs_cytoBand.txt', 4, 'addtoplot', gca, 'unit', 2)
```



The `pancrea_oligocgh.mat` file used in this example contains data from Aguirre et al., 2004.

References

[1] Snijders, A.M., Nowak, N., Segraves, R., Blackwood, S., Brown, N., Conroy, J., Hamilton, G., Hindle, A.K., Huey, B., Kimura, K., Law, S., Myambo, K., Palmer, J., Ylstra, B., Yue, J.P., Gray, J.W., Jain, A.N., Pinkel, D., and Albertson, D.G. (2001). Assembly of microarrays for genome-wide measurement of DNA copy number. Nature Genetics *29*, 263–264.

[2] Aguirre, A.J., Brennan, C., Bailey, G., Sinha, R., Feng, B., Leo, C., Zhang, Y., Zhang, J., Gans, J.D., Bardeesy, N., Cauwels, C., Cordon-Cardo, C., Redston, M.S., DePinho, R.A., and Chin, L. (2004).

High-resolution characterization of the pancreatic adenocarcinoma genome. PNAS *101, 24*, 9067–9072.

See Also

Bioinformatics Toolbox functions: `cghcbs`, `chromosomeplot`, `cytobandread`

chromosomeplot

Purpose

Plot chromosome ideogram with G-banding pattern

Syntax

```
chromosomeplot(CytoData)
chromosomeplot(CytoData, ChromNum)
chromosomeplot(CytoData, ChromNum, ...,'Orientation',
OrientationValue, ...)
chromosomeplot(CytoData, ChromNum, ...,'ShowBandLabel',
   ShowBandLabelValue, ...)
chromosomeplot(CytoData, ChromNum, ...,'AddToPlot',
   AddToPlotValue, ...)
chromosomeplot(..., 'Unit', UnitValue, ...)
chromosomeplot(..., 'CNV', CNVValue, ...)
```

Arguments

CytoData

Either of the following:

- String specifying a file containing cytogenetic G-banding data (in bp units), such as an NCBI ideogram text file or a UCSC Genome Browser cytoband text file.
- Structure containing cytogenetic G-banding data (in bp units) in the following fields:
  - `ChromLabels`
  - `BandStartBPs`
  - `BandEndBPs`
  - `BandLabels`
  - `GieStains`

Tip Use the `cytobandread` function to create the structure to use for *`CytoData`*.

`ChromNum`

Scalar or string specifying a single chromosome to plot. Valid entries are integers, `'X'`, and `'Y'`.

Note Setting *`ChromNum`* to `0` will plot ideograms for all chromosomes.

`OrientationValue`

String or number that specifies the orientation of the ideogram of a single chromosome specified by *`ChromNum`*. Choices are `'Vertical'` or `1` (default) and `'Horizontal'` or `2`.

`ShowBandLabelValue`

Controls the display of band labels (such as `q25.3`) when plotting a single chromosome ideogram, specified by *`ChromNum`*. Choices are `true` (default) or `false`.

`AddToPlotValue`

Variable name of a figure axis to which to add the single chromosome ideogram, specified by *`ChromNum`*.

Note If you use this property to add the ideogram to a plot of genomic data that is in units other than bp, use the `'Unit'` property to convert the ideogram data to the appropriate units.

Tip Before printing a figure containing an added chromosome ideogram, change the background to white by issuing the following command:

```
set(gcf,'color','w')
```

UnitValue	Integer that specifies the units (base pairs, kilo base pairs, or mega base pairs) for the starting and ending genomic positions. This unit is used in the data tip displayed when you hover the cursor over chromosomes in the ideogram. This unit can also be used when using the `'AddToPlot'` property to add the ideogram to a plot that is in units other than bp. Choices are `1` (bp), `2` (kb), or `3` (mb). Default is `1` (bp).
CNVValue	Controls the display of copy number variance (CNV) data, provided by *CNVValue*, aligned to the chromosome ideogram. Gains are shown in green to the right or above the ideogram, while losses are shown in red to the left or below the ideogram. *CNVValue* is a structure array containing the four fields described in the table below.

Description

`chromosomeplot(`*CytoData*`)` plots the ideogram of all chromosomes, using information from *CytoData*, a structure containing cytogenetic G-banding data (in bp units), or a string specifying a file containing cytogenetic G-banding data (in bp units), such as an NCBI ideogram text file or a UCSC Genome Browser cytoband text file. The G bands

distinguish different areas of the chromosome. For example, for the *Homo sapiens* ideogram, possible G bands are:

- `gneg` — white
- `gpos25` — light gray
- `gpos50` — medium gray
- `gpos75` — dark gray
- `gpos100` — black
- `acen` — red (centromere)
- `stalk` — light blue (regions with repeats)
- `gvar` — indented region

Darker bands are AT-rich, while lighter bands are GC-rich.

`chromosomeplot(`*`CytoData`*`, `*`ChromNum`*`)` plots the ideogram of a single chromosome specified by *`ChromNum`*.

`chromosomeplot(..., '`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `chromosomeplot` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`chromosomeplot(`*`CytoData`*`, `*`ChromNum`*`, ...,'Orientation',` *`OrientationValue`*`, ...)` specifies the orientation of the ideogram of a single chromosome specified by *`ChromNum`*. Choices are `'Vertical'` or `1` (default) and `'Horizontal'` or `2`.

Note When plotting the ideogram of all chromosomes, the orientation is always vertical.

`chromosomeplot(CytoData, ChromNum, ...,'ShowBandLabel', ShowBandLabelValue, ...)` displays band labels (such as q25.3) when plotting a single chromosome ideogram, specified by *`ChromNum`*. Choices are `true` (default) or `false`.

`chromosomeplot(CytoData, ChromNum, ...,'AddToPlot', AddToPlotValue, ...)` adds the single chromosome ideogram, specified by *`ChromNum`*, to a figure axis specified by *`AddToPlotValue`*.

Note If you use this property to add the ideogram to a plot of genomic data that is in units other than bp, use the `'Unit'` property to convert the ideogram data to the appropriate units.

Tip Before printing a figure containing an added chromosome ideogram, change the background to white by issuing the following command:

```
set(gcf,'color','w')
```

`chromosomeplot(..., 'Unit', UnitValue, ...)` specifies the units (base pairs, kilo base pairs, or mega base pairs) for the starting and ending genomic positions. This unit is used in the data tip displayed when you hover the cursor over chromosomes in the ideogram. This unit can also be used when using the `'AddToPlot'` property to add the ideogram to a plot that is in units other than bp. Choices are `1` (bp), `2` (kb), or `3` (mb). Default is `1` (bp).

`chromosomeplot(..., 'CNV', CNVValue, ...)` displays copy number variance (CNV) data, provided by *`CNVValue`*, aligned to the chromosome ideogram. Gains are shown in green to the right or above the ideogram, while losses are shown in red to the left or below the ideogram. *`CNVValue`* is a structure array containing the following fields. Each field must contain the same number of elements.

Field	Description

`Chromosome`	Either of the following:
	
	• Numeric vector containing the chromosome number on which each CNV is located.
	
	Note For the sex chromosome, `X`, use *N*, where *N* = number of autosomes + 1. For the sex chromosome, `Y`, use *M*, where *M* = number of autosomes + 2. For example, for *Homo sapiens* use `23` for `X` and `24` for `Y`, and for *Mus musculus* (lab mouse), use `20` for `X` and `21` for `Y`.
	
	• Character array containing the chromosome number on which each CNV is located.
	
	Note Using a character array lets you use the characters `X` and `Y` (instead of numbers) for sex chromosomes. However, all elements in the array must be the same width, which may require you to add spaces to the strings. For example:
	
	`[' 1'; ' 2'; '10'; ' X']`
	
	Or you can use the `char` function with a cell array to create a character array of the chromosome numbers and letters. For example: .
	
	`char({'1', '2', '10', 'X'})`

Field	Description
`CNVType`	Numeric vector containing the type of each CNV, either `1` (loss) or `2` (gain).
`Start`	Numeric vector containing the starting genomic position of each CNV. Units must be in base pairs.
`End`	Numeric vector containing the ending genomic position of each CNV. Units must be in base pairs.

Examples

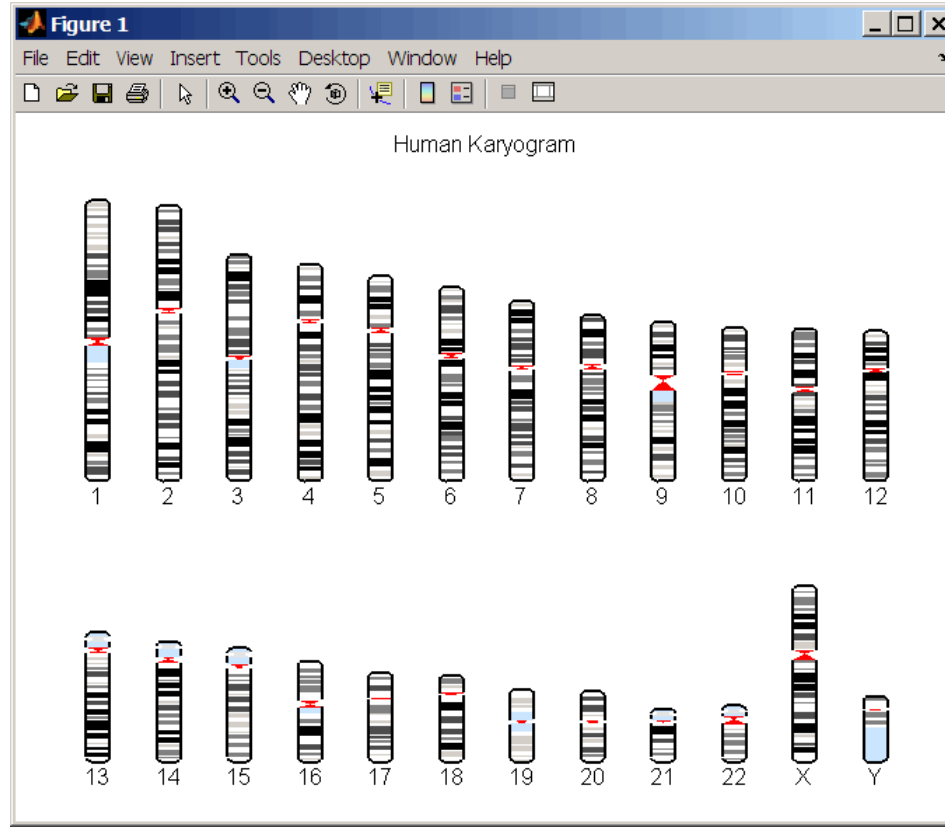
Plotting Chromosome Ideograms

1 Read the cytogenetic banding information for *Homo sapiens* into a structure.

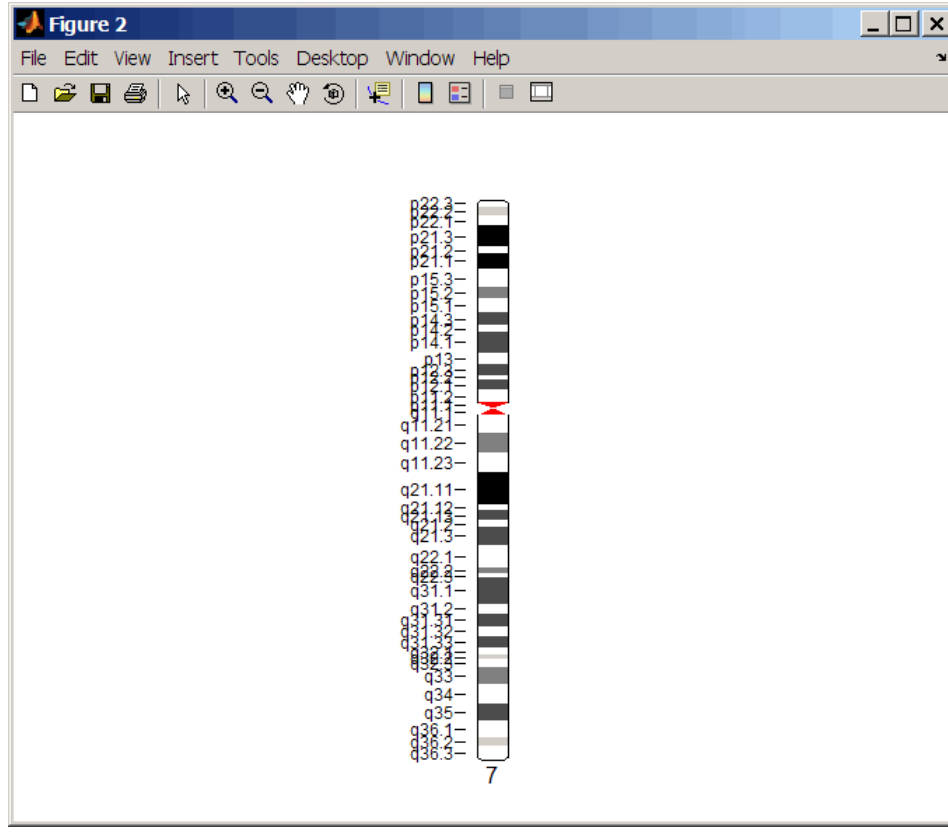
```
hs_cytobands = cytobandread('hs_cytoBand.txt')

hs_cytobands =

     ChromLabels: {862x1 cell}
    BandStartBPs: [862x1 int32]
      BandEndBPs: [862x1 int32]
      BandLabels: {862x1 cell}
       GieStains: {862x1 cell}
```

2 Plot the entire chromosome ideogram for *Homo sapiens*.

```
chromosomeplot(hs_cytobands);
title('Human Karyogram')
```

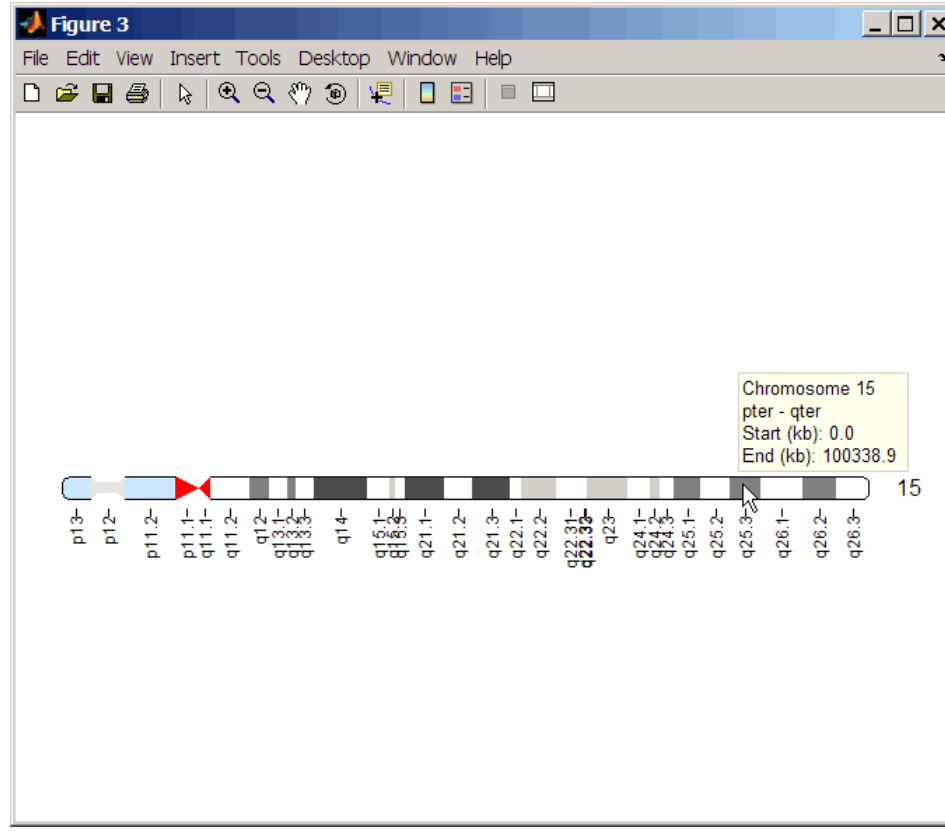


3 Display the ideogram of only chromosome 7 for *Homo sapiens* by right-clicking chromosome 7 in the plot, then selecting **Display in New Figure > Vertical**.



4 Plot the ideogram of only chromosome 15 for *Homo sapiens* in a horizontal orientation. Set the units used in the data tip to kilo base pairs.

```
chromosomeplot(hs_cytobands, 15, 'Orientation', 2, 'Unit', 2);
```



5 View a data tip with information about the chromosome by hovering the cursor over the chromosome. View a data tip with detailed information about a specific band by clicking the Data Cursor  button on the toolbar, then clicking the band in the plot. To delete this data tip, right-click it, then select **Delete Current Datatip**.

Tip You can change the orientation of a single chromosome ideogram by right-clicking, selecting **Display > Vertical** or **Horizontal**. You can show or hide the band labels of a single chromosome ideogram by right-clicking, then selecting **Show G-band Labels** or **Hide G-band Labels**.

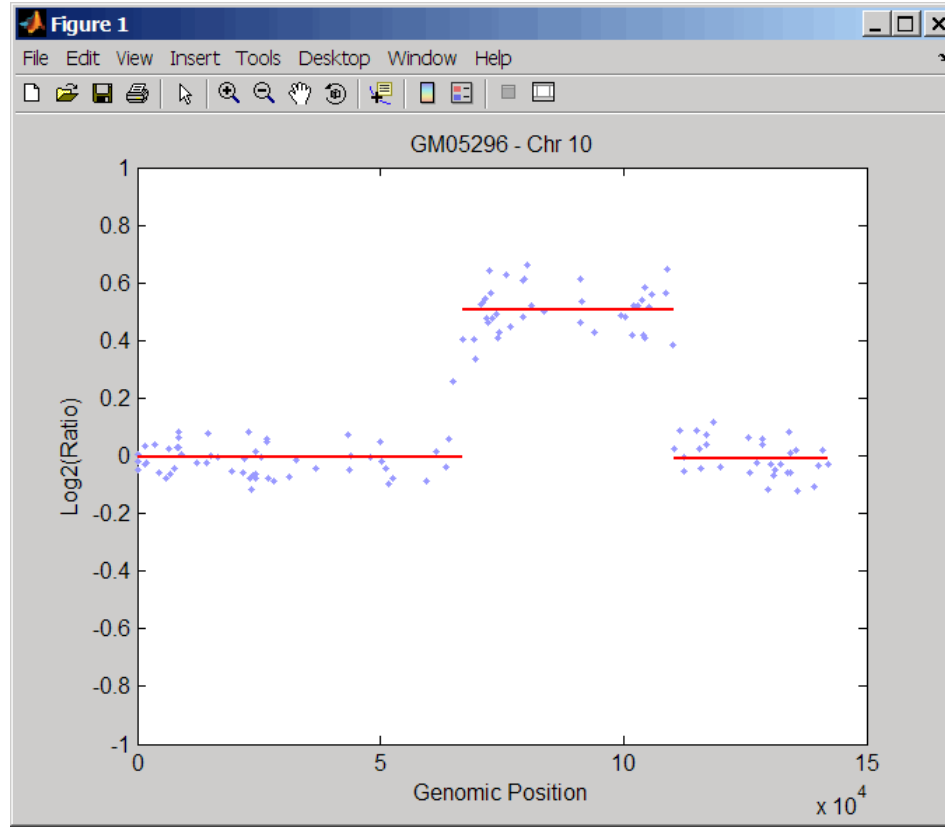
Adding a Chromosome Ideogram to a Plot

1. Load a MAT-file, included with the Bioinformatics Toolbox software, which contains `coriell_data`, a structure of CGH data.

```
load coriell_baccgh
```

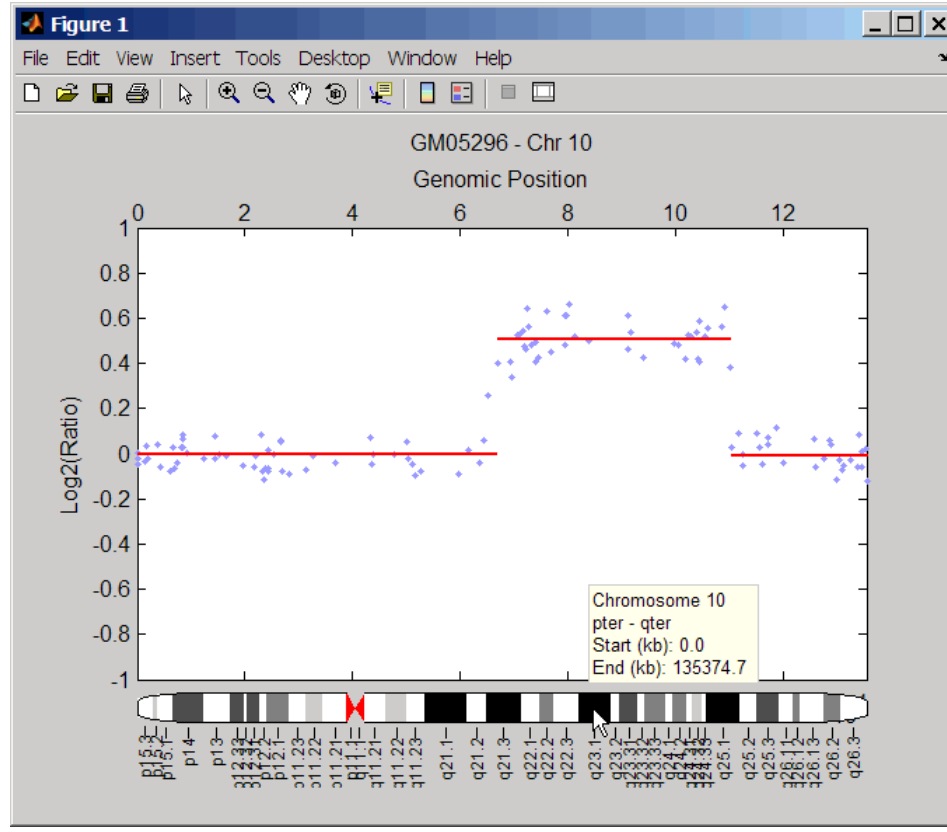
2. Use the `cghcbs` function to analyze chromosome 10 of sample 3 (GM05296) of the CGH data and return copy number variance (CNV) data in a structure, `S`. Plot the segment means over the original data for only chromosome 10 of sample 3.

```
S = cghcbs(coriell_data,'sampleindex',3,'chromosome',10,...
           'showplot',10);
```



3 Use the `chromosomeplot` function with the `'addtoplot'` property to add the ideogram of chromosome 10 for *Homo sapiens* to the plot. Because the plot of the CNV data from the Coriell cell line study is in kb units, use the `'Unit'` property to convert the ideogram data to kb units.

```
chromosomeplot('hs_cytoBand.txt', 10, 'addtoplot', gca,...
               'Unit', 2)
```



Tip Before printing the above figure containing an added chromosome ideogram, change the background to white by issuing the following command:

```
set(gcf,'color','w')
```

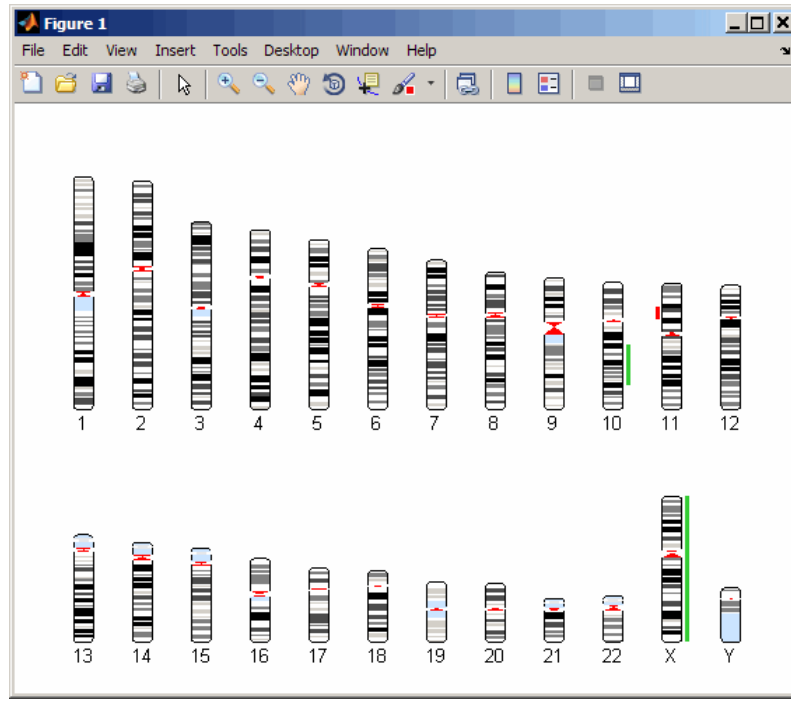
Displaying Copy Number Alteration Regions Aligned to a Chromosome Ideogram

1. Create a structure containing segment gain and loss information for chromosomes 10, 11, and X from sample 3 from the Coriell cell line study, making sure the segment data is in bp units. (You can determine copy number variance (CNV) information by exploring `S`, the structure of segments returned by the `cghcbs` function in step 2 in Adding a Chromosome Ideogram to a Plot on page 3-274.) For the `'CNVType'` field, use `1` to indicate a loss and `2` to indicate a gain.

   ```
   cnvStruct = struct('Chromosome', char({'10', '11', 'X'}),...
                      'CNVType', [2 1 2],...
                      'Start', [66905000 25416000 1],...
                      'End',   [110412000 39389000 154913755]);
   ```

2. Pass the structure to the `chromosomeplot` function using the `'CNV'` property to display the copy number gains (green) and losses (red) aligned to the human chromosome ideogram.

   ```
   chromosomeplot('hs_cytoBand.txt', 'cnv', cnvStruct);
   ```



The `coriell_baccgh.mat` file used in this example contains data from Snijders et al., 2001.

References

[1] Snijders, A.M., Nowak, N., Segraves, R., Blackwood, S., Brown, N., Conroy, J., Hamilton, G., Hindle, A.K., Huey, B., Kimura, K., Law, S., Myambo, K., Palmer, J., Ylstra, B., Yue, J.P., Gray, J.W., Jain, A.N., Pinkel, D., and Albertson, D.G. (2001). Assembly of microarrays for genome-wide measurement of DNA copy number. Nature Genetics *29*, 263–264.

See Also

Bioinformatics Toolbox functions: `cghcbs`, `cytobandread`

Purpose

Evaluate performance of classifier

Syntax

```
classperf
CP = classperf(truelabels)
CP = classperf(truelabels, classout)
CP = classperf(..., 'Positive', PositiveValue, 'Negative',
   NegativeValue)
classperf(CP, classout)
classperf(CP, classout, testidx)
```

Arguments

truelabels

True class labels for each observation, specified by one of the following:

- Numeric vector
- Cell array of strings

Note When used in a cross-validation design experiment, *truelabels* should have the same size as the total number of observations.

classout

Classifier output, specified by one of the following:

- Numeric vector
- Cell array of strings

Note *classout* must contain the same number of elements as *truelabels*.

PositiveValue	Numeric vector or cell array of strings that specifies the positive labels to identify the target class(es). Default is the first class returned by `grp2idx(truelabels)`.
NegativeValue	Numeric vector or cell array of strings that specifies the negative labels to identify the control class(es). Default is all classes other than the first class returned by `grp2idx(truelabels)`.
testidx	Vector that indicates the observations that were used in the current validation. Choices are: • Index vector • Logical index vector of the same size as *truelabels* used to construct the classifier performance object

Return Values

CP	Classifier performance object with performance properties listed in the following table.

Description

`classperf` provides an interface to keep track of the performance during the validation of classifiers. `classperf` creates and, optionally, updates a classifier performance object, *CP*, which accumulates the results of the classifier. The performance properties of a classifier performance object are listed in the following table.

`classperf`, without input arguments, displays all the performance properties of a classifier performance object.

CP = `classperf(`*truelabels*`)` creates and initializes an empty classifier performance object. *CP* is the handle to the object. *truelabels* is a vector or cell array of strings containing the true class labels for every observation. When used in a cross-validation design experiment, *truelabels* must have the same size as the total number of observations.

CP = classperf(*truelabels*, *classout*) creates *CP* using *truelabels*, then updates *CP* using the classifier output, *classout*.

Tip This syntax is useful when you want to know the performance of a single validation.

CP = classperf(..., 'Positive', *PositiveValue*, 'Negative', *NegativeValue*) specifies the positive and negative labels to identify the target and the control classes, respectively. These labels are used to compute clinical diagnostic test performance.

If *truelabels* is a numeric vector, *PositiveValue* and *NegativeValue* must be numeric vectors whose entries are subsets of grp2idx(*truelabels*). If *truelabels* is a cell array of strings, *PositiveValue* and *NegativeValue* can be cell arrays of strings or numeric vectors whose entries are subsets of grp2idx(*truelabels*). *PositiveValue* defaults to the first class returned by grp2idx(*truelabels*), while *NegativeValue* defaults to all other classes.

PositiveValue and *NegativeValue* must consist of disjoint sets of the labels used in *truelabels*. For example, if

```
truelabels = [1 2 2 1 3 4 4 1 3 3 3 2]
```

you could set

```
p = [1 2];
n = [3 4];
```

For example, if you have a data set with data from six samples: five different types of cancer (ovarian, lung, prostate, skin, brain) and no cancer, then ClassLabels = {'Ovarian', 'Lung', 'Prostate', 'Skin', 'Brain', 'Healthy'}.

You could test a detector for lung cancer by using a *PositiveValue* of 2, and a *NegativeValue* = [1 3 4 5 6].

Or you can test for any type of cancer by using *PositiveValue* = [1 2 3 4 5] and a *NegativeValue* of 6.

In clinical tests, inconclusive values such as '' or NaN are counted as false negatives for the computation of the specificity, and as false positives for the computation of the sensitivity. That is, inconclusive results may decrease the diagnostic value of the test. Tested observations for which *truelabels* is not within the union of *PositiveValue* and *NegativeValue* are not considered. However, tested observations that result in a class not covered by the vector *truelabels* are counted as inconclusive.

classperf(*CP*, *classout*) updates *CP*, the classifier performance object, with the classifier output *classout*. *classout* must be the same size as *truelabels*, the vector or cell array used to construct the classifier performance object. When *classout* is a cell array of strings, an empty string, '', represents an inconclusive result of the classifier. For numeric arrays, NaN represents an inconclusive result.

classperf(*CP*, *classout*, *testidx*) updates *CP*, the classifier performance object, with the classifier output *classout*. *classout* has a smaller size than *truelabels*. *testidx* is an index vector or a logical index vector of the same size as *truelabels*, the vector or cell array used to construct the classifier performance object. *testidx* indicates the observations that were used in the current validation.

Note In the two previous syntaxes, you do not need to create a separate output variable to update the classifier performance object, *CP*.

Properties of a Classifier Performance Object

You can access classifier performance object properties by using the get function

```
get(CP, 'ControlClasses')
```

or using dot notation

```
CP.ControlClasses
```

You cannot directly modify the classifier performance object properties by using the `set` function, with the exception of the `Label` and `Description` properties.

Tip To modify properties, use either of the following syntaxes:

```
classperf(CP, classout)
classperf(CP, classout, testidx)
```

Property	Description
`Label`	String to label the classifier performance object. Default is `''`.
`Description`	String to describe the classifier performance object. Default is `''`.
`ClassLabels`	Numeric vector or cell array of strings specifying a unique set of class labels from `unique(truelabels)`.
`GroundTruth`	Numeric vector or cell array of strings that specifies the true class labels for each observation. The number of elements = `NumberOfObservations`.
`NumberOfObservations`	Positive integer specifying the number of observations in the study.

Property	Description
`ControlClasses`	Indices to the `ClassLabels` vector or cell array, indicating which classes to be considered as the control or negative classes in a diagnostic test. **Tip** You set the `ControlClasses` property with the `'Negative'` property name/value pair. If you do not specify the `'Negative'` property, `ControlClasses` defaults to all classes other than the first class returned by `grp2idx(truelabels)`.
`TargetClasses`	Indices to the `ClassLabels` vector or cell array, indicating which classes to be considered as the target or positive classes in a diagnostic test. **Tip** You set the `TargetClasses` property with the `'Positive'` property name/value pair. If you do not specify the `'Positive'` property, `TargetClasses` defaults to the first class returned by `grp2idx(truelabels)`.
`ValidationCounter`	Positive integer specifying the number of validations performed.

Property	Description
`SampleDistribution`	Numeric vector indicating how many times each sample was considered in the validation. For example, if you use resubstitution, `SampleDistribution` is a vector of ones and `ValidationCounter` = 1. If you have a ten-fold cross-validation, `SampleDistribution` is also a vector of ones, but `ValidationCounter` = 10. **Tip** `SampleDistribution` is more useful when doing Monte Carlo partitions of the test sets, as this will help determine if all the samples are being equally tested.
`ErrorDistribution`	Numeric vector indicating how many times each sample was misclassified.
`SampleDistributionByClass`	Numeric vector indicating the frequency of the true classes in the validation.
`ErrorDistributionByClass`	Numeric vector indicating the frequency of errors for each class in the validation.

Property	Description
`CountingMatrix`	The classification confusion matrix. The order of rows and columns is the same as `grp2idx(truelabels)`. Columns represent the true classes, and rows represent the classifier prediction. The last row in `CountingMatrix` is reserved to count inconclusive results. There are some families of classifiers that can reserve the right to make a hard class assignment; this can be based on metrics, such as the posterior probabilities, or on how close a sample is to the class boundaries.
`CorrectRate`	Correctly Classified Samples / Classified Samples **Note** Inconclusive results are not counted.
`ErrorRate`	Incorrectly Classified Samples / Classified Samples **Note** Inconclusive results are not counted.

Property	Description
`LastCorrectRate`	The following equation applies only to samples considered the last time the classifier performance object was updated: Correctly Classified Samples / Classified Samples
`LastErrorRate`	The following equation applies only to samples considered the last time the classifier performance object was updated: Incorrectly Classified Samples / Classified Samples
`InconclusiveRate`	Nonclassified Samples / Total Number of Samples
`ClassifiedRate`	Classified Samples / Total Number of Samples
`Sensitivity`	Correctly Classified Positive Samples / True Positive Samples **Note** Inconclusive results that are true positives are counted as errors for computing `Sensitivity` (following a conservative approach). This is the same as being incorrectly classified as negatives.

Property	Description
`Specificity`	Correctly Classified Negative Samples / True Negative Samples **Note** Inconclusive results that are true negatives are counted as errors for computing `Specificity` (following a conservative approach). This is the same as being incorrectly classified as positives.
`PositivePredictiveValue`	Correctly Classified Positive Samples / Positive Classified Samples **Note** Inconclusive results are classified as negatives when computing `PositivePredictiveValue`.
`NegativePredictiveValue`	Correctly Classified Negative Samples / Negative Classified Samples **Note** Inconclusive results are classified as positives when computing `NegativePredictiveValue`.
`PositiveLikelihood`	`Sensitivity` / (1 – `Specificity`)
`NegativeLikelihood`	(1 – `Sensitivity`) / `Specificity`

Property	Description
`Prevalence`	True Positive Samples / Total Number of Samples
`DiagnosticTable`	A 2-by-2 numeric array with diagnostic counts. The first row indicates the number of samples that were classified as positive, with the number of true positives in the first column, and the number of false positives in the second column. The second row indicates the number of samples that were classified as negative, with the number of false negatives in the first column, and the number of true negatives in the second column. Correct classifications appear in the diagonal elements, and errors appear in the off-diagonal elements. Inconclusive results are considered errors and counted in the off-diagonal elements. For an illustration of a diagnostic table, see below.

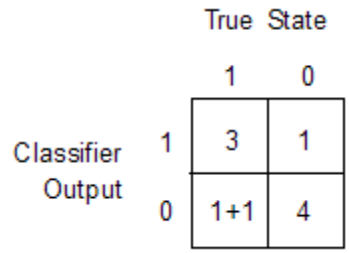
Example Diagnostic Table

In a cancer study of ten patients, suppose we get the following results:

Patient	Classifier Output	Has Cancer
1	Positive	Yes
2	Positive	Yes
3	Positive	Yes
4	Positive	No

Patient	Classifier Output	Has Cancer
5	Negative	Yes
6	Negative	No
7	Negative	No
8	Negative	No
9	Negative	No
10	Inconclusive	Yes

The diagnostic table would look as follows:



Examples

```
% Classify the fisheriris data with a K-Nearest Neighbor classifier
load fisheriris
c = knnclassify(meas,meas,species,4,'euclidean','Consensus');
cp = classperf(species,c)
get(cp)

% 10-fold cross-validation on the fisheriris data using linear
% discriminant analysis and the third column as only feature for
% classification
load fisheriris
indices = crossvalind('Kfold',species,10);
cp = classperf(species); % initializes the CP object
for i = 1:10
    test = (indices == i); train = ~test;
```

```
    class = classify(meas(test,3),meas(train,3),species(train));
    % updates the CP object with the current classification results
    classperf(cp,class,test)
end
cp.CorrectRate % queries for the correct classification rate


cp =

 biolearning.classperformance

                      Label: ''
                Description: ''
                ClassLabels: {3x1 cell}
                truelabels: [150x1 double]
        NumberOfObservations: 150
              ControlClasses: [2x1 double]
               TargetClasses: 1
           ValidationCounter: 1
          SampleDistribution: [150x1 double]
           ErrorDistribution: [150x1 double]
   SampleDistributionByClass: [3x1 double]
    ErrorDistributionByClass: [3x1 double]
              CountingMatrix: [4x3 double]
                 CorrectRate: 1
                   ErrorRate: 0
             InconclusiveRate: 0.0733
               ClassifiedRate: 0.9267
                 Sensitivity: 1
                 Specificity: 0.8900
      PositivePredictiveValue: 0.8197
      NegativePredictiveValue: 1
           PositiveLikelihood: 9.0909
           NegativeLikelihood: 0
                   Prevalence: 0.3333
            DiagnosticTable: [2x2 double]
```

```
ans =
    0.9467
```

See Also

Bioinformatics Toolbox functions: `crossvalind`, `knnclassify`, `svmclassify`

Statistics Toolbox™ functions: `classify`, `grp2idx`

Purpose

Cleave amino acid sequence with enzyme

Syntax

```
Fragments = cleave(SeqAA, Enzyme)
Fragments = cleave(SeqAA, PeptidePattern, Position)
[Fragments, CuttingSites] = cleave(...)
[Fragments, CuttingSites, Lengths] = cleave(...)
[Fragments, CuttingSites, Lengths, Missed] = cleave(...)
cleave(..., 'PartialDigest', PartialDigestValue, ...)
cleave(..., 'MissedSites', MissedSitesValue, ...)
cleave(..., 'Exception', ExceptionValue, ...)
```

Arguments

SeqAA

One of the following:

- String of single-letter codes specifying an amino acid sequence.
- Row vector of integers specifying an amino acid sequence.
- MATLAB structure containing a `Sequence` field that contains an amino acid sequence, such as returned by `fastaread`, `getgenpept`, `genpeptread`, `getpdb`, or `pdbread`.

Examples: `'ARN'` or `[1 2 3]`.

Enzyme

String specifying a name or abbreviation code for an enzyme or compound for which the literature specifies a cleavage rule.

Tip Use the `cleavelookup` function to display the names of enzymes and compounds in the cleavage rule library.

PeptidePattern	Short amino acid sequence to search for in *SeqAA*, a larger sequence. *PeptidePattern* can be any of the following: • Character string • Vector of integers • Regular expression
Position	Integer from 0 to the length of the *PeptidePattern*, that specifies a position in the *PeptidePattern* to cleave. **Note** Position 0 corresponds to the N terminal end of *PeptidePattern*.
PartialDigestValue	Value from 0 to 1 (default) specifying the probability that a cleavage site will be cleaved.
MissedSitesValue	Nonnegative integer specifying the maximum number of missed cleavage sites. The output includes all possible peptide fragments that can result from missing *MissedSitesValue* or less cleavage sites. Default is 0, which is equivalent to an ideal digestion.
ExceptionValue	Regular expression specifying an exception rule to the cleavage rule associated with *Enzyme*. By default, cleave applies no exception rule.

Return Values

Fragments	Cell array of strings representing the fragments from the cleavage.
CuttingSites	Numeric vector containing indices representing the cleavage sites.

Note The `cleave` function adds a `0` to the list, so `numel(`*`CuttingSites`*`)==numel(`*`Fragments`*`)`. Use *`CuttingSites`* `+ 1` to point to the first amino acid of every fragment respective to the original sequence.

Lengths	Numeric vector containing the length of each fragment.
Missed	Numeric vector containing the number of missed cleavage sites for every peptide fragment.

Description

Fragments `= cleave(`*SeqAA*`, `*Enzyme*`)` cuts *SeqAA*, an amino acid sequence, into parts at the cleavage sites specific for *Enzyme*, a string specifying a name or abbreviation code for an enzyme or compound for which the literature specifies a cleavage rule. It returns *Fragments*, a cell array of strings representing the fragments from the cleavage.

Tip Use the `cleavelookup` function to display the names of enzymes and compounds in the cleavage rule library.

Fragments `= cleave(`*SeqAA*`, `*PeptidePattern*`, `*Position*`)` cuts *SeqAA*, an amino acid sequence, into parts at the cleavage sites specified by a peptide pattern and position.

`[Fragments, CuttingSites] = cleave(...)` returns a numeric vector containing indices representing the cleavage sites.

Note The `cleave` function adds a `0` to the list, so `numel(CuttingSites)==numel(Fragments)`. Use `CuttingSites + 1` to point to the first amino acid of every fragment respective to the original sequence.

`[Fragments, CuttingSites, Lengths] = cleave(...)` returns a numeric vector containing the length of each fragment.

`[Fragments, CuttingSites, Lengths, Missed] = cleave(...)` returns a numeric vector containing the number of missed cleavage sites for every fragment.

`cleave(..., 'PropertyName', PropertyValue, ...)` calls `cleave` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each *`PropertyName`* in single quotation marks. Each *`PropertyName`* is case insensitive. These property name/property value pairs are as follows:

`cleave(..., 'PartialDigest', PartialDigestValue, ...)` simulates a partial digestion where *`PartialDigestValue`* is the probability of a cleavage site being cut. *`PartialDigestValue`* is a value from `0` to `1` (default).

This table lists some common proteases and their cleavage sites.

Protease	Peptide Pattern	Position
Aspartic acid N	`D`	1
Chymotrypsin	`[WYF](?!P)`	1
Glutamine C	`[ED](?!P)`	1
Lysine C	`[K](?!P)`	1
Trypsin	`[KR](?!P)`	1

`cleave(..., 'MissedSites', MissedSitesValue, ...)` returns all possible peptide fragments that can result from missing *`MissedSitesValue`* or less cleavage sites. *`MissedSitesValue`* is a nonnegative integer. Default is `0`, which is equivalent to an ideal digestion.

`cleave(..., 'Exception', ExceptionValue, ...)` specifies an exception rule to the cleavage rule associated with *`Enzyme`*. *`ExceptionValue`* is a regular expression. By default, `cleave` applies no exception rule.

Examples

1 Retrieve a protein sequence from the GenPept database.

```
S = getgenpept('AAA59174');
```

2 Cleave the sequence using proteinase K.

```
[partsPK, sitesPK, lengthsPK] = cleave(S.Sequence, ...
 'proteinase K');
```

3 Display the indices of the cleavage sites, lengths, and sequences of the first ten fragments.

```
for i=1:10
       fprintf('%5d%5d %s\n',sitesPK(i),lengthsPK(i),partsPK{i})
   end
```

```
 0    3   MGT
 3    6   GGRRGA
 9    1   A
10    1   A
11    1   A
12    2   PL
14    1   L
15    1   V
16    1   A
17    1   V
```

4 Cleave the same sequence using one of trypsin's cleavage rules (cleave after K or R when the next residue is not P).

```
[partsT, sitesT, lengthsT] = cleave(S.Sequence,'[KR](?!P)',1);
```

5 Display the indices of the cleavage sites, lengths, and sequences of the first ten fragments.

```
for i=1:10
       fprintf('%5d%5d   %s\n',sitesT(i),lengthsT(i),partsT{i})
   end
```

```
  0    6   MGTGGR
  6    1   R
  7   34   GAAAAPLLVAVAALLLGAAGHLYPGEVCPGMDIR
 41    5   NNLTR
 46   21   LHELENCSVIEGHLQILLMFK
 67    7   TRPEDFR
 74    6   DLSFPK
 80   12   LIMITDYLLLFR
 92    8   VYGLESLK
100   10   DLFPNLTVIR
```

6 Cleave the same sequence using trypsin's cleavage rule, but allow for one missed cleavage site.

```
[partsT2, sitesT2, lengthsT2, missedT2] = cleave(S.Sequence, ...
                                          'trypsin','missedsites',1);
```

7 Cleave the same sequence using trypsin's cleavage rule, except do not to cleave after K when K is following by a D.

```
partsT3 = cleave(S.Sequence, 'trypsin', 'exception', 'KD');
```

See Also

Bioinformatics Toolbox functions: `cleavelookup`, `rebasecuts`, `restrict`, `seqshowwords`

MATLAB function: `regexp`

Purpose

Find cleavage rule for enzyme or compound

Syntax

```
cleavelookup
cleavelookup('Code', CodeValue)
cleavelookup('Name', NameValue)
```

Arguments

CodeValue	String specifying a code representing an abbreviation code for an enzyme or compound. For valid codes, see the table Cleave Lookup on page 3-299.
NameValue	String specifying an enzyme or compound name. For valid names, see the table Cleave Lookup on page 3-299.

Description

`cleavelookup` displays a table of abbreviation codes, cleavage positions, cleavage patterns, and full names of enzymes and compounds for which cleavage rules are specified by the cleavage rule library. For more information, see the ExPASy PeptideCutter tool.

Cleave Lookup

Code	Position	Pattern	Full Name
ARG-C	1	R	ARG-C proteinase
ASP-N	2	D	ASP-N endopeptidase
BNPS	1	W	BNPS-Skatole
CASP1	1	(?<=[FWYL]\w[HAT])D(?=[^PEDQKR])	Caspase 1
CASP2	1	(?<=DVA)D(?=[^PEDQKR])	Caspase 2
CASP3	1	(?<=DMQ)D(?=[^PEDQKR])	Caspase 3

Cleave Lookup (Continued)

Code	Position	Pattern	Full Name
CASP4	1	(?<=LEV)D(?=[^PEDQKR])	Caspase 4
CASP5	1	(?<=[LW]EH)D	Caspase 5
CASP6	1	(?<=VE[HI])D(?=[^PEDQKR])	Caspase 6
CASP7	1	(?<=DEV)D(?=[^PEDQKR])	Caspase 7
CASP8	1	(?<=[IL]ET)D(?=[^PEDQKR])	Caspase 8
CASP9	1	(?<=LEH)D	Caspase 9
CASP10	1	(?<=IEA)D	Caspase 10
CH-HI	1	([FY](?=[^P]))|(W(?=[^MP]))	Chymotrypsin-high specificity
CH-LO	1	([FLY](?=[^P]))|(W(?=[^MP]))| (M(?=[^PY]))|(H(?=[^DMPW]))	Chymotrypsin-low specificity
CLOST	1	R	Clostripain
CNBR	1	M	CNBR
ENTKIN	1	(?<=[DN][DN][DN])K	Enterokinase
FACTXA	1	(?<=[AFGILTVM][DE]G)R	Factor XA
FORMIC	1	D	Formic acid
GLUEND	1	E	Glutamyl endopeptidase
GRANB	1	(?<=IEP)D	Granzyme B
HYDROX	1	N(?=G)	Hydroxylamine
IODOB	1	W	Iodosobenzoic acid
LYSC	1	K	Lysc

Cleave Lookup (Continued)

Code	Position	Pattern	Full Name
NTCB	1	C	NTCB
PEPS	1	((?<=[^HKR][^P])[^R](?=[FLWY][^P]))| ((?<=[^HKR][^P])[FLWY](?=\w[^P]))	Pepsin PH = 1.3
PEPS2	1	((?<=[^HKR][^P])[^R](?=[FL][^P]))| ((?<=[^HKR][^P])[FL](?=\w[^P]))	Pepsin PH > 2
PROEND	1	(?<=[HKR])P(?=[^P])	Proline endopeptidase
PROTK	1	[AEFILTVWY]	Proteinase K
STAPHP	1	(?<=[^E])E	Staphylococcal peptidase I
THERMO	1	[^DE](?=[AFILMV])	Thermolysin
THROMB	1	((?<=\w\wG)R(?=G))| ((?<=[AFGILTVM][AFGILTVWA]P)R(?=[^DE][^DE]))	Thrombin
TRYPS	1	((?<=\w)[KR](?=[^P]))| ((?<=W)K(?=P))|((?<=M)R(?=P))	Trypsin

`cleavelookup('Code', CodeValue)` displays the cleavage position, cleavage pattern, and full name of the enzyme or compound specified by *`CodeValue`*, a string specifying an abbreviation code.

`cleavelookup('Name', NameValue)` displays the cleavage position, cleavage pattern, and abbreviation code of the enzyme or compound specified by *`NameValue`*, a string specifying an enzyme or compound name.

Examples

Using cleavelookup with an Enzyme Name

Display the cleavage position, cleavage pattern, and abbreviation code of the enzyme Caspase 1.

```
cleavelookup('name', 'CASPASE 1')
```

```
ans =

1 (?<=[FWYL]\w[HAT])D(?=[^PEDQKR]) CASP1
```

Using cleavelookup with an Abbreviation Code

Display the cleavage position, cleavage pattern, and full name of the enzyme with a abbreviation code of CASP1.

```
cleavelookup('code', 'CASP1')

ans =

1 (?<=[FWYL]\w[HAT])D(?=[^PEDQKR]) CASPASE 1
```

See Also

Bioinformatics Toolbox functions: `cleave`, `rebasecuts`, `restrict`

Purpose

Validate clusters in phylogenetic tree

Syntax

```
LeafClusters = cluster(Tree, Threshold)
[LeafClusters, NodeClusters] = cluster(Tree, Threshold)
[LeafClusters, NodeClusters, Branches] = cluster(Tree,
   Threshold)
cluster(..., 'Criterion', CriterionValue, ...)
cluster(..., 'MaxClust', MaxClustValue, ...)
cluster(..., 'Distances', DistancesValue, ...)
```

Arguments

Tree	Phylogenetic tree object created, such as created with the `phytree` constructor function.
Threshold	Scalar specifying a threshold value.
CriterionValue	String specifying the criterion to determine the number of clusters as a function of the species pairwise distances. Choices are:

- `'maximum'` (default) — Maximum within cluster pairwise distance (W_{max}). Cluster splitting stops when $W_{max} \le$ *Threshold*.
- `'median'` — Median within cluster pairwise distance (W_{med}). Cluster splitting stops when $W_{med} \le$ *Threshold*.
- `'average'` — Average within cluster pairwise distance (W_{avg}). Cluster splitting stops when $W_{avg} \le$ *Threshold*.
- `'ratio'` — Between/within cluster pairwise distance ratio, defined as

  $$BW_{rat} = (\text{trace}(B)/(k - 1)) / (\text{trace}(W)/(n - k))$$

  where B and W are the between- and within-scatter matrices, respectively. k is the

number of clusters, and n is the number of species in the tree. Cluster splitting stops when $BW_{rat} \geq$ *Threshold*.

- `'gain'` — Within cluster pairwise distance gain, defined as

  $$W_{gain} = (\text{trace}(W_{old})/ (\text{trace}(W) - 1) * (n - k - 1))$$

  where W and W_{old} are the within-scatter matrices for k and k - 1, respectively. k is the number of clusters, and n is the number of species in the tree. Cluster splitting stops when $W_{gain} \leq$ *Threshold*.

- `'silhouette'` — Average silhouette width (SW_{avg}). SW_{avg} ranges from `-1` to `+1`. Cluster splitting stops when $SW_{avg} \geq$ *Threshold*. For more information, see `silhouette`.

MaxClustValue Positive integer specifying the maximum number of possible clusters for the tested partitions. Default is the number of leaves in the tree.

Tip When using the `'maximum'`, `'median'`, or `'average'` criteria, set *Threshold* to `[]` (empty) to force `cluster` to return *MaxClustValue* clusters. It does so because such metrics monotonically decrease as k increases.

Tip When using the `'ratio'`, `'gain'`, or `'silhouette'` criteria, you may find it hard to estimate an appropriate *`Threshold`* in advance. Set *`Threshold`* to `[]` (empty) to find the optimal number of clusters below *`MaxClustValue`*. Also, set *`MaxClustValue`* to a small value to avoid expensive computation due to testing all possible number of clusters.

`DistancesValue` Matrix of pairwise distances, such as returned by the `seqpdist` function, containing biological distances between each pair of sequences. `cluster` substitutes this matrix for the patristic distances in *`Tree`*. For example, this matrix can contain the real sample pairwise distances.

Return Values

`LeafClusters` Column vector containing a cluster index for each species (leaf) in *`Tree`*, a phylogenetic tree object.

`NodeClusters` Column vector containing the cluster index for each leaf node and branch node in *`Tree`*.

Tip Use the *`LeafClusters`* or *`NodeClusters`* output vectors with the handle returned by the `plot` method to modify graphic elements of the phylogenetic tree object. For more information, see "Examples" on page 3-307.

`Branches` Two-column matrix containing, for each step in the algorithm, the index of the branch being considered and the value of the criterion. Each row corresponds to a step in the algorithm. The first

column contains branch indices, and the second column contains criterion values.

Tip To obtain the whole curve of the criterion versus the number of clusters in *Branches*, set *Threshold* to [] (empty) and do not specify a *MaxClustValue*. Be aware that computation of some criteria can be computationally intensive.

Description

LeafClusters = cluster(*Tree*, *Threshold*) returns a column vector containing a cluster index for each species (leaf) in a phylogenetic tree object. It determines the optimal number of clusters as follows:

- Starting with two clusters (k = 2), selects the partition that optimizes the criterion specified by the 'Criterion' property
- Increments k by 1 and again selects the optimal partition
- Continues incrementing k and selecting the optimal partition until a criterion value = *Threshold* or k = the maximum number of clusters (that is, number of leaves)
- From all possible k values, selects the k value whose partition optimizes the criterion

[*LeafClusters*, *NodeClusters*] = cluster(*Tree*, *Threshold*) returns a column vector containing the cluster index for each leaf node and branch node in *Tree*.

[*LeafClusters*, *NodeClusters*, *Branches*] = cluster(*Tree*, *Threshold*) returns a two-column matrix containing, for each step in the algorithm, the index of the branch being considered and the value of the criterion. Each row corresponds to a step in the algorithm. The first column contains branch indices, and the second column contains criterion values.

`cluster(..., '`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `cluster` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each *`PropertyName`* in single quotation marks. Each *`PropertyName`* is case insensitive. These property name/property value pairs are as follows:.

`cluster(..., 'Criterion', `*`CriterionValue`*`, ...)` specifies the criterion to determine the number of clusters as a function of the species pairwise distances.

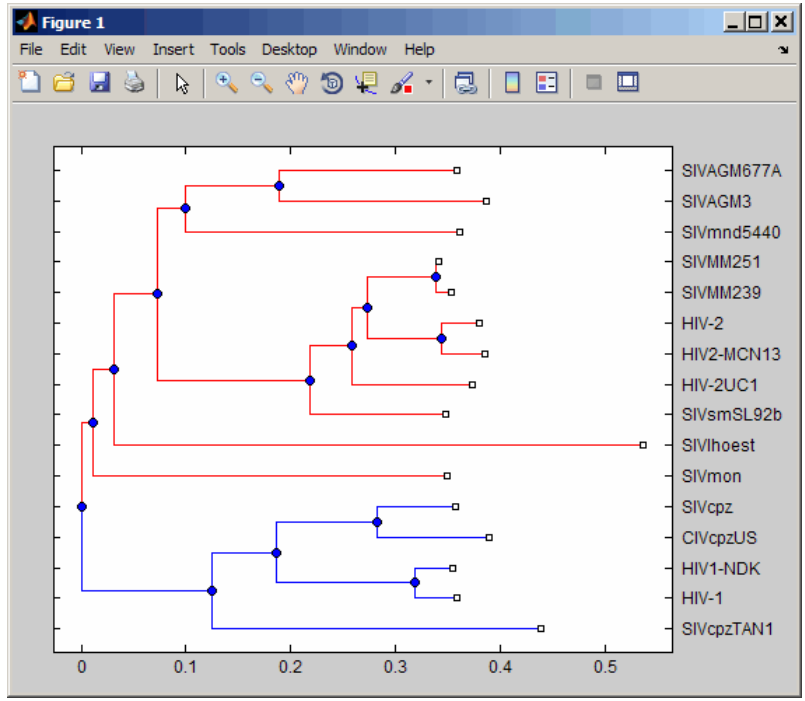
`cluster(..., 'MaxClust', `*`MaxClustValue`*`, ...)` specifies the maximum number of possible clusters for the tested partitions. Default is the number of leaves in the tree.

`cluster(..., 'Distances', `*`DistancesValue`*`, ...)` substitutes the patristic distances in *`Tree`* with a user-provided pairwise distance matrix.

Examples

Validate the clusters in a phylogenetic tree:

```
% Read sequences from a multiple alignment file into a MATLAB
% structure
gagaa = multialignread('aagag.aln');

% Build a phylogenetic tree from the sequences
gag_tree = seqneighjoin(seqpdist(gagaa),'equivar',gagaa);

% Validate the clusters in the tree and find the best partition
% using the 'gain' criterion
[i,j] = cluster(gag_tree,[],'criterion','gain','maxclust',10);

% Use the returned vector of indices to color the branches of each
% cluster in a plot of the tree
h = plot(gag_tree);
set(h.BranchLines(j==2),'Color','b')
set(h.BranchLines(j==1),'Color','r')
```



References

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[2] Theodoridis, S. and Koutroumbas, K. (1999). Pattern Recognition (Academic Press), pp. 434–435.

[3] Kaufman, L. and Rousseeuw, P.J. (1990). Finding Groups in Data: An Introduction to Cluster Analysis (New York, Wiley).

[4] Calinski, R. and Harabasz, J. (1974). A dendrite method for cluster analysis. Commun Statistics *3*, 1–27.

[5] Hartigan, J.A. (1985). Statistical theory in clustering. J Classification *2*, 63–76.

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreeread`, `phytreetool`, `seqlinkage`, `seqneighjoin`, `seqpdist`

Bioinformatics Toolbox object: phytree object

Bioinformatics Toolbox methods of phytree object: `plot`, `view`

Statistics Toolbox functions: `cluster`, `silhouette`

clustergram object

Purpose

Object containing hierarchical clustering analysis data

Description

A clustergram object contains hierarchical clustering analysis data that you can view in a heat map and dendrograms.

Create a clustergram object using the object constructor function `clustergram`. View a graphical representation of the clustergram object in a heat map and dendrograms using the `view` method.

The clustergram class is a subclass of the HeatMap class.

Method Summary

Following are methods of a clustergram object:

addTitle (clustergram)	Add title to clustergram
addXLabel (clustergram)	Label *x*-axis of clustergram
addYLabel (clustergram)	Label *y*-axis of clustergram
clusterGroup (clustergram)	Select cluster group
get (clustergram)	Retrieve information about clustergram object
plot (clustergram)	Render clustergram and dendrograms for clustergram object
set (clustergram)	Set property of clustergram object
view (clustergram)	View clustergram and dendrograms of clustergram object

Property Summary

Properties for Clustering Analysis and Clustergram Creation

Property Name	Description
`Standardize`	String or number specifying the dimension for standardizing the data values. This property transforms the standardized values so that the mean is `0` and the standard deviation is `1` in the specified dimension. Choices are: • `'column'` or `1` — Standardize along the columns of data. • `'row'` or `2` (default) — Standardize along the rows of data. • `'none'` or `3` — Do not standardize.
`Cluster`	String or number specifying the dimension for clustering the values in the data. Choices are: • `'column'` or `1` — Cluster along the columns of data only, which results in clustered rows. • `'row'` or `2` — Cluster along the rows of data only, which results in clustered columns. • `'all'` or `3` (default) — Cluster along the columns of data, then cluster along the rows of row-clustered data.

Properties for Clustering Analysis and Clustergram Creation (Continued)

Property Name	Description
`RowPDist`	String specifying the distance metric to pass to the `pdist` function (Statistics Toolbox software) to calculate the pairwise distances between rows. For information on choices, see the `pdist` function. Default is `'euclidean'`. **Note** If the distance metric requires extra arguments, then *`RowPDistValue`* is a cell array. For example, to use the Minkowski distance with exponent `P`, you would use `{'minkowski', P}`.
`ColumnPDist`	String specifying the distance metric to pass to the `pdist` function (Statistics Toolbox software) to calculate the pairwise distances between columns. For information on choices, see the `pdist` function. Default is `'euclidean'`. **Note** If the distance metric requires extra arguments, then *`ColumnPDistValue`* is a cell array. For example, to use the Minkowski distance with exponent `P`, you would use `{'minkowski', P}`.

Properties for Clustering Analysis and Clustergram Creation (Continued)

Property Name	Description
`Linkage`	String or two-element cell array of strings specifying the linkage method to pass to the `linkage` function (Statistics Toolbox software) to create the hierarchical cluster tree for rows and columns. If a two-element cell array of strings, this property uses the first element for linkage between rows, and the second element for linkage between columns. For information on choices, see the `linkage` function. Default is `'average'`.
`Dendrogram`	Scalar or two-element numeric vector or cell array of strings specifying the `'colorthreshold'` property to pass to the `dendrogram` function (Statistics Toolbox software) to create the dendrogram plot. If a two-element numeric vector or cell array, the first element is for the rows, and the second element is for the columns. For more information, see the `dendrogram` function.
`OptimalLeafOrder`	Enables or disables the optimal leaf ordering calculation, which determines the leaf order that maximizes the similarity between neighboring leaves. Choices are `true` (enable) or `false` (disable). Default depends on the size of *`Data`*, the matrix of data used to create the clustergram object. If the number of rows or columns in *`Data`* exceeds 1000, default is `false`; otherwise, default is `true`.

Properties for Clustering Analysis and Clustergram Creation (Continued)

Property Name	Description
	Tip Disabling the optimal leaf ordering calculation can be useful when working with large data sets, because this calculation consumes a lot of memory and time.
`Colormap`	Either of the following: • *M*-by-3 matrix of RGB values • Name or function handle of a function that returns a colormap, such as `redgreencmap` or `redbluecmap` Default is `redgreencmap`.
`DisplayRange`	Positive scalar specifying the display range of standardized values. Default is `3`, which means there is a color variation for values between –3 and 3, but values >3 are the same color as 3, and values < –3 are the same color as –3. For example, if you specify `redgreencmap` for the `'Colormap'` property, pure red represents values ≥ *`DisplayRangeValue`*, and pure green represents values ≤ –*`DisplayRangeValue`*.
`Symmetric`	Forces the color scale of the heat map to be symmetric around zero. Choices are `true` (default) or `false`.

Properties for Clustering Analysis and Clustergram Creation (Continued)

Property Name	Description
`LogTrans`	Controls the $\log_2$ transform of the data from natural scale. Choices are `true` or `false` (default).
`DisplayRatio`	Either of the following: • Scalar • Two-element vector This property specifies the ratio of space that the row and column dendrograms occupy relative to the heat map. If `DisplayRatio` is a scalar, it is used as the ratio for both dendrograms. If `DisplayRatio` is a two-element vector, the first element is used for the ratio of the row dendrogram width to the heat map width, and the second element is used for the ratio of the column dendrogram height to the heat map height. The second element is ignored for one-dimensional clustergrams. Default is `1/5`.

Properties for Clustering Analysis and Clustergram Creation (Continued)

Property Name	Description
`ImputeFun`	One of the following: • Name of a function that imputes missing data. • Handle to a function that imputes missing data. • Cell array where the first element is the name of or handle to a function that imputes missing data. The remaining elements are property name/property value pairs used as inputs to the function.
`ShowDendrogram`	Shows and hides the dendrogram tree diagrams with the clustergram. Choices are `'on'` (default) or `'off'`. **Tip** After displaying a clustergram in a Clustergram window, click the Show Dendrogram  button on the toolbar to show and hide the dendrograms.

Properties for Group Labels

Property Name	Description
`RowGroupMarker`	Structure or structure array containing information for annotating the groups (clusters) of rows determined by the `clustergram` function. The structure or structures contain the following fields. If a single structure, then the fields contain a cell array of elements. If a structure array, then the fields contain one element: • `GroupNumber` — Scalar specifying the row group number to annotate. • `Annotation` — String specifying text to annotate the row group. • `Color` — String or three-element vector of RGB values specifying a color to label the row group. For more information on specifying colors, see `ColorSpec`. If this field is empty, default is `'blue'`.
`ColumnGroupMarker`	Structure or structure array containing information for annotating the groups (clusters) of columns determined by the `clustergram` function. The structure or structures contain the following fields. If a single structure, then the fields contain a cell array of elements. If a structure array, then the fields contain one element: • `GroupNumber` — Scalar specifying the column group number to annotate. • `Annotation` — String specifying text to annotate the column group.

Properties for Group Labels (Continued)

Property Name	Description
	• `Color` — String or three-element vector of RGB values specifying a color to label the column group. For more information on specifying colors, see `ColorSpec`. If this field is empty, default is `'blue'`.

Properties for Row and Column Labels

Property Name	Description
`RowLabels`	Vector of numbers or cell array of text strings to label the rows in the dendrogram and heat map. Default is a vector of values `1` through *M*, where *M* is the number of rows in *`Data`*, the matrix of data used by the `clustergram` function to create the clustergram object.
`ColumnLabels`	Vector of numbers or cell array of text strings to label the columns in the dendrogram and heat map. Default is a vector of values `1` through *M*, where *M* is the number of columns in *`Data`*, the matrix of data used by the `clustergram` function to create the clustergram object.
`ColumnLabelsLocation`	Read-only string specifying the location of the column labels. For clustergram objects, it is always `'bottom'` (default).
`RowLabelsLocation`	Read-only string specifying the location of the row labels. For clustergram objects, it is always `'right'` (default).

Properties for Row and Column Labels (Continued)

Property Name	Description
`RowLabelsColor`	Structure or structure array containing color information for labeling the rows (*y*-axis) of the clustergram. The structure or structures contain the following fields. If a single structure, then the fields contain a cell array of elements. If a structure array, then the fields contain one element: • `Labels` — String specifying a row label listed in the `RowLabels` vector. • `Colors` — String or three-element vector of RGB values specifying a color for the row label specified in the `Labels` field. For more information on specifying colors, see `ColorSpec`. If this field is empty, default colors are assigned to the row label.
`ColumnLabelsColor`	Structure or structure array containing color information for labeling the columns (*x*-axis) of the clustergram. The structure or structures contain the following fields. If a single structure, then the fields contain a cell array of elements. If a structure array, then the fields contain one element: • `Labels` — String specifying a column label listed in the `ColumnLabels` vector. • `Colors` — String or three-element vector of RGB values specifying a color for the column label specified in the `Labels` field. For more information on specifying colors,

Properties for Row and Column Labels (Continued)

Property Name	Description
	see `ColorSpec`. If this field is empty, default colors are assigned to the column label.
`LabelsWithMarkers`	Controls the display of colored markers instead of colored text for the row labels and column labels. Choices are `true` or `false` (default).
`RowLabelsRotate`	Numeric value in degrees rotation specifying the orientation of row (*y*-axis) labels. Default is `0` degrees, which is horizontal. Positive values cause counterclockwise rotation.
`ColumnLabelsRotate`	Numeric value in degrees rotation specifying the orientation of column (*x*-axis) labels. Default is `90` degrees, which is vertical. Values greater than `90` degrees cause counterclockwise rotation.

Properties for Annotating Data

Property Name	Description
`Annotate`	Controls the display of intensity values on each area of the heat map. Choices are `true` or `false` (default). **Tip** After displaying a clustergram in a Clustergram window, click the Annotate  button on the toolbar to show and hide the intensity values.

Properties for Annotating Data (Continued)

Property Name	Description
`AnnotPrecision`	Positive integer specifying the precision of the intensity values when displayed on the heat map. Default is `2`.
`AnnotColor`	String or three-element vector of RGB values specifying a color, which is used for the text of the intensity values when displayed on the heat map. Default is `'white'`. For more information on specifying colors, see `ColorSpec`.

Examples

Note The following examples use the `get` and `set` methods with property names and values of a clustergram object. When supplying a *`PropertyName`*, be aware that it is case sensitive.

Determining Properties and Property Values of a Clustergram Object

Display all properties and their current values of a clustergram object, *`CGobj`*:

```
get(CGobj)
```

Return all properties and their current values of *`CGobj`*, a clustergram object, to *`CGstruct`*, a scalar structure, in which each field name is a property of a clustergram object, and each field contains the value of that property:

```
CGstruct = get(CGobj)
```

Return the value of a specific property of a clustergram object, *`CGobj`*, using either:

```
PropertyValue = get(CGobj, 'PropertyName')
```

```
PropertyValue = CGobj.PropertyName
```

Return the value of specific properties of a clustergram object, *CGobj*:

```
[Property1Value, Property2Value, ...] = get(CGobj, ...
'Property1Name', 'Property2Name', ...)
```

Determining Possible Values of Clustergram Object Properties

Display possible values for all properties that have a fixed set of property values in a clustergram object, *CGobj*:

```
set(CGobj)
```

Display possible values for a specific property that has a fixed set of property values in a clustergram object, *CGobj*:

```
set(CGobj,  'PropertyName')
```

Specifying Properties of a Clustergram Object

Set a specific property of a clustergram object, *CGobj*, using either:

```
set(CGobj, 'PropertyName', PropertyValue)
```

```
CGobj.PropertyName = PropertyValue
```

Set multiple properties of a clustergram object, *CGobj*:

```
set(CGobj,  'Property1Name', Property1Value, ...
    'Property2Name', Property2Value, ...)
```

See Also

Bioinformatics Toolbox function: `clustergram` (object constructor)

Bioinformatics Toolbox methods of a clustergram object: `addTitle`, `addXLabel`, `addYLabel`, `clusterGroup`, `get`, `plot`, `set`, `view`

MATLAB function: `display`

Bioinformatics Toolbox object: HeatMap object

Purpose

Compute hierarchical clustering, display dendrogram and heat map, and create clustergram object

Syntax

```
CGobj = clustergram(Data)
CGobj = clustergram(Data, ...'RowLabels',
RowLabelsValue, ...)
CGobj = clustergram(Data, ...'ColumnLabels',
   ColumnLabelsValue, ...)
CGobj = clustergram(Data, ...'Standardize',
StandardizeValue,
   ...)
CGobj = clustergram(Data, ...'Cluster', ClusterValue, ...)
CGobj = clustergram(Data, ...'RowPDist',
RowPDistValue, ...)
CGobj = clustergram(Data, ...'ColumnPDist',
ColumnPDistValue,
   ...)
CGobj = clustergram(Data, ...'Linkage', LinkageValue, ...)
CGobj = clustergram(Data, ...'Dendrogram', DendrogramValue,
   ...)
CGobj = clustergram(Data, ...'OptimalLeafOrder',
   OptimalLeafOrderValue, ...)
CGobj = clustergram(Data, ...'Colormap',
ColormapValue, ...)
CGobj = clustergram(Data, ...'DisplayRange',
   DisplayRangeValue, ...)
CGobj = clustergram(Data, ...'Symmetric', SymmetricValue,
   ...)
CGobj = clustergram(Data, ...'LogTrans',
LogTransValue, ...)
CGobj = clustergram(Data, ...'DisplayRatio',
   DisplayRatioValue, ...)
CGobj = clustergram(Data, ...'ImputeFun', ImputeFunValue,
   ...)
CGobj = clustergram(Data, ...'RowGroupMarker',
   RowGroupMarkerValue, ...)
CGobj = clustergram(Data, ...'ColumnGroupMarker',
```

```
   ColumnGroupMarkerValue, ...)
CGobj = clustergram(Data, ...'ShowDendrogram',
   ShowDendrogramValue, ...)
```

Arguments

Data	DataMatrix object or numeric matrix of data. If the matrix contains gene expression data, typically each row corresponds to a gene and each column corresponds to a sample.
RowLabelsValue	Vector of numbers or cell array of text strings to label the rows in the dendrogram and heat map. Default is a vector of values `1` through *M*, where *M* is the number of rows in *Data*.
ColumnLabelsValue	Vector of numbers or cell array of text strings to label the columns in the dendrogram and heat map. Default is a vector of values `1` through *N*, where *N* is the number of columns in *Data*.
StandardizeValue	String or number specifying the dimension for standardizing the values in *Data*. The `clustergram` function transforms the standardized values so that the mean is `0` and the standard deviation is `1` in the specified dimension. Choices are: • `'column'` or `1` — Standardize along the columns of data. • `'row'` or `2` (default) — Standardize along the rows of data. • `'none'` or `3` — Do not standardize.

ClusterValue

String or number specifying the dimension for clustering the values in *Data*. Choices are:

- `'column'` or `1` — Cluster along the columns of data only, which results in clustered rows.
- `'row'` or `2` — Cluster along the rows of data only, which results in clustered columns.
- `'all'` or `3` (default) — Cluster along the columns of data, then cluster along the rows of row-clustered data.

RowPDistValue

String, function handle, or cell array specifying the distance metric to pass to the `pdist` function (Statistics Toolbox software) to calculate the pairwise distances between rows. For information on choices, see the `pdist` function. Default is `'euclidean'`.

Note If the distance metric requires extra arguments, then *RowistValue* is a cell array. For example, to use the Minkowski distance with exponent `P`, you would use `{'minkowski', P}`.

ColumnPDistValue

String, function handle, or cell array specifying the distance metric to pass to the `pdist` function (Statistics Toolbox software) to use to calculate the pairwise distances between columns. For information on choices, see the `pdist` function. Default is `'euclidean'`.

Note If the distance metric requires extra arguments, then *ColumnPDistValue* is a cell array. For example, to use the Minkowski distance with exponent `P`, you would use `{'minkowski', P}`.

LinkageValue

String or two-element cell array of strings specifying the linkage method to pass to the `linkage` function (Statistics Toolbox software) to create the hierarchical cluster tree for rows and columns. If a two-element cell array of strings, the `clustergram` function uses the first element for linkage between rows, and the second element for linkage between columns. For information on choices, see the `linkage` function. Default is `'average'`.

Tip To specify the linkage method for only one dimension, set the other dimension to `''`.

DendrogramValue

Scalar or two-element numeric vector or cell array of strings specifying the `'colorthreshold'` property to pass to the `dendrogram` function (Statistics Toolbox software) to create the dendrogram plot. If a two-element numeric vector or cell array, the first element is for the rows, and the second element is for the columns. For more information, see the `dendrogram` function.

Tip To specify the `'colorthreshold'` property for only one dimension, set the other dimension to `''`.

OptimalLeafOrderValue

Enables or disables the optimal leaf ordering calculation, which determines the leaf order that maximizes the similarity between neighboring leaves. Choices are `true` (enable) or `false` (disable). Default depends on the size of *`Data`*. If the number of rows or columns in *`Data`* exceeds 1000, default is `false`; otherwise, default is `true`.

Note Disabling the optimal leaf ordering calculation can be useful when working with large data sets, because this calculation consumes a lot of memory and time.

ColormapValue	Either of the following: • *M*-by-3 matrix of RGB values • Name of or handle to a function that returns a colormap, such as `redgreencmap` or `redbluecmap` Default is `redgreencmap`, in which red represents values above the mean, black represents the mean, and green represents values below the mean of a row (gene) across all columns (samples).
DisplayRangeValue	Positive scalar that specifies the display range of standardized values. Default is `3`, which means there is a color variation for values between –3 and 3, but values >3 are the same color as 3, and values < –3 are the same color as –3. For example, if you specify `redgreencmap` for the `'Colormap'` property, pure red represents values ≥ *DisplayRangeValue*, and pure green represents values ≤ –*DisplayRangeValue*.
SymmetricValue	Forces the color scale of the heat map to be symmetric around zero. Choices are `true` (default) or `false`.
LogTransValue	Controls the $\log_2$ transform of *Data* from natural scale. Choices are `true` or `false` (default).

DisplayRatioValue

Either of the following:

- Scalar
- Two-element vector

This property specifies the ratio of space that the row and column dendrograms occupy relative to the heat map. If *DisplayRatioValue* is a scalar, the `clustergram` function uses it as the ratio for both dendrograms. If *DisplayRatioValue* is a two-element vector, the `clustergram` function uses the first element for the ratio of the row dendrogram width to the heat map width, and the second element for the ratio of the column dendrogram height to the heat map height. The `clustergram` function ignores the second element for one-dimensional clustergrams. Default is `1/5`.

ImputeFunValue

One of the following:

- Name of a function that imputes missing data.
- Handle to a function that imputes missing data.
- Cell array where the first element is the name of or handle to a function that imputes missing data. The remaining elements are property name/property value pairs used as inputs to the function.

Caution If data points are missing, use the `'ImputeFun'` property. Otherwise, the `clustergram` function errors.

`RowGroupMarkerValue`

Structure or structure array containing information for annotating the groups (clusters) of rows determined by the `clustergram` function. The structure or structures contain the following fields. If a single structure, then the fields contain a cell array of elements. If a structure array, then the fields contain a single element.

- `GroupNumber` — Scalar specifying the row group number to annotate.
- `Annotation` — String specifying text to annotate the row group.
- `Color` — String or three-element vector of RGB values specifying a color, which the `clustergram` function uses to label the row group. For more information on specifying colors, see `ColorSpec`. If this field is empty, default is `'blue'`.

ColumnGroupMarkerValue Structure or structure array containing information for annotating the groups (clusters) of columns determined by the `clustergram` function. The structure or structures contain the following fields. If a single structure, then the fields contain a cell array of elements. If a structure array, then the fields contain a single element.

- `GroupNumber` — Scalar specifying the column group number to annotate.
- `Annotation` — String specifying text to annotate the column group.
- `Color` — String or three-element vector of RGB values specifying a color, which the `clustergram` function uses to label the column group. For more information on specifying colors, see `ColorSpec`. If this field is empty, default is `'blue'`.

ShowDendrogramValue String controlling the display of dendrogram tree diagrams with the clustergram. Choices are `'on'` (default) or `'off'`.

Tip After displaying a clustergram in a Clustergram window, click the Show Dendrogram  button on the toolbar to show and hide the dendrograms.

Description

CGobj = clustergram(*Data*) performs hierarchical clustering analysis on the values in *Data*, a DataMatrix object or numeric matrix. It creates *CGobj*, an object containing the analysis data, and displays a dendrogram and heat map. It uses hierarchical clustering with Euclidean distance metric and average linkage to generate the hierarchical tree. It clusters first along the columns (producing row-clustered data), and then along the rows in the matrix *Data*. If *Data* contains gene expression data, typically the rows correspond to genes and the columns correspond to samples.

CGobj = clustergram(*Data*, ...'*PropertyName*', *PropertyValue*, ...) calls clustergram with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each *PropertyName* in single quotation marks. Each *PropertyName* is case insensitive. These property name/property value pairs are as follows:

CGobj = clustergram(*Data*, ...'RowLabels', *RowLabelsValue*, ...) uses the contents of *RowLabelsValue*, a vector of numbers or cell array of text strings, as labels for the rows in the dendrogram and heat map. Default is a vector of values 1 through *M*, where *M* is the number of rows in *Data*.

CGobj = clustergram(*Data*, ...'ColumnLabels', *ColumnLabelsValue*, ...) uses the contents of *ColumnLabelsValue*, a vector of numbers or cell array of text strings, as labels for the columns in the dendrogram and heat map. Default is a vector of values 1 through *M*, where *M* is the number of columns in *Data*.

CGobj = clustergram(*Data*, ...'Standardize', *StandardizeValue*, ...) specifies the dimension for standardizing the values in *Data*. The clustergram function transforms the standardized values so that the mean is 0 and the standard deviation is 1 in the specified dimension. *StandardizeValue* can be:

- 'column' or 1 — Standardize along the columns of data.
- 'row' or 2 (default) — Standardize along the rows of data.
- 'none' or 3 — Do not standardize.

CGobj = clustergram(*Data*, ...'Cluster', *ClusterValue*, ...) specifies the dimension for clustering the values in *Data*. *ClusterValue* can be:

- 'column' or 1 — Cluster along the columns of data only, which results in clustered rows.
- 'row' or 2 — Cluster along the rows of data only, which results in clustered columns.
- 'all' or 3 (default) — Cluster along the columns of data, then cluster along the rows of row-clustered data.

CGobj = clustergram(*Data*, ...'RowPDist', *RowPDistValue*, ...) specifies the distance metric to pass to the pdist function (Statistics Toolbox software) to use to calculate the pairwise distances between rows. *RowPDistValue* is a string, function handle, or cell array. For information on choices, see the pdist function. Default is 'euclidean'.

CGobj = clustergram(*Data*, ...'ColumnPDist', *ColumnPDistValue*, ...) specifies the distance metric to pass to the pdist function (Statistics Toolbox software) to use to calculate the pairwise distances between columns. *ColumnPDistValue* is a string, function handle, or cell array. For information on choices, see the pdist function. Default is 'euclidean'.

Note If the distance metric requires extra arguments, then *RowPDistValue* or *ColumnPDistValue* is a cell array. For example, to use the Minkowski distance with exponent P, you would use {'minkowski', P}.

CGobj = clustergram(*Data*, ...'Linkage', *LinkageValue*, ...) specifies the linkage method to pass to the linkage function (Statistics Toolbox software) to use to create the hierarchical cluster tree for rows and columns. *LinkageValue* is a string or two-element cell array of

strings. If a two-element cell array of strings, the `clustergram` function uses first element for linkage between rows, and the second element for linkage between columns. For information on choices, see the `linkage` function. Default is `'average'`.

Tip To specify the linkage method for only one dimension, set the other dimension to `''`.

CGobj = clustergram(*Data*, ...'Dendrogram', *DendrogramValue*, ...) specifies the `'colorthreshold'` property to pass to the `dendrogram` function (Statistics Toolbox software) to create the dendrogram plot. *DendrogramValue* is a scalar or two-element numeric vector or cell array of strings that specifies the `'colorthreshold'` property. If a two-element numeric vector or cell array, the first element is for the rows, and the second element is for the columns. For more information, see the `dendrogram` function.

Tip To specify the `'colorthreshold'` property for only one dimension, set the other dimension to `''`.

CGobj = clustergram(*Data*, ...'OptimalLeafOrder', *OptimalLeafOrderValue*, ...) enables or disables the optimal leaf ordering calculation, which determines the leaf order that maximizes the similarity between neighboring leaves. Choices are `true` (enable) or `false` (disable). Default depends on the size of *Data*. If the number of rows or columns in *Data* exceeds 1000, default is `false`; otherwise, default is `true`.

Tip Disabling the optimal leaf ordering calculation can be useful when working with large data sets, because this calculation consumes a lot of memory and time.

CGobj = clustergram(*Data*, ...'Colormap', *ColormapValue*, ...) specifies the colormap to use to create the clustergram. The colormap controls the colors used to display the heat map. *ColormapValue* is either an *M*-by-3 matrix of RGB values or the name of or handle to a function that returns a colormap, such as redgreencmap or redbluecmap. Default is redgreencmap.

Note In redgreencmap, red represents values above the mean, black represents the mean, and green represents values below the mean of a row (gene) across all columns (samples). In redbluecmap, red represents values above the mean, white represents the mean, and blue represents values below the mean of a row (gene) across all columns (samples).

CGobj = clustergram(*Data*, ...'DisplayRange', *DisplayRangeValue*, ...) specifies the display range of standardized values. *DisplayRangeValue* must be a positive scalar. Default is 3, which means there is a color variation for values between –3 and 3, but values >3 are the same color as 3, and values < –3 are the same color as –3.

For example, if you specify redgreencmap for the 'Colormap' property, pure red represents values ≥ *DisplayRangeValue*, and pure green represents values ≤ –*DisplayRangeValue*.

CGobj = clustergram(*Data*, ...'Symmetric', *SymmetricValue*, ...) controls whether the color scale of the heat map is symmetric around zero. *SymmetricValue* can be true (default) or false.

CGobj = clustergram(*Data*, ...'LogTrans', *LogTransValue*, ...) controls the $\log_2$ transform of *Data* from natural scale. Choices are true or false (default).

CGobj = clustergram(*Data*, ...'DisplayRatio', *DisplayRatioValue*, ...) specifies the ratio of space that the row and column dendrograms occupy relative to the heat map. If *DisplayRatioValue* is a scalar, the clustergram function uses it as the ratio for both dendrograms. If *DisplayRatioValue* is a two-element

vector, the `clustergram` function uses the first element for the ratio of the row dendrogram width to the heat map width, and the second element for the ratio of the column dendrogram height to the heat map height. The `clustergram` function ignores the second element for one-dimensional clustergrams. Default is `1/5`.

`CGobj` `= clustergram(`*`Data`*`, ...'ImputeFun', `*`ImputeFunValue`*`, ...)` specifies a function and optional inputs that impute missing data. *`ImputeFunValue`* can be any of the following:

- Name of a function that imputes missing data.
- Handle to a function that imputes missing data.
- Cell array where the first element is the name of or handle to a function that imputes missing data. The remaining elements are property name/property value pairs used as inputs to the function.

Tip If data points are missing, use the `'ImputeFun'` property. Otherwise, the `clustergram` function errors.

`CGobj` `= clustergram(`*`Data`*`, ...'RowGroupMarker', `*`RowGroupMarkerValue`*`, ...)` specifies a structure or structure array containing information for annotating the groups (clusters) of rows determined by the `clustergram` function.

`CGobj` `= clustergram(`*`Data`*`, ...'ColumnGroupMarker', `*`ColumnGroupMarkerValue`*`, ...)` specifies a structure or structure array containing information for annotating the groups of columns determined by the `clustergram` function.

Tip If necessary, view row labels (right) and column labels (bottom) by clicking the Zoom In  button on the toolbar to zoom the clustergram.

CGobj = clustergram(*Data*, ...'ShowDendrogram', *ShowDendrogramValue*, ...) controls the display of dendrogram tree diagrams with the clustergram. Choices are 'on' (default) or 'off'.

Examples

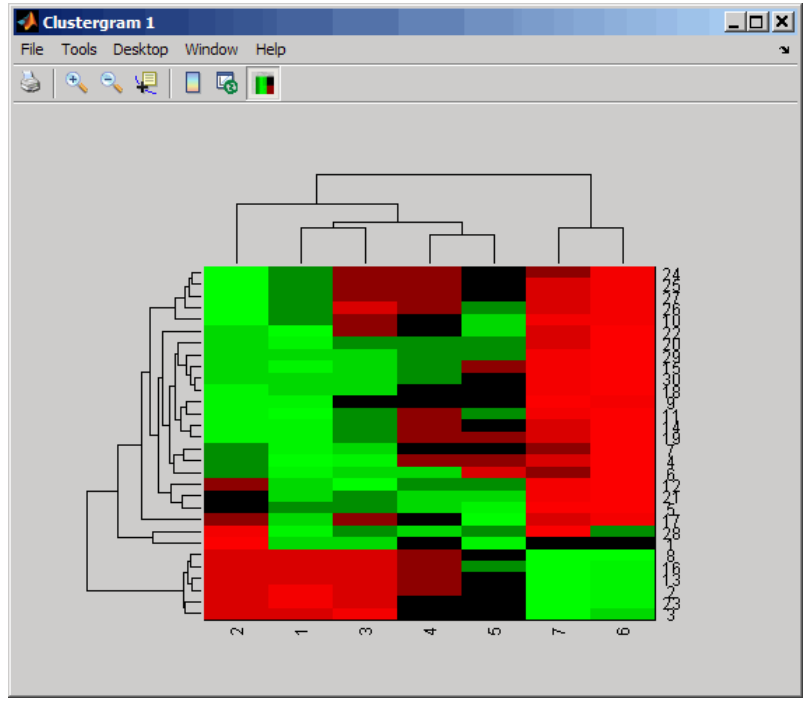
The following example uses data from an experiment (DeRisi et al., 1997) that used DNA microarrays to study temporal gene expression of almost all genes in *Saccharomyces cerevisiae* during the metabolic shift from fermentation to respiration. Expression levels were measured at seven time points during the diauxic shift.

1. Load the MAT-file, provided with the Bioinformatics Toolbox software, that contains filtered yeast data. This MAT-file includes three variables: yeastvalues, a matrix of gene expression data, genes, a cell array of GenBank accession numbers for labeling the rows in yeastvalues, and times, a vector of time values for labeling the columns in yeastvalues.

   ```
   load filteredyeastdata
   ```

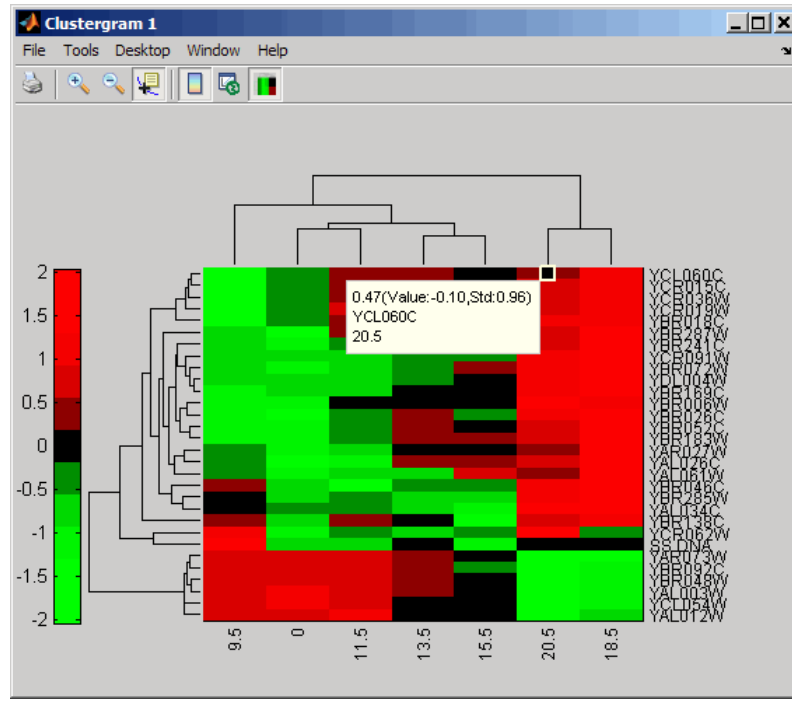
2. Create a clustergram object and display the dendrograms and heat map from the gene expression data in the first 30 rows of the yeastvalues matrix.

   ```
   cgo = clustergram(yeastvalues(1:30,:))
   Clustergram object with 30 rows of nodes and 7 columns of nodes.
   ```



3 Use the `set` method and the `genes` and `times` vectors to add meaningful row and column labels to the clustergram.

```
set(cgo,'RowLabels',genes(1:30),'ColumnLabels',times)
```



4 Add a color bar to the clustergram by clicking the Insert Colorbar button on the toolbar.

5 View a data tip containing the intensity value, row label, and column label for a specific area of the heat map by clicking the Data Cursor button on the toolbar, then clicking an area in the heat map. To delete this data tip, right-click it, then select **Delete Current Datatip**.

6 Display intensity values for each area of the heat map by clicking the Annotate button on the toolbar. Click the Annotate button again to remove the intensity values.

Tip If the amount of data is large enough, the cells within the clustergram are too small to display the intensity annotations. Zoom the clustergram to see the intensity annotations.

7 Remove the dendrogram tree diagrams from the figure by clicking the Show Dendrogram  button on the toolbar. Click the Show Dendrogram button again to display the dendrograms.

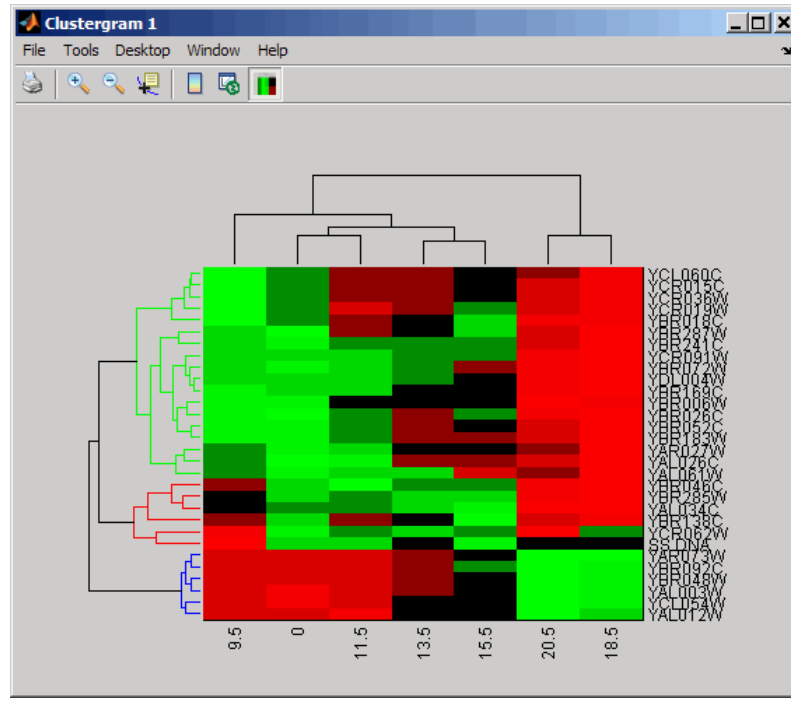
8 Use the `get` method to display the properties of the clustergram object, `cgo`:

```
get(cgo)

                Cluster: 'ALL'
              RowPDist: {'Euclidean'}
           ColumnPDist: {'Euclidean'}
               Linkage: {'Average'}
            Dendrogram: {}
      OptimalLeafOrder: 1
              LogTrans: 0
          DisplayRatio: [0.2000 0.2000]
         RowGroupMarker: []
      ColumnGroupMarker: []
        ShowDendrogram: 'on'
          ColumnLabels: {' 9.5'  '   0'  '11.5'  '13.5'  '15.5'  '20.5'  '18.5'}
             RowLabels: {30x1 cell}
    ColumnLabelsRotate: 90
       RowLabelsRotate: 0
 ColumnLabelsLocation: 'bottom'
    RowLabelsLocation: 'right'
          Standardize: 'ROW'
            Symmetric: 1
         DisplayRange: 3
             Colormap: [11x3 double]
            ImputeFun: []
```

```
              Annotate: 'off'
         AnnotPrecision: 2
             AnnotColor: 'w'
       ColumnLabelsColor: []
          RowLabelsColor: []
       LabelsWithMarkers: 0
```

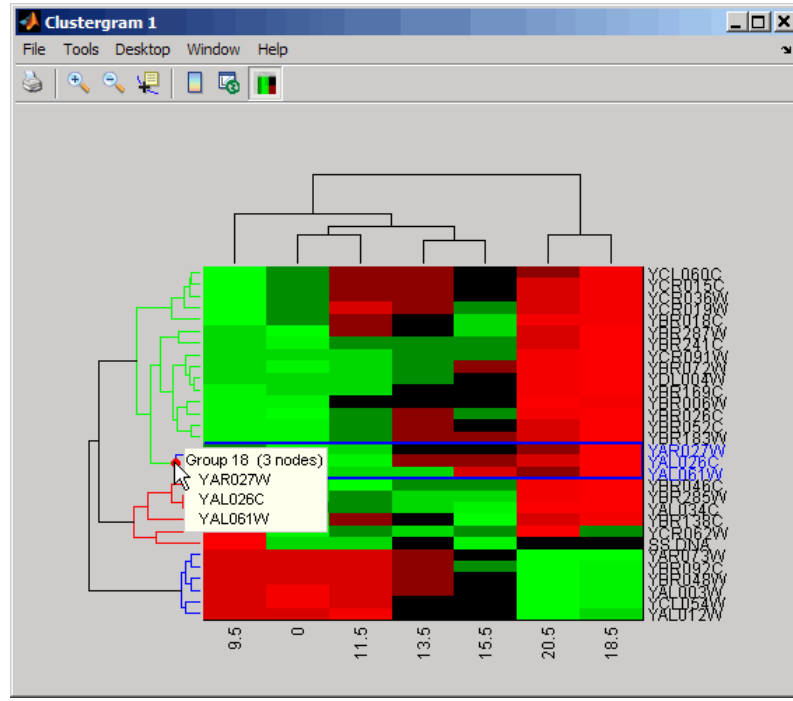
9 Change the clustering parameters by changing the linkage method and changing the color of the groups of nodes in the dendrogram whose linkage is less than a threshold of 3.

```
set(cgo,'Linkage','complete','Dendrogram',3)
```

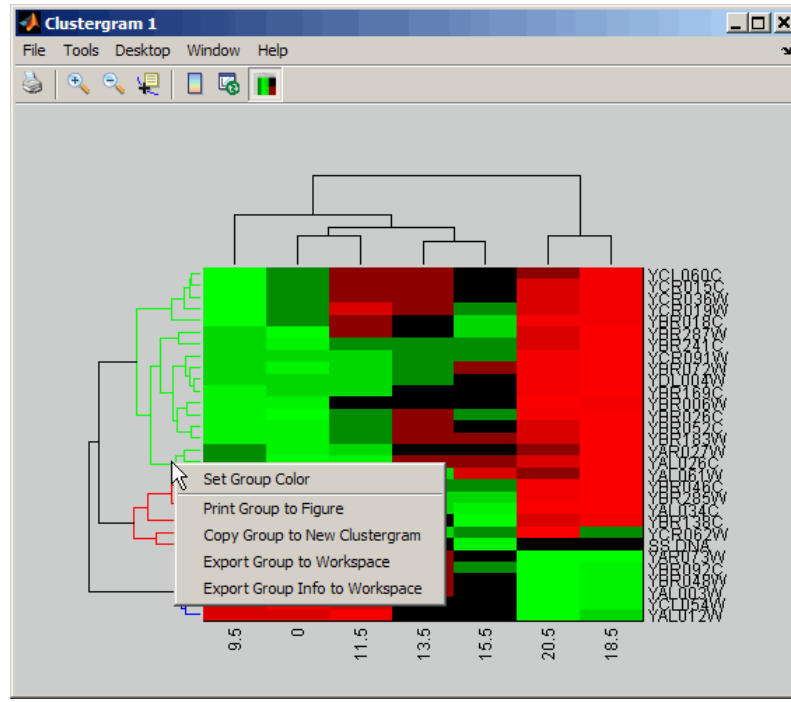


10 Place the cursor on a branch node in the dendrogram to highlight (in blue) the group associated with it. Press and hold the mouse button

to display a data tip listing the group number and the nodes (genes or samples) in the group.



11 Right-click a branch node in the dendrogram to display a menu of options.



The following options are available:

- **Set Group Color** — Change the cluster group color.
- **Print Group to Figure** — Print the group to a Figure window.
- **Copy Group to New Clustergram** — Copy the group to a new Clustergram window.
- **Export Group to Workspace** — Create a clustergram object of the group in the MATLAB Workspace.
- **Export Group Info to Workspace** — Create a structure containing information about the group in the MATLAB Workspace. The structure contains these fields:

- `GroupNames` — Cell array of text strings containing the names of the row or column groups.
- `RowNodeNames` — Cell array of text strings containing the names of the row nodes.
- `ColumnNodeNames` — Cell array of text strings containing the names of the column nodes.
- `ExprValues` — An *M*-by-*N* matrix of intensity values, where *M* and *N* are the number of row nodes and of column nodes respectively. If the matrix contains gene expression data, typically each row corresponds to a gene and each column corresponds to sample.

12 Create a clustergram object in the MATLAB Workspace of Group 18 by right-clicking it, then selecting **Export Group to Workspace**. In the Export to Workspace dialog box, type **Group18**, then click **OK**.

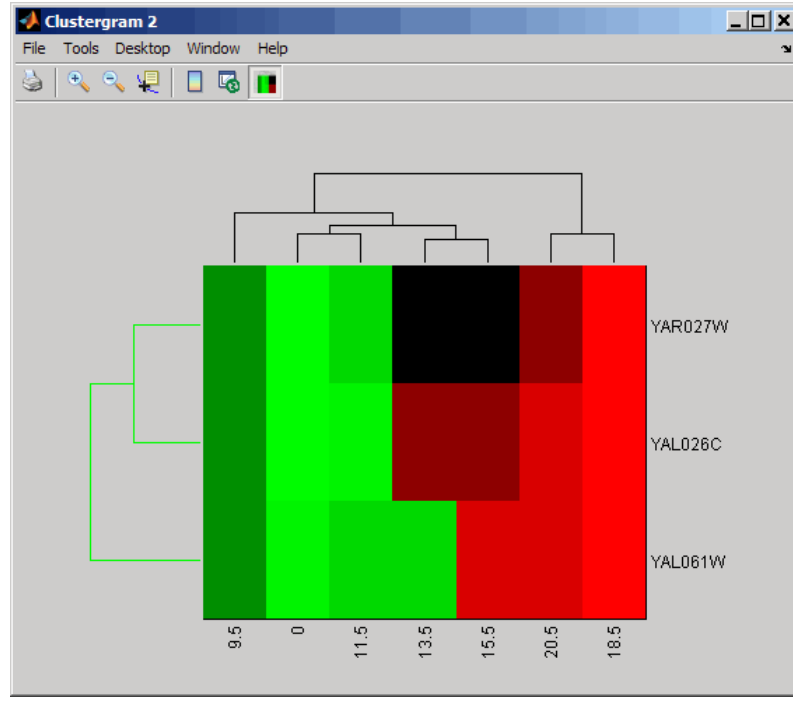
13 Use the `get` method to display the properties of the clustergram object, `Group18`.

```
get(Group18)

                Cluster: 'ALL'
              RowPDist: {'Euclidean'}
           ColumnPDist: {'Euclidean'}
               Linkage: 'complete'
            Dendrogram: 3
      OptimalLeafOrder: 1
              LogTrans: 0
          DisplayRatio: [0.2000 0.2000]
        RowGroupMarker: []
     ColumnGroupMarker: []
        ShowDendrogram: 'on'
          ColumnLabels: {' 9.5'  '   0'  '11.5'  '13.5'  '15.5'  '20.5'  '18.5'}
             RowLabels: {3x1 cell}
    ColumnLabelsRotate: 90
       RowLabelsRotate: 0
```

```
ColumnLabelsLocation: 'bottom'
   RowLabelsLocation: 'right'
         Standardize: 'ROW'
           Symmetric: 1
        DisplayRange: 3
            Colormap: [11x3 double]
           ImputeFun: []
            Annotate: 'off'
      AnnotPrecision: 2
          AnnotColor: 'w'
   ColumnLabelsColor: []
      RowLabelsColor: []
   LabelsWithMarkers: 0
```

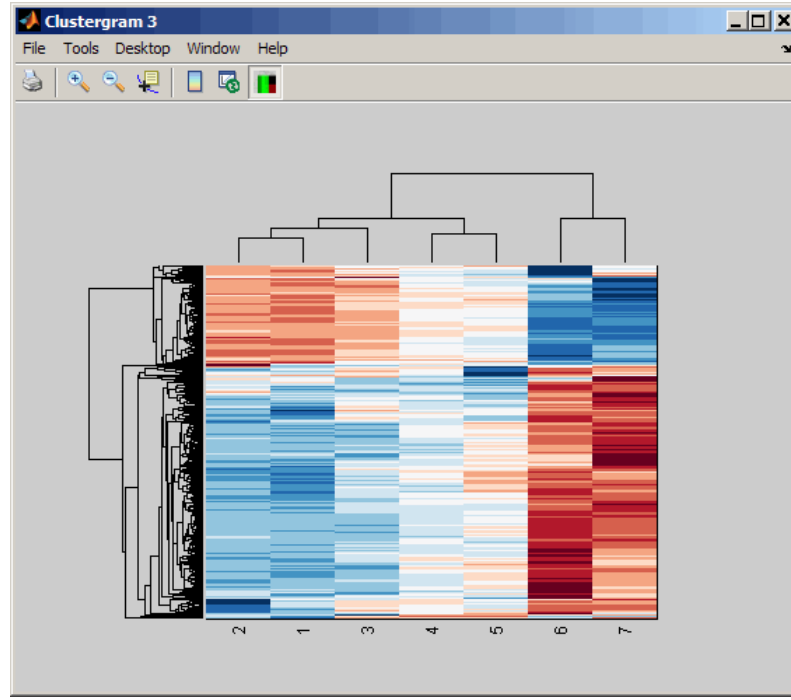
14 Use the `view` method to view the clustergram (dendrograms and heat map) of the clustergram object, `Group18`.

```
view(Group18)
```



15 View all the gene expression data using a diverging red and blue colormap.

```
cgo_all = clustergram(yeastvalues,'Colormap',redbluecmap)
Clustergram object with 614 rows of nodes and 7 columns of nodes.
```

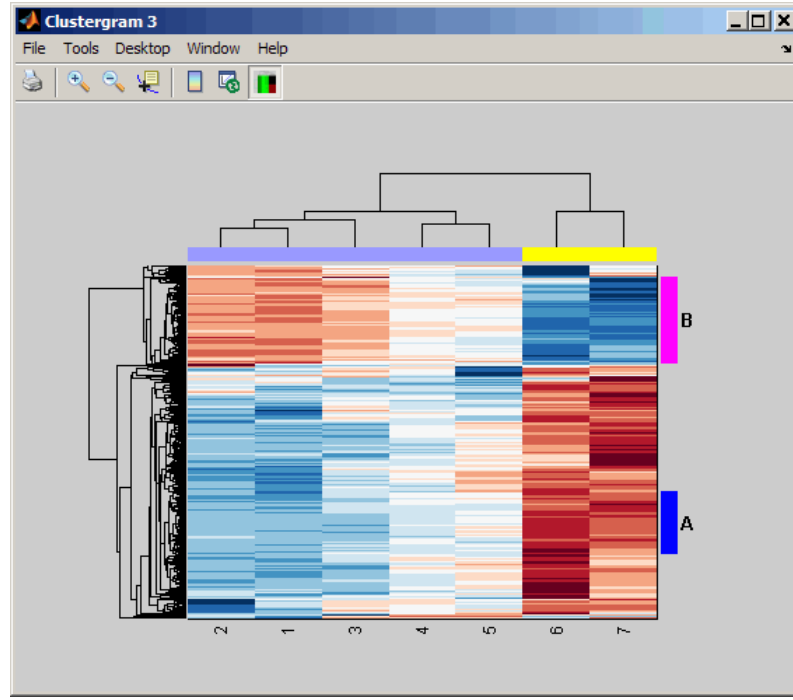


16 Create structure arrays to specify marker colors and annotations for two groups of rows (510 and 593) and two groups of columns (4 and 5).

```
rm = struct('GroupNumber',{510,593},'Annotation',{'A','B'},...
     'Color',{'b','m'});
cm = struct('GroupNumber',{4,5},'Annotation',{'Time1','Time2'},..
     'Color',{[1 1 0],[0.6 0.6 1]});
```

17 Use the `'RowGroupMarker'` and `'ColumnGroupMarker'` properties to add the color markers and annotations to the clustergram.

```
set(cgo_all,'RowGroupMarker',rm,'ColumnGroupMarker',cm)
```



18 Click the color column markers to display the annotations.

References

[1] Bar-Joseph, Z., Gifford, D.K., and Jaakkola, T.S. (2001). Fast optimal leaf ordering for hierarchical clustering. Bioinformatics *17*, Suppl 1:S22 – 9. PMID: 11472989.

[2] Eisen, M.B., Spellman, P.T., Brown, P.O., and Botstein, D. (1998). Cluster analysis and display of genome-wide expression patterns. Proc Natl Acad Sci USA *95*, 14863–8.

[3] DeRisi, J.L., Iyer, V.R., and Brown, P.O. (1997). Exploring the metabolic and genetic control of gene expression on a genomic scale. Science *278*, 680–686s.

[4] Golub, T.R., Slonim, D.K., and Tamayo, P., et al. (1999). Molecular classification of cancer: class discovery and class prediction by gene expression monitoring. Science *286 (15)*, 531–537.

See Also

Bioinformatics Toolbox functions: `redbluecmap`, `redgreencmap`

Bioinformatics Toolbox object: clustergram object

Bioinformatics Toolbox methods of a clustergram object: `addTitle`, `addXLabel`, `addYLabel`, `clustergroup`, `get`, `plot`, `set`, `view`

Statistics Toolbox functions: `cluster`, `dendrogram`, `linkage`, `pdist`

clusterGroup (clustergram)

Purpose

Select cluster group

Syntax

```
clusterGroup(CGobj1, GroupIndex, Dim)
CGobj2 = clusterGroup(CGobj1, GroupIndex, Dim)
CGStruct = clusterGroup(CGobj1, GroupIndex,
Dim, 'InfoOnly',
   InfoOnlyValue)
CGStruct = clusterGroup(CGobj1, GroupIndex, Dim, 'Color',
   ColorValue)
```

Arguments

CGobj1	Clustergram object created with the function `clustergram`.
GroupIndex	Positive integer specifying a group index for a cluster in *CGobj1*.
Dim	String specifying the dimension of the cluster group. Choices are `'column'` or `'row'`.
InfoOnlyValue	Controls the return of a structure (instead of a clustergram object) containing information about the cluster group. Choices are `true` or `false` (default).
ColorValue	Color to highlight the dendrogram of the selected cluster group. Specify the color with one of the following: • Three-element numeric vector of RGB values • String containing a predefined single-letter color code • String containing a predefined color name For example, to use cyan, enter `[0 1 1]`, `'c'`, or `'cyan'`. For more information on specifying colors, see `ColorSpec`.

Return Values

CGobj2 — Clustergram object created from the selected cluster group in *CGobj1*.

CGStruct — Structure containing information about the cluster group in the following fields:

- `GroupNames` — Cell array of text strings containing the names of the row or column groups in the selected cluster group.
- `RowNodeNames` — Cell array of text strings containing the names of the row nodes in the selected cluster group.
- `ColumnNodeNames` — Cell array of text strings containing the names of the column nodes in the selected cluster group.
- `ExprValues` — An *M*-by-*N* matrix of intensity values, where *M* and *N* are the number of row nodes and of column nodes respectively in the selected cluster group. If the matrix contains gene expression data, typically each row corresponds to a gene and each column corresponds to a sample.

Description

`clusterGroup(`*`CGobj1`*`, `*`GroupIndex`*`, `*`Dim`*`)` selects and highlights a cluster group in the Clustergram window, specified by a clustergram object, group index, and dimension.

`CGobj2` `= clusterGroup(`*`CGobj1`*`, `*`GroupIndex`*`, `*`Dim`*`)` creates a clustergram object from the specified cluster group. This syntax is equivalent to selecting the **Export Group to Workspace** command from the context menu after right-clicking a group in the Clustergram window.

`CGStruct` `= clusterGroup(`*`CGobj1`*`, `*`GroupIndex`*`, `*`Dim`*`, 'InfoOnly', `*`InfoOnlyValue`*`)` controls the return of a structure (instead of a clustergram object) containing information about the

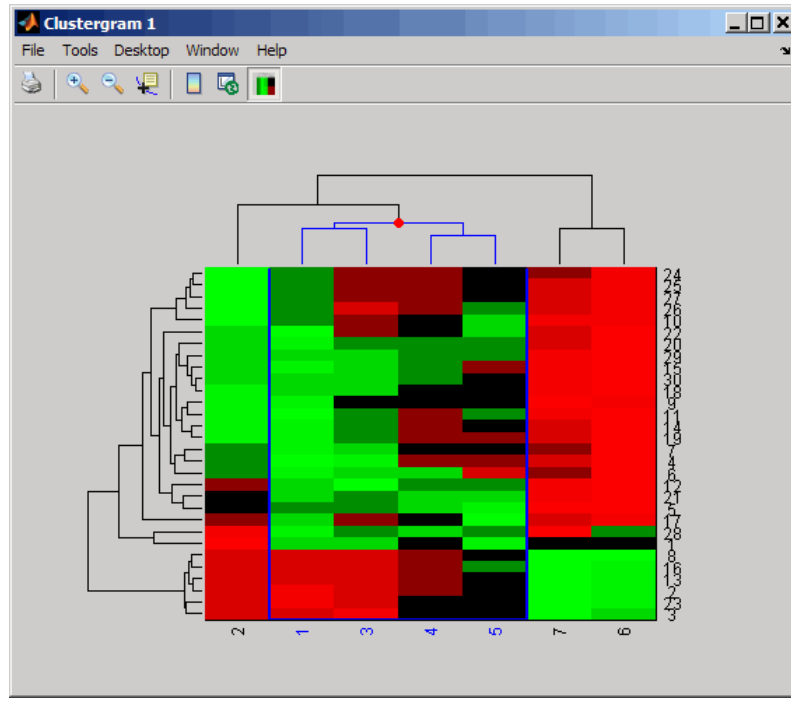
cluster group. Choices are `true` or `false` (default). Setting this property to `true` is equivalent to selecting the **Export Group Info to Workspace** command from the context menu after right-clicking a group in the Clustergram window.

`CGStruct` `= clusterGroup(`*`CGobj1`*`, `*`GroupIndex`*`, `*`Dim`*`, 'Color', `*`ColorValue`*`)` specifies a color for the dendrogram of the selected cluster group.

Examples

Select and highlight column cluster Group 4 in the Clustergram window, from the clustergram object created in the Examples section of the `clustergram` function.

```
clusterGroup(cgo,4,'column')
```



See Also

Bioinformatics Toolbox function: `clustergram` (object constructor)

Bioinformatics Toolbox object: clustergram object

Bioinformatics Toolbox methods of a clustergram object: `get`, `set`, `view`

codonbias

Purpose

Calculate codon frequency for each amino acid coded for in nucleotide sequence

Syntax

```
CodonFreq = codonbias(SeqNT)
CodonFreq = codonbias(SeqNT, ...'GeneticCode',
GeneticCodeValue, ...)
CodonFreq = codonbias(SeqNT, ...'Frame', FrameValue, ...)
CodonFreq = codonbias(SeqNT, ...'Reverse',
ReverseValue, ...)
CodonFreq = codonbias(SeqNT, ...'Pie', PieValue, ...)
```

Arguments

SeqNT	One of the following: • String of codes specifying a nucleotide sequence • Row vector of integers specifying a nucleotide sequence • MATLAB structure containing a `Sequence` field that contains a nucleotide sequence, such as returned by `fastaread`, `fastqread`, `emblread`, `getembl`, `genbankread`, or `getgenbank` Valid characters include `A`, `C`, `G`, `T`, and `U`. `codonbias` does not count ambiguous nucleotides or gaps.
GeneticCodeValue	Integer or string specifying a genetic code number or code name from the table Genetic Code on page 3-356. Default is `1` or `'Standard'`.

Tip If you use a code name, you can truncate the name to the first two letters of the name.

FrameValue	Integer specifying a reading frame in the nucleotide sequence. Choices are 1 (default), 2, or 3.
ReverseValue	Controls the return of the codon frequency for the reverse complement sequence of the nucleotide sequence specified by *SeqNT*. Choices are `true` or `false` (default).
PieValue	Controls the creation of a figure of 20 pie charts, one for each amino acid. Choices are `true` or `false` (default).

Return Values

CodonFreq	MATLAB structure containing a field for each amino acid, each of which contains the associated codon frequencies as percentages.

Description

Many amino acids are coded by two or more nucleic acid codons. However, the probability that a specific codon (from all possible codons for an amino acid) is used to code an amino acid varies between sequences. Knowing the frequency of each codon in a protein coding sequence for each amino acid is a useful statistic.

CodonFreq = codonbias(*SeqNT*) calculates the codon frequency in percent for each amino acid coded for in *SeqNT*, a nucleotide sequence, and returns the results in *CodonFreq*, a MATLAB structure containing a field for each amino acid.

CodonFreq = codonbias(*SeqNT*, ...'*PropertyName*', *PropertyValue*, ...) calls codonbias with optional properties that use property name/property value pairs. You can specify one or more

properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

CodonFreq = codonbias(*SeqNT*, ...'GeneticCode', *GeneticCodeValue*, ...) specifies a genetic code. Choices for *GenetidCodeValue* are an integer or string specifying a code number or code name from the table Genetic Code on page 3-356. If you use a code name, you can truncate the name to the first two characters of the name. Default is 1 or 'Standard'.

Tip If you use a code name, you can truncate the name to the first two letters of the name.

CodonFreq = codonbias(*SeqNT*, ...'Frame', *FrameValue*, ...) calculates the codon frequency in the reading frame specified by *FrameValue*, which can be 1 (default), 2, or 3.

CodonFreq = codonbias(*SeqNT*, ...'Reverse', *ReverseValue*, ...) controls the return of the codon frequency for the reverse complement of the nucleotide sequence specified by *SeqNT*. Choices are true or false (default).

CodonFreq = codonbias(*SeqNT*, ...'Pie', *PieValue*, ...) controls the creation of a figure of 20 pie charts, one for each amino acid. Choices are true or false (default).

Genetic Code

Code Number	Code Name
1	Standard
2	Vertebrate Mitochondrial
3	Yeast Mitochondrial

Genetic Code (Continued)

Code Number	Code Name
4	Mold, Protozoan, Coelenterate Mitochondrial, and Mycoplasma/Spiroplasma
5	Invertebrate Mitochondrial
6	Ciliate, Dasycladacean, and Hexamita Nuclear
9	Echinoderm Mitochondrial
10	Euplotid Nuclear
11	Bacterial and Plant Plastid
12	Alternative Yeast Nuclear
13	Ascidian Mitochondrial
14	Flatworm Mitochondrial
15	Blepharisma Nuclear
16	Chlorophycean Mitochondrial
21	Trematode Mitochondrial
22	Scenedesmus Obliquus Mitochondrial
23	Thraustochytrium Mitochondrial

Examples

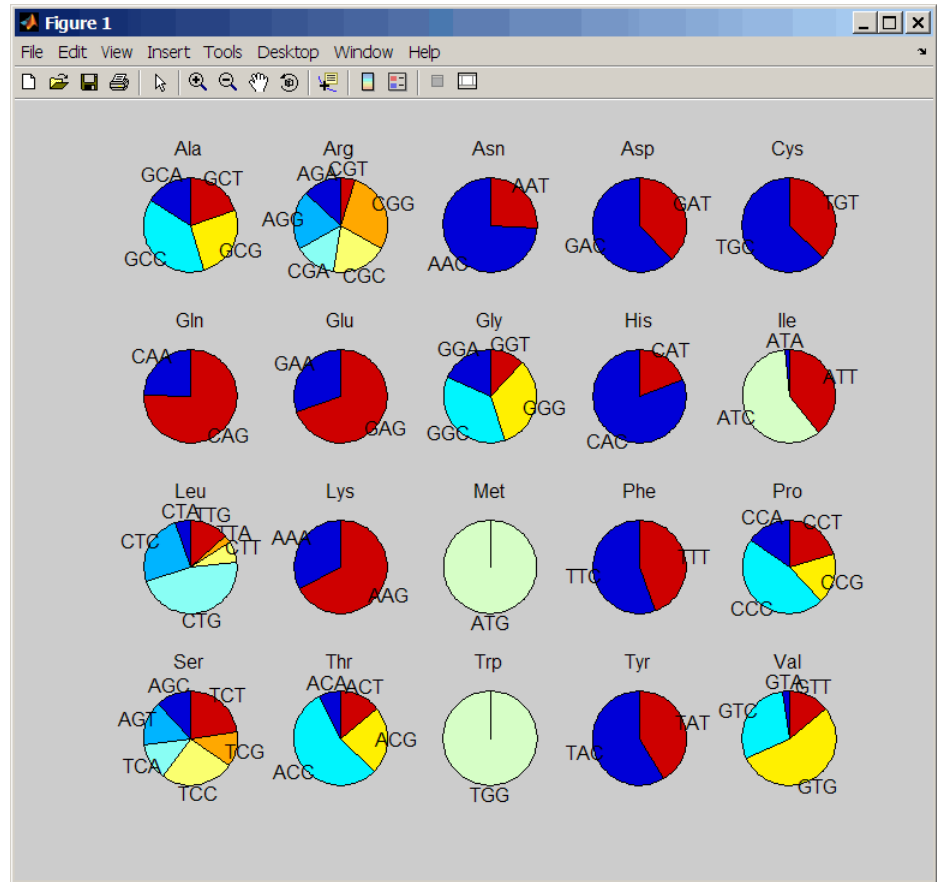
1 Import a nucleotide sequence from the GenBank database into the MATLAB software. For example, retrieve the DNA sequence that codes for a human insulin receptor.

```
S = getgenbank('M10051');
```

2 Calculate the codon frequency for each amino acid coded for by the DNA sequence, and then plot the results.

```
cb = codonbias(S.Sequence,'PIE',true)
```

A figure with 20 pie charts for the 20 amino acids displays.



3 Get the codon frequency for the alanine (A) amino acid.

```
cb.Ala

ans =

    Codon: {'GCA' 'GCC' 'GCG' 'GCT'}
```

```
Freq: [0.1600 0.3867 0.2533 02000]
```

See Also

Bioinformatics Toolbox functions: `aminolookup`, `codoncount`, `geneticcode`, `nt2aa`

codoncount

Purpose

Count codons in nucleotide sequence

Syntax

```
Codons = codoncount(SeqNT)
[Codons, CodonArray] = codoncount(SeqNT)
... = codoncount(SeqNT, ...'Frame', FrameValue, ...)
... = codoncount(SeqNT, ...'Reverse', ReverseValue, ...)
... = codoncount(SeqNT, ...'Figure', FigureValue, ...)
```

Arguments

SeqNT	One of the following: • String of codes specifying a nucleotide sequence. For valid letter codes, see the table Mapping Nucleotide Letter Codes to Integers on page 3-1121 • Row vector of integers specifying a nucleotide sequence. For valid integers, see the table Mapping Nucleotide Integers to Letter Codes on page 3-809 • MATLAB structure containing a `Sequence` field that contains a nucleotide sequence, such as returned by `fastaread`, `fastqread`, `emblread`, `getembl`, `genbankread`, or `getgenbank`. Examples: `'ACGT'` or `[1 2 3 4]`
FrameValue	Integer specifying a reading frame in the nucleotide sequence. Choices are `1` (default), `2`, or `3`.
ReverseValue	Controls the return of the codon count for the reverse complement sequence of the nucleotide sequence specified by *SeqNT*. Choices are `true` or `false` (default).
FigureValue	Controls the display of a heat map of the codon counts. Choices are `true` or `false` (default).

Return Values

Codons	MATLAB structure containing fields for the 64 possible codons (AAA, AAC, AAG, ..., TTG, TTT), which contain the codon counts in *SeqNT*.
CodonArray	A 4-by-4-by-4 array containing the raw count data for each codon. The three dimensions correspond to the three positions in the codon, and the indices to each element are represented by 1 = A, 2 = C, 3 = G, and 4 = T. For example, the element (2,3,4) in the array contains the number of CGT codons.

Description

Codons = codoncount(*SeqNT*) counts the codons in *SeqNT*, a nucleotide sequence, and returns the codon counts in *Codons*, a MATLAB structure containing fields for the 64 possible codons (AAA, AAC, AAG, ..., TTG, TTT).

- For sequences that have codons with the character U, these codons are added to the corresponding codons containing a T.
- If the sequence contains ambiguous nucleotide characters (R, Y, K, M, S, W, B, D, H, V, or N), or gaps indicated by a hyphen (-), then these characters are counted in the field Others, and the following warning message appears:

```
Warning: Ambiguous symbols appear in the sequence. These will be in Others.
```

- If the sequence contains undefined nucleotide characters (E, F, H, I, J, L, O, P, Q, X, or Z), then codons containing these characters are counted in the field Others, and the following warning message appears:

```
Warning: Unknown symbols appear in the sequence. These will be in Others.
```

[*Codons, CodonArray*] = codoncount(*SeqNT*) returns *CodonArray*, a 4-by-4-by-4 array containing the raw count data for each codon. The three dimensions correspond to the three positions in the codon, and the indices to each element are represented by 1 = A, 2 = C, 3 = G, and 4 = T. For example, the element (2,3,4) in the array contains the number of CGT codons.

`... = codoncount(SeqNT, ...'PropertyName', PropertyValue, ...)` calls `codoncount` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = codoncount(SeqNT, ...'Frame', FrameValue, ...)` counts the codons in the reading frame specified by *`FrameValue`*, which can be `1` (default), `2`, or `3`.

`... = codoncount(SeqNT, ...'Reverse', ReverseValue, ...)` controls the return of the codon count for the reverse complement sequence of *`SeqNT`*. Choices are `true` or `false` (default).

`... = codoncount(SeqNT, ...'Figure', FigureValue, ...)` controls the display of a heat map of the codon counts. Choices are `true` or `false` (default).

Examples

- Count the codons in a nucleotide sequence.

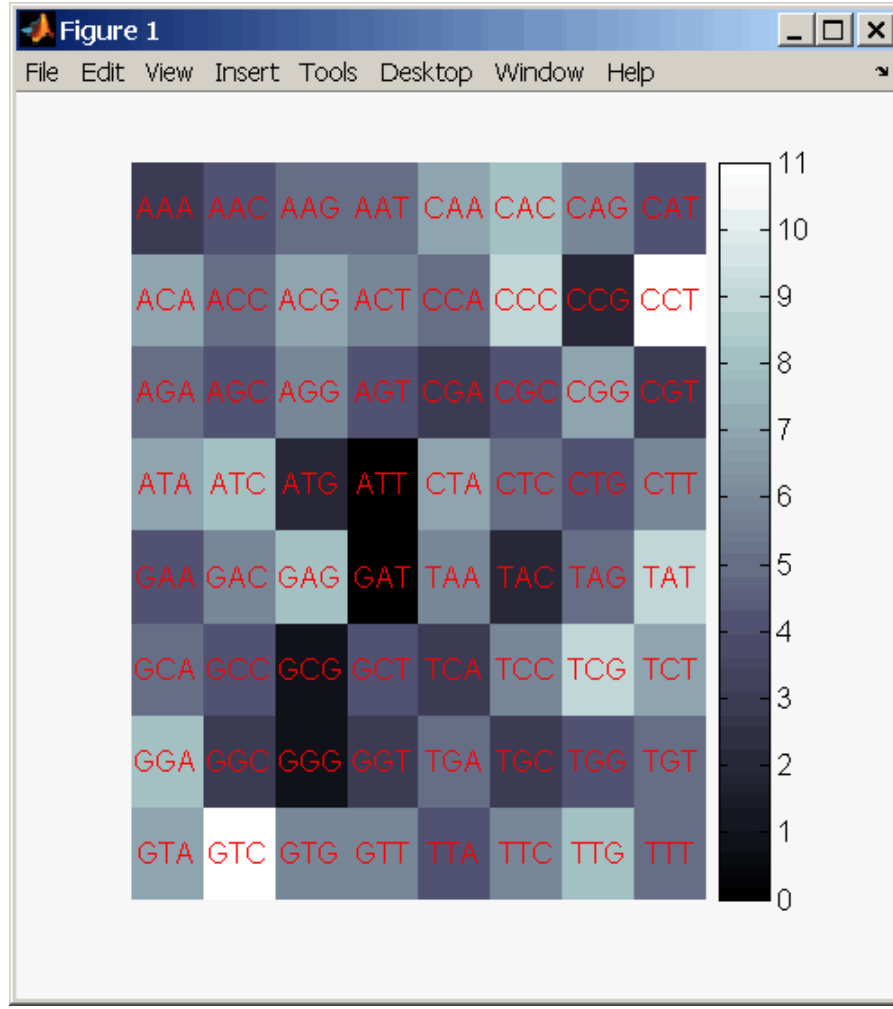
```
codons = codoncount('AAACGTTA')

codons =
       AAA: 1  ATC: 0  CGG: 0  GCT: 0  TCA: 0
       AAC: 0  ATG: 0  CGT: 1  GGA: 0  TCC: 0
       AAG: 0  ATT: 0  CTA: 0  GGC: 0  TCG: 0
       AAT: 0  CAA: 0  CTC: 0  GGG: 0  TCT: 0
       ACA: 0  CAC: 0  CTG: 0  GGT: 0  TGA: 0
       ACC: 0  CAG: 0  CTT: 0  GTA: 0  TGC: 0
       ACG: 0  CAT: 0  GAA: 0  GTC: 0  TGG: 0
       ACT: 0  CCA: 0  GAC: 0  GTG: 0  TGT: 0
       AGA: 0  CCC: 0  GAG: 0  GTT: 0  TTA: 0
       AGC: 0  CCG: 0  GAT: 0  TAA: 0  TTC: 0
       AGG: 0  CCT: 0  GCA: 0  TAC: 0  TTG: 0
       AGT: 0  CGA: 0  GCC: 0  TAG: 0  TTT: 0
       ATA: 0  CGC: 0  GCG: 0  TAT: 0
```

- Count the codons in the second frame for the reverse complement of a sequence.

```
r2codons = codoncount('AAACGTTA','Frame',2,'Reverse',true)
```

- Create a heat map of the codons in a random nucleotide sequence.

```
a = randseq(1000);
codoncount(a,'Figure', true);
```



See Also

Bioinformatics Toolbox functions: `aacount`, `basecount`, `baselookup`, `codonbias`, `dimercount`, `nmercount`, `ntdensity`, `seqcomplement`, `seqrcomplement`, `seqreverse`, `seqwordcount`

Purpose

Retrieve or set column names of DataMatrix object

Syntax

```
ReturnColNames = colnames(DMObj)
ReturnColNames = colnames(DMObj, ColIndices)
DMObjNew = colnames(DMObj, ColIndices, ColNames)
```

Arguments

DMObj	DataMatrix object, such as created by `DataMatrix` (object constructor).
ColIndices	One or more columns in *DMObj*, specified by any of the following: • Positive integer • Vector of positive integers • String specifying a column name • Cell array of strings • Logical vector
ColNames	Column names specified by any of the following: • Numeric vector • Cell array of strings • Character array • Single string, which is used as a prefix for column names, with column numbers appended to the prefix • Logical `true` or `false` (default). If `true`, unique column names are assigned using the format `col1`, `col2`, `col3`, etc. If `false`, no column names are assigned.

Note The number of elements in *ColNames* must equal the number of elements in *ColIndices*.

Return Values

ReturnColNames	String or cell array of strings containing column names in *DMObj*.
DMObjNew	DataMatrix object created with names specified by *ColIndices* and *ColNames*.

Description

ReturnColNames = colnames(*DMObj*) returns *ReturnColNames*, a cell array of strings specifying the column names in *DMObj*, a DataMatrix object.

ReturnColNames = colnames(*DMObj*, *ColIndices*) returns the column names specified by *ColIndices*. *ColIndices* can be a positive integer, vector of positive integers, string specifying a column name, cell array of strings, or a logical vector.

DMObjNew = colnames(*DMObj*, *ColIndices*, *ColNames*) returns *DMObjNew*, a DataMatrix object with columns specified by *ColIndices* set to the names specified by *ColNames*. The number of elements in *ColIndices* must equal the number of elements in *ColNames*.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: rownames

Purpose

Combine two ExptData objects

Syntax

```
NewEDObj = combine(EDObj1, EDObj2)
```

Description

`NewEDObj = combine(EDObj1, EDObj2)` combines data from two ExptData objects and returns a new ExptData object. The number and names of features (rows) in both ExptData objects must match. The number and names of samples (columns) in both ExptData objects must match.

Inputs

EDObj#

Object of the `bioma.data.ExptData` class.

See Also

`bioma.data.ExptData`

How To

- "Working with ExptData Objects"

bioma.data.MetaData.combine

Purpose

Combine two MetaData objects

Syntax

```
NewMDObj = combine(MDObj1, MDObj2)
```

Description

`NewMDObj = combine(MDObj1, MDObj2)` combines data from two MetaData objects and returns a new MetaData object. The sample or feature names in the two MetaData objects being combined must be unique. The variable names in the two MetaData objects can be unique or the same. If a variable name is common to the two MetaData objects, then the variable occupies one column in the new MetaData object. Variable names unique to either of the two MetaData objects occupy their own column and contain values only for the samples or features where the variable is present.

Inputs

MDObj#

Object of the `bioma.data.MetaData` class.

See Also

`bioma.data.MetaData`

How To

- "Working with MetaData Objects"

Purpose

Combine two MIAME objects

Syntax

```
NewMIAMEObj = combine(MIAMEObj1, MIAMEObj2)
```

Description

`NewMIAMEObj = combine(MIAMEObj1, MIAMEObj2)` combines data from two MIAME objects and returns a new MIAME object. The `combine` method concatenates the properties of the two objects together.

Inputs

`MIAMEObj#`

Object of the `bioma.data.MIAME` class.

Examples

Construct two MIAME objects, and then combine them:

```
% Create a MATLAB structure containing GEO Series data
geoStruct1 = getgeodata('GSE4616');
% Create a second MATLAB structure containing GEO Series data
geoStruct2 = getgeodata('GSE11287');
% Import bioma.data package to make constructor function
% available
import bioma.data.*
% Construct MIAME object from the first structure
MIAMEObj1 = MIAME(geoStruct1);
% Construct MIAME object from the second structure
MIAMEObj2 = MIAME(geoStruct2);
% Combine the two MIAME objects
newMIAMEObj = combine(MIAMEObj1, MIAMEObj2)
```

See Also

`bioma.data.MIAME`

How To

- "Working with MIAME Objects"

conncomp (biograph)

Purpose

Find strongly or weakly connected components in biograph object

Syntax

```
[S, C] = conncomp(BGObj)
[S, C] = conncomp(BGObj, ...'Directed', DirectedValue, ...)
[S, C] = conncomp(BGObj, ...'Weak', WeakValue, ...)
```

Arguments

BGObj	Biograph object created by `biograph` (object constructor).
DirectedValue	Property that indicates whether the graph is directed or undirected. Enter `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`. A DFS-based algorithm computes the connected components. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.
WeakValue	Property that indicates whether to find weakly connected components or strongly connected components. A weakly connected component is a maximal group of nodes that are mutually reachable by violating the edge directions. Set *WeakValue* to `true` to find weakly connected components. Default is `false`, which finds strongly connected components. The state of this parameter has no effect on undirected graphs because weakly and strongly connected components are the same in undirected graphs. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

`[S, C] = conncomp(BGObj)` finds the strongly connected components of an N-by-N adjacency matrix extracted from a biograph object, *`BGObj`* using Tarjan's algorithm. A strongly connected component is a maximal group of nodes that are mutually reachable without violating the edge directions. The N-by-N sparse matrix represents a directed graph; all nonzero entries in the matrix indicate the presence of an edge.

The number of components found is returned in *`S`*, and *`C`* is a vector indicating to which component each node belongs.

Tarjan's algorithm has a time complexity of `O(N+E)`, where `N` and `E` are the number of nodes and edges respectively.

`[S, C] = conncomp(BGObj, ...'PropertyName', PropertyValue, ...)` calls `conncomp` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[S, C] = conncomp(BGObj, ...'Directed', DirectedValue, ...)` indicates whether the graph is directed or undirected. Set *`DirectedValue`* to `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`. A DFS-based algorithm computes the connected components. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.

`[S, C] = conncomp(BGObj, ...'Weak', WeakValue, ...)` indicates whether to find weakly connected components or strongly connected components. A weakly connected component is a maximal group of nodes that are mutually reachable by violating the edge directions. Set *`WeakValue`* to `true` to find weakly connected components. Default is `false`, which finds strongly connected components. The state of this parameter has no effect on undirected graphs because weakly and strongly connected components are the same in undirected graphs. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.

Note By definition, a single node can be a strongly connected component.

Note A directed acyclic graph (DAG) cannot have any strongly connected components larger than one.

References

[1] Tarjan, R.E., (1972). Depth first search and linear graph algorithms. SIAM Journal on Computing *1(2)*, 146–160.

[2] Sedgewick, R., (2002). Algorithms in C++, Part 5 Graph Algorithms (Addison-Wesley).

[3] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphconncomp`

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `isdag`, `isomorphism`, `isspantree`, `maxflow`, `minspantree`, `shortestpath`, `topoorder`, `traverse`

Purpose

Locate CpG islands in DNA sequence

Syntax

```
cpgStruct = cpgisland(SeqDNA)
cpgStruct = cpgisland(SeqDNA, ...'Window',
WindowValue, ...)
cpgStruct = cpgisland(SeqDNA, ...'MinIsland',
MinIslandValue,
   ...)
cpgStruct = cpgisland(SeqDNA, ...'GCmin', GCminValue, ...)
cpgStruct = cpgisland(SeqDNA, ...'CpGoe', CpGoeValue, ...)
cpgStruct = cpgisland(SeqDNA, ...'Plot', PlotValue, ...)
```

Arguments

SeqDNA	One of the following: • String of codes specifying a DNA nucleotide sequence • Row vector of integers specifying a DNA nucleotide sequence • MATLAB structure containing a `Sequence` field that contains a DNA nucleotide sequence, such as returned by `fastaread`, `fastqread`, `emblread`, `getembl`, `genbankread`, or `getgenbank` Valid characters include `A`, `C`, `G`, and `T`. `cpgisland` does not count ambiguous nucleotides or gaps.
WindowValue	Integer specifying the window size for calculating GC content and CpGobserved/CpGexpected ratios. Default is `100` bases. A smaller window size increases the noise in a plot.
MinIslandValue	Integer specifying the minimum number of consecutive marked bases to report as a CpG island. Default is `200` bases.

GCminValue	Value specifying the minimum GC percent in a window needed to mark a base. Choices are a value between 0 and 1. Default is 0.5.
CpGoeValue	Value specifying the minimum CpGobserved/CpGexpected ratio in each window needed to mark a base. Choices are a value between 0 and 1. Default is 0.6. This ratio is defined as: `CPGobs/CpGexp = (NumCpGs*Length)/(NumGs*NumCs)`
PlotValue	Controls the plotting of GC content, CpGoe content, CpG islands greater than the minimum island size, and all potential CpG islands for the specified criteria. Choices are `true` or `false` (default).

Return Values

cpgStruct	MATLAB structure containing the starting and ending bases of the CpG islands greater than the minimum island size.

Description

cpgStruct = cpgisland(*SeqDNA*) searches *SeqDNA*, a DNA nucleotide sequence, for CpG islands with a GC content greater than 50% and a CpGobserved/CpGexpected ratio greater than 60%. It marks bases meeting this criteria within a moving window of 100 DNA bases and then returns the results in *cpgStruct*, a MATLAB structure containing the starting and ending bases of the CpG islands greater than the minimum island size of 200 bases.

cpgStruct = cpgisland(*SeqDNA*, ...'*PropertyName*', *PropertyValue*, ...) calls cpgisland with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

cpgStruct = cpgisland(*SeqDNA*, ...'Window', *WindowValue*, ...) specifies the window size for calculating GC content and CpGobserved/CpGexpected ratios. Default is 100 bases. A smaller window size increases the noise in a plot.

cpgStruct = cpgisland(*SeqDNA*, ...'MinIsland', *MinIslandValue*, ...) specifies the minimum number of consecutive marked bases to report as a CpG island. Default is 200 bases.

cpgStruct = cpgisland(*SeqDNA*, ...'GCmin', *GCminValue*, ...) specifies the minimum GC percent in a window needed to mark a base. Choices are a value between 0 and 1. Default is 0.5.

cpgStruct = cpgisland(*SeqDNA*, ...'CpGoe', *CpGoeValue*, ...) specifies the minimum CpGobserved/CpGexpected ratio in each window needed to mark a base. Choices are a value between 0 and 1. Default is 0.6. This ratio is defined as:

```
CPGobs/CpGexp = (NumCpGs*Length)/(NumGs*NumCs)
```

cpgStruct = cpgisland(*SeqDNA*, ...'Plot', *PlotValue*, ...) controls the plotting of GC content, CpGoe content, CpG islands greater than the minimum island size, and all potential CpG islands for the specified criteria. Choices are true or false (default).

Examples

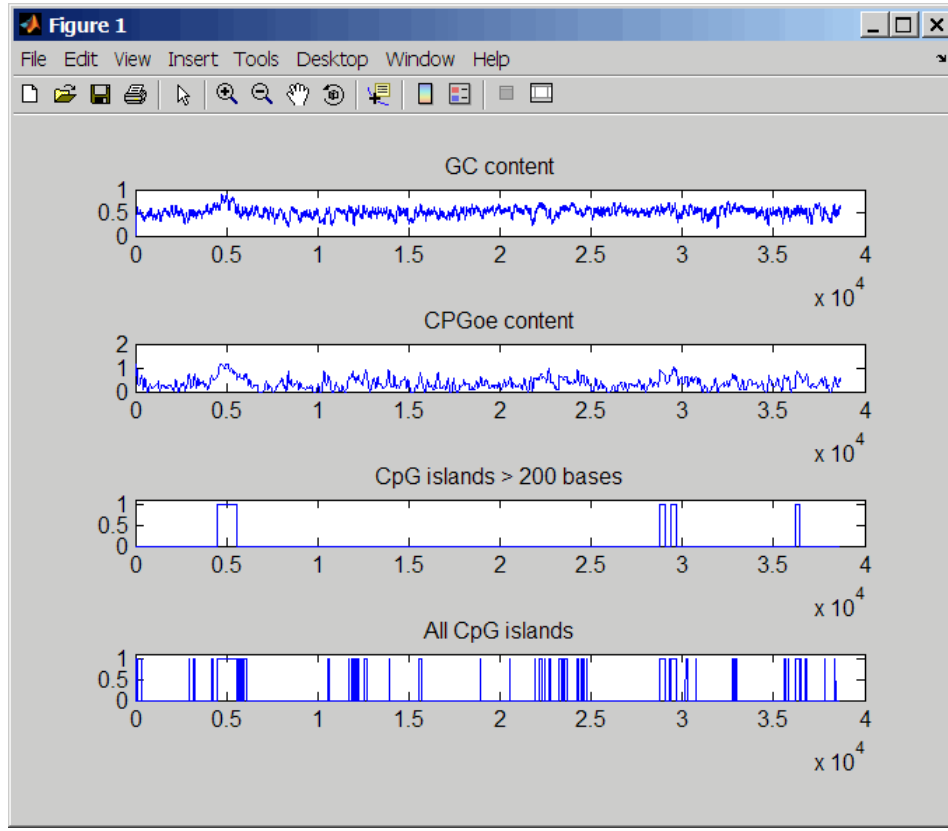
1. Import a nucleotide sequence from the GenBank database. For example, retrieve a sequence from *Homo sapiens* chromosome 12.

```
S = getgenbank('AC156455');
```

2. Calculate the CpG islands in the sequence and plot the results.

```
cpgisland(S.Sequence,'PLOT',true)

ans =

   Starts: [4470 28753 29347 36229]
   Stops: [5555 29064 29676 36450]
```

The CpG islands greater than 200 bases in length are listed and a plot displays.



See Also

Bioinformatics Toolbox functions: `basecount`, `ntdensity`, `seqshoworfs`

Purpose

Generate cross-validation indices

Syntax

```
Indices = crossvalind('Kfold', N, K)
[Train, Test] = crossvalind('HoldOut', N, P)
[Train, Test] = crossvalind('LeaveMOut', N, M)
[Train, Test] = crossvalind('Resubstitution', N, [P,Q])
[...] = crossvalind(Method, Group, ...)
[...] = crossvalind(Method, Group, ..., 'Classes', C)
[...] = crossvalind(Method, Group, ..., 'Min', MinValue)
```

Description

`Indices = crossvalind('Kfold', N, K)` returns randomly generated indices for a K-fold cross-validation of `N` observations. `Indices` contains equal (or approximately equal) proportions of the integers `1` through `K` that define a partition of the `N` observations into `K` disjoint subsets. Repeated calls return different randomly generated partitions. `K` defaults to `5` when omitted. In K-fold cross-validation, `K-1` folds are used for training and the last fold is used for evaluation. This process is repeated `K` times, leaving one different fold for evaluation each time.

`[Train, Test] = crossvalind('HoldOut', N, P)` returns logical index vectors for cross-validation of `N` observations by randomly selecting `P*N` (approximately) observations to hold out for the evaluation set. `P` must be a scalar between `0` and `1`. P defaults to `0.5` when omitted, corresponding to holding `50%` out. Using holdout cross-validation within a loop is similar to K-fold cross-validation one time outside the loop, except that non-disjointed subsets are assigned to each evaluation.

`[Train, Test] = crossvalind('LeaveMOut', N, M)`, where `M` is an integer, returns logical index vectors for cross-validation of `N` observations by randomly selecting `M` of the observations to hold out for the evaluation set. `M` defaults to `1` when omitted. Using `LeaveMOut` cross-validation within a loop does not guarantee disjointed evaluation sets. Use K-fold instead.

`[Train, Test] = crossvalind('Resubstitution', N, [P,Q])` returns logical index vectors of indices for cross-validation of `N` observations by randomly selecting `P*N` observations for the evaluation set and `Q*N` observations for training. Sets are selected in order to

minimize the number of observations that are used in both sets. `P` and `Q` are scalars between `0` and `1`. `Q=1-P` corresponds to holding out `(100*P)%`, while `P=Q=1` corresponds to full resubstitution. `[P,Q]` defaults to `[1,1]` when omitted.

`[...] = crossvalind(Method, Group, ...)` takes the group structure of the data into account. `Group` is a grouping vector that defines the class for each observation. `Group` can be a numeric vector, a string array, or a cell array of strings. The partition of the groups depends on the type of cross-validation: For K-fold, each group is divided into `K` subsets, approximately equal in size. For all others, approximately equal numbers of observations from each group are selected for the evaluation set. In both cases the training set contains at least one observation from each group.

`[...] = crossvalind(Method, Group, ..., 'Classes', C)` restricts the observations to only those values specified in `C`. `C` can be a numeric vector, a string array, or a cell array of strings, but it is of the same form as `Group`. If one output argument is specified, it contains the value `0` for observations belonging to excluded classes. If two output arguments are specified, both will contain the logical value false for observations belonging to excluded classes.

`[...] = crossvalind(Method, Group, ..., 'Min', MinValue)` sets the minimum number of observations that each group has in the training set. `Min` defaults to `1`. Setting a large value for `Min` can help to balance the training groups, but adds partial resubstitution when there are not enough observations. You cannot set `Min` when using K-fold cross-validation.

Examples

Create a 10-fold cross-validation to compute classification error.

```
load fisheriris
indices = crossvalind('Kfold',species,10);
cp = classperf(species);
for i = 1:10
    test = (indices == i); train = ~test;
    class = classify(meas(test,:),meas(train,:),species(train,:));
```

```
    classperf(cp,class,test)
end
cp.ErrorRate
```

Approximate a leave-one-out prediction error estimate.

```
load carbig
x = Displacement; y = Acceleration;
N = length(x);
sse = 0;
for i = 1:100
    [train,test] = crossvalind('LeaveMOut',N,1);
    yhat = polyval(polyfit(x(train),y(train),2),x(test));
    sse = sse + sum((yhat - y(test)).^2);
end
CVerr = sse / 100
```

Divide cancer data 60/40 without using the `'Benign'` observations. Assume groups are the true labels of the observations.

```
labels = {'Cancer','Benign','Control'};
groups = labels(ceil(rand(100,1)*3));
[train,test] = crossvalind('holdout',groups,0.6,'classes',...
                           {'Control','Cancer'});
sum(test) % Total groups allocated for testing
sum(train) % Total groups allocated for training
```

See Also

Bioinformatics Toolbox functions: `classperf`, `knnclassify`, `svmclassify`

Statistics Toolbox functions: `classify`, `grp2idx`

cytobandread

Purpose

Read cytogenetic banding information

Syntax

```
CytoStruct = cytobandread(File)
```

Arguments

File	String specifying a file containing cytogenetic G-banding data, such as an NCBI ideogram text file or a UCSC Genome Browser cytoband text file.

Return Values

CytoStruct	Structure containing cytogenetic G-banding data in the following fields: • `ChromLabels` • `BandStartBPs` • `BandEndBPs` • `BandLabels` • `GieStains`

Description

CytoStruct = `cytobandread(`*File*`)` reads *File*, which is a string specifying a file containing cytogenetic G-banding data, and returns *CytoStruct*, which is a structure containing the following fields.

Field	Description
`ChromLabels`	Cell array containing the chromosome label (number or letter) on which each band is located.
`BandStartBPs`	Column vector containing the number of the base pair at the start of each band.
`BandEndBPs`	Column vector containing the number of the base pair at the end of each band.

Field	Description
`BandLabels`	Cell array containing the FISH label of each band, for example, `p32.3`.
`GieStains`	Cell array containing the Giemsa staining result for each band. Possible stain results depend on the species. For example, for *Homo sapiens*, the possibilities are: • `gneg` • `gpos25` • `gpos50` • `gpos75` • `gpos100` • `acen` • `stalk` • `gvar`

Tip You can download files containing cytogenetic G-banding data from the NCBI or UCSC Genome Browser ftp site. For example, you can download the cytogenetic banding data for *Homo sapiens* from:

```
ftp://ftp.ncbi.nlm.nih.gov/genomes/H_sapiens/mapview/ideogram.gz
```

or

```
ftp://hgdownload.cse.ucsc.edu/goldenPath/hg18/database/cytoBandIdeo.txt.gz
```

Examples

Read the cytogenetic banding information for *Homo sapiens* into a structure.

```
hs_cytobands = cytobandread('hs_cytoBand.txt')

hs_cytobands =

     ChromLabels: {862x1 cell}
    BandStartBPs: [862x1 int32]
      BandEndBPs: [862x1 int32]
      BandLabels: {862x1 cell}
       GieStains: {862x1 cell}
```

See Also

Bioinformatics Toolbox function: `chromosomeplot`

Purpose

Data structure encapsulating data and metadata from microarray experiment so that it can be indexed by gene or probe identifiers and by sample identifiers

Description

A DataMatrix object is a data structure encapsulating measurement data and feature metadata from a microarray experiment so that it can be indexed by gene or probe identifiers and by sample identifiers. A DataMatrix object stores experimental data in a matrix, with rows typically corresponding to gene names or probe identifiers, and columns typically corresponding to sample identifiers. A DataMatrix object also stores metadata, such as the gene names or probe identifiers and sample identifiers, in row names and column names.

You create a DataMatrix object using the object constructor function `DataMatrix`.

Property Summary

Properties of a DataMatrix Object

Property	Description
`Name`	String that describes the DataMatrix object. Default is `''`.
`RowNames`	Empty array or cell array of strings that specifies the names for the rows, typically gene names or probe identifiers. The number of elements in the cell array must equal the number of rows in the matrix. Default is an empty array.
`ColNames`	Empty array or cell array of strings that specifies the names for the columns, typically sample identifiers. The number of elements in the cell array must equal the number of columns in the matrix.

Properties of a DataMatrix Object (Continued)

Property	Description
`NRows`	Read-only. Positive number that specifies the number of rows in the matrix. **Note** You cannot modify this property directly. You can access it using the `get` method.
`NCols`	Read-only. Positive number that specifies the number of columns in the matrix. **Note** You cannot modify this property directly. You can access it using the `get` method.
`NDims`	Read-only. Positive number that specifies the number of dimensions in the matrix. **Note** You cannot modify this property directly. You can access it using the `get` method.
`ElementClass`	Read-only. String that specifies the class type of the elements in the DataMatrix object, such as `single` or `double`. **Note** You cannot modify this property directly. You can access it using the `get` method.

Method Summary

General Methods of a DataMatrix Object

Method	Description
`colnames`	Retrieve or set column names of DataMatrix object.
`disp`	Display DataMatrix object.
`display`	Display DataMatrix object, printing DataMatrix object name. To invoke this method, enter the name of a DataMatrix object at the command prompt.
`dmwrite`	Write DataMatrix object to text file.
`double`	Convert DataMatrix object to double-precision array.
`get`	Retrieve information about DataMatrix object.
`isempty`	Determine if DataMatrix object is empty.
`isfinite`	Determine if DataMatrix object elements are finite.
`isinf`	Determine if DataMatrix object elements are infinite.
`isnan`	Determine if DataMatrix object elements are NaN.
`isscalar`	Determine if DataMatrix object is scalar.
`isequal`	Test DataMatrix objects for equality.
`isequalwithequalnans`	Test DataMatrix objects for equality, treating NaNs as equal.
`isvector`	Determine if DataMatrix object is vector.
`length`	Return length of DataMatrix object.

General Methods of a DataMatrix Object (Continued)

Method	Description
ndims	Return number of dimensions in DataMatrix object.
numel	Return number of elements in DataMatrix object.
plot	Draw 2-D line plot of DataMatrix object.
rownames	Retrieve or set row names of DataMatrix object.
set	Set property of DataMatrix object.
single	Convert DataMatrix object to single-precision array.
size	Return size of DataMatrix object.

Methods for Manipulating the Data in a DataMatrix Object

Method	Description
cat	Concatenate DataMatrix objects. The horzcat and vertcat methods implement special cases.
horzcat	Concatenate DataMatrix objects horizontally.
sortcols	Sort columns of DataMatrix object in ascending or descending order.
sortrows	Sort rows of DataMatrix object in ascending or descending order.
subsasgn	Subscripted assignment for DataMatrix object. To invoke this method, use parentheses or dot indexing described in “Accessing DataMatrix Objects” in the Bioinformatics Toolbox User’s Guide.

Methods for Manipulating the Data in a DataMatrix Object (Continued)

Method	Description
subsref	Subscripted reference for DataMatrix object. To invoke this method, use parentheses or dot indexing described in "Accessing DataMatrix Objects" in the Bioinformatics Toolbox User's Guide.
transpose	Transpose DataMatrix object.
vertcat	Concatenate DataMatrix objects vertically.

Descriptive Statistics and Statistical Learning Methods

Method	Description
kmeans	K-means clustering.
max	Return maximum values in DataMatrix object.
mean	Return average or mean values in DataMatrix object.
median	Return median values in DataMatrix object.
min	Return minimum values in DataMatrix object.
nanmax	Return maximum values in DataMatrix object ignoring NaN values.
nanmean	Return average or mean values in DataMatrix object ignoring NaN values.
nanmedian	Return median values in DataMatrix object ignoring NaN values.
nanmin	Return minimum values in DataMatrix object ignoring NaN values.

Descriptive Statistics and Statistical Learning Methods (Continued)

Method	Description
nanstd	Return standard deviation values in DataMatrix object ignoring NaN values.
nansum	Return sum of elements in DataMatrix object ignoring NaN values.
nanvar	Return variance values in DataMatrix object ignoring NaN values.
pdist	Pairwise distance.
princomp	Principal component analysis on data.
std	Return standard deviation values in DataMatrix object.
sum	Return sum of elements in DataMatrix object.
var	Return variance values in DataMatrix object.

Unary Methods — Exponential

Method	Description
exp	Exponential.
log	Natural logarithm.
log10	Common (base 10) logarithm.
log2	Base 2 logarithm and dissect floating-point numbers into exponent and mantissa.
pow2	Base 2 power and scale floating-point numbers.
sqrt	Square root.

Unary Methods — Integer

Method	Description
`ceil`	Round DataMatrix object toward infinity.
`fix`	Round DataMatrix object toward zero.
`floor`	Round DataMatrix object toward minus infinity.
`round`	Round DataMatrix object to nearest integer.

Unary Methods — Custom

Method	Description
`dmarrayfun`	Apply function to each element in DataMatrix object.

Binary Methods — Arithmetic Operator

Operator	Method	Description
`+`	`plus`	Add DataMatrix objects
`-`	`minus`	Subtract DataMatrix objects.
`.*`	`times`	Multiply DataMatrix objects.
`./`	`rdivide`	Right array divide DataMatrix objects.
`.\`	`ldivide`	Left array divide DataMatrix objects.
`.^`	`power`	Array power DataMatrix objects.

Binary Methods — Relational Operator

Operator	Method	Description
`<`	`lt`	Test DataMatrix objects for less than.

Binary Methods — Relational Operator (Continued)

Operator	Method	Description
<=	le	Test DataMatrix objects for less than or equal to.
>	gt	Test DataMatrix objects for greater than.
>=	ge	Test DataMatrix objects for greater than or equal to.
==	eq	Test DataMatrix objects for equality.
~=	ne	Test DataMatrix objects for inequality.

Binary Methods — Custom

Method	Description
dmbsxfun	Apply element-by-element binary operation to two DataMatrix objects with singleton expansion enabled.

Examples

Determining Properties and Property Values of a DataMatrix Object

You can display all properties and their current values of a DataMatrix object, *DMobj*, by using the following syntax:

```
get(DMobj)
```

You can return all properties and their current values of *DMobj*, a DataMatrix object, to *DMstruct*, a scalar structure in which each field name is a property of a DataMatrix object, and each field contains the value of that property, by using the following syntax:

```
DMstruct = get(DMobj)
```

You can return the value of a specific property of a DataMatrix object, *DMobj*, by using either of the following syntaxes:

```
PropertyValue = get(DMObj, 'PropertyName')

PropertyValue = DMObj.PropertyName
```

You can return the value of specific properties of a DataMatrix object, *DMobj*, by using the following syntax:

```
[Property1Value, Property2Value, ...] = get(DMobj, ...
'Property1Name', 'Property2Name', ...)
```

Determining Possible Values of DataMatrix Object Properties

You can display possible values for all properties that have a fixed set of property values in a DataMatrix object, *DMobj*, by using the following syntax:

```
set(DMobj)
```

You can display possible values for a specific property that has a fixed set of property values in a DataMatrix object, *DMobj*, by using the following syntax:

```
set(DMObj,  'PropertyName')
```

Specifying Properties of a DataMatrix Object

You can set a specific property of a DataMatrix object, *DMObj*, by using either of the following syntaxes:

```
DMObj = set(DMObj,  'PropertyName', PropertyValue)

DMObj.PropertyName = PropertyValue
```

You can set multiple properties of a DataMatrix object, *DMobj*, by using the following syntax:

```
set(DMobj,  'PropertyName1', PropertyValue1, ...
    'PropertyName2', PropertyValue2, ...)
```

Note For more examples of creating and using DataMatrix objects, see "Working with DataMatrix Objects" in the Bioinformatics Toolbox User's Guide.

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox methods of a DataMatrix object: `colnames`, `disp`, `dmarrayfun`, `dmbsxfun`, `dmwrite`, `double`, `eq`, `ge`, `get`, `gt`, `horzcat`, `isequal`, `isequalwithequalnans`, `ldivide`, `le`, `lt`, `max`, `mean`, `median`, `min`, `minus`, `ndims`, `ne`, `numel`, `plot`, `plus`, `power`, `rdivide`, `rownames`, `set`, `single`, `sortcols`, `sortrows`, `std`, `sum`, `times`, `var`, `vertcat`

Purpose

Create DataMatrix object

Syntax

```
DMobj = DataMatrix(Matrix)
DMobj = DataMatrix(Matrix, RowNames, ColumnNames)
DMobj = DataMatrix('File', FileName)
DMobj = DataMatrix(..., 'RowNames', RowNamesValue, ...)
DMobj = DataMatrix(..., 'ColNames', ColNamesValue, ...)
DMobj = DataMatrix(..., 'Name', NameValue, ...)
DMobj = DataMatrix('File', FileName, ...'Delimiter',
   DelimiterValue, ...)
DMobj = DataMatrix('File', FileName, ...'HLine',
HLineValue,
   ...)
DMobj = DataMatrix('File', FileName, ...'Rows', RowsValue,
   ...)
DMobj = DataMatrix('File', FileName, ...'Columns',
   ColumnsValue, ...)
```

Arguments

Matrix

Two-dimensional numeric or logical array.

RowNames

Row names for the DataMatrix object, specified by a numeric vector, character array, or cell array of strings, whose elements are equal in number to the number of rows in *Matrix*. *RowNames* are typically gene names or probe identifiers from a microarray experiment.

Note The row names do not need to be unique.

ColumnNames

Column names for the DataMatrix object, specified by a numeric vector, character array, or cell array of strings, whose elements are equal in number to the number of columns in *Matrix*. *ColumnNames* are typically sample identifiers from a microarray experiment.

Note The column names do not need to be unique.

FileName

String specifying a file name or a path and file name of a tab-delimited TXT or XLS file that contains table-oriented data and metadata.

Note Typically, the first row of the table contains column names, the first column contains row names, and the numeric data starts at the `2,2` position. The `DataMatrix` function will detect if the first column does not contain row names, and read data from the first column. However, if the first row does not contain header text (column names), set the `HLine` property to `0`.

RowNamesValue, *ColNamesValue*

Row names or column names for the DataMatrix object. Choices are:

- Numeric vector, character array, or a cell array of strings, whose elements are equal in number to the number of rows or number of columns of numeric data in the input matrix.
- A single string, which is used as a prefix for row or column names. Numbers will be appended to the prefix.
- `true` — Unique row or column names will be assigned using the formats `row1`, `row2`, `row3`, etc., or `col1`, `col2`, `col3`, etc.
- `false` — Default. No row or column names are assigned.

Note The row or column names do not need to be unique.

NameValue

String specifying a name for the DataMatrix object. Default is `''`.

DelimiterValue

String specifying a delimiter symbol to use for the input file. Typical choices are:

- `' '`
- `'\t'` (default)
- `','`
- `';'`
- `'|'`

HLineValue	Positive integer that specifies which row of the input file contains the column header text (column names). Default is 1. When creating the DataMatrix object *DMobj*, the DataMatrix function loads data from (*HLineValue* + 1) to the end of the file. **Tip** If the input file does not contain column header text (column names), set *HLineValue* to 0.
RowsValue, *ColumnsValue*	A subset of rows or columns in File, for the DataMatrix function to use to create the DataMatrix object. Choices are: • Cell array of strings • Character array • Numeric or logical vector

Description

A DataMatrix object encapsulates measurement data and feature metadata from a microarray experiment so that it can be indexed by gene names or probe identifiers and by sample identifiers. For examples of creating and using DataMatrix objects, see "Working with DataMatrix Objects" in the Bioinformatics Toolbox User's Guide.

Note The DataMatrix constructor function is part of the microarray object package. To make it available, type the following in the MATLAB command line:

```
import bioma.data.*
```

Otherwise, use `bioma.data.DataMatrix` instead of `DataMatrix`, in the following syntaxes.

`DMobj` = `DataMatrix(`*`Matrix`*`)` creates a DataMatrix object, *`DMobj`*, from *`Matrix`*, a two-dimensional numeric or logical array. *`Matrix`* can also be a DataMatrix object.

`DMobj` = `DataMatrix(`*`Matrix`*`, `*`RowNames`*`, `*`ColumnNames`*`)` creates a DataMatrix object, *`DMobj`*, from *`Matrix`*, a two-dimensional numeric or logical array, with row names and column names specified by *`RowNames`* and *`ColumnNames`*. *`RowNames`* and *`ColumnNames`* can be a numeric vector, character array, or cell array of strings, whose elements are equal in number to the number of rows and number of columns, respectively, in *`Matrix`*. *`RowNames`* are typically gene names or probe identifiers, while *`ColumnNames`* are typically sample identifiers.

Note The row or column names do not need to be unique.

`DMobj` = `DataMatrix('File', `*`FileName`*`)` creates a DataMatrix object, *`DMobj`*, from *`FileName`*, a string specifying a file name or a path and file name of a tab-delimited TXT or XLS file that contains table-oriented data and metadata.

Note Typically, the first row of the table contains column names, the first column contains row names, and the numeric data starts at the `2,2` position. The `DataMatrix` function will detect if the first column does not contain row names, and read data from the first column. However, if the first row does not contain header text (column names), set the `HLine` property to `0`.

`DMobj` `= DataMatrix(..., '`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `DataMatrix` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`DMobj` `= DataMatrix(..., 'RowNames', `*`RowNamesValue`*`, ...)` specifies row names for *`DMobj`*. *`RowNamesValue`* can be any of the following:

- Numeric vector, character array, or a cell array of strings, whose elements are equal in number to the number of rows of numeric data in the input matrix.
- A single string, which is used as a prefix for row names. Row numbers will be appended to the prefix.
- `true` — Unique row names will be assigned using the format `row1`, `row2`, `row3`, etc.
- `false` — Default. No row names are assigned.

Note The row names do not need to be unique.

`DMobj` `= DataMatrix(..., 'ColNames', `*`ColNamesValue`*`, ...)` specifies column names for *`DMobj`*. *`ColNamesValue`* can be any of the following:

- Numeric vector, character array, or a cell array of strings, whose elements are equal in number to the number of columns of numeric data in the input matrix.
- A single string, which is used as a prefix for column names. Column numbers will be appended to the prefix.
- `true` — Unique column names will be assigned using the format `col1`, `col2`, `col3`, etc.
- `false` — Default. No column names are assigned.

Note The column names do not need to be unique.

`DMobj` `= DataMatrix(..., 'Name',` *`NameValue`*`, ...)` specifies a name for *`DMobj`*. Default is `''`.

`DMobj` `= DataMatrix('File',` *`FileName`*`, ...'Delimiter',` *`DelimiterValue`*`, ...)` specifies a delimiter symbol to use for the input file. Typical choices are:

- `' '`
- `'\t'` (default)
- `','`
- `';'`
- `'|'`

`DMobj` `= DataMatrix('File',` *`FileName`*`, ...'HLine',` *`HLineValue`*`, ...)` specifies which row of the input file contains the column header text (column names). *`HLineValue`* is a positive integer. Default is `1`. When creating the DataMatrix object *`DMobj`*, the `DataMatrix` function loads data from (*`HLineValue`* `+ 1`) to the end of the file.

Tip If the input file does not contain column header text (column names), set *HLineValue* to 0.

DMobj = DataMatrix('File', *FileName*, ...'Rows', *RowsValue*, ...) specifies a subset of row names in File for the DataMatrix function to use to create *DMobj*. *RowsValue* can be a cell array of strings, a character array, or a numeric or logical vector.

DMobj = DataMatrix('File', *FileName*, ...'Columns', *ColumnsValue*, ...) specifies a subset of column names in File for the DataMatrix function to use to create *DMobj*. *ColumnsValue* can be a cell array of strings, a character array, or a numeric or logical vector.

Examples

For examples of creating and using DataMatrix objects, see "Working with DataMatrix Objects" in the Bioinformatics Toolbox User's Guide.

See Also

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox methods of a DataMatrix object: colnames, disp, dmarrayfun, dmbsxfun, dmwrite,double, eq, ge, get, gt, horzcat, isequal, isequalwithequalnans, ldivide, le, lt, max, mean, median, min, minus, ndims, ne, numel, plot, plus, power, rdivide, rownames, set, single, sortcols, sortrows, std, sum, times, var, vertcat

Purpose

Return Dayhoff scoring matrix

Syntax

```
ScoringMatrix = dayhoff
```

Description

`ScoringMatrix = dayhoff` returns a `PAM250` type scoring matrix. The order of amino acids in the matrix is `A R N D C Q E G H I L K M F P S T W Y V B Z X *`.

See Also

Bioinformatics Toolbox functions: `blosum`, `gonnet`, `localalign`, `nuc44`, `nwalign`, `pam`, `swalign`

dimercount

Purpose

Count dimers in nucleotide sequence

Syntax

```
Dimers = dimercount(SeqNT)
[Dimers, Percent] = dimercount(SeqNT)
... = dimercount(SeqNT, 'Chart', ChartValue)
```

Arguments

SeqNT One of the following:

- String of codes specifying a nucleotide sequence. For valid letter codes, see the table Mapping Nucleotide Letter Codes to Integers on page 3-1121.
- Row vector of integers specifying a nucleotide sequence. For valid integers, see the table Mapping Nucleotide Integers to Letter Codes on page 3-809.
- MATLAB structure containing a `Sequence` field that contains a nucleotide sequence, such as returned by `fastaread`, `fastqread`, `emblread`, `getembl`, `genbankread`, or `getgenbank`.

Examples: `'ACGT'` or `[1 2 3 4]`

ChartValue String specifying a chart type. Choices are `'pie'` or `'bar'`.

Return Values

Dimers — MATLAB structure containing the fields AA, AC, AG, AT, CA, CC, CG, CT, GA, GC, GG, GT, TA, TC, TG, and TT, which contain the dimer counts in *SeqNT*.

Percent — A 4-by-4 matrix with the relative proportions of the dimers in *SeqNT*. The rows correspond to A, C, G, and T in the first element of the dimer, and the columns correspond to A, C, G, and T in the second element of the dimer.

Description

Dimers = dimercount(*SeqNT*) counts the nucleotide dimers in *SeqNT*, a nucleotide sequence, and returns the dimer counts in *Dimers*, a MATLAB structure containing the fields AA, AC, AG, AT, CA, CC, CG, CT, GA, GC, GG, GT, TA, TC, TG, and TT.

- For sequences that have dimers with the character U, these dimers are added to the corresponding dimers containing a T.
- If the sequence contains ambiguous nucleotide characters (R, Y, K, M, S, W, B, D, H, V, or N), or gaps indicated by a hyphen (-), then these characters are counted in the field Others, and the following warning message appears.

```
Warning: Ambiguous symbols appear in the sequence. These will be in Others.
```

- If the sequence contains undefined nucleotide characters (E, F, H, I, J, L, O, P, Q, X, or Z), then dimers containing these characters are counted in the field Others, and the following warning message appears:

```
Warning: Unknown symbols appear in the sequence. These will be in Others.
```

[*Dimers*, *Percent*] = dimercount(*SeqNT*) returns *Percent*, a 4-by-4 matrix with the relative proportions of the dimers in *SeqNT*. The rows correspond to A, C, G, and T in the first element of the dimer, and the columns correspond to A, C, G, and T in the second element of the dimer.

`... = dimercount(SeqNT, 'Chart', ChartValue)` creates a chart showing the relative proportions of the dimers. `ChartValue` can be `'pie'` or `'bar'`.

Examples

Count the dimers in a nucleotide sequence and display a matrix of the percentage of each dimer.

```
[Dimers, Percent] = dimercount('TAGCTGGCCAAGCGAGCTTG')

Dimers =

    AA: 1
    AC: 0
    AG: 3
    AT: 0
    CA: 1
    CC: 1
    CG: 1
    CT: 2
    GA: 1
    GC: 4
    GG: 1
    GT: 0
    TA: 1
    TC: 0
    TG: 2
    TT: 1


Percent =

    0.0526         0    0.1579         0
    0.0526    0.0526    0.0526    0.1053
    0.0526    0.2105    0.0526         0
    0.0526         0    0.1053    0.0526
```

See Also

Bioinformatics Toolbox functions: `aacount`, `basecount`, `baselookup`, `codoncount`, `nmercount`, `ntdensity`

disp (DataMatrix)

Purpose

Display DataMatrix object

Syntax

```
disp(DMObj)
```

Arguments

DMObj	DataMatrix object, such as created by `DataMatrix` (object constructor).

Description

`disp(DMObj)` displays the DataMatrix object *DMObj*, including row names and column names, without printing the DataMatrix object name.

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Purpose

Apply function to each element in DataMatrix object

Syntax

```
DMObjNew1 = dmarrayfun(Func, DMObj1)
DMObjNew1 = dmarrayfun(Func, DMObj1, DMObj2, ...)
[DMObjNew1, DMObjNew2, ...] = dmarrayfun(Func, DMObj1, ...)
[DMObjNew1, ...] = dmarrayfun(Func, DMObj1,
...'UniformOutput', UniformOutputValue, ...)
[DMObjNew1, ...] = dmarrayfun(Func, DMObj1,
   ...'DataMatrixOutput', DataMatrixOutputValue, ...)
[DMObjNew1, ...] = dmarrayfun(Func, DMObj1, ...'Rows',
   RowsValue, ...)
[DMObjNew1, ...] = dmarrayfun(Func, DMObj1, ...'Columns',
   ColumnsValue, ...)
[DMObjNew1, ...] = dmarrayfun(Func, DMObj1,
...'ErrorHandler',
   ErrorHandlerValue, ...)
```

Arguments

Func	Function handle for a function that returns one or more scalars, and returns values of the same class each time it is called.
DMObj1	DataMatrix object, such as created by `DataMatrix` (object constructor).
DMObj2	Either of the following: • DataMatrix object, such as created by `DataMatrix` (object constructor) • MATLAB numeric array

Note *DMObj2* and subsequent input objects or arrays must be the same size (number of rows and columns) as *DMObj1*.

UniformOutputValue	Specifies whether *Func* must return output values without encapsulation in a cell array. Choices are `true` (default) or `false`. If `true`, `dmarrayfun` must return scalar values that can be concatenated into an array. These values can also be a cell array. If `false`, `dmarrayfun` returns a cell array (or multiple cell arrays), where the `I,J`th cell contains the value equal to *Func*`(`*DMObj1*`(I,J),...)`.
DataMatrixOutputValue	Specifies whether return values must be DataMatrix objects. Choices are `true` (default) or `false`. If you set the `'UniformOutput'` property to `false`, this property is ignored.
RowsValue, *ColumnsValue*	Specifies the rows or columns to which to apply the function. Choices are: • Positive integer • Vector of positive integers • String specifying a row or column name • Cell array of strings • Logical vector
ErrorHandlerValue	Specifies a function handle to a function that `dmarrayfun` calls if the call to *Func* fails.

Return Values

DMObjNew1, *DMObjNew2*	DataMatrix objects created from applying the function to each element in one or more DataMatrix objects. The size (number of rows and columns), row names, and column names will be the same as *DMObj1*.

Description

DMObjNew1 = dmarrayfun(*Func*, *DMObj1*) applies the function specified by *Func* to each element in *DMObj1*, a DataMatrix object, and returns the results in *DMObjNew1*, a new DataMatrix object. *DMObjNew1* has the same size (number of rows and columns), row names, and column names as *DMObj1*. The I,Jth element of *DMObjNew1* is equal to *Func*(*DMObj1*(I,J)), where *Func* is a function handle for a function that takes one input argument, returns one scalar value, and returns values of the same class each time it is called.

DMObjNew1 = dmarrayfun(*Func*, *DMObj1*, *DMObj2*, ...) evaluates the function specified by *Func* using elements in *DMObj1*, *DMObj2*, etc. as input arguments. The I,Jth element of *DMObjNew1* is equal to *Func*(*DMObj1*(I,J), *DMObj2*(I,J), ...), where *Func* is a function handle for a function that takes multiple input arguments, returns one scalar, and returns values of the same class each time it is called.

[*DMObjNew1*, *DMObjNew2*, ...] = dmarrayfun(*Func*, *DMObj1*, ...) evaluates the function specified by *Func* using elements in *DMObj1*, and possibly other input arguments. *Func* is a function handle for a function that takes one or more input arguments, returns multiple scalars, and returns values of the same class each time it is called. It returns DataMatrix objects *DMObjNew1*, *DMObjNew2*, etc. with each one corresponding to one of the outputs of *Func*. The outputs of *Func* may be of different classes, however, but each output must be the same each time it is called.

[*DMObjNew1*, ...] = dmarrayfun(*Func*, *DMObj1*, ...'*PropertyName*', *PropertyValue*, ...) calls dmarrayfun with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName*

must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`[DMObjNew1, ...] = dmarrayfun(Func, DMObj1, ...'UniformOutput', UniformOutputValue, ...)` specifies whether *`Func`* must return output values without encapsulation in a cell array. Choices are `true` (default) or `false`. If `true`, `dmarrayfun` must return scalar values that can be concatenated into an array. These values can also be a cell array. If `false`, `dmarrayfun` returns a cell array (or multiple cell arrays), where the `I,J`th cell contains the value equal to *`Func`*`(`*`DMObj1`*`(I,J),...)`.

`[DMObjNew1, ...] = dmarrayfun(Func, DMObj1, ...'DataMatrixOutput', DataMatrixOutputValue, ...)` specifies whether return values must be DataMatrix objects. Choices are `true` (default) or `false`. If you set the `'UniformOutput'` property to `false`, this property is ignored.

`[DMObjNew1, ...] = dmarrayfun(Func, DMObj1, ...'Rows', RowsValue, ...)` applies the function only to the rows in the DataMatrix object specified by *`RowsValue`*, which can be a positive integer, vector of positive integers, string specifying a row name, cell array of strings, or a logical vector.

`[DMObjNew1, ...] = dmarrayfun(Func, DMObj1, ...'Columns', ColumnsValue, ...)` applies the function only to the columns in the DataMatrix object specified by *`ColsValue`*, which can be a positive integer, vector of positive integers, string specifying a column name, cell array of strings, or a logical vector.

`[DMObjNew1, ...] = dmarrayfun(Func, DMObj1, ...'ErrorHandler', ErrorHandlerValue, ...)` specifies a function handle to a function that `dmarrayfun` calls if the call to *`Func`* fails. The error handling function will be called with these input arguments:

- Structure with the following fields:
  - `identifier` — Identifier of the error

  - `message` — Error message text
  - `index` — Linear index into the input array(s) at which the error occurred
- Set of input arguments at which the call to the function failed

If you do not specify *`ErrorHandlerValue`*, `dmarrayfun` rethrows the error from the call to *`Func`*.

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: `dmbsxfun`

MATLAB function: `arrayfun`

dmbsxfun (DataMatrix)

Purpose

Apply element-by-element binary operation to two DataMatrix objects with singleton expansion enabled

Syntax

```
DMObjNew = dmbsxfun(Func, DMObj1, DMObj2)
```

Arguments

Func	Function handle for an M-file function or a built-in function. For more information on built-in functions, see `bsxfun`.
DMObj1, *DMObj2*	Either of the following: • DataMatrix object, such as created by `DataMatrix` (object constructor) • MATLAB numeric array At least one of these input arguments must be a DataMatrix object.

Return Values

DMObjNew	DataMatrix object or MATLAB numeric array created from element-by-element binary operation of two DataMatrix objects with singleton expansion enabled.

Description

DMObjNew = dmbsxfun(*Func*, *DMObj1*, *DMObj2*) applies an element-by-element binary operation to the DataMatrix objects *DMObj1* and *DMObj2*, with singleton expansion enabled. *Func* is a function handle, and can be for an M-file function or a built-in function. For more information on built-in functions, see `bsxfun`.

DMObj1 and *DMObj2* can be DataMatrix objects or MATLAB numeric arrays; however, at least one of these input arguments must be a DataMatrix object. *DMObj1* and *DMObj2* must have the same number of rows or the same number or columns. If they don't have the same number of rows, then one must be a row vector and its rows are expanded down to be equal to the larger matrix. If they don't have the

same number of columns, then one must be a column vector and its columns are expanded across to be equal to the larger matrix.

DMObjNew is a DataMatrix object, unless the larger input argument is a MATLAB numeric array; then *DMObjNew* is also a numeric array. The size (number of rows and columns) of *DMObjNew* is equal to the larger of the two input arguments. The row names and column names of *DMObjNew* come from the larger input argument, or, if both inputs are the same size, from the first input argument.

Examples

1 Use the `DataMatrix` constructor function to create a DataMatrix object.

```
A = bioma.data.DataMatrix(magic(3), 'RowNames', true, ...
                                'ColNames',true)
```

2 Use the built-in function `@minus` to subtract the column means from this DataMatrix object.

```
A = dmbsxfun(@minus, A, mean(A))
```

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

MATLAB function: `bsxfun`

bioma.data.ExptData.dmNames

Purpose

Retrieve or set `Name` properties of DataMatrix objects in ExptData object

Syntax

```
DMNames = dmNames(EDObj)
DMNames = dmNames(EDObj, Subset)
NewEDObj = dmNames(EDObj, Subset, NewDMNames)
```

Description

`DMNames = dmNames(EDObj)` returns a cell array of strings specifying the `Name` properties of all the DataMatrix objects in an ExptData object.

`DMNames = dmNames(EDObj, Subset)` returns a cell array of strings specifying the `Name` properties of a subset of the DataMatrix objects in an ExptData object.

`NewEDObj = dmNames(EDObj, Subset, NewDMNames)` replaces the `Name` properties of DataMatrix objects specified by *`Subset`* in *`EDObj`*, an ExptData object, with *`NewDMNames`*, and returns *`NewEDObj`*, a new ExptData object.

Inputs

`EDObj`

Object of the `bioma.data.ExptData` class.

`Subset`

One of the following to specify the names of a subset of the DataMatrix objects in an ExptData object:

- String specifying a name
- Cell array of strings specifying names
- Positive integer
- Vector of positive integers
- Logical vector

`NewDMNames`

New names for specific DataMatrix objects within an ExptData object, specified by one of the following:

- Numeric vector
- String or cell array of strings
- String, which `dmNames` uses as a prefix for the DataMatrix object names, with numbers appended to the prefix
- Logical `true` or `false` (default). If `true`, `dmNames` assigns unique names using the format `DM1`, `DM2`, etc.

The number of elements in *`NewDMNames`* must equal the number of DataMatrix objects specified by *`Subset`*.

Outputs

`DMNames`

Cell array of strings specifying the names of all or some of the DataMatrix objects in an ExptData object.

`NewEDObj`

Object of the `bioma.data.ExptData` class, returned after replacing names of specific DataMatrix objects.

Examples

Construct an ExptData object, and then retrieve the names of DataMatrix objects from it:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Retrieve DataMatrix object names
DMNames = dmNames(EDObj);
```

See Also

`bioma.data.ExptData` | `DataMatrix` | `elementNames` | `featureNames` | `sampleNames`

How To

- “Working with ExptData Objects”

Purpose

Write DataMatrix object to text file

Syntax

```
dmwrite(DMObj, File)
dmwrite(..., 'Delimiter', DelimiterValue, ...)
dmwrite(..., 'Precision', PrecisionValue, ...)
dmwrite(..., 'Header', HeaderValue, ...)
dmwrite(..., 'Annotated', AnnotatedValue, ...)
dmwrite(..., 'Append', AppendValue, ...)
```

Arguments

DMObj	DataMatrix object, such as created by `DataMatrix` (object constructor).
File	String specifying either a file name or a path and file name for saving the text file.
DelimiterValue	String specifying a delimiter symbol to use as a matrix column separator. Typical choices are: • `' '` • `'\t'` (default) • `','` • `';'` • `'|'`
PrecisionValue	Precision for writing the data to the text file, specified by either: • Positive integer specifying the number of significant digits • C-style format string starting with `%`, such as `'%6.5f'` Default is `5`.

HeaderValue	String specifying the first line of the text file. Default is the Name property for the DataMatrix object.
AnnotatedValue	Controls the writing of row and column names to the text file. Choices are true (default) or false.
AppendValue	Controls the appending of *DMObj* to *File* when it is an existing file. Choices are true or false (default). If false, dmwrite overwrites *File*.

Description

dmwrite(*DMObj*, *File*) writes a DataMatrix object to a text file using the delimiter \t to separate DataMatrix columns. dmwrite writes the data starting at the first column of the first row in the destination file.

dmwrite(..., '*PropertyName*', *PropertyValue*, ...) calls dmwrite with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each *PropertyName* in single quotation marks. Each *PropertyName* is case insensitive. These property name/property value pairs are as follows:

dmwrite(..., 'Delimiter', *DelimiterValue*, ...) specifies a delimiter symbol to use as a column separator for separating matrix columns. Default is '\t'.

dmwrite(..., 'Precision', *PrecisionValue*, ...) specifies the precision for writing the data to the text file. Default is 5.

dmwrite(..., 'Header', *HeaderValue*, ...) specifies the first line of the text file. Default is the Name property for the DataMatrix object.

dmwrite(..., 'Annotated', *AnnotatedValue*, ...) controls the writing of row and column names to the text file. Choices are true (default) or false.

dmwrite(..., 'Append', *AppendValue*, ...) controls the appending of *DMObj* to *File* when it is an existing file. Choices are true or false (default). If false, dmwrite overwrites *File*.

Examples

Create a DataMatrix object and write the contents to a text file:

```
% Create a DataMatrix object
dmobj = bioma.data.DataMatrix(rand(2,3), {'Row1', 'Row2'}, ...
                                         {'Col1', 'Col2', 'Col3'})
% Write the DataMatrix object to a text file
dmwrite(dmobj,'testdm.txt')
```

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

dna2rna

Purpose

Convert DNA sequence to RNA sequence

Syntax

```
SeqRNA = dna2rna(SeqDNA)
```

Arguments

SeqDNA — DNA sequence specified by any of the following:

- Character string with the characters `A`, `C`, `G`, `T`, and ambiguous characters `R`, `Y`, `K`, `M`, `S`, `W`, `B`, `D`, `H`, `V`, `N`,
- Row vector of integers from the table Mapping Nucleotide Integers to Letter Codes on page 3-809.
- MATLAB structure containing a `Sequence` field that contains a DNA sequence, such as returned by `fastaread`, `fastqread`, `emblread`, `getembl`, `genbankread`, or `getgenbank`.

Description

SeqRNA = `dna2rna(`*SeqDNA*`)` converts a DNA sequence to an RNA sequence by converting any thymine nucleotides (`T`) in the DNA sequence to uracil nucleotides (`U`). The RNA sequence is returned in the same format as the DNA sequence. For example, if *SeqDNA* is a vector of integers, then so is *SeqRNA*.

Examples

Convert a DNA sequence to an RNA sequence.

```
rna = dna2rna('ACGATGAGTCATGCTT')

rna =
ACGAUGAGUCAUGCUU
```

See Also

Bioinformatics Toolbox function: `rna2dna`

MATLAB functions: `regexp`, `strrep`

Purpose

Estimate synonymous and nonsynonymous substitution rates

Syntax

```
[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2)
[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2,
...'GeneticCode', GeneticCodeValue, ...)
[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2, ...'Method',
   MethodValue, ...)
[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2, ...'Window',
   WindowValue, ...)
[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2,
   ...'AdjustStops', AdjustStopsValue, ...)
[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2, ...'Verbose',
   VerboseValue, ...)
```

Arguments

SeqNT1, *SeqNT2*	Nucleotide sequences. Enter either a string or a structure with the field `Sequence`.
GeneticCodeValue	Property to specify a genetic code. Enter a Code Number or a string with a Code Name from the table Genetic Code on page 3-8. If you use a Code Name, you can truncate it to the first two characters. Default is `1` or `Standard`.
MethodValue	String specifying the method for calculating substitution rates. Choices are: • `NG` (default) — Nei-Gojobori method (1986) uses the number of synonymous and nonsynonymous substitutions and the number of potentially synonymous and nonsynonymous sites. Based on the Jukes-Cantor model. • `LWL` — Li-Wu-Luo method (1985) uses the number of transitional and transversional substitutions at three different levels of

degeneracy of the genetic code. Based on Kimura's two-parameter model.

- `PBL` — Pamilo-Bianchi-Li method (1993) is similar to the Li-Wu-Luo method, but with bias correction. Use this method when the number of transitions is much larger than the number of transversions.

`WindowValue`	Integer specifying the sliding window size, in codons, for calculating substitution rates and variances.
`AdjustStopsValue`	Controls whether stop codons are excluded from calculations. Choices are `true` (default) or `false`.
`VerboseValue`	Property to control the display of the codons considered in the computations and their amino acid translations. Choices are `true` or `false` (default).

Tip Specify `true` to use this display to manually verify the codon alignment of the two input sequences. The presence of stop codons (`*`) in the amino acid translation can indicate that *`SeqNT1`* and *`SeqNT2`* are not codon-aligned.

Return Values

`Dn`	Nonsynonymous substitution rate(s).
`Ds`	Synonymous substitution rate(s).

Vardn	Variance for the nonsynonymous substitution rate(s).
Vards	Variance for the synonymous substitutions rate(s).

Description

`[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2)` estimates the synonymous and nonsynonymous substitution rates per site between the two homologous nucleotide sequences, *SeqNT1* and *SeqNT2*, by comparing codons using the Nei-Gojobori method.

`dnds` returns:

- *Dn* — Nonsynonymous substitution rate(s).
- *Ds* — Synonymous substitution rate(s).
- *Vardn* — Variance for the nonsynonymous substitution rate(s).
- *Vards* — Variance for the synonymous substitutions rate(s).

This analysis:

- Assumes that the nucleotide sequences, *SeqNT1* and *SeqNT2*, are codon-aligned, that is, do not have frame shifts

  Tip If your sequences are not codon-aligned, use the `nt2aa` function to convert them to amino acid sequences, use the `nwalign` function to globally align them, then use the `seqinsertgaps` function to recover the corresponding codon-aligned nucleotide sequences. See Estimating Synonymous and Nonsynonymous Substitution Rates Between Two Nucleotide Sequences That Are Not Codon-Aligned on page 3-427.

- Excludes codons that include ambiguous nucleotide characters or gaps

- Considers the number of codons in the shorter of the two nucleotide sequences

Caution

If *SeqNT1* and *SeqNT2* are too short or too divergent, saturation can be reached, and `dnds` returns `NaN`s and a warning message.

`[`*Dn, Ds, Vardn, Vards*`] = dnds(`*SeqNT1*`, `*SeqNT2*`, ...'`*PropertyName*`', `*PropertyValue*`, ...)` calls `dnds` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`[`*Dn, Ds, Vardn, Vards*`] = dnds(`*SeqNT1*`, `*SeqNT2*`, ...'GeneticCode', `*GeneticCodeValue*`, ...)` calculates synonymous and nonsynonymous substitution rates using the specified genetic code. Enter a Code Number or a string with a Code Name from the table Genetic Code on page 3-8. If you use a Code Name, you can truncate it to the first two characters. Default is `1` or `Standard`.

`[`*Dn, Ds, Vardn, Vards*`] = dnds(`*SeqNT1*`, `*SeqNT2*`, ...'Method', `*MethodValue*`, ...)` allows you to calculate synonymous and nonsynonymous substitution rates using the following algorithms:

- `NG` (default) — Nei-Gojobori method (1986) uses the number of synonymous and nonsynonymous substitutions and the number of potentially synonymous and nonsynonymous sites. Based on the Jukes-Cantor model.
- `LWL` — Li-Wu-Luo method (1985) uses the number of transitional and transversional substitutions at three different levels of degeneracy of the genetic code. Based on Kimura's two-parameter model.

- `PBL` — Pamilo-Bianchi-Li method (1993) is similar to the Li-Wu-Luo method, but with bias correction. Use this method when the number of transitions is much larger than the number of transversions.

`[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2, ...'Window', WindowValue, ...)` performs the calculations over a sliding window, specified in codons. Each output is an array containing a rate or variance for each window.

`[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2, ...'AdjustStops', AdjustStopsValue, ...)` controls whether stop codons are excluded from calculations. Choices are `true` (default) or `false`.

Tip When the `'AdjustStops'` property is set to `true`, the following are true:

- Stop codons are excluded from frequency tables.
- Paths containing stop codons are not counted in the Nei-Gojobori method.

`[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2, ...'Verbose', VerboseValue, ...)` controls the display of the codons considered in the computations and their amino acid translations. Choices are `true` or `false` (default).

Tip Specify `true` to use this display to manually verify the codon alignment of the two input sequences, *`SeqNT1`* and *`SeqNT2`*. The presence of stop codons (`*`) in the amino acid translation can indicate that *`SeqNT1`* and *`SeqNT2`* are not codon-aligned.

Examples

Estimating Synonymous and Nonsynonymous Substitution Rates Between the gag Genes of Two HIV Viruses

1 Retrieve two sequences from the GenBank database for the gag genes of two HIV viruses.

```
gag1 = getgenbank('L11768');
gag2 = getgenbank('L11770');
```

2 Estimate the synonymous and nonsynonymous substitution rates between the two sequences.

```
[dn ds vardn vards] = dnds(gag1, gag2)

dn =

    0.0244

ds =

    0.0697

vardn =

  2.3509e-005

vards =

  2.3438e-004
```

Estimating Synonymous and Nonsynonymous Substitution Rates Between Two Nucleotide Sequences That Are Not Codon-Aligned

1 Retrieve two nucleotide sequences from the GenBank database for the neuraminidase (NA) protein of two strains of the influenza A virus (H5N1).

```
hk01 = getgenbank('AF509094');
vt04 = getgenbank('DQ094287');
```

2 Extract the coding region from the two nucleotide sequences.

```
hk01_cds = featuresparse(hk01,'feature','CDS','Sequence',true);
vt04_cds = featuresparse(vt04,'feature','CDS','Sequence',true);
```

3 Align the amino acids sequences converted from the nucleotide sequences.

```
[sc,al] = nwalign(nt2aa(hk01_cds),nt2aa(vt04_cds),'extendgap',1);
```

4 Use the `seqinsertgaps` function to copy the gaps from the aligned amino acid sequences to their corresponding nucleotide sequences, thus codon-aligning them.

```
hk01_aligned = seqinsertgaps(hk01_cds,al(1,:))
vt04_aligned = seqinsertgaps(vt04_cds,al(3,:))
```

5 Estimate the synonymous and nonsynonymous substitutions rates of the codon-aligned nucleotide sequences and also display the codons considered in the computations and their amino acid translations.

```
[dn,ds] = dnds(hk01_aligned,vt04_aligned,'verbose',true)
```

References

[1] Li, W., Wu, C., and Luo, C. (1985). A new method for estimating synonymous and nonsynonymous rates of nucleotide substitution considering the relative likelihood of nucleotide and codon changes. Molecular Biology and Evolution *2(2)*, 150–174.

[2] Nei, M., and Gojobori, T. (1986). Simple methods for estimating the numbers of synonymous and nonsynonymous nucleotide substitutions. Molecular Biology and Evolution *3(5)*, 418–426.

[3] Nei, M., and Jin, L. (1989). Variances of the average numbers of nucleotide substitutions within and between populations. Molecular Biology and Evolution *6(3)*, 290–300.

[4] Nei, M., and Kumar, S. (2000). Synonymous and nonsynonymous nucleotide substitutions" in Molecular Evolution and Phylogenetics (Oxford University Press).

[5] Pamilo, P., and Bianchi, N. (1993). Evolution of the Zfx And Zfy genes: rates and interdependence between the genes. Molecular Biology and Evolution *10(2)*, 271–281.

See Also

Bioinformatics Toolbox functions: `dndsml`, `featuresparse`, `geneticcode`, `nt2aa`, `nwalign`, `seqinsertgaps`, `seqpdist`

Purpose

Estimate synonymous and nonsynonymous substitution rates using maximum likelihood method

Syntax

```
[Dn, Ds, Like] = dndsml(SeqNT1, SeqNT2)
[Dn, Ds, Like] = dndsml(SeqNT1, SeqNT2, ...'GeneticCode',
GeneticCodeValue, ...)
[Dn, Ds, Like] = dndsml(SeqNT1, SeqNT2, ...'Verbose',
   VerboseValue, ...)
```

Arguments

SeqNT1, *SeqNT2*	Nucleotide sequences. Enter either a string or a structure with the field `Sequence`.
GeneticCodeValue	Property to specify a genetic code. Enter a Code Number or a string with a Code Name from the table Genetic Code on page 3-8. If you use a Code Name, you can truncate it to the first two characters. Default is `1` or `Standard`.
VerboseValue	Property to control the display of the codons considered in the computations and their amino acid translations. Choices are `true` or `false` (default).

Tip Specify `true` to use this display to manually verify the codon alignment of the two input sequences. The presence of stop codons (`*`) in the amino acid translation can indicate that *SeqNT1* and *SeqNT2* are not codon-aligned.

Return Values

Dn	Nonsynonymous substitution rate(s).
Ds	Synonymous substitution rate(s).
Like	Likelihood of estimate of substitution rates.

Description

`[Dn, Ds, Like] = dndsml(SeqNT1, SeqNT2)` estimates the synonymous and nonsynonymous substitution rates between the two homologous sequences, *SeqNT1* and *SeqNT2*, using the Goldman-Yang method (1994). This maximum likelihood method estimates an explicit model for codon substitution that accounts for transition/transversion rate bias and base/codon frequency bias. Then it uses the model to correct synonymous and nonsynonymous counts to account for multiple substitutions at the same site. The maximum likelihood method is best suited when the sample size is significant (larger than 100 bases) and when the sequences being compared can have transition/transversion rate biases and base/codon frequency biases.

`dndsml` returns:

- *Dn* — Nonsynonymous substitution rate(s).
- *Ds* — Synonymous substitution rate(s).
- *Like* — Likelihood of this estimate.

This analysis:

- Assumes that the nucleotide sequences, *SeqNT1* and *SeqNT2*, are codon-aligned, that is, do not have frame shifts.

  Tip If your sequences are not codon-aligned, use the `nt2aa` function to convert them to amino acid sequences, use the `nwalign` function to globally align them, then use the `seqinsertgaps` function to recover the corresponding codon-aligned nucleotide sequences. See Estimating Synonymous and Nonsynonymous Substitution Rates Between Two Nucleotide Sequences That Are Not Codon-Aligned on page 3-432

- Excludes any ambiguous nucleotide characters or codons that include gaps.

- Considers the number of codons in the shorter of the two nucleotide sequences.

Caution

If *SeqNT1* and *SeqNT2* are too short or too divergent, saturation can be reached, and `dndsml` returns `NaN`s and a warning message.

`[`*`Dn, Ds, Like`*`] = dndsml(`*`SeqNT1`*`, `*`SeqNT2`*`, ...'`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `dnds` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`[`*`Dn, Ds, Like`*`] = dndsml(`*`SeqNT1`*`, `*`SeqNT2`*`, ...'GeneticCode', `*`GeneticCodeValue`*`, ...)` calculates synonymous and nonsynonymous substitution rates using the specified genetic code. Enter a Code Number or a string with a Code Name from the table Genetic Code on page 3-8. If you use a Code Name, you can truncate it to the first two characters. Default is `1` or `Standard`.

`[`*`Dn, Ds, Like`*`] = dndsml(`*`SeqNT1`*`, `*`SeqNT2`*`, ...'Verbose', `*`VerboseValue`*`, ...)` controls the display of the codons considered in the computations and their amino acid translations. Choices are `true` or `false` (default).

Tip Specify `true` to use this display to manually verify the codon alignment of the two input sequences, *`SeqNT1`* and *`SeqNT2`*. The presence of stop codons (`*`) in the amino acid translation can indicate that *`SeqNT1`* and *`SeqNT2`* are not codon-aligned.

Examples

Estimating Synonymous and Nonsynonymous Substitution Rates Between the gag Genes of Two HIV Viruses

1 Retrieve two sequences from the GenBank database for the gag genes of two HIV viruses

```
gag1 = getgenbank('L11768');
gag2 = getgenbank('L11770');
```

2 Estimate the synonymous and nonsynonymous substitution rates between the two sequences.

```
[dn ds like] = dndsml(gag1, gag2)

dn =
    0.0259
ds =
    0.0623
like =
   -2.1857e+003
```

Estimating Synonymous and Nonsynonymous Substitution Rates Between Two Nucleotide Sequences That Are Not Codon-Aligned

1 Retrieve two nucleotide sequences from the GenBank database for the neuraminidase (NA) protein of two strains of the Influenza A virus (H5N1).

```
hk01 = getgenbank('AF509094');
vt04 = getgenbank('DQ094287');
```

2 Extract the coding region from the two nucleotide sequences.

```
hk01_cds = featuresparse(hk01,'feature','CDS','Sequence',true);
vt04_cds = featuresparse(vt04,'feature','CDS','Sequence',true);
```

3 Align the amino acids sequences converted from the nucleotide sequences.

```
[sc,al]=nwalign(nt2aa(hk01_cds),nt2aa(vt04_cds),'extendgap',1);
```

4 Use the `seqinsertgaps` function to copy the gaps from the aligned amino acid sequences to their corresponding nucleotide sequences, thus codon-aligning them.

```
hk01_aligned = seqinsertgaps(hk01_cds,al(1,:));
vt04_aligned = seqinsertgaps(vt04_cds,al(3,:));
```

5 Estimate the synonymous and nonsynonymous substitutions rates of the codon-aligned nucleotide sequences and also display the codons considered in the computations and their amino acid translations.

```
[dn,ds] = dndsml(hk01_aligned,vt04_aligned,'verbose',true)

dn =
    0.0445

ds =
    0.1576
```

References

[1] Tamura, K., and Mei, M. (1993). Estimation of the number of nucleotide substitutions in the control region of mitochondrial DNA in humans and chimpanzees. Molecular Biology and Evolution *10*, 512–526.

[2] Yang, Z., and Nielsen, R. (2000). Estimating synonymous and nonsynonymous substitution rates under realistic evolutionary models. Molecular Biology and Evolution *17*, 32–43.

[3] Goldman, N., and Yang, Z. (1994). A Codon-based Model of Nucleotide Substitution for Protein-coding DNA Sequences. Mol. Biol. Evol. *11(5)*, 725–736.

See Also

Bioinformatics Toolbox functions: `dnds`, `featuresparse`, `geneticcode`, `nt2aa`, `nwalign`, `seqinsertgaps`, `seqpdist`

Purpose

Calculate node positions and edge trajectories

Syntax

```
dolayout(BGobj)
dolayout(BGobj, 'Paths', PathsOnlyValue)
```

Arguments

BGobj	Biograph object created by the `biograph` function (object constructor).
PathsOnlyValue	Controls the calculation of only the edge paths, leaving the nodes at their current positions. Choices are `true` or `false` (default).

Description

Note To use the `dolayout` method, you must have accepted a Graphviz software license (free). If you have not, you will be prompted to do so.

`dolayout(BGobj)` calls the layout engine to calculate the optimal position for each node so that its 2-D rendering is clean and uncluttered, and then calculates the best curves to represent the edges. The layout engine uses the following properties of the biograph object:

- `LayoutType` — Specifies the layout engine as `'hierarchical'`, `'equilibrium'`, or `'radial'`.
- `LayoutScale` — Rescales the sizes of the node before calling the layout engine. This gives more space to the layout and reduces the overlapping of nodes.
- `NodeAutoSize` — Controls precalculating the node size before calling the layout engine. When `NodeAutoSize` is set to `'on'`, the layout engine uses the node properties `FontSize` and `Shape`, and the biograph object property `LayoutScale` to precalculate the actual size of each node. When `NodeAutoSize` is set to `'off'`, the layout engine uses the node property `Size`.

For more information on the above properties, see Properties of a Biograph Object on page 3-128. For information on accessing and specifying the above properties of a biograph object, see Determining Properties and Property Values of a Biograph Object on page 3-134 and Specifying Properties of a Biograph Object on page 3-135.

`dolayout(`*`BGobj`*`, 'Paths', `*`PathsOnlyValue`*`)` controls the calculation of only the edge paths, leaving the nodes at their current positions. Choices are `true` or `false` (default).

Examples

1 Create a biograph object.

```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];
bg = biograph(cm)
Biograph object with 5 nodes and 9 edges.
bg.nodes(1).Position

ans =

     []
```

Nodes do not have a position yet.

2 Call the layout engine and render the graph.

```
dolayout(bg)
bg.nodes(1).Position

ans =

   112   224

view(bg)
```

3 Manually modify a node position and recalculate the paths only.

```
bg.nodes(1).Position = [150 150];
dolayout(bg, 'Pathsonly', true)
```

```
view(bg)
```

See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: `dolayout`, `get`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `set`, `view`

double (DataMatrix)

Purpose

Convert DataMatrix object to double-precision array

Syntax

```
B = double(DMObj)
B = double(DMObj, Rows)
B = double(DMObj, Rows, Cols)
```

Arguments

DMObj	DataMatrix object, such as created by `DataMatrix` (object constructor).
Rows, *Cols*	Row(s) or column(s) in *DMObj*, specified by one of the following: • Scalar • Vector of positive integers • String specifying a row or column name • Cell array of row or column names • Logical vector

Return Values

B	MATLAB numeric array.

Description

B = `double(`*DMObj*`)` converts *DMObj*, a DataMatrix object, to a double-precision array, which it returns in *B*.

B = `double(`*DMObj*`, `*Rows*`)` converts a subset of *DMObj*, a DataMatrix object, specified by *Rows*, to a double-precision array, which it returns in*B*. *Rows* can be a positive integer, vector of positive integers, string specifying a row name, cell array of row names, or a logical vector.

B = `double(`*DMObj*`, `*Rows*`, `*Cols*`)` converts a subset of *DMObj*, a DataMatrix object, specified by *Rows* and *Cols*, to a double-precision array, which it returns in*B*. *Cols* can be a positive integer, vector of

positive integers, string specifying a column name, cell array of column names, or a logical vector.

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: `single`

bioma.ExpressionSet.elementData

Purpose

Retrieve or set data element (DataMatrix object) in ExpressionSet object

Syntax

```
DMObj = elementData(ESObj, Element)
NewESObj = elementData(ESObj, Element, NewDMObj)
```

Description

`DMObj = elementData(ESObj, Element)` returns the DataMatrix object from an ExpressionSet object, specified by *`Element`*, a positive integer or a string specifying an element name.

`NewESObj = elementData(ESObj, Element, NewDMObj)` replaces the DataMatrix object specified by *`Element`* in *`ESObj`*, an ExpressionSet object, with *`NewDMObj`*, a new DataMatrix object, and returns *`NewESObj`*, a new ExpressionSet object.

Inputs

`ESObj`

Object of the `bioma.ExpressionSet` class.

`Element`

Element (DataMatrix object) in an ExpressionSet object, specified by either of the following:

- Positive integer
- String specifying the element name

`NewDMObj`

Object of the DataMatrix class. The sample names and feature names in *`NewDMObj`* must match the sample names and feature names in the DataMatrix object specified by *`Element`*.

Outputs

`DMObj`

Object of the DataMatrix class, returned from the ExptData object of an ExpressionSet object.

`NewESObj`

Object of the `bioma.ExpressionSet` class, returned after replacing a specified data element (DataMatrix object).

Examples

Construct an ExpressionSet object from `EDObj`, an ExptData object, `MDObj2`, a MetaData object containing sample variable information, and `MIAMEObj`, a MIAME object. Extract a DataMatrix object from it:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Construct MIAME object
MIAMEObj = MIAME(geoStruct);
% Import bioma package to make constructor function
% available
import bioma.*
% Construct ExpressionSet object
ESObj = ExpressionSet(EDObj, 'SData', MDObj2, 'EInfo', MIAMEObj);
% Extract first DataMatrix object
ExtractedDMObj = elementData(ESObj, 1);
```

See Also

`bioma.ExpressionSet` | `bioma.data.ExptData` | `DataMatrix`

How To

- "Working with ExpressionSet Objects"

bioma.data.ExptData.elementData

Purpose

Retrieve or set data element (DataMatrix object) in ExptData object

Syntax

```
DMObj = elementData(EDObj, Element)
NewEDObj = elementData(EDObj, Element, NewDMObj)
```

Description

`DMObj = elementData(EDObj, Element)` returns the DataMatrix object from an ExptData object, specified by `Element`, a positive integer or string specifying an element name.

`NewEDObj = elementData(EDObj, Element, NewDMObj)` replaces the element (DataMatrix object) specified by `Element` in `EDObj`, an ExptData object, with `NewDMObj`, a new DataMatrix object, and returns `NewEDObj`, a new ExptData object.

Inputs

EDObj

Object of the `bioma.data.ExptData` class.

Element

Element (DataMatrix object) in an ExptData object, specified by either of the following:

- Positive integer
- String specifying the element name

NewDMObj

Object of the DataMatrix class. The sample names and feature names in *NewDMObj* must match the sample names and feature names of *EDObj*.

Outputs

DMObj

Object of the DataMatrix class, returned from an ExptData object.

NewEDObj

Object of the `bioma.data.ExptData` class, returned after replacing a data element (DataMatrix object).

Examples

Construct an ExptData object, and then extract a DataMatrix object from it:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Extract first DataMatrix object
ExtractedDMObj = elementData(EDObj, 1);
```

See Also

`bioma.data.ExptData` | `DataMatrix`

How To

- "Working with ExptData Objects"

bioma.ExpressionSet.elementNames

Purpose

Retrieve or set element names of DataMatrix objects in ExpressionSet object

Syntax

```
ElmtNames = elementNames(ESObj)
ElmtNames = elementNames(ESObj, Subset)
NewESObj = elementNames(ESObj, Subset, NewElmtNames)
```

Description

`ElmtNames = elementNames(ESObj)` returns a cell array of strings specifying the element names of all the data elements (DataMatrix objects) stored in the ExptData object in an ExpressionSet object.

`ElmtNames = elementNames(ESObj, Subset)` returns a cell array of strings specifying the element names of a subset of the data elements (DataMatrix objects) in the ExptData object in an ExpressionSet object.

`NewESObj = elementNames(ESObj, Subset, NewElmtNames)` replaces the element names of the data elements (DataMatrix objects) specified by `Subset` in `ESObj`, an ExpressionSet object, with `NewElmtNames`, and returns `NewESObj`, a new ExpressionSet object.

Inputs

ESObj

Object of the `bioma.ExpressionSet` class.

Subset

One of the following to specify the element names of a subset of the data elements (DataMatrix objects) in the ExptData object of an ExpressionSet object:

- String specifying an element name
- Cell array of strings specifying element names
- Positive integer
- Vector of positive integers
- Logical vector

NewElmtNames

New element names for specific data elements (DataMatrix objects) within an ExpressionSet object, specified by one of the following:

- Numeric vector
- String or cell array of strings
- String, which `elementNames` uses as a prefix for the element names, with element numbers appended to the prefix
- Logical `true` or `false` (default). If `true`, `elementNames` assigns unique element names using the format `Elmt1`, `Elmt2`, etc.

The number of elements in *`NewElmtNames`* must equal the number of elements specified by *`Subset`*.

Outputs

`ElmtNames`

Cell array of strings specifying the element names of all or some of the data elements (DataMatrix objects) in the ExptData object of an ExpressionSet object.

`NewESObj`

Object of the `bioma.ExpressionSet` class, returned after replacing element names of specific data elements (DataMatrix objects).

Examples

Construct an ExpressionSet object from `EDObj`, an ExptData object, `MDObj2`, a MetaData object containing sample variable information, and `MIAMEObj`, a MIAME object. Retrieve the element names of the DataMatrix objects in it:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
```

```
EDObj = ExptData(dmObj);
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Construct MIAME object
MIAMEObj = MIAME(geoStruct);
% Import bioma package to make constructor function
% available
import bioma.*
% Construct ExpressionSet object
ESObj = ExpressionSet(EDObj, 'SData', MDObj2, 'EInfo', MIAMEObj);
% Retrieve element names of DataMatrix objects
ENames = elementNames(ESObj);
```

See Also

bioma.ExpressionSet | bioma.data.ExptData | DataMatrix | exptData

How To

- “Working with ExpressionSet Objects”

Purpose

Retrieve or set element names of DataMatrix objects in ExptData object

Syntax

```
ElmtNames = elementNames(EDObj)
ElmtNames = elementNames(EDObj, Subset)
NewEDObj = elementNames(EDObj, Subset, NewElmtNames)
```

Description

`ElmtNames = elementNames(EDObj)` returns a cell array of strings specifying the element names of all the data elements (DataMatrix objects) stored in an ExptData object.

`ElmtNames = elementNames(EDObj, Subset)` returns a cell array of strings specifying the element names of a subset of the data elements (DataMatrix objects) stored in an ExptData object.

`NewEDObj = elementNames(EDObj, Subset, NewElmtNames)` replaces the element names of the data elements (DataMatrix objects) specified by `Subset` in `EDObj`, an ExptData object, with `NewElmtNames`, and returns `NewEDObj`, a new ExptData object.

Inputs

EDObj

Object of the `bioma.data.ExptData` class.

Subset

One of the following to specify the element names of a subset of the data elements (DataMatrix objects) in an ExptData object:

- String specifying an element name
- Cell array of strings specifying element names
- Positive integer
- Vector of positive integers
- Logical vector

NewElmtNames

New element names for specific data elements (DataMatrix objects) within an ExptData object, specified by one of the following:

- Numeric vector
- String or cell array of strings
- String, which `elementNames` uses as a prefix for the element names, with element numbers appended to the prefix
- Logical `true` or `false` (default). If `true`, `elementNames` assigns unique element names using the format `Elmt1`, `Elmt2`, etc.

The number of elements in *`NewElmtNames`* must equal the number of elements specified by *`Subset`*.

Outputs

`ElmtNames`

Cell array of strings specifying the element names of all or some of the data elements (DataMatrix objects) in an ExptData object.

`NewEDObj`

Object of the `bioma.data.ExptData` class, returned after replacing element names of specific data elements (DataMatrix objects).

Examples

Construct an ExptData object, and then retrieve the element names of DataMatrix objects from it:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Retrieve element names of DataMatrix objects
ENames = elementNames(EDObj);
```

See Also

`bioma.data.ExptData` | `DataMatrix` | `dmNames` | `featureNames` | `sampleNames`

How To

- "Working with ExptData Objects"

emblread

Purpose

Read data from EMBL file

Syntax

```
EMBLData = emblread(File)
EMBLSeq = emblread (File, 'SequenceOnly',
SequenceOnlyValue)
```

Arguments

File	Either of the following: • String specifying a file name, a path and file name, or a URL pointing to a file. The referenced file is an EMBL-formatted file. • MATLAB character array that contains the text of an EMBL-formatted file
SequenceOnlyValue	Controls the reading of only the sequence without the metadata. Choices are `true` or `false` (default).

Return Values

EMBLData	MATLAB structure with fields corresponding to EMBL data.
EMBLSeq	MATLAB character string representing the sequence.

Description

EMBLData = emblread(*File*) reads data from *File*, an EMBL-formatted file, and creates *EMBLData*, a MATLAB structure with fields corresponding to the EMBL two-character line type code. Each line type code is stored as a separate element in the structure.

EMBLData contains the following fields.

Field
Identification.EntryName

Field
Identification.Version
Identification.Topology
Identification.Molecule
Identification.DataClass
Identification.Division
Identification.SequenceLength
Accession
SequenceVersion
DateCreated
DateUpdated
Description
Keyword
OrganismSpecies
OrganismClassification
Organelle
Reference{#}.Number
Reference{#}.Comment
Reference{#}.Position
Reference{#}.MedLine
Reference{#}.PubMed
Reference{#}.Group
Reference{#}.Authors
Reference{#}.Title
Reference{#}.Location
DatabaseCrossReference

Field
Comments
Assembly
Feature
Basecount.BP
Basecount.A
Basecount.C
Basecount.G
Basecount.T
Basecount.Other
Sequence

Note Topology information was not included in EMBL flat files before release 87 of the database. When reading a file created before release 87, EMBLREAD returns an empty `Identification.Topology` field.

Note The entry name is no longer displayed in the ID line of EMBL flat files in release 87. When reading a file created in release 87, EMBLREAD returns the accession number in the `Identification.EntryName` field.

`EMBLSeq` `= emblread (`*`File`*`, 'SequenceOnly',` *`SequenceOnlyValue`*`)` controls the reading of only the sequence without the metadata. Choices are `true` or `false` (default).

Examples

Retrieve sequence information from the Web, save to a file, and then read back into the MATLAB software.

1 Use the `getembl` function and `ToFile` property to retrieve sequence information from the Web and save to an EMBL-formatted file.

```
getembl('X00558','ToFile','rat_protein.txt');
```

2 Read data from the EMBL-formatted file and create a MATLAB structure.

```
EMBLData = emblread('rat_protein.txt')

EMBLData =

            Identification: [1x1 struct]
                 Accession: 'X00558'
           SequenceVersion: 'X00558.1'
               DateCreated: '13-JUN-1985 (Rel. 06, Created)'
               DateUpdated: [1x46 char]
               Description: [1x75 char]
                   Keyword: [1x75 char]
           OrganismSpecies: [1x75 char]
    OrganismClassification: [3x75 char]
                 Organelle: ''
                 Reference: {[1x1 struct]}
    DatabaseCrossReference: ''
                  Comments: ''
                  Assembly: ''
                   Feature: [23x75 char]
                 BaseCount: [1x1 struct]
                  Sequence: [1x877 char]
```

See Also

Bioinformatics Toolbox functions: `fastaread`, `genbankread`, `genpeptread`, `getembl`, `pdbread`, `seqtool`

eq (DataMatrix)

Purpose

Test DataMatrix objects for equality

Syntax

```
T = eq(DMObj1, DMObj2)
T = DMObj1 == DMObj2
T = eq(DMObj1, B)
T = DMObj1 == B
T = eq(B, DMObj1)
T = B == DMObj1
```

Arguments

DMObj1, *DMObj2*	DataMatrix objects, such as created by `DataMatrix` (object constructor).
B	MATLAB numeric or logical array.

Return Values

T	Logical matrix of the same size as *DMObj1* and *DMObj2* or *DMObj1* and *B*. It contains logical `1` (true) where elements in the first input are equal to the corresponding element in the second input, and logical `0` (false) when they are not equal.

Description

T = `eq(`*DMObj1*`,` *DMObj2*`)` or the equivalent *T* = *DMObj1* == *DMObj2* compares each element in DataMatrix object *DMObj1* to the corresponding element in DataMatrix object *DMObj2*, and returns *T*, a logical matrix of the same size as *DMObj1* and *DMObj2*, containing logical `1` (true) where elements in *DMObj1* are equal to the corresponding element in *DMObj2*, and logical `0` (false) when they are not equal. *DMObj1* and *DMObj2* must have the same size (number of rows and columns), unless one is a scalar (1-by-1 DataMatrix object). *DMObj1* and *DMObj2* can have different `Name` properties.

T = `eq(`*DMObj1*`,` *B*`)` or the equivalent *T* = *DMObj1* == *B* compares each element in DataMatrix object *DMObj1* to the corresponding element in *B*, a numeric or logical array, and returns *T*, a logical matrix of the same size as *DMObj1* and *B*, containing logical `1` (true) where elements

in *DMObj1* are equal to the corresponding element in *B*, and logical 0 (false) when they are not equal. *DMObj1* and *B* must have the same size (number of rows and columns), unless one is a scalar.

T = eq(*B*, *DMObj1*) or the equivalent *T* = *B* == *DMObj1* compares each element in *B*, a numeric or logical array, to the corresponding element in DataMatrix object *DMObj1*, and returns *T*, a logical matrix of the same size as *B* and *DMObj1*, containing logical 1 (true) where elements in *B* are equal to the corresponding element in *DMObj1*, and logical 0 (false) when they are not equal. *B* and *DMObj1* must have the same size (number of rows and columns), unless one is a scalar.

MATLAB calls *T* = eq(*X*, *Y*) for the syntax *T* = *X* == *Y* when *X* or *Y* is a DataMatrix object.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: ne

evalrasmolscript

Purpose

Send RasMol script commands to Molecule Viewer window

Syntax

```
evalrasmolscript(FigureHandle, Command)
evalrasmolscript(FigureHandle, 'File', FileValue)
```

Arguments

FigureHandle — Figure handle to a molecule viewer returned by the `molviewer` function.

Command — Either of the following:

- String specifying one or more RasMol script commands. Use a `;` to separate commands.
- Character array or cell array containing strings specifying RasMol script commands.

Note For a complete list of RasMol script commands, see

```
http://www.stolaf.edu/academics/chemapps/jmol/docs/
```

FileValue — String specifying a file name or a path and file name of a text file containing Jmol script commands. If you specify only a file name, that file must be on the MATLAB search path or in the MATLAB Current Directory.

Description

`evalrasmolscript(FigureHandle, Command)` sends the RasMol script commands specified by *`Command`* to *`FigureHandle`*, the figure handle of a Molecule Viewer window created using the `molviewer` function.

`evalrasmolscript(FigureHandle, 'File', FileValue)` sends the RasMol script commands specified by *`FileValue`* to *`FigureHandle`*,

the figure handle of a Molecule Viewer window created using the `molviewer` function.

Examples

1. Use the `molviewer` function to create a figure handle to a Molecule Viewer window.

   ```
   FH = molviewer('2DHB')
   ```

2. Use the `evalrasmolscript` function to send script commands to the molecule viewer that change the background to black and spin the molecule.

   ```
   evalrasmolscript(FH, 'background white; spin')
   ```

See Also

Bioinformatics Toolbox functions: `getpdb`, `molviewer`, `pdbread`, `pdbwrite`

bioma.ExpressionSet.expressions

Purpose

Retrieve or set `Expressions` DataMatrix object from ExpressionSet object

Syntax

```
ExpressionsDMObj = expressions(ESObj)
NewESObj = expressions(ESObj, NewDMObj)
```

Description

`ExpressionsDMObj = expressions(ESObj)` returns the `Expressions` element (DataMatrix object), which contains expression values, from an ExpressionSet object.

`NewESObj = expressions(ESObj, NewDMObj)` replaces the `Expressions` element (DataMatrix object) in *`ESObj`*, an ExpressionSet object, with *`NewDMObj`*, a new DataMatrix object, and returns *`NewESObj`*, a new ExpressionSet object.

Inputs

`ESObj`

Object of the `bioma.ExpressionSet` class.

`NewDMObj`

Object of the DataMatrix class.

Outputs

`ExpressionsDMObj`

DataMatrix object containing the expression values from the `Expressions` DataMatrix object within an ExpressionSet object.

`NewESObj`

ExpressionSet object returned after replacing the `Expressions` DataMatrix object.

Examples

Construct an ExpressionSet object from `EDObj`, an ExptData object, `MDObj2`, a MetaData object containing sample variable information, and `MIAMEObj`, a MIAME object. Extract the `Expressions` DataMatrix object from it:

```
% Import bioma.data package to make constructor functions
% available
```

```
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Construct MIAME object
MIAMEObj = MIAME(geoStruct);
% Import bioma package to make constructor function
% available
import bioma.*
% Construct ExpressionSet object
ESObj = ExpressionSet(EDObj, 'SData', MDObj2, 'EInfo', MIAMEObj);
% Extract expression values from Expressions DataMatrix object
ExpressionsDMObj = expressions(ESObj);
```

See Also

bioma.ExpressionSet | bioma.data.ExptData | DataMatrix

How To

- “Working with ExpressionSet Objects”

exprprofrange

Purpose

Calculate range of gene expression profiles

Syntax

```
Range = exprprofrange(Data)
[Range, LogRange] = exprprofrange(Data)
... = exprprofrange(Data, 'ShowHist', ShowHistValue)
```

Arguments

Data	DataMatrix object or numeric matrix of expression values, where each row corresponds to a gene.
ShowHistValue	Controls the display of a histogram with range data. Choices are `true` or `false` (default).

Description

Range = `exprprofrange(`*Data*`)` calculates the range of each expression profile in *Data*, a DataMatrix object or numeric matrix of expression values, where each row corresponds to a gene.

`[`*Range, LogRange*`] = exprprofrange(`*Data*`)` returns the log range, that is, `log(max(prof))- log(min(prof))`, of each expression profile. If you do not specify output arguments, `exprprofrange` displays a histogram bar plot of the range.

`... = exprprofrange(`*Data*`, 'ShowHist', `*ShowHistValue*`)` controls the display of a histogram with range data. Choices for *ShowHistValue* are `true` or `false` (default).

Examples

1. Load the MAT-file, provided with the Bioinformatics Toolbox software, that contains yeast data. This MAT-file includes three variables: `yeastvalues`, a matrix of gene expression data, `genes`, a cell array of GenBank accession numbers for labeling the rows in `yeastvalues`, and `times`, a vector of time values for labeling the columns in `yeastvalues`

   ```
   load yeastdata
   ```

2. Calculate the range of expression profiles for yeast data as gene expression changes during the metabolic shift from fermentation to respiration. Display a histogram of the data.

```
range = exprprofrange(yeastvalues,'ShowHist',true);
```

See Also

Bioinformatics Toolbox functions: `exprprofvar`, `generangefilter`

exprprofvar

Purpose

Calculate variance of gene expression profiles

Syntax

```
Variance = exprprofvar(Data)
exprprofvar(..., 'PropertyName', PropertyValue,...)
exprprofvar(..., 'ShowHist', ShowHistValue)
```

Arguments

Data	DataMatrix object or numeric matrix of expression values, where each row corresponds to a gene.
ShowHistValue	Property to control the display of a histogram with variance data. Enter either `true` or `false` (default).

Description

Variance = exprprofvar(*Data*) calculates the variance of each expression profile in *Data*, a DataMatrix object or numeric matrix of expression values, where each row corresponds to a gene. If you do not specify output arguments, this function displays a histogram bar plot of the range.

exprprofvar(..., '*PropertyName*', *PropertyValue*,...) defines optional properties using property name/value pairs.

exprprofvar(..., 'ShowHist', *ShowHistValue*), when ShowHist is `true`, displays a histogram of the range data .

Examples

1. Load the MAT-file, provided with the Bioinformatics Toolbox software, that contains yeast data. This MAT-file includes three variables: `yeastvalues`, a matrix of gene expression data, `genes`, a cell array of GenBank accession numbers for labeling the rows in `yeastvalues`, and `times`, a vector of time values for labeling the columns in `yeastvalues`

   ```
   load yeastdata
   ```

2. Calculate the variance of expression profiles for yeast data as gene expression changes during the metabolic shift from fermentation to respiration. Display a histogram of the data.

```
datavar = exprprofvar(yeastvalues,'ShowHist',true);
```

See Also

Bioinformatics Toolbox functions: `exprprofrange`, `generangefilter`, `genevarfilter`

bioma.ExpressionSet.exprWrite

Purpose

Write expression values in ExpressionSet object to text file

Syntax

```
exprWrite(ESObj, File)
exprWrite(..., 'Delimiter', DelimiterValue, ...)
exprWrite(..., 'Precision', PrecisionValue, ...)
exprWrite(..., 'Header', HeaderValue, ...)
exprWrite(..., 'Annotated', AnnotatedValue, ...)
exprWrite(..., 'Append', AppendValue, ...)
```

Description

`exprWrite(ESObj, File)` writes the expression values in the `Expressions` element (DataMatrix object) from an ExpressionSet object to a text file, using the delimiter `\t` to separate columns. `exprWrite` writes the data starting at the first column of the first row in the destination file.

`exprWrite(..., 'PropertyName', PropertyValue, ...)` calls `exprWrite` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each *`PropertyName`* in single quotation marks. Each *`PropertyName`* is case insensitive. These property name/property value pairs are as follows:

`exprWrite(..., 'Delimiter', DelimiterValue, ...)` specifies a delimiter symbol to use as a column separator. Default is `'\t'`.

`exprWrite(..., 'Precision', PrecisionValue, ...)` specifies the precision for writing the data to the text file. Default is `5`.

`exprWrite(..., 'Header', HeaderValue, ...)` specifies the first line of the text file. Default is the `Name` property for the DataMatrix object.

`exprWrite(..., 'Annotated', AnnotatedValue, ...)` controls the writing of row and column names to the text file. Choices are `true` (default) or `false`.

`exprWrite(..., 'Append', AppendValue, ...)` controls the appending of the expression values to *`File`* when it is an existing file. Choices are `true` or `false` (default). If `false`, `exprWrite` overwrites *`File`*.

Inputs

ESObj

Object of the `bioma.ExpressionSet` class.

File

String specifying either a file name or a path and file name for saving the expression values. If you specify only a file name, `exprWrite` saves the file to the MATLAB Current Folder.

DelimiterValue

String specifying a delimiter symbol to use as a matrix column separator. Typical choices are:

- `' '`
- `'\t'` (default)
- `','`
- `';'`
- `'|'`

PrecisionValue

Precision for writing the data to the text file, specified by either:

- Positive integer specifying the number of significant digits
- C-style format string starting with `%`, such as `'%6.5f'`

Default: `5`

HeaderValue

String specifying the first line of the text file. Default is the `Name` property for the DataMatrix object.

AnnotatedValue

Controls the writing of row and column names to the text file. Choices are `true` (default) or `false`.

AppendValue

Controls the appending of the expression values to *File* when it is an existing file. Choices are `true` or `false` (default). If `false`, `exprWrite` overwrites *File*.

Examples

Construct an ExpressionSet object from `EDObj`, an ExptData object, `MDObj2`, a MetaData object containing sample variable information, and `MIAMEObj`, a MIAME object. Write the expression values in the ExpressionSet object to a text file:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Construct MIAME object
MIAMEObj = MIAME(geoStruct);
% Import bioma package to make constructor function
% available
import bioma.*
% Construct ExpressionSet object
ESObj = ExpressionSet(EDObj, 'SData', MDObj2, 'EInfo', MIAMEObj);
% Write expression values to text file
exprWrite(ESObj, 'myexpressiondata.txt')
```

See Also

`bioma.ExpressionSet` | `bioma.data.ExptData` | `DataMatrix` | `dmwrite`

How To

- "Working with ExpressionSet Objects"

Purpose

Retrieve or set experiment data in ExpressionSet object

Syntax

```
ExptDataObj = exptData(ESObj)
NewESObj = exptData(ESObj, NewExptDataObj)
```

Description

`ExptDataObj = exptData(ESObj)` returns the ExptData object stored in an ExpressionSet object.

`NewESObj = exptData(ESObj, NewExptDataObj)` replaces the ExptData object in *`ESObj`*, an ExpressionSet object, with *`NewExptDataObj`*, a new ExptData object, and returns *`NewESObj`*, a new ExpressionSet object.

Inputs

`ESObj`

Object of the `bioma.ExpressionSet` class.

`NewExptDataObj`

Object of the `bioma.data.ExptData` class.

Outputs

`ExptDataObj`

Object of the `bioma.data.ExptData` class.

`NewESObj`

Object of the `bioma.ExpressionSet` class, returned after replacing the ExptData object.

Examples

Construct an ExpressionSet object from `EDObj`, an ExptData object, `MDObj2`, a MetaData object containing sample variable information, and `MIAMEObj`, a MIAME object. Retrieve the ExptData object stored in the ExpressionSet object:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
```

```
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Construct MIAME object
MIAMEObj = MIAME(geoStruct);
% Import bioma package to make constructor function
% available
import bioma.*
% Construct ExpressionSet object
ESObj = ExpressionSet(EDObj, 'SData', MDObj2, 'EInfo', MIAMEObj);
% Retrieve the ExptData object
NewEDObj = exptData(ESObj);
```

See Also

bioma.ExpressionSet | bioma.data.ExptData | DataMatrix | featureData | sampleData

How To

- "Working with ExpressionSet Objects"

Purpose

Retrieve or set experiment information in ExpressionSet object

Syntax

```
MIAMEObj = exptInfo(ESObj)
NewESObj = exptInfo(ESObj, NewMIAMEObj)
```

Description

`MIAMEObj = exptInfo(ESObj)` returns a MIAME object containing experiment information from an ExpressionSet object.

`NewESObj = exptInfo(ESObj, NewMIAMEObj)` replaces the MIAME object in *`ESObj`*, an ExpressionSet object, with *`NewMIAMEObj`*, a new MIAME object, and returns *`NewESObj`*, a new ExpressionSet object.

Inputs

`ESObj`

Object of the `bioma.ExpressionSet` class.

`NewMIAMEObj`

Object of the `bioma.data.MIAME` class.

Outputs

`MIAMEObj`

Object of the `bioma.data.MIAME` class.

`NewESObj`

Object of the `bioma.ExpressionSet` class, returned after replacing the MIAME object.

Examples

Construct an ExpressionSet object from `EDObj`, an ExptData object, `MDObj2`, a MetaData object containing sample variable information, and `MIAMEObj`, a MIAME object. Retrieve the MIAME object stored in the ExpressionSet object:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
```

```
% Construct ExptData object
EDObj = ExptData(dmObj);
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Construct MIAME object
MIAMEObj = MIAME(geoStruct);
% Import bioma package to make constructor function
% available
import bioma.*
% Construct ExpressionSet object
ESObj = ExpressionSet(EDObj, 'SData', MDObj2, 'EInfo', MIAMEObj);
% Retrieve the MIAME object
NewMIAMEObj = exptInfo(ESObj);
```

See Also

`bioma.ExpressionSet` | `bioma.data.MIAME`

How To

- "Working with ExpressionSet Objects"
- http://www.mged.org/Workgroups/MIAME/miame.html

Purpose

Return information about FASTA file

Syntax

```
InfoStruct = fastainfo(File)
```

Description

`InfoStruct = fastainfo(File)` returns a MATLAB structure containing summary information about a FASTA-formatted file.

Inputs

`File`

FASTA-formatted file specified by one of the following:

- String specifying a file name or path and file name of a FASTA-formatted file. If you specify only a file name, that file must be on the MATLAB search path or in the current folder.
- URL pointing to a FASTA-formatted file.
- MATLAB character array containing the text of a FASTA-formatted file.

Outputs

`InfoStruct`

MATLAB structure containing summary information about a FASTA-formatted file. The structure contains the following fields.

Field	Description
`Filename`	Name of the file.
`FileModDate`	Modification date of the file.
`FileSize`	Size of the file in bytes.
`NumberOfEntries`	Number of sequence entries in the file.

Examples

Return a summary of the contents of a FASTA file:

```
info = fastainfo('p53nt.txt')
```

```
info =

           Filename: 'p53nt.txt'
        FileModDate: '31-Mar-2003 11:44:27'
           FileSize: 2764
    NumberOfEntries: 1
```

See Also

fastaread | fastawrite | fastqinfo | fastqread | fastqwrite | sffinfo | sffread

Purpose

Read data from FASTA file

Syntax

```
FASTAData = fastaread(File)
[Header, Sequence] = fastaread(File)
... = fastaread(File, ...'IgnoreGaps',
IgnoreGapsValue, ...)
... = fastaread(File, ...'Blockread', BlockreadValue, ...)
```

Arguments

File	FASTA-formatted file (ASCII text file). Enter a file name, a path and file name, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text for a file name.
IgnoreGapsValue	Property to control removing gap symbols. Enter either `true` or `false` (default).
BlockreadValue	Property to control reading a single sequence entry or block of sequence entries from a file containing multiple sequences. Enter a scalar *N*, to read the *N*th entry in the file. Enter a 1-by-2 vector [*M1, M2*], to read the block of entries starting at the *M1* entry and ending at the *M2* entry. To read all remaining entries in the file starting at the *M1* entry, enter a positive value for *M1* and enter `Inf` for *M2*.

Return Values

FASTAData	MATLAB structure with the fields `Header` and `Sequence`.

Description

`fastaread` reads data from a FASTA-formatted file into a MATLAB structure with the following fields.

Field
Header
Sequence

A file with a FASTA format begins with a right angle bracket (>) and a single line description. Following this description is the sequence as a series of lines with fewer than 80 characters. Sequences are expected to use the standard IUB/IUPAC amino acid and nucleotide letter codes.

For a list of codes, see `aminolookup` and `baselookup`.

`FASTAData` `= fastaread(`*`File`*`)` reads a file with a FASTA format and returns the data in a structure. `FASTAData.Header` is the header information, while `FASTAData.Sequence` is the sequence stored as a string of letters.

`[`*`Header, Sequence`*`] = fastaread(`*`File`*`)` reads data from a file into separate variables. If the file contains more than one sequence, then `header` and `sequence` are cell arrays of header and sequence information.

`...  = fastaread(`*`File`*`, ...'PropertyName',` *`PropertyValue`*`, ...)` calls `fastaread` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. The property name/value pairs can be in any format supported by the function `set` (for example, name-value string pairs, structures, and name-value cell array pairs). These property name/property value pairs are as follows:

`...  = fastaread(`*`File`*`, ...'IgnoreGaps',` *`IgnoreGapsValue`*`, ...)`, when *`IgnoreGapsValue`* is `true`, removes any gap symbol (`'-'` or `'.'`) from the sequences. Default is `false`.

`...  = fastaread(`*`File`*`, ...'Blockread',` *`BlockreadValue`*`, ...)` lets you read in a single sequence entry or block of sequence entries from a file containing multiple sequences. If *`BlockreadValue`* is a scalar *`N`*, then `fastaread` reads the *`N`*th entry in the file. If *`BlockreadValue`* is a 1-by-2 vector [*`M1, M2`*], then `fastaread` reads the block of entries

starting at the *M1* entry and ending at the *M2* entry. To read all remaining entries in the file starting at the *M1* entry, enter a positive value for *M1* and enter `Inf` for *M2*.

Examples

Read the sequence for the human p53 tumor gene.

```
p53nt = fastaread('p53nt.txt')
```

Read the sequence for the human p53 tumor protein.

```
p53aa = fastaread('p53aa.txt')
```

Read the human mitochondrion genome in FASTA format.

```
entrezSite = 'http://www.ncbi.nlm.nih.gov/entrez/viewer.fcgi?';
textOptions = '&txt=on&view=fasta';
genbankID = '&list_uids=NC_001807';
mitochondrion = fastaread([entrezSite textOptions genbankID])
```

See Also

Bioinformatics Toolbox functions: `emblread`, `fastainfo`, `fastawrite`, `fastqinfo`, `fastqread`, `fastqwrite`, `genbankread`, `genpeptread`, `multialignread`, `seqprofile`, `seqtool`, `sffinfo`, `sffread`

fastawrite

Purpose

Write to file using FASTA format

Syntax

```
fastawrite(File, Data)
fastawrite(File, Header, Sequence)
```

Arguments

File	String specifying either a file name or a path and file name for saving the FASTA-formatted data. If you specify only a file name, `fastawrite` saves the file to the MATLAB Current Folder. If you specify an existing file, `fastawrite` appends the data to the file, instead of overwriting the file.
Data	Any of the following: • String containing a sequence • MATLAB structure containing the fields `Header` and `Sequence` • MATLAB structure containing sequence information from the GenBank or GenPept database, such as returned by `genbankread`, `getgenbank`, `genpeptread`, or `getgenpept`.
Header	String or name of variable containing information about the sequence. This text appears in the header of the FASTA-formatted file, *File*.
Sequence	String or name of variable containing an amino acid or nucleotide sequence using the standard IUB/IUPAC letter or integer codes. For a list of valid characters, see Amino Acid Lookup on page 3-111 or Nucleotide Lookup on page 3-122.

Description

`fastawrite(File, Data)` writes the contents of *Data* to *File*, a FASTA-formatted file. If you specify an existing FASTA-formatted file,`fastawrite` appends the data to the file, instead of overwriting the file.

`fastawrite(File, Header, Sequence)` writes the specified header and sequence information to `File`, a FASTA-formatted file.

Tip To append FASTA-formatted data to an existing file, simply specify that file name. `fastawrite` adds the data to the end of the file.

If you are using `fastawrite` in a script, you can disable the append warning message by entering the following command lines before the `fastawrite` command:

```
warnState = warning %Save the current warning state
warning('off','Bioinfo:fastawrite:AppendToFile');
```

Then enter the following command line after the `fastawrite` command:

```
warning(warnState) %Reset warning state to previous settings
```

Examples

Writing a Coding Region to a FASTA-Formatted File

1. Retrieve the sequence for the human p53 gene from the GenBank database.

   ```
   seq = getgenbank('NM_000546');
   ```

2. Find the CDS line in the FEATURES information.

   ```
   cdsline = strmatch('CDS',seq.Features)

   cdsline =

       23
   ```

3. Read the coordinates of the coding region in the CDS line.

   ```
   [start,stop] = strread(seq.Features(cdsline,:),'%*s%d..%d')
   ```

```
start =

   252

stop =

   1433
```

4 Extract the coding region.

```
codingSeq = seq.Sequence(start:stop);
```

5 Write the coding region to a FASTA-formatted file, specifying `Coding region for p53` for the Header in the file, and `p53coding.txt` for the file name.

```
fastawrite('p53coding.txt','Coding region for p53',codingSeq);
```

Saving Multiple Sequences to a FASTA-Formatted File

1 Write two nucleotide sequences to a MATLAB structure containing the fields `Header` and `Sequence`.

```
data(1).Sequence = 'ACACAGGAAA';
data(1).Header = 'First sequence';
data(2).Sequence = 'ACGTCAGGTC';
data(2).Header = 'Second sequence';
```

2 Write the sequences to a FASTA-formatted file, specifying `my_sequences.txt` for the file name.

```
fastawrite('my_sequences.txt', data)
```

3 Display the FASTA-formatted file, `my_sequences.txt`.

```
type('my_sequences.txt')

>First sequence
ACACAGGAAA
```

```
>Second sequence
ACGTCAGGTC
```

Appending Sequences to a FASTA-Formatted File

1. If you haven't already done so, create the FASTA-formatted file, `my_sequences.txt`, described in Saving Multiple Sequences to a FASTA-Formatted File on page 3-478.

2. Append a third sequence to the file.

```
fastawrite('my_sequences.txt','Third sequence','TACTGACTTC')
```

3. Display the FASTA-formatted file, `my_sequences.txt`.

```
type('my_sequences.txt')

>First sequence
ACACAGGAAA

>Second sequence
ACGTCAGGTC

>Third sequence
TACTGACTTC
```

See Also

Bioinformatics Toolbox functions: `fastainfo`, `fastaread`, `fastqinfo`, `fastqread`, `fastqwrite`, `genbankread`, `genpeptread`, `getgenbank`, `getgenpept`, `multialignwrite`, `seqtool`, `sffinfo`, `sffread`

fastqinfo

Purpose

Return information about FASTQ file

Syntax

```
InfoStruct = fastqinfo(File)
```

Description

`InfoStruct = fastqinfo(File)` returns a MATLAB structure containing summary information about a FASTQ-formatted file.

Inputs

`File`

String specifying a file name or path and file name of a FASTQ-formatted file. If you specify only a file name, that file must be on the MATLAB search path or in the current folder.

Outputs

`InfoStruct`

MATLAB structure containing summary information about a FASTQ-formatted file. The structure contains the following fields.

Field	Description
`Filename`	Name of the file.
`FileModDate`	Modification date of the file.
`FileSize`	Size of the file in bytes.
`NumberOfEntries`	Number of sequence reads in the file.

Examples

Return a summary of the contents of a FASTQ file:

```
info = fastqinfo('SRR005164_1_50.fastq')

info =

           Filename: 'SRR005164_1_50.fastq'
        FileModDate: '03-Mar-2009 14:21:51'
           FileSize: 16702
    NumberOfEntries: 50
```

See Also

`fastqread` | `fastqwrite` | `fastainfo` | `fastaread` | `fastawrite` | `sffinfo` | `sffread`

Tutorials

- Working with Illumina/Solexa Next-Generation Sequencing Data

Related Links

-

fastqread

Purpose

Read data from FASTQ file

Syntax

```
FASTQStruct = fastqread(File)
[Header, Sequence] = fastqread(File)
[Header, Sequence, Qual] = fastqread(File)
fastqread(..., 'Blockread', BlockreadValue, ...)
fastqread(..., 'HeaderOnly', HeaderOnlyValue, ...)
```

Description

`FASTQStruct = fastqread(File)` reads a FASTQ-formatted file and returns the data in a MATLAB array of structures.

`[Header, Sequence] = fastqread(File)` returns only the header and sequence data in two separate variables.

`[Header, Sequence, Qual] = fastqread(File)` returns the data in three separate variables.

`fastqread(..., 'PropertyName', PropertyValue, ...)` calls `fastqread` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each *`PropertyName`* in single quotation marks. Each *`PropertyName`* is case insensitive. These property name/property value pairs are as follows:

`fastqread(..., 'Blockread', BlockreadValue, ...)` reads a single sequence entry or block of sequence entries from a FASTQ-formatted file containing multiple sequences.

`fastqread(..., 'HeaderOnly', HeaderOnlyValue, ...)` specifies whether to return only the header information.

Inputs

`File`

String specifying a file name or path and file name of a FASTQ-formatted file. If you specify only a file name, that file must be on the MATLAB search path or in the current folder.

`BlockreadValue`

Scalar or vector that controls the reading of a single sequence entry or block of sequence entries from a FASTQ-formatted file containing multiple sequences. Enter a scalar *N*, to read the *N*th entry in the file. Enter a 1-by-2 vector [*M1, M2*], to read a block of entries starting at the *M1* entry and ending at the *M2* entry. To read all remaining entries in the file starting at the *M1* entry, enter a positive value for *M1* and enter `Inf` for *M2*.

HeaderOnlyValue

Specifies whether to return only the header information. Choices are `true` or `false` (default).

Outputs

FASTQStruct

Array of structures containing information from a FASTQ-formatted file. There is one structure for each read or entry in the file. Each structure contains the following fields.

Field	Description
`Header`	Header information.
`Sequence`	Single letter-code representation of nucleotide sequence.
`Quality`	ASCII representation of per-base quality scores for a nucleotide sequence.

Header

Variable containing header information or, if the FASTQ-formatted file contains multiple sequences, a cell array containing header information.

Sequence

Variable containing sequence information or, if the FASTQ-formatted file contains multiple sequences, a cell array containing sequence information.

Qual

Variable containing quality information or, if the FASTQ-formatted file contains multiple sequences, a cell array containing quality information.

Definitions

A FASTQ-formatted file contains nucleotide sequence and quality information on four lines:

- **Line 1** — Header information prefixed with an `@` symbol
- **Line 2** — Nucleotide sequence
- **Line 3** — Header information prefixed with a `+` symbol
- **Line 4** — ASCII representation of per-base quality scores for the nucleotide sequence using Phred or Solexa encoding

Examples

Read a FASTQ file into an array of structures:

```
% Read the contents of a FASTQ-formatted file into
% an array of structures
reads = fastqread('SRR005164_1_50.fastq')

reads =

1x50 struct array with fields:
    Header
    Sequence
    Quality
```

Read a FASTQ file into three separate variables:

```
% Read the contents of a FASTQ-formatted file into
% three separate variables
[h,s,q] = fastqread('SRR005164_1_50.fastq');
```

Read a block of entries from a FASTQ file:

```
% Read the contents of reads 5 through 10 into
% an array of structures
reads_5_10 = fastqread('SRR005164_1_50.fastq', 'blockread', [5 10])

1x6 struct array with fields:
    Header
    Sequence
    Quality
```

See Also

fastqwrite | fastaread | fastawrite | fastainfo | fastqinfo | sffinfo | sffread

Tutorials

- Working with Illumina/Solexa Next-Generation Sequencing Data

Related Links

-

fastqwrite

Purpose

Write to file using FASTQ format

Syntax

```
fastqwrite(File, FASTQStruct)
fastqwrite(File, Header, Sequence, Qual)
```

Description

`fastqwrite(File, FASTQStruct)` writes the contents of a MATLAB structure or array of structures to a FASTQ-formatted file. If you specify an existing FASTQ-formatted file, `fastqwrite` appends the data to the file, instead of overwriting the file.

`fastqwrite(File, Header, Sequence, Qual)` writes header, sequence, and quality information to a FASTQ-formatted file.

Tip To append FASTQ-formatted data to an existing file, simply specify that file name. `fastqwrite` adds the data to the end of the file.

If you are using `fastqwrite` in a script, you can disable the append warning message by entering the following command lines before the `fastqwrite` command:

```
warnState = warning %Save the current warning state
warning('off','Bioinfo:fastqwrite:AppendToFile');
```

Then enter the following command line after the `fastqwrite` command:

```
warning(warnState) %Reset warning state to previous settings
```

Inputs

File

String specifying either a file name or a path and file name for saving the FASTQ-formatted data. If you specify only a file name, `fastqwrite` saves the file to the MATLAB Current Folder. If you specify an existing file, `fastqwrite` appends the data to the file, instead of overwriting the file.

FASTQStruct

MATLAB structure or array of structures containing the fields `Header`, `Sequence`, and `Quality`, such as returned by `fastqread`.

`Header`

String or name of a variable containing information about the nucleotide sequence. This text appears in the header of the FASTQ-formatted file, *`File`*.

`Sequence`

String or name of a variable containing a nucleotide sequence using the standard IUB/IUPAC letter or integer codes. For a list of valid characters, see Amino Acid Lookup on page 3-111 or Nucleotide Lookup on page 3-122.

`Qual`

String or name of a variable containing ASCII representation of per-base quality scores for a nucleotide sequence.

Definitions

A FASTQ-formatted file contains nucleotide sequence and quality information on four lines:

- **Line 1** — Header information prefixed with an `@` symbol
- **Line 2** — Nucleotide sequence
- **Line 3** — Header information prefixed with a `+` symbol
- **Line 4** — ASCII representation of per-base quality scores for the nucleotide sequence using Phred or Solexa encoding

Examples

Write multiple sequences to a FASTQ file from an array of structures:

```
% Read the contents of a FASTQ-formatted file into
% an array of structures
reads = fastqread('SRR005164_1_50.fastq');
% Create another array of structures for the first five reads
reads5 = reads(1:5);
% Write the first five reads to a separate FASTQ-formatted file
```

```
fastqwrite('fiveReads.fastq', reads5)
```

Write a single sequence to a FASTQ file from separate variables:

```
% Create separate variables for the header, sequence, and
% quality information of a nucleotide sequence
h = 'MYSEQ-000_1_1_1_953_493';
s = 'GTTACCATGATGTTATTTCTTCATTTGGAGGTAAAA';
q = ']]]]]]]]]]]]]]]]]]]]]]T]]]]RJRZTQLOA';
% Write the information to a FASTQ-formatted file
fastqwrite('oneRead.fastq', h, s, q)
```

See Also

`fastqread` | `fastqinfo` | `fastaread` | `fastawrite` | `fastainfo` | `sffinfo` | `sffread`

Tutorials

- Working with Illumina/Solexa Next-Generation Sequencing Data

How To

- Amino Acid Lookup on page 3-111
- Nucleotide Lookup on page 3-122

Related Links

-

Purpose

Retrieve or set feature metadata in ExpressionSet object

Syntax

```
MetaDataObj = featureData(ESObj)
NewESObj = featureData(ESObj, NewMetaDataObj)
```

Description

`MetaDataObj = featureData(ESObj)` returns a MetaData object containing the feature metadata from an ExpressionSet object.

`NewESObj = featureData(ESObj, NewMetaDataObj)` replaces the feature metadata in *`ESObj`*, an ExpressionSet object, with *`NewMetaDataObj`*, and returns *`NewESObj`*, a new ExpressionSet object.

Inputs

`ESObj`

Object of the `bioma.ExpressionSet` class.

`NewMetaDataObj`

Object of the `bioma.data.MetaData` class, containing feature metadata, stored in two dataset arrays. The feature names and variable names in *`NewMetaDataObj`* must match the feature names and variable names in the *`MetaDataObj`* being replaced in the ExpressionSet object, *`ESObj`*.

Outputs

`MetaDataObj`

Object of the `bioma.data.MetaData` class, containing the feature metadata, stored in two dataset arrays.

`NewESObj`

Object of the `bioma.ExpressionSet` class, returned after replacing the MetaData object containing the feature metadata.

See Also

`bioma.ExpressionSet` | `bioma.data.MetaData` | `featureNames` | `sampleData`

How To

- "Working with ExpressionSet Objects"

bioma.ExpressionSet.featureNames

Purpose

Retrieve or set feature names in ExpressionSet object

Syntax

```
FeatNames = featureNames(ESObj)
FeatNames = featureNames(ESObj, Subset)
NewESObj = featureNames(ESObj, Subset, NewFeatNames)
```

Description

`FeatNames = featureNames(ESObj)` returns a cell array of strings specifying all feature names in an ExpressionSet object.

`FeatNames = featureNames(ESObj, Subset)` returns a cell array of strings specifying a subset the feature names in an ExpressionSet object.

`NewESObj = featureNames(ESObj, Subset, NewFeatNames)` replaces the feature names specified by `Subset` in `ESObj`, an ExpressionSet object, with `NewFeatNames`, and returns `NewESObj`, a new ExpressionSet object.

Inputs

`ESObj`

Object of the `bioma.ExpressionSet` class.

`Subset`

One of the following to specify a subset of the feature names in an ExpressionSet object:

- String specifying a feature name
- Cell array of strings specifying feature names
- Positive integer
- Vector of positive integers
- Logical vector

`NewFeatNames`

New feature names for specific feature names within an ExpressionSet object, specified by one of the following:

- Numeric vector
- String or cell array of strings
- String, which `featureNames` uses as a prefix for the feature names, with feature numbers appended to the prefix
- Logical `true` or `false` (default). If `true`, `featureNames` assigns unique feature names using the format `Feature1`, `Feature2`, etc.

The number of feature names in *`NewFeatNames`* must equal the number of features specified by *`Subset`*.

Outputs

`FeatNames`

Cell array of strings specifying all or some of the feature names in an ExpressionSet object. The feature names are the row names in the DataMatrix objects in the ExpressionSet object. The feature names are also the row names of the *`VarValues`* dataset array in the MetaData object in the ExpressionSet object.

`NewESObj`

Object of the `bioma.ExpressionSet` class, returned after replacing specific feature names.

See Also

`bioma.ExpressionSet` | `bioma.data.ExptData` | `DataMatrix` | `bioma.data.MetaData` | `sampleNames`

How To

- "Working with ExpressionSet Objects"

bioma.data.ExptData.featureNames

Purpose

Retrieve or set feature names in ExptData object

Syntax

```
FeatNames = featureNames(EDObj)
FeatNames = featureNames(EDObj, Subset)
NewESObj = featureNames(EDObj, Subset, NewFeatNames)
```

Description

`FeatNames = featureNames(EDObj)` returns a cell array of strings specifying all feature names in an ExptData object.

`FeatNames = featureNames(EDObj, Subset)` returns a cell array of strings specifying a subset the feature names in an ExptData object.

`NewESObj = featureNames(EDObj, Subset, NewFeatNames)` replaces the feature names specified by `Subset` in `EDObj`, an ExptData object, with `NewFeatNames`, and returns `NewEDObj`, a new ExptData object.

Inputs

`EDObj`

Object of the `bioma.data.ExptData` class.

`Subset`

One of the following to specify a subset of the feature names in an ExptData object:

- String specifying a feature name
- Cell array of strings specifying feature names
- Positive integer
- Vector of positive integers
- Logical vector

`NewFeatNames`

New feature names for specific feature names within an ExptData object, specified by one of the following:

- Numeric vector

- String or cell array of strings
- String, which `featureNames` uses as a prefix for the feature names, with feature numbers appended to the prefix
- Logical `true` or `false` (default). If `true`, `featureNames` assigns unique feature names using the format `Feature1`, `Feature2`, etc.

The number of feature names in *`NewFeatNames`* must equal the number of features specified by *`Subset`*.

Outputs

`FeatNames`

Cell array of strings specifying all or some of the feature names in an ExptData object. The feature names are the row names in the DataMatrix objects in the ExptData object.

`NewEDObj`

Object of the `bioma.data.ExptData` class, returned after replacing specific feature names.

Examples

Construct an ExptData object, and then retrieve the feature names from it:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Retrieve feature names
FNames = featureNames(EDObj);
```

See Also

`bioma.data.ExptData` | `DataMatrix` | `dmNames` | `elementNames` | `sampleNames`

How To

- "Working with ExptData Objects"

Purpose

Draw linear or circular map of features from GenBank structure

Syntax

```
featuresmap(GBStructure)
featuresmap(GBStructure, FeatList)
featuresmap(GBStructure, FeatList, Levels)
featuresmap(GBStructure, Levels)
[Handles, OutFeatList] = featuresmap(...)
featuresmap(..., 'FontSize', FontSizeValue, ...)
featuresmap(..., 'ColorMap', ColorMapValue, ...)
featuresmap(..., 'Qualifiers', QualifiersValue, ...)
featuresmap(..., 'ShowPositions', ShowPositionsValue, ...)
```

Arguments

GBStructure

GenBank structure, typically created using the `getgenbank` or the `genbankread` function.

FeatList

Cell array of features (from the list of all features in the GenBank structure) to include in or exclude from the map.

- If *FeatList* is a cell array of features, these features are mapped. Any features in *FeatList* not found in the GenBank structure are ignored.
- If *FeatList* includes `'-'` as the first string in the cell array, then the remaining strings (features) are not mapped.

By default, *FeatList* is the a list of all features in the GenBank structure.

Levels	Vector of N integers, where N is the number of features. Each integer represents the level in the map for the corresponding feature. For example, if *Levels* = [1, 1, 2, 3, 3], the first two features would appear on level 1, the third feature on level 2, and the fourth and fifth features on level 3. By default, *Levels* = [1:N].
FontSizeValue	Scalar that sets the font size (points) for the annotations of the features. Default is 9.
ColorMapValue	Three-column matrix, to specify a list of colors to use for each feature. This matrix replaces the default matrix, which specifies the following colors and order: blue, green, red, cyan, magenta, yellow, brown, light green, orange, purple, gold, and silver. In the matrix, each row corresponds to a color, and each column specifies red, green, and blue intensity respectively. Valid values for the RGB intensities are 0.0 to 1.0.
QualifiersValue	Cell array of strings to specify an ordered list of qualifiers to search for in the structure and use as annotations. For each feature, the first matching qualifier found from the list is used for its annotation. If a feature does not include any of the qualifiers, no annotation displays for that feature. By default, *QualifiersValue* = {*'gene', 'product', 'locus_tag', 'note', 'db_xref', 'protein_id'*}. Provide your own *QualifiersValue* to limit or expand the list of qualifiers or change the search order.

Tip Set *QualifiersValue* = {} to create a map with no annotations.

Tip To determine all qualifiers available for a given feature, do either of the following:

- Create the map, and then click a feature or its annotation to list all qualifiers for that feature.
- Use the `featuresparse` command to parse all the features into a new structure, and then use the `fieldnames` command to list the qualifiers for a specific feature. See Determining Qualifiers for a Specific Feature on page 3-502.

ShowPositionsValue Property to add the sequence position to the annotation label for each feature. Enter `true` to add the sequence position. Default is `false`.

Description

`featuresmap(`*`GBStructure`*`)` creates a linear or circular map of all features from a GenBank structure, typically created using the `getgenbank` or the `genbankread` function.

`featuresmap(`*`GBStructure`*`, `*`FeatList`*`)` creates a linear or circular map of a subset of features from a GenBank structure. *`FeatList`* lets you specify features (from the list of all features in the GenBank structure) to include in or exclude from the map.

- If *FeatList* is a cell array of features, these features are mapped. Any features in *FeatList* not found in the GenBank structure are ignored.
- If *FeatList* includes '-' as the first string in the cell array, then the remaining strings (features) are not mapped.

By default, *FeatList* is a list of all features in the GenBank structure.

featuresmap(*GBStructure*, *FeatList*, *Levels*) or featuresmap(*GBStructure*, *Levels*) indicates which level on the map each feature is drawn. Level 1 is the left-most (linear map) or inner-most (circular map) level, and level N is the right-most (linear map) or outer-most (circular map) level, where N is the number of features.

Levels is a vector of N integers, where N is the number of features. Each integer represents the level in the map for the corresponding feature. For example, if *Levels* = [1, 1, 2, 3, 3], the first two features would appear on level 1, the third feature on level 2, and the fourth and fifth features on level 3. By default, *Levels* = [1:N].

[*Handles, OutFeatList*] = featuresmap(...) returns a list of handles for each feature in *OutFeatList*. It also returns *OutFeatList*, which is a cell array of the mapped features.

Tip Use *Handles* and *OutFeatList* with the legend command to create a legend of features.

---

featuresmap(..., '*PropertyName*', *PropertyValue*, ...) defines optional properties that use property name/value pairs in any order. These property name/value pairs are as follows:

featuresmap(..., 'FontSize', *FontSizeValue*, ...) sets the font size (points) for the annotations of the features. Default *FontSizeValue* is 9.

featuresmap(..., 'ColorMap', *ColorMapValue*, ...) specifies a list of colors to use for each feature. This matrix replaces the default matrix,

which specifies the following colors and order: blue, green, red, cyan, magenta, yellow, brown, light green, orange, purple, gold, and silver. *ColorMapValue* is a three-column matrix, where each row corresponds to a color, and each column specifies red, green, and blue intensity respectively. Valid values for the RGB intensities are `0.0` to `1.0`.

`featuresmap(..., 'Qualifiers', QualifiersValue, ...)` lets you specify an ordered list of qualifiers to search for and use as annotations. For each feature, the first matching qualifier found from the list is used for its annotation. If a feature does not include any of the qualifiers, no annotation displays for that feature. *QualifiersValue* is a cell array of strings. By default, *QualifiersValue* = {*'gene', 'product', 'locus_tag', 'note', 'db_xref', 'protein_id'*}. Provide your own *QualifiersValue* to limit or expand the list of qualifiers or change the search order.

Tip Set *QualifiersValue* = {} to create a map with no annotations.

Tip To determine all qualifiers available for a given feature, do either of the following:

- Create the map, and then click a feature or its annotation to list all qualifiers for that feature.
- Use the `featuresparse` command to parse all the features into a new structure, and then use the `fieldnames` command to list the qualifiers for a specific feature. See Determining Qualifiers for a Specific Feature on page 3-502.

`featuresmap(..., 'ShowPositions', ShowPositionsValue, ...)` lets you add the sequence position to the annotation label. If *ShowPositionsValue* is `true`, sequence positions are added to the annotation labels. Default is `false`.

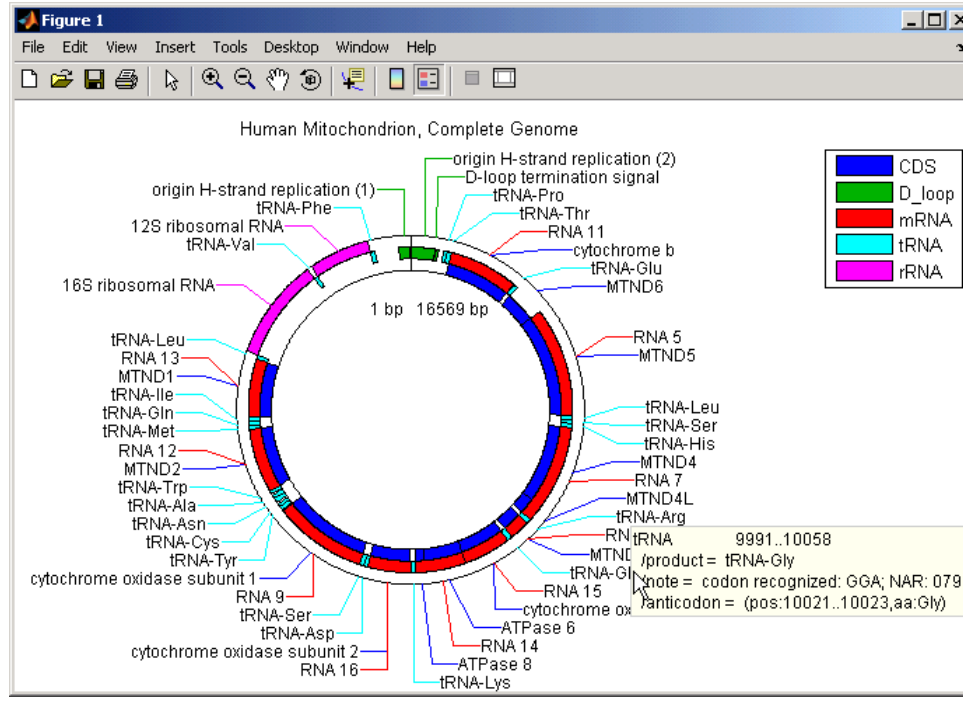


Figure 1
File Edit View Insert Tools Desktop Window Help
Human Mitochondrion, Complete Genome
origin H-strand replication (2)
D-loop termination signal
tRNA-Pro
tRNA-Thr
RNA 11
cytochrome b
tRNA-Glu
MTND6
RNA 5
MTND5
tRNA-Leu
tRNA-Ser
tRNA-His
MTND4
RNA 7
MTND4L
tRNA-Arg
ATPase 6
RNA 14
ATPase 8
tRNA-Lys
RNA 16
cytochrome oxidase subunit 2
tRNA-Asp
tRNA-Ser
RNA 9
cytochrome oxidase subunit 1
tRNA-Tyr
tRNA-Cys
tRNA-Asn
tRNA-Ala
tRNA-Trp
MTND2
RNA 12
tRNA-Met
tRNA-Gln
tRNA-Ile
MTND1
RNA 13
tRNA-Leu
16S ribosomal RNA
12S ribosomal RNA
tRNA-Val
tRNA-Phe
origin H-strand replication (1)
1 bp 16569 bp
CDS
D_loop
mRNA
tRNA
rRNA
tRNA 9991..10058
/product = tRNA-Gly
/note = codon recognized: GGA; NAR: 0797
/anticodon = (pos:10021..10023,aa:Gly)

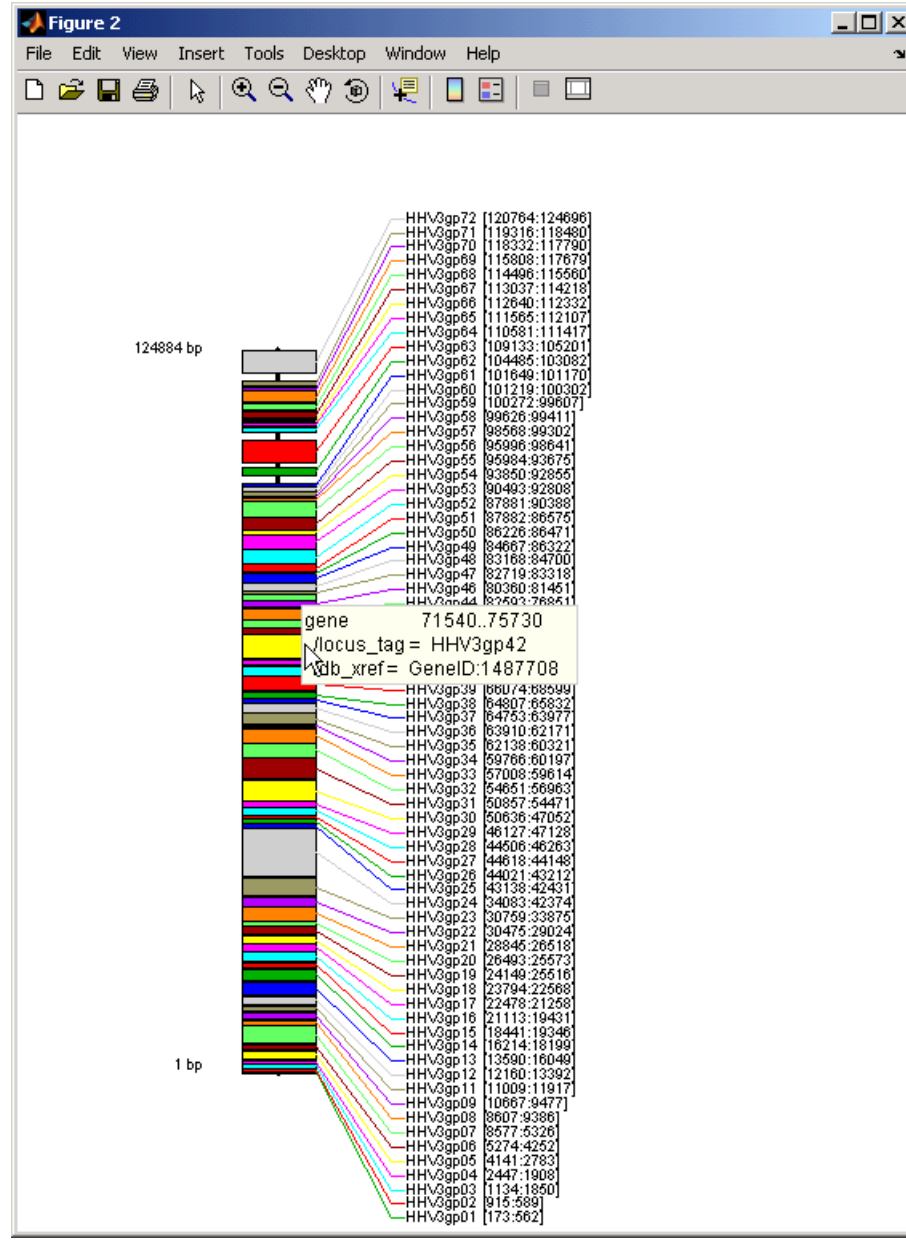


Figure 2
File Edit View Insert Tools Desktop Window Help
124884 bp
1 bp
HHV3gp72 [120764:124696]
HHV3gp71 [119316:118480]
HHV3gp70 [118332:117790]
HHV3gp69 [115808:117679]
HHV3gp68 [114496:115560]
HHV3gp67 [113037:114218]
HHV3gp66 [112640:112332]
HHV3gp65 [111565:112107]
HHV3gp64 [110581:111417]
HHV3gp63 [109133:105201]
HHV3gp62 [104485:103082]
HHV3gp61 [101649:101170]
HHV3gp60 [101219:100302]
HHV3gp59 [100272:99607]
HHV3gp58 [99626:99411]
HHV3gp57 [98568:99302]
HHV3gp56 [95996:98641]
HHV3gp55 [95984:93675]
HHV3gp54 [93850:92855]
HHV3gp53 [90493:92808]
HHV3gp52 [87881:90388]
HHV3gp51 [87882:86575]
HHV3gp50 [86226:86471]
HHV3gp49 [84667:86322]
HHV3gp48 [83168:84700]
HHV3gp47 [82719:83318]
HHV3gp46 [80360:81451]
gene 71540..75730
/locus_tag= HHV3gp42
/db_xref= GeneID:1487708
HHV3gp38 [64807:65832]
HHV3gp37 [64753:63977]
HHV3gp36 [63910:62171]
HHV3gp35 [62138:60321]
HHV3gp34 [59766:60197]
HHV3gp33 [57008:59614]
HHV3gp32 [54651:56963]
HHV3gp31 [50857:54471]
HHV3gp30 [50636:47052]
HHV3gp29 [46127:47128]
HHV3gp28 [44506:46263]
HHV3gp27 [44618:44148]
HHV3gp26 [44021:43212]
HHV3gp25 [43138:42431]
HHV3gp24 [34083:42374]
HHV3gp23 [30759:33875]
HHV3gp22 [30475:29024]
HHV3gp21 [28845:26518]
HHV3gp20 [26493:25573]
HHV3gp19 [24149:25516]
HHV3gp18 [23794:22568]
HHV3gp17 [22478:21258]
HHV3gp16 [21113:19431]
HHV3gp15 [18441:19346]
HHV3gp14 [16214:18199]
HHV3gp13 [13590:16049]
HHV3gp12 [12160:13392]
HHV3gp11 [11009:11917]
HHV3gp09 [10667:9477]
HHV3gp08 [8607:9386]
HHV3gp07 [8577:5326]
HHV3gp06 [5274:4252]
HHV3gp05 [4141:2783]
HHV3gp04 [2447:1908]
HHV3gp03 [1134:1850]
HHV3gp02 [915:589]
HHV3gp01 [173:562]

After creating a map:

- Click a feature or annotation to display a list of all qualifiers for that feature.
- Zoom the plot by clicking the following buttons:

 or 

Examples

Creating a Circular Map with a Legend

The following example creates a circular map of five different features mapped on three levels. It also uses outputs from the `featuresmap` function as inputs to the `legend` function to add a legend to the map.

```
GBStructure = getgenbank('J01415');
[Handles, OutFeatList] = featuresmap(GBStructure, ...
     {'CDS','D_loop','mRNA','tRNA','rRNA'}, [1 2 2 2 3])
legend(Handles, OutFeatList, 'interpreter', 'none', ...
     'location','bestoutside')
title('Human Mitochondrion, Complete Genome')
```

Creating a Linear Map with Sequence Position Labels and Changed Font Size

The following example creates a linear map showing only the gene feature. It changes the font of the labels to seven points and includes the sequence position in the labels.

```
herpes = getgenbank('NC_001348');
featuresmap(herpes,{'gene'},'fontsize',7,'showpositions',true)
title('Genes in Human herpesvirus 3 (strain Dumas)')
```

Determining Qualifiers for a Specific Feature

The following example uses the `getgenbank` function to create a GenBank structure, `GBStructure`. It then uses the `featuresparse` function to parse the features in the GenBank structure into a new

structure, `features`. It then uses the `fieldnames` function to return all qualifiers for one of the features, `D_loop`.

```
GenBankStructure = getgenbank('J01415');
features = featuresparse (GenBankStructure)
features =

         source: [1x1 struct]
         D_loop: [1x2 struct]
     rep_origin: [1x3 struct]
    repeat_unit: [1x4 struct]
    misc_signal: [1x1 struct]
       misc_RNA: [1x1 struct]
      variation: [1x17 struct]
           tRNA: [1x22 struct]
           rRNA: [1x2 struct]
           mRNA: [1x10 struct]
            CDS: [1x13 struct]
       conflict: [1x1 struct]

fieldnames(features.D_loop)

ans =

    'Location'
    'Indices'
    'note'
    'citation'
```

See Also

`featuresparse`, `genbankread`, `getgenbank`, `seqtool`

featuresparse

Purpose

Parse features from GenBank, GenPept, or EMBL data

Syntax

```
FeatStruct = featuresparse(Features)
FeatStruct = featuresparse(Features, ...'Feature',
FeatureValue, ...)
FeatStruct = featuresparse(Features, ...'Sequence',
   SequenceValue, ...)
```

Arguments

Features	Any of the following: • String containing GenBank, GenPept, or EMBL features • MATLAB character array including text describing GenBank, GenPept, or EMBL features • MATLAB structure with fields corresponding to GenBank, GenPept, or EMBL data, such as those returned by `genbankread`, `genpeptread`, `emblread`, `getgenbank`, `getgenpept`, or `getembl`
FeatureValue	Name of a feature contained in *Features*. When specified, `featuresparse` returns only the substructure that corresponds to this feature. If there are multiple features with the same *FeatureValue*, then *FeatStruct* is an array of structures.
SequenceValue	Property to control the extraction, when possible, of the sequences respective to each feature, joining and complementing pieces of the source sequence and storing them in the `Sequence` field of the returned structure, *FeatStruct*. When extracting the sequence from an incomplete CDS feature, `featuresparse` uses the `codon_start` qualifier to adjust the frame of the sequence. Choices are `true` or `false` (default).

Return Values

FeatStruct — Output structure containing a field for every database feature. Each field name in *FeatStruct* matches the corresponding feature name in the GenBank, GenPept, or EMBL database, with the exceptions listed in the table below. Fields in *FeatStruct* contain substructures with feature qualifiers as fields. In the GenBank, GenPept, and EMBL databases, for each feature, the only mandatory qualifier is its location, which `featuresparse` translates to the field `Location`. When possible, `featuresparse` also translates this location to numeric indices, creating an `Indices` field.

Note If you use the `Indices` field to extract sequence information, you may need to complement the sequences.

Description

FeatStruct = `featuresparse(`*Features*`)` parses the features from *Features*, which contains GenBank, GenPept, or EMBL features. *Features* can be a:

- String containing GenBank, GenPept, or EMBL features
- MATLAB character array including text describing GenBank, GenPept, or EMBL features
- MATLAB structure with fields corresponding to GenBank, GenPept, or EMBL data, such as those returned by `genbankread`, `genpeptread`, `emblread`, `getgenbank`, `getgenpept`, or `getembl`

FeatStruct is the output structure containing a field for every database feature. Each field name in *FeatStruct* matches the corresponding

feature name in the GenBank, GenPept, or EMBL database, with the following exceptions.

Feature Name in GenBank, GenPept, or EMBL Database	Field Name in MATLAB Structure
-10_signal	minus_10_signal
-35_signal	minus_35_signal
3'UTR	three_prime_UTR
3'clip	three_prime_clip
5'UTR	five_prime_UTR
5'clip	five_prime_clip
D-loop	D_loop

Fields in *FeatStruct* contain substructures with feature qualifiers as fields. In the GenBank, GenPept, and EMBL databases, for each feature, the only mandatory qualifier is its location, which `featuresparse` translates to the field `Location`. When possible, `featuresparse` also translates this location to numeric indices, creating an `Indices` field.

Note If you use the `Indices` field to extract sequence information, you may need to complement the sequences.

FeatStruct = `featuresparse (`*Features*`, ...'`*PropertyName*`',` *PropertyValue*`, ...)` calls `featuresparse` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

FeatStruct = `featuresparse(`*Features*`, ...'Feature',` *FeatureValue*`, ...)` returns only the substructure that corresponds to *FeatureValue*,

the name of a feature contained in *Features*. If there are multiple features with the same *FeatureValue*, then *FeatStruct* is an array of structures.

FeatStruct = featuresparse(*Features*, ...'Sequence', *SequenceValue*, ...) controls the extraction, when possible, of the sequences respective to each feature, joining and complementing pieces of the source sequence and storing them in the field Sequence. When extracting the sequence from an incomplete CDS feature, featuresparse uses the codon_start qualifier to adjust the frame of the sequence. Choices are true or false (default).

Examples

Obtaining All Features from a GenBank File

The following example obtains all the features stored in the GenBank file nm175642.txt:

```
gbkStruct = genbankread('nm175642.txt');
features = featuresparse(gbkStruct)

features =

    source: [1x1 struct]
      gene: [1x1 struct]
       CDS: [1x1 struct]
```

Obtaining a Subset of Features from a GenBank Record

The following example obtains only the coding sequences (CDS) feature of the *Caenorhabditis elegans* cosmid record (accession number Z92777) from the GenBank database:

```
worm = getgenbank('Z92777');
CDS = featuresparse(worm,'feature','cds')

CDS =

1x12 struct array with fields:
    Location
```

```
Indices
locus_tag
standard_name
note
codon_start
product
protein_id
db_xref
translation
```

Extracting Sequences for Each Feature

1. Retrieve two nucleotide sequences from the GenBank database for the neuraminidase (NA) protein of two strains of the Influenza A virus (H5N1).

```
hk01 = getgenbank('AF509094');
vt04 = getgenbank('DQ094287');
```

2. Extract the sequence of the coding region for the neuraminidase (NA) protein from the two nucleotide sequences. The sequences of the coding regions are stored in the `Sequence` fields of the returned structures, `hk01_cds` and `vt04_cds`.

```
hk01_cds = featuresparse(hk01,'feature','CDS','Sequence',true);
vt04_cds = featuresparse(vt04,'feature','CDS','Sequence',true);
```

3. Once you have extracted the nucleotide sequences, you can use the `nt2aa` and `nwalign` functions to align the amino acids sequences converted from the nucleotide sequences.

```
[sc,al]=nwalign(nt2aa(hk01_cds),nt2aa(vt04_cds),'extendgap',1);
```

4. Then you can use the `seqinsertgaps` function to copy the gaps from the aligned amino acid sequences to their corresponding nucleotide sequences, thus codon-aligning them.

```
hk01_aligned = seqinsertgaps(hk01_cds,al(1,:))
```

```
vt04_aligned = seqinsertgaps(vt04_cds,al(3,:))
```

5 Once you have code aligned the two sequences, you can use them as input to other functions such as `dnds`, which calculates the synonymous and nonsynonymous substitutions rates of the codon-aligned nucleotide sequences. By setting `Verbose` to `true`, you can also display the codons considered in the computations and their amino acid translations.

```
[dn,ds] = dnds(hk01_aligned,vt04_aligned,'verbose',true)
```

See Also

Bioinformatics Toolbox functions: `emblread`, `genbankread`, `genpeptread`, `getgenbank`, `getgenpept`

bioma.ExpressionSet.featureVarDesc

Purpose

Retrieve or set feature variable descriptions in ExpressionSet object

Syntax

```
DSVarDescriptions = featureVarDesc(ESObj)
NewESObj = featureVarDesc(ESObj, NewDSVarDescriptions)
```

Description

`DSVarDescriptions = featureVarDesc(ESObj)` returns a dataset array containing the feature variable names and descriptions from the MetaData object in an ExpressionSet object.

`NewESObj = featureVarDesc(ESObj, NewDSVarDescriptions)` replaces the feature variable descriptions in *`ESObj`*, an ExpressionSet object, with *`NewDSVarDescriptions`*, and returns *`NewESObj`*, a new ExpressionSet object.

Inputs

`ESObj`

Object of the `bioma.ExpressionSet` class.

`NewDSVarDescriptions`

Descriptions of the feature variable names, specified by either of the following:

- A new dataset array containing the feature variable names and descriptions. In this dataset array, each row corresponds to a variable. The first column contains the variable name, and the second column (`VariableDescription`) contains a description of the variable. The row names (variable names) must match the row names (variable names) in *`DSVarDescriptions`*, the dataset array being replaced in the MetaData object in the ExpressionSet object, *`ESObj`*.
- Cell array of strings containing descriptions of the feature variables. The number of elements in *`VarDesc`* must equal the number of row names (variable names) in *`DSVarDescriptions`*, the dataset array being replaced in the MetaData object in the ExpressionSet object, *`ESObj`*.

Outputs

DSVarDescriptions

A dataset array containing the feature variable names and descriptions from the MetaData object of an ExpressionSet object. In this dataset array, each row corresponds to a variable. The first column contains the variable name, and the second column (`VariableDescription`) contains a description of the variable.

NewESObj

Object of the `bioma.ExpressionSet` class, returned after replacing the dataset array containing the feature variable descriptions.

See Also

`bioma.ExpressionSet` | `bioma.data.MetaData` | `variableDesc`

How To

- "Working with ExpressionSet Objects"

bioma.ExpressionSet.featureVarNames

Purpose

Retrieve or set feature variable names in ExpressionSet object

Syntax

```
FeatVarNames = featureVarNames(ESObj)
FeatVarNames = featureVarNames(ESObj, Subset)
NewESObj = featureVarNames(ESObj, Subset, NewFeatVarNames)
```

Description

`FeatVarNames = featureVarNames(ESObj)` returns a cell array of strings specifying all feature variable names in an ExpressionSet object.

`FeatVarNames = featureVarNames(ESObj, Subset)` returns a cell array of strings specifying a subset the feature variable names in an ExpressionSet object.

`NewESObj = featureVarNames(ESObj, Subset, NewFeatVarNames)` replaces the feature variable names specified by `Subset` in `ESObj`, an ExpressionSet object, with `NewFeatVarNames`, and returns `NewESObj`, a new ExpressionSet object.

Inputs

`ESObj`

Object of the `bioma.ExpressionSet` class.

`Subset`

One of the following to specify a subset of the feature variable names in an ExpressionSet object:

- String specifying a feature variable name
- Cell array of strings specifying feature variable names
- Positive integer
- Vector of positive integers
- Logical vector

`NewFeatVarNames`

New feature variable names for specific feature variable names within an ExpressionSet object, specified by one of the following:

- Numeric vector
- Cell array of strings
- Character array
- String, which `featureVarNames` uses as a prefix for the feature variable names, with feature variable numbers appended to the prefix
- Logical `true` or `false` (default). If `true`, `featureVarNames` assigns unique feature variable names using the format `Var1`, `Var2`, etc.

The number of feature variable names in *`NewFeatVarNames`* must equal the number of feature variable names specified by *`Subset`*.

Outputs

`FeatVarNames`

Cell array of strings specifying all or some of the feature variable names in an ExpressionSet object. The feature variable names are the column names of the *`VarValues`* dataset array. The feature variable names are also the row names of the *`VarDescriptions`* dataset array. Both dataset arrays are in the MetaData object in the ExpressionSet object.

`NewESObj`

Object of the `bioma.ExpressionSet` class, returned after replacing specific feature names.

See Also

`bioma.ExpressionSet` | `bioma.data.MetaData` | `sampleNames` | `featureNames` | `sampleVarNames`

How To

- "Working with ExpressionSet Objects"

bioma.ExpressionSet.featureVarValues

Purpose

Retrieve or set feature variable data values in ExpressionSet object

Syntax

```
DSVarValues = featureVarValues(ESObj)
NewESObj = featureVarValues(ESObj, NewDSVarValues)
```

Description

`DSVarValues = featureVarValues(ESObj)` returns a dataset array containing the measured value of each variable per feature from the MetaData object of an ExpressionSet object.

`NewESObj = featureVarValues(ESObj, NewDSVarValues)` replaces the feature variable values in *`ESObj`*, an ExpressionSet object, with *`NewDSVarValues`*, and returns *`NewESObj`*, a new ExpressionSet object.

Inputs

`ESObj`

Object of the `bioma.ExpressionSet` class.

`NewDSVarValues`

A dataset array containing a value for each variable per feature. In this dataset array, the columns correspond to variables and rows correspond to feature. The row names (feature names) must match the row names (feature names) in *`DSVarValues`*, the dataset array being replaced in the MetaData object in the ExpressionSet object, *`ESObj`*.

Outputs

`DSVarValues`

A dataset array containing the measured value of each variable per feature from the MetaData object of an ExpressionSet object. In this dataset array, the columns correspond to variables and rows correspond to features.

`NewESObj`

Object of the `bioma.ExpressionSet` class, returned after replacing the dataset array containing the feature variable values.

See Also

`bioma.ExpressionSet` | `bioma.data.MetaData` | `variableValues`

How To

- "Working with ExpressionSet Objects"

galread

Purpose

Read microarray data from GenePix array list file

Syntax

```
GALData = galread('File')
```

Arguments

File	GenePix array list formatted file (GAL). Enter a file name, or enter a path and file name.

Description

`galread` reads data from a GenePix formatted file into a MATLAB structure.

GALData = `galread('`*File*`')` reads in a GenePix array list formatted file (*File*) and creates a structure (`GALData`) containing the following fields.

Field
`Header`
`BlockData`
`IDs`
`Names`

The field `BlockData` is an `N`-by-`3` array. The columns of this array are the block data, the column data, and the row data respectively. For more information on the GAL format, see

```
http://www.moleculardevices.com/pages/software/gn_genepix_file_formats.html#gal
```

For a list of supported file format versions, see

```
http://www.moleculardevices.com/pages/software/gn_genepix_file_formats.html
```

See Also

Bioinformatics Toolbox functions: `affyread`, `geoseriesread`, `geosoftread`, `gprread`, `ilmnbsread`, `imageneread`, `sptread`

Purpose

Perform GC Robust Multi-array Average (GCRMA) background adjustment, quantile normalization, and median-polish summarization on Affymetrix microarray probe-level data

Syntax

```
ExpressionMatrix = gcrma(PMMatrix, MMMatrix, ProbeIndices,
   AffinPM, AffinMM)
ExpressionMatrix = gcrma(PMMatrix, MMMatrix, ProbeIndices,
   SequenceMatrix)
ExpressionMatrix = gcrma(..., 'ChipIndex',
ChipIndexValue, ...)
ExpressionMatrix = gcrma(..., 'OpticalCorr',
   OpticalCorrValue, ...)
ExpressionMatrix = gcrma(..., 'CorrConst', CorrConstValue,
   ...)
ExpressionMatrix = gcrma(..., 'Method', MethodValue, ...)
ExpressionMatrix = gcrma(..., 'TuningParam',
   TuningParamValue, ...)
ExpressionMatrix = gcrma(..., 'GSBCorr', GSBCorrValue, ...)
ExpressionMatrix = gcrma(..., 'Normalize', NormalizeValue,
   ...)
ExpressionMatrix = gcrma(..., 'Verbose', VerboseValue, ...)
```

Arguments

PMMatrix

Matrix of intensity values where each row corresponds to a perfect match (PM) probe and each column corresponds to an Affymetrix CEL file. (Each CEL file is generated from a separate chip. All chips should be of the same type.)

Tip You can use the `PMIntensities` matrix returned by the `celintensityread` function.

MMMatrix

Matrix of intensity values where each row corresponds to a mismatch (MM) probe and each column corresponds to an Affymetrix CEL

file. (Each CEL file is generated from a separate chip. All chips should be of the same type.)

Tip You can use the `MMIntensities` matrix returned by the `celintensityread` function.

`ProbeIndices` Column vector containing probe indices. Probes within a probe set are numbered 0 through *N* - 1, where *N* is the number of probes in the probe set.

Tip You can use the `affyprobeseqread` function to generate this column vector.

`AffinPM` Column vector of PM probe affinities.

Tip You can use the `affyprobeaffinities` function to generate this column vector.

`AffinMM` Column vector of MM probe affinities.

Tip You can use the `affyprobeaffinities` function to generate this column vector.

SequenceMatrix An *N*-by-25 matrix of sequence information for the perfect match (PM) probes on the Affymetrix GeneChip array, where *N* is the number of probes on the array. Each row corresponds to a probe, and each column corresponds to one of the 25 sequence positions. Nucleotides in the sequences are represented by one of the following integers:

- `0` — None
- `1` — A
- `2` — C
- `3` — G
- `4` — T

Tip You can use the `affyprobeseqread` function to generate this matrix. If you have this sequence information in letter representation, you can convert it to integer representation using the `nt2int` function.

ChipIndexValue Positive integer specifying a column index in *MMMatrix*, which specifies a chip. This chip intensity data is used to compute probe affinities. Default is `1`.

OpticalCorrValue Controls the use of optical background correction on the PM and MM intensity values in *PMMatrix* and *MMMatrix*. Choices are `true` (default) or `false`.

CorrConstValue	Value that specifies the correlation constant, rho, for background intensity for each PM/MM probe pair. Choices are any value ≥ `0` and ≤ `1`. Default is `0.7`.
MethodValue	String that specifies the method to estimate the signal. Choices are `MLE`, a faster, ad hoc Maximum Likelihood Estimate method, or `EB`, a slower, more formal, empirical Bayes method. Default is `MLE`.
TuningParamValue	Value that specifies the tuning parameter used by the estimate method. This tuning parameter sets the lower bound of signal values with positive probability. Choices are a positive value. Default is `5` (MLE) or `0.5` (EB). **Tip** For information on determining a setting for this parameter, see Wu et al., 2004.
GSBCorrValue	Specifies whether to perform gene-specific binding (GSB) correction using probe affinity data. Choices are `true` (default) or `false`. If there is no probe affinity information, this property is ignored.
NormalizeValue	Controls whether quantile normalization is performed on background adjusted data. Choices are `true` (default) or `false`.
VerboseValue	Controls the display of a progress report showing the number of each chip as it is completed. Choices are `true` (default) or `false`.

Return Values

ExpressionMatrix	Matrix of $\log_2$ expression values where each row corresponds to a gene (probe set) and each column corresponds to an Affymetrix CEL file, which represents a single chip.

Description

ExpressionMatrix = gcrma(*PMMatrix*, *MMMatrix*, *ProbeIndices*, *AffinPM*, *AffinMM*) performs GCRMA background adjustment, quantile normalization, and median-polish summarization on Affymetrix microarray probe-level data using probe affinity data. *ExpressionMatrix* is a matrix of $\log_2$ expression values where each row corresponds to a gene (probe set) and each column corresponds to an Affymetrix CEL file, which represents a single chip.

Note There is no column in *ExpressionMatrix* that contains probe set or gene information.

ExpressionMatrix = gcrma(*PMMatrix*, *MMMatrix*, *ProbeIndices*, *SequenceMatrix*) performs GCRMA background adjustment, quantile normalization, and Robust Multi-array Average (RMA) summarization on Affymetrix microarray probe-level data using probe sequence data to compute probe affinity data. *ExpressionMatrix* is a matrix of $\log_2$ expression values where each row corresponds to a gene (probe set) and each column corresponds to an Affymetrix CEL file, which represents a single chip.

Note If *AffinPM* and *AffinMM* affinity data and *SequenceMatrix* sequence data are not available, you can still use the gcrma function by entering an empty matrix for these inputs in the syntax.

ExpressionMatrix = gcrma(...'*PropertyName*', *PropertyValue*, ...) calls gcrma with optional properties that use property

name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

ExpressionMatrix = gcrma(..., 'ChipIndex', *ChipIndexValue*, ...) computes probe affinities from MM probe intensity data from the chip with the specified column index in *MMMatrix*. Default *ChipIndexValue* is 1. If *AffinPM* and *AffinMM* affinity data are provided, this property is ignored.

ExpressionMatrix = gcrma(..., 'OpticalCorr', *OpticalCorrValue*, ...) controls the use of optical background correction on the PM and MM intensity values in *PMMatrix* and *MMMatrix*. Choices are true (default) or false.

ExpressionMatrix = gcrma(..., 'CorrConst', *CorrConstValue*, ...) specifies the correlation constant, rho, for background intensity for each PM/MM probe pair. Choices are any value ≥ 0 and ≤ 1. Default is 0.7.

ExpressionMatrix = gcrma(..., 'Method', *MethodValue*, ...) specifies the method to estimate the signal. Choices are MLE, a faster, ad hoc Maximum Likelihood Estimate method, or EB, a slower, more formal, empirical Bayes method. Default is MLE.

ExpressionMatrix = gcrma(..., 'TuningParam', *TuningParamValue*, ...) specifies the tuning parameter used by the estimate method. This tuning parameter sets the lower bound of signal values with positive probability. Choices are a positive value. Default is 5 (MLE) or 0.5 (EB).

Tip For information on determining a setting for this parameter, see Wu et al., 2004.

ExpressionMatrix = gcrma(..., 'GSBCorr', *GSBCorrValue*, ...) specifies whether to perform gene specific binding (GSB) correction

using probe affinity data. Choices are `true` (default) or `false`. If there is no probe affinity information, this property is ignored.

`ExpressionMatrix` `= gcrma(..., 'Normalize', ` *`NormalizeValue`*`, ...)` controls whether quantile normalization is performed on background adjusted data. Choices are `true` (default) or `false`.

`ExpressionMatrix` `= gcrma(..., 'Verbose', ` *`VerboseValue`*`, ...)` controls the display of a progress report showing the number of each chip as it is completed. Choices are `true` (default) or `false`.

Examples

1. Load the MAT-file, included with the Bioinformatics Toolbox software, that contains Affymetrix data from a prostate cancer study. The variables in the MAT-file include `seqMatrix`, a matrix containing sequence information for PM probes, `pmMatrix` and `mmMatrix`, matrices containing PM and MM probe intensity values, and `probeIndices`, a column vector containing probe indexing information.

   ```
   load prostatecancerrawdata
   ```

2. Compute the Affymetrix PM and MM probe affinities from their sequences and MM probe intensities.

   ```
   [apm, amm] = affyprobeaffinities(seqMatrix, mmMatrix(:,1),...
                'ProbeIndices', probeIndices);
   ```

3. Perform GCRMA background adjustment, quantile normalization, and Robust Multi-array Average (RMA) summarization on the Affymetrix microarray probe-level data and create a matrix of expression values.

   ```
   expdata = gcrma(pmMatrix, mmMatrix, probeIndices, seqMatrix);
   ```

The `prostatecancerrawdata.mat` file used in this example contains data from Best et al., 2005.

References

[1] Wu, Z., Irizarry, R.A., Gentleman, R., Murillo, F.M., and Spencer, F. (2004). A Model Based Background Adjustment for Oligonucleotide

Expression Arrays. Journal of the American Statistical Association *99(468)*, 909–917.

[2] Wu, Z., and Irizarry, R.A. (2005). Stochastic Models Inspired by Hybridization Theory for Short Oligonucleotide Arrays. Proceedings of RECOMB 2004. J Comput Biol. *12(6)*, 882–93.

[3] Wu, Z., and Irizarry, R.A. (2005). A Statistical Framework for the Analysis of Microarray Probe-Level Data. Johns Hopkins University, Biostatistics Working Papers 73.

[4] Speed, T. (2006). Background models and GCRMA. Lecture 10, Statistics 246, University of California Berkeley. `http://www.stat.berkeley.edu/users/terry/Classes/s246.2006/-Week10/Week10L1.pdf`.

[5] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L., Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan, W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823–6834.

See Also

Bioinformatics Toolbox functions: `affygcrma`, `affyprobeseqread`, `affyread`, `affyrma`, `celintensityread`, `gcrmabackadj`, `quantilenorm`, `rmabackadj`, `rmasummary`

Purpose

Perform GC Robust Multi-array Average (GCRMA) background adjustment on Affymetrix microarray probe-level data using sequence information

Syntax

```
PMMatrix_Adj = gcrmabackadj(PMMatrix, MMMatrix, AffinPM,
   AffinMM)
[PMMatrix_Adj, nsbStruct] = gcrmabackadj(PMMatrix,
MMMatrix,
   AffinPM, AffinMM)
... = gcrmabackadj( ...'OpticalCorr',
OpticalCorrValue, ...)
... = gcrmabackadj( ...'CorrConst', CorrConstValue, ...)
... = gcrmabackadj( ...'Method', MethodValue, ...)
... = gcrmabackadj( ...'TuningParam',
TuningParamValue, ...)
... = gcrmabackadj( ...'AddVariance',
AddVarianceValue, ...)
... = gcrmabackadj( ...'GSBCorr', GSBCorrValue, ...)
... = gcrmabackadj( ...'Showplot', ShowplotValue, ...)
... = gcrmabackadj( ...'Verbose', VerboseValue, ...)
```

Arguments

PMMatrix

Matrix of intensity values where each row corresponds to a perfect match (PM) probe and each column corresponds to an Affymetrix CEL file. (Each CEL file is generated from a separate chip. All chips should be of the same type.)

Tip You can use the `PMIntensities` matrix returned by the `celintensityread` function.

MMMatrix

Matrix of intensity values where each row corresponds to a mismatch (MM) probe and each column corresponds to an Affymetrix CEL

file. (Each CEL file is generated from a separate chip. All chips should be of the same type.)

Tip You can use the `MMIntensities` matrix returned by the `celintensityread` function.

AffinPM	Column vector of PM probe affinities, such as returned by the `affyprobeaffinities` function. Each row corresponds to a probe.
AffinMM	Column vector of MM probe affinities, such as returned by the `affyprobeaffinities` function. Each row corresponds to a probe.
OpticalCorrValue	Controls the use of optical background correction on the PM and MM probe intensity values in *PMMatrix* and *MMMatrix*. Choices are `true` (default) or `false`.
CorrConstValue	Value that specifies the correlation constant, rho, for log background intensity for each PM/MM probe pair. Choices are any value ≥ `0` and ≤ `1`. Default is `0.7`.
MethodValue	String that specifies the method to estimate the signal. Choices are `MLE`, a faster, ad hoc Maximum Likelihood Estimate method, or `EB`, a slower, more formal, empirical Bayes method. Default is `MLE`.

TuningParamValue Value that specifies the tuning parameter used by the estimate method. This tuning parameter sets the lower bound of signal values with positive probability. Choices are a positive value. Default is `5` (MLE) or `0.5` (EB).

Tip For information on determining a setting for this parameter, see Wu et al., 2004.

AddVarianceValue Controls whether the signal variance is added to the weight function for smoothing low signal edge. Choices are `true` or `false` (default).

GSBCorrValue Specifies whether to perform gene-specific binding (GSB) correction using probe affinity data. Choices are `true` (default) or `false`. If there is no probe affinity information, this property is ignored.

ShowplotValue Controls the display of a plot showing the $\log_2$ of probe intensity values from a specified column (chip) in *`MMMatrix`*, versus probe affinities in *`AffinMM`*. Choices are `true`, `false`, or *`I`*, an integer specifying a column in *`MMMatrix`*. If set to `true`, the first column in *`MMMatrix`* is plotted. Default is:

- `false` — When return values are specified.
- `true` — When return values are not specified.

VerboseValue Controls the display of a progress report showing the number of each chip as it is completed. Choices are `true` (default) or `false`.

Return Values

PMMatrix_Adj	Matrix of background adjusted PM (perfect match) intensity values.
nsbStruct	Structure containing nonspecific binding background parameters, estimated from the intensities and affinities of probes on an Affymetrix GeneChip array. *nsbStruct* includes the following fields: • sigma • mu_pm • mu_mm

Description

PMMatrix_Adj = gcrmabackadj(*PMMatrix*, *MMMatrix*, *AffinPM*, *AffinMM*) performs GCRMA background adjustment (including optical background correction and nonspecific binding correction) on Affymetrix microarray probe-level data, using probe sequence information and returns *PMMatrix_Adj*, a matrix of background adjusted PM (perfect match) intensity values.

Note If *AffinPM* and *AffinMM* data are not available, you can still use the gcrmabackadj function by entering empty column vectors for both of these inputs in the syntax.

[*PMMatrix_Adj*, *nsbStruct*] = gcrmabackadj(*PMMatrix*, *MMMatrix*, *AffinPM*, *AffinMM*) returns *nsbStruct*, a structure containing nonspecific binding background parameters, estimated from the intensities and affinities of probes on an Affymetrix GeneChip array. *nsbStruct* includes the following fields:

- sigma
- mu_pm

- `mu_mm`

`... = gcrmabackadj( ...'PropertyName', PropertyValue, ...)` calls `gcrmabackadj` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = gcrmabackadj( ...'OpticalCorr', OpticalCorrValue, ...)` controls the use of optical background correction on the PM and MM probe intensity values in *`PMMatrix`* and *`MMMatrix`*. Choices are `true` (default) or `false`.

`... = gcrmabackadj( ...'CorrConst', CorrConstValue, ...)` specifies the correlation constant, rho, for log background intensity for each PM/MM probe pair. Choices are any value ≥ `0` and ≤ `1`. Default is `0.7`.

`... = gcrmabackadj( ...'Method', MethodValue, ...)` specifies the method to estimate the signal. Choices are `MLE`, a faster, ad hoc Maximum Likelihood Estimate method, or `EB`, a slower, more formal, empirical Bayes method. Default is `MLE`.

`... = gcrmabackadj( ...'TuningParam', TuningParamValue, ...)` specifies the tuning parameter used by the estimate method. This tuning parameter sets the lower bound of signal values with positive probability. Choices are a positive value. Default is `5` (MLE) or `0.5` (EB).

Tip For information on determining a setting for this parameter, see Wu et al., 2004.

`... = gcrmabackadj( ...'AddVariance', AddVarianceValue, ...)` controls whether the signal variance is added to the weight function for smoothing low signal edge. Choices are `true` or `false` (default).

`... = gcrmabackadj( ...'GSBCorr', GSBCorrValue, ...)` specifies whether to perform gene specific binding (GSB) correction using probe affinity data. Choices are `true` (default) or `false`. If there is no probe affinity information, this property is ignored.

`... = gcrmabackadj( ...'Showplot', ShowplotValue, ...)` controls the display of a plot showing the $\log_2$ of probe intensity values from a specified column (chip) in *`MMMatrix`*, versus probe affinities in *`AffinMM`*. Choices are `true`, `false`, or *`I`*, an integer specifying a column in *`MMMatrix`*. If set to `true`, the first column in *`MMMatrix`* is plotted. Default is:

- `false` — When return values are specified.
- `true` — When return values are not specified.

`... = gcrmabackadj( ...'Verbose', VerboseValue, ...)` controls the display of a progress report showing the number of each chip as it is completed. Choices are `true` (default) or `false`.

Examples

1. Load the MAT-file, included with the Bioinformatics Toolbox software, that contains Affymetrix data from a prostate cancer study. The variables in the MAT-file include `seqMatrix`, a matrix containing sequence information for PM probes, `pmMatrix` and `mmMatrix`, matrices containing PM and MM probe intensity values, and `probeIndices`, a column vector containing probe indexing information.

   ```
   load prostatecancerrawdata
   ```

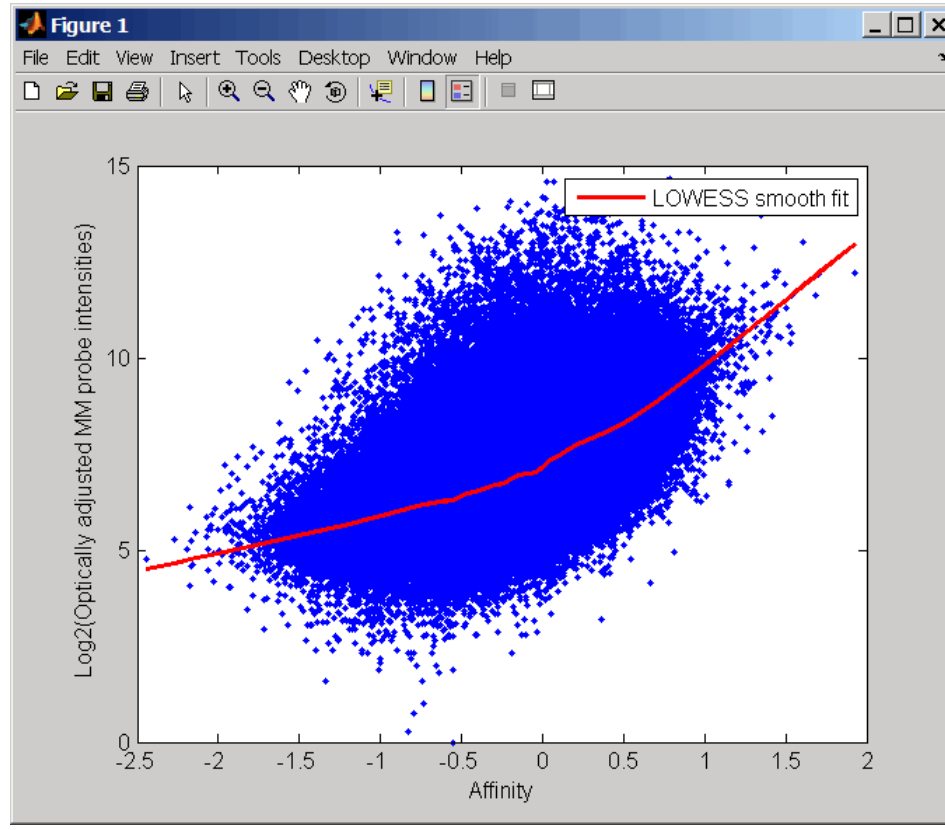
2. Compute the Affymetrix PM and MM probe affinities from their sequences and MM probe intensities.

   ```
   [apm, amm] = affyprobeaffinities(seqMatrix, mmMatrix(:,1),...
                'ProbeIndices', probeIndices);
   ```

3. Perform GCRMA background adjustment on the Affymetrix microarray probe-level data, creating a matrix of background adjusted PM intensity values. Also, display a plot showing the $\log_2$

of probe intensity values from column 3 (chip 3) in `mmMatrix`, versus probe affinities in `amm`.

```
pms_adj = gcrmabackadj(pmMatrix, mmMatrix, apm, amm, 'showplot', 3);
```



4 Perform GCRMA background adjustment again, using the slower, more formal, empirical Bayes method.

```
pms_adj2 = gcrmabackadj(pmMatrix, mmMatrix, apm, amm, 'method', 'EB');
```

The prostatecancerrawdata.mat file used in this example contains data from Best et al., 2005.

References

[1] Wu, Z., Irizarry, R.A., Gentleman, R., Murillo, F.M., and Spencer, F. (2004). A Model Based Background Adjustment for Oligonucleotide Expression Arrays. Journal of the American Statistical Association *99(468)*, 909–917.

[2] Wu, Z., and Irizarry, R.A. (2005). Stochastic Models Inspired by Hybridization Theory for Short Oligonucleotide Arrays. Proceedings of RECOMB 2004. J Comput Biol. *12(6)*, 882–93.

[3] Wu, Z., and Irizarry, R.A. (2005). A Statistical Framework for the Analysis of Microarray Probe-Level Data. Johns Hopkins University, Biostatistics Working Papers 73.

[4] Wu, Z., and Irizarry, R.A. (2003). A Model Based Background Adjustment for Oligonucleotide Expression Arrays. RSS Workshop on Gene Expression, Wye, England, http://biosun01.biostat.jhsph.edu/%7Eririzarr/Talks/gctalk.pdf.

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See Also

Bioinformatics Toolbox functions: affygcrma, affyprobeseqread, affyread, celintensityread, probelibraryinfo

Purpose

Test DataMatrix objects for greater than or equal to

Syntax

```
T = ge(DMObj1, DMObj2)
T = DMObj1 >= DMObj2
T = ge(DMObj1, B)
T = DMObj1 >= B
T = ge(B, DMObj1)
T = B >= DMObj1
```

Arguments

DMObj1, *DMObj2*	DataMatrix objects, such as created by `DataMatrix` (object constructor).
B	MATLAB numeric or logical array.

Return Values

T	Logical matrix of the same size as *DMObj1* and *DMObj2* or *DMObj1* and *B*. It contains logical `1` (true) where elements in the first input are greater than or equal to the corresponding element in the second input, and logical `0` (false) otherwise.

Description

`T = ge(DMObj1, DMObj2)` or the equivalent `T = DMObj1 >= DMObj2` compares each element in DataMatrix object *DMObj1* to the corresponding element in DataMatrix object *DMObj2*, and returns *T*, a logical matrix of the same size as *DMObj1* and *DMObj2*, containing logical `1` (true) where elements in *DMObj1* are greater than or equal to the corresponding element in *DMObj2*, and logical `0` (false) otherwise. *DMObj1* and *DMObj2* must have the same size (number of rows and columns), unless one is a scalar (1-by-1 DataMatrix object). *DMObj1* and *DMObj2* can have different `Name` properties.

`T = ge(DMObj1, B)` or the equivalent `T = DMObj1 >= B` compares each element in DataMatrix object *DMObj1* to the corresponding element in *B*, a numeric or logical array, and returns *T*, a logical matrix of the same size as *DMObj1* and *B*, containing logical `1` (true) where elements

in *DMObj1* are greater than or equal to the corresponding element in *B*, and logical 0 (false) otherwise. *DMObj1* and *B* must have the same size (number of rows and columns), unless one is a scalar.

T = ge(*B*, *DMObj1*) or the equivalent *T* = *B* >= *DMObj1* compares each element in *B*, a numeric or logical array, to the corresponding element in DataMatrix object *DMObj1*, and returns *T*, a logical matrix of the same size as *B* and *DMObj1*, containing logical 1 (true) where elements in *B* are greater than or equal to the corresponding element in *DMObj1*, and logical 0 (false) otherwise. *B* and *DMObj1* must have the same size (number of rows and columns), unless one is a scalar.

MATLAB calls *T* = ge(*X*, *Y*) for the syntax *T* = *X* >= *Y* when *X* or *Y* is a DataMatrix object.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: le

Purpose

Read data from GenBank file

Syntax

```
GenBankData = genbankread(File)
```

Arguments

File	Either of the following: • String specifying a file name, a path and file name, or a URL pointing to a file. The referenced file is a GenBank-formatted file (ASCII text file). If you specify only a file name, that file must be on the MATLAB search path or in the MATLAB Current Directory. • MATLAB character array that contains the text of a GenBank-formatted file.
GenBankData	MATLAB structure with fields corresponding to GenBank keywords.

Description

GenBankData = genbankread(*File*) reads in a GenBank-formatted file, *File*, and creates a structure, *GenBankData*, containing fields corresponding to the GenBank keywords. Each separate sequence listed in the output structure *GenBankData* is stored as a separate element of the structure.

Examples

1 Retrieve sequence information for a gene (HEXA), store data in a file, and then read back into the MATLAB software.

```
getgenbank('nm_000520', 'ToFile', 'TaySachs_Gene.txt')
s = genbankread('TaySachs_Gene.txt')

s =

                LocusName: 'NM_000520'
      LocusSequenceLength: '2437'
     LocusNumberofStrands: ''
```

```
            LocusTopology: 'linear'
        LocusMoleculeType: 'mRNA'
     LocusGenBankDivision: 'PRI'
    LocusModificationDate: '18-FEB-2009'
               Definition: [1x63 char]
                Accession: 'NM_000520'
                  Version: 'NM_000520.4'
                       GI: '189181665'
                  Project: []
                   DBLink: []
                 Keywords: []
                  Segment: []
                   Source: 'Homo sapiens (human)'
           SourceOrganism: [4x65 char]
                Reference: {1x10 cell}
                  Comment: [32x67 char]
                 Features: [147x74 char]
                      CDS: [1x1 struct]
                 Sequence: [1x2437 char]
```

2 Display the source organism for this sequence.

```
s.SourceOrganism

ans =

Homo sapiens
Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi;
Mammalia; Eutheria; Euarchontoglires; Primates; Haplorrhini;
Catarrhini; Hominidae; Homo.
```

See Also

Bioinformatics Toolbox functions: `emblread`, `fastaread`, `genpeptread`, `getgenbank`, `scfread`, `seqtool`

Purpose

Remove genes with low entropy expression values

Syntax

```
Mask = geneentropyfilter(Data)
[Mask, FData] = geneentropyfilter(Data)
[Mask, FData, FNames] = geneentropyfilter(Data, Names)
geneentropyfilter(..., 'Percentile', PercentileValue)
```

Arguments

Data	DataMatrix object or numeric matrix where each row corresponds to the experimental results for one gene. Each column is the results for all genes from one experiment.
Names	Cell array with the name of a gene for each row of experimental data. *Names* has same number of rows as *Data* with each row containing the name or ID of the gene in the data set.
PercentileValue	Property to specify a percentile below which gene data is removed. Enter a value from 0 to 100.

Description

Mask = geneentropyfilter(*Data*) identifies gene expression profiles in *Data* with entropy values less than the 10th percentile.

Mask is a logical vector with one element for each row in *Data*. The elements of *Mask* corresponding to rows with a variance greater than the threshold have a value of 1, and those with a variance less then the threshold are 0.

[*Mask*, *FData*] = geneentropyfilter(*Data*) returns *FData*, a filtered data matrix. You can also create *FData* using *FData* = Data(*Mask*,:).

[*Mask*, *FData*, *FNames*] = geneentropyfilter(*Data*, *Names*) returns *FNames*, a filtered names array, where *Names* is a cell array of the names of the genes corresponding to each row of *Data*. You can also create *FNames* using *FNames* = Names(*Mask*).

Note If *Data* is a DataMatrix object with specified row names, you do not need to provide the second input *Names* to return the third output *FNames*.

`geneentropyfilter(..., 'Percentile', PercentileValue)` removes from *Data*, the experimental data, gene expression profiles with entropy values less than *PercentileValue*, the specified percentile.

Examples

1. Load the MAT-file, provided with the Bioinformatics Toolbox software, that contains yeast data. This MAT-file includes three variables: `yeastvalues`, a matrix of gene expression data, `genes`, a cell array of GenBank accession numbers for labeling the rows in `yeastvalues`, and `times`, a vector of time values for labeling the columns in `yeastvalues`

   ```
   load yeastdata
   ```

2. Remove genes with low entropy expression values.

   ```
   [fyeastvalues, fgenes] = geneentropyfilter(yeastvalues,genes);
   ```

References

[1] Kohane I.S., Kho A.T., Butte A.J. (2003), Microarrays for an Integrative Genomics, Cambridge, MA:MIT Press.

See Also

Bioinformatics Toolbox functions: `exprprofrange`, `exprprofvar`, `genelowvalfilter`, `generangefilter`, `genevarfilter`

Purpose

Remove gene profiles with low absolute values

Syntax

```
Mask = genelowvalfilter(Data)
[Mask, FData] = genelowvalfilter(Data)
[Mask, FData, FNames] = genelowvalfilter(Data, Names)
genelowvalfilter(..., 'Percentile', PercentileValue, ...)
genelowvalfilter(..., 'AbsValue', AbsValueValue, ...)
genelowvalfilter(..., 'AnyVal', AnyValValue, ...)
```

Arguments

Data	DataMatrix object or numeric matrix where each row corresponds to the experimental results for one gene. Each column is the results for all genes from one experiment.
Names	Cell array with the same number of rows as *Data*. Each row contains the name or ID of the gene in the data set.
PercentileValue	Property to specify a percentile below which gene expression profiles are removed. Enter a value from 0 to 100.
AbsValueValue	Property to specify an absolute value below which gene expression profiles are removed.
AnyValValue	Property to select the minimum or maximum absolute value for comparison with *AbsValueValue*. If *AnyValValue* is true, selects the minimum absolute value. If *AnyValValue* is false, selects the maximum absolute value. The default value is false.

Description

Gene expression profile experiments have data where the absolute values are very low. The quality of this type of data is often bad due to large quantization errors or simply poor spot hybridization.

Mask = genelowvalfilter(*Data*) identifies gene expression profiles in *Data* with all absolute values less than the 10th percentile.

Mask is a logical vector with one element for each row in *Data*. The elements of *Mask* corresponding to rows with absolute expression levels greater than the threshold have a value of 1, and those with absolute expression levels less then the threshold are 0.

[*Mask*, *FData*] = genelowvalfilter(*Data*) returns *FData*, a filtered data matrix. You can also create *FData* using *FData* = Data(*Mask*,:).

[*Mask*, *FData*, *FNames*] = genelowvalfilter(*Data*, *Names*) returns *FNames*, a filtered names array, where *Names* is a cell array of the names of the genes corresponding to each row of *Data*. You can also create *FNames* using *FNames* = Names(*Mask*).

Note If *Data* is a DataMatrix object with specified row names, you do not need to provide the second input *Names* to return the third output *FNames*.

---

genelowvalfilter(..., '*PropertyName*', *PropertyValue*, ...) calls genelowvalfilter with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

genelowvalfilter(..., 'Percentile', *PercentileValue*, ...) removes from *Data*, the experimental data, the gene expression profiles with all absolute values less than *PercentileValue*, the specified percentile.

genelowvalfilter(..., 'AbsValue', *AbsValueValue*, ...) calculates the maximum absolute value for each gene expression profile and removes the profiles with maximum absolute values less than *AbsValValue*.

genelowvalfilter(..., 'AnyVal', *AnyValValue*, ...), when *AnyValValue* is true, calculates the minimum absolute value for

each gene expression profile and removes the profiles with minimum absolute values less than *AnyValValue*.

Examples

```
[data, labels, I, FI] = genelowvalfilter(data,labels,'AbsValue',5);
```

References

[1] Kohane I.S., Kho A.T., Butte A.J. (2003), Microarrays for an Integrative Genomics, Cambridge, MA:MIT Press.

See Also

Bioinformatics Toolbox functions: `exprprofrange`, `exprprofvar`, `geneentropyfilter`, `generangefilter`, `genevarfilter`

geneont class

Purpose

Data structure containing Gene Ontology (GO) information

Description

A geneont object is a data structure containing Gene Ontology information. You can explore and traverse Gene Ontology terms using “is_a” and “part_of” relationships.

Construction

geneont	Create geneont object and term objects

Methods

getancestors	Find terms that are ancestors of specified Gene Ontology (GO) term
getdescendants	Find terms that are descendants of specified Gene Ontology (GO) term
getmatrix	Convert geneont object into relationship matrix
getrelatives	Find terms that are relatives of specified Gene Ontology (GO) term

Properties

date	Read-only string containing date and time OBO file was last updated
default_namespace	Read-only string containing namespace to which GO terms are assigned

format_version	Read-only string containing version of encoding of OBO file
terms	Read-only column vector with handles to term objects of geneont object

Instance Hierarchy

A geneont object contains term objects.

Copy Semantics

Handle. To learn how this affects your use of the class, see Copying Objects in the MATLAB Programming Fundamentals documentation.

Indexing

You can use parenthesis () indexing with either GO identifiers (numbers) or by GO terms (term objects) to create a subontology. See "Examples" on page 3-543 below.

Examples

Indexing into a geneont Object Using the GO Identifier

You can create a subontology by indexing into a geneont object by using the GO identifier.

1 Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

```
GeneontObj = geneont('LIVE', true)
```

The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

```
Gene Ontology object with 27769 Terms.
```

2 Create a subontology by returning the terms with GO identifiers of `GO:000005` through `GO:000010`.

```
subontology1 = GeneontObj(5:10)

Gene Ontology object with 6 Terms.
```

3 Create a subontology by returning the term with a GO identifier of `GO:000100`.

```
subontology2 = GeneontObj(100)

Gene Ontology object with 1 Terms.
```

Indexing into a geneont Object Using the GO Term

You can create a subontology by indexing into a geneont object by using the GO term.

1 Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

```
GeneontObj = geneont('LIVE', true)
```

The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

```
Gene Ontology object with 27769 Terms.
```

2 Create an array of term objects containing the fifth through tenth terms of the geneont object.

```
termObject = GeneontObj.terms(5:10)

6x1 struct array with fields:
    id
    name
    ontology
    definition
    comment
    synonym
    is_a
    part_of
    obsolete
```

Note The GO term of `5` is the position of the term object in the geneont object, and is not necessarily the same as the term object with a GO identifier of `GO:000005` used in the first example. This is because there are many terms that are obsolete and are not included as term objects in the geneont object.

3 Create a subontology by returning the fifth through tenth terms of the geneont object.

```
subontology3 = GeneontObj(termObject)

Gene Ontology object with 6 Terms.
```

See Also

Bioinformatics Toolbox functions: `goannotread`, `num2goid`

Bioinformatics Toolbox class: `term`

Purpose

Create geneont object and term objects

Syntax

```
GeneontObj = geneont
GeneontObj = geneont('File', FileValue)
GeneontObj = geneont('Live', LiveValue)
GeneontObj = geneont('Live', LiveValue, 'ToFile',
   ToFileValue)
```

Description

`GeneontObj = geneont` creates *`GeneontObj`*, a geneont object, from the `gene_ontology.obo` file in the MATLAB current directory. It also creates multiple term objects, one for each term in the geneont object.

`GeneontObj = geneont('File', FileValue)` creates *`GeneontObj`*, a geneont object, from *`FileValue`*, a string specifying the file name of an Open Biomedical Ontology (OBO)-formatted file that is on the MATLAB search path.

`GeneontObj = geneont('Live', LiveValue)` controls the creation of *`GeneontObj`*, a geneont object, from the current version of the Gene Ontology database, which is the file at:

```
http://www.geneontology.org/ontology/gene_ontology.obo
```

Choices are `true` or `false` (default).

Note The full Gene Ontology database may take several minutes to download when you run this function using the `'Live'` property.

`GeneontObj = geneont('Live', LiveValue, 'ToFile', ToFileValue)`, when *`LiveValue`* is `true`, creates *`GeneontObj`*, a geneont object, from the most recent version of the Gene Ontology database, which is the file at:

```
http://www.geneontology.org/ontology/gene_ontology.obo
```

and saves the contents of this file to *ToFileValue*, a string specifying a file name or a path and file name.

Inputs

FileValue	String specifying the file name of an OBO-formatted file that is on the MATLAB search path.
LiveValue	Controls the creation of the most up-to-date geneont object. Enter `true` to create *GeneontObj*, a geneont object, from the most recent version of the Gene Ontology database. Default is `false`.
ToFileValue	String specifying a file name or path and file name to which to save the contents of the current version of the Gene Ontology database.

Outputs

GeneontObj	MATLAB object containing gene ontology information.

Examples

1 Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

```
GeneontObj = geneont('LIVE', true)
```

The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

```
Gene Ontology object with 27769 Terms.
```

2 Display information about the geneont object.

```
get(GeneontObj)

default_namespace: 'gene_ontology'
```

```
                    format_version: '1.0'
                           version: '4.509'
                              date: '28:11:2008 19:30'
                         saved_by: 'gocvs'
                auto_generated_by: 'OBO-Edit 1.101'
                        subsetdef: {7x1 cell}
                           import: ''
                     synonymtypedef: ''
                           idspace: ''
    default_relationship_id_prefix: ''
                       id_mapping: ''
                           remark: [1x31 char]
                          typeref: ''
                   unrecognized_tag: {1x2 cell}
                            Terms: [27769x1 geneont.term]
```

3 Search for all GO terms in the geneont object that contain the string `ribosome` in the field `name`, and use the `geneont.terms` property to create a MATLAB structure array of term objects containing those terms.

```
comparison = regexpi(get(GeneontObj.terms,'name'),'ribosome');
indices = find(~cellfun('isempty',comparison));
terms_with_ribosmome = GeneontObj.terms(indices)

22x1 struct array with fields:
    id
    name
    ontology
    definition
    comment
    synonym
    is_a
    part_of
    obsolete
```

Note Although the `terms` property is a column vector with handles to term objects, in the MATLAB Command Window, it displays as a structure array, with one structure for each GO term in the geneont object.

See Also

Bioinformatics Toolbox functions: `goannotread`, `num2goid`

Bioinformatics Toolbox class: `term`

Bioinformatics Toolbox property of geneont class: `geneont.terms`

generangefilter

Purpose

Remove gene profiles with small profile ranges

Syntax

```
Mask = generangefilter(Data)
[Mask, FData] = generangefilter(Data)
[Mask, FData, FNames] = generangefilter(Data, Names)
generangefilter(..., 'Percentile', PercentileValue, ...)
generangefilter(..., 'AbsValue', AbsValueValue, ...)
generangefilter(..., 'LogPercentile', LogPercentileValue,
   ...)
generangefilter(..., 'LogValue', LogValueValue, ...)
```

Arguments

Data	DataMatrix object or numeric matrix where each row corresponds to the experimental results for one gene. Each column is the results for all genes from one experiment.
Names	Cell array with the name of a gene for each row of experimental data. *Names* has same number of rows as *Data* with each row containing the name or ID of the gene in the data set.
PercentileValue	Property to specify a percentile below which gene expression profiles are removed. Enter a value from 0 to 100.
AbsValueValue	Property to specify an absolute value below which gene expression profiles are removed.
LogPercentileValue	Property to specify the logarithm of a percentile.
LogValueValue	Property to specify the logarithm of an absolute value.

Description

Mask = generangefilter(*Data*) calculates the range for each gene expression profile in *Data*, a DataMatrix object or matrix of the

experimental data, and then identifies the expression profiles with ranges less than the 10th percentile.

Mask is a logical vector with one element for each row in *Data*. The elements of *Mask* corresponding to rows with a range greater then the threshold have a value of 1, and those with a range less then the threshold are 0.

[*Mask*, *FData*] = generangefilter(*Data*) returns *FData*, a filtered data matrix. You can also create *FData* using *FData* = Data(*Mask*,:).

[*Mask*, *FData*, *FNames*] = generangefilter(*Data*, *Names*) returns *FNames*, a filtered names array, where *Names* is a cell array of the names of the genes corresponding to each row in *Data*. You can also create *FNames* using *FNames* = Names(*Mask*).

Note If *Data* is a DataMatrix object with specified row names, you do not need to provide the second input *Names* to return the third output *FNames*.

---

generangefilter(..., '*PropertyName*', *PropertyValue*, ...) calls generangefilter with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

generangefilter(..., 'Percentile', *PercentileValue*, ...) removes from the experimental data (*Data*) gene expression profiles with ranges less than a specified percentile (*PercentileValue*).

generangefilter(..., 'AbsValue', *AbsValueValue*, ...) removes from *Data* gene expression profiles with ranges less than *AbsValueValue*.

generangefilter(..., 'LogPercentile', *LogPercentileValue*, ...) filters genes with profile ranges in the lowest percent of the log range (*LogPercentileValue*).

`generangefilter(..., 'LogValue', LogValueValue, ...)` filters genes with profile log ranges lower than *`LogValueValue`*.

Examples

1. Load the MAT-file, provided with the Bioinformatics Toolbox software, that contains yeast data. This MAT-file includes three variables: `yeastvalues`, a matrix of gene expression data, `genes`, a cell array of GenBank accession numbers for labeling the rows in `yeastvalues`, and `times`, a vector of time values for labeling the columns in `yeastvalues`

   ```
   load yeastdata
   ```

2. Remove gene profiles with small profile ranges.

   ```
   [mask, fyeastvalues, fgenes] = generangefilter(yeastvalues,genes);
   ```

References

[1] Kohane I.S., Kho A.T., Butte A.J. (2003), Microarrays for an Integrative Genomics, Cambridge, MA:MIT Press.

See Also

Bioinformatics Toolbox functions: `exprprofrange`, `exprprofvar`, `geneentropyfilter`, `genelowvalfilter`, `genevarfilter`

Purpose

Return nucleotide codon to amino acid mapping for genetic code

Syntax

```
Map = geneticcode
Map = geneticcode(GeneticCode)
```

Arguments

GeneticCode Integer or string specifying a genetic code number or code name from the table Genetic Code on page 3-554. Default is `1` or `'Standard'`.

Tip If you use a code name, you can truncate the name to the first two letters of the name.

Return Values

Map Structure containing the mapping of nucleotide codons to amino acids for the standard genetic code. The *Map* structure contains a field for each nucleotide codon.

Description

Map = `geneticcode` returns a structure containing the mapping of nucleotide codons to amino acids for the standard genetic code. The *Map* structure contains a field for each nucleotide codon.

Map = `geneticcode(`*GeneticCode*`)` returns a structure containing the mapping of nucleotide codons to amino acids for the specified genetic code. *GeneticCode* is either:

- An integer or string specifying a code number or code name from the table Genetic Code on page 3-554
- The `transl_table` (code) number from the NCBI Web page describing genetic codes:

  ```
  http://www.ncbi.nlm.nih.gov/Taxonomy/Utils/wprintgc.cgi?mode=c
  ```

Tip If you use a code name, you can truncate the name to the first two letters of the name.

Genetic Code

Code Number	Code Name
1	Standard
2	Vertebrate Mitochondrial
3	Yeast Mitochondrial
4	Mold, Protozoan, Coelenterate Mitochondrial, and Mycoplasma/Spiroplasma
5	Invertebrate Mitochondrial
6	Ciliate, Dasycladacean, and Hexamita Nuclear
9	Echinoderm Mitochondrial
10	Euplotid Nuclear
11	Bacterial and Plant Plastid
12	Alternative Yeast Nuclear
13	Ascidian Mitochondrial
14	Flatworm Mitochondrial
15	Blepharisma Nuclear
16	Chlorophycean Mitochondrial
21	Trematode Mitochondrial
22	Scenedesmus Obliquus Mitochondrial
23	Thraustochytrium Mitochondrial

Examples

Return the mapping of nucleotide codons to amino acids for the Flatworm Mitochondrial genetic code.

```
wormmap = geneticcode('Flatworm Mitochondrial');
```

References

[1] NCBI Web page describing genetic codes:

```
http://www.ncbi.nlm.nih.gov/Taxonomy/Utils/wprintgc.cgi?mode=c
```

See Also

Bioinformatics Toolbox functions: `aa2nt`, `aminolookup`, `baselookup`, `codonbias`, `dnds`, `dndsml`, `nt2aa`, `revgeneticcode`, `seqshoworfs`, `seqtool`

genevarfilter

Purpose

Filter genes with small profile variance

Syntax

```
Mask = genevarfilter(Data)
[Mask, FData] = genevarfilter(Data)
[Mask, FData, FNames] = genevarfilter(Data, Names)
genevarfilter(..., 'Percentile', PercentileValue, ...)
genevarfilter(..., 'AbsValue', AbsValueValue, ...)
```

Arguments

Data	DataMatrix object or numeric matrix where each row corresponds to a gene. If a matrix, the first column is the names of the genes, and each additional column is the results from an experiment.
Names	Cell array with the name of a gene for each row of experimental data. *Names* has same number of rows as *Data* with each row containing the name or ID of the gene in the data set.
PercentileValue	Specifies a percentile below which gene expression profiles are removed. Enter a value from 0 to 100.
AbsValueValue	Property to specify an absolute value below which gene expression profiles are removed.

Description

Gene profiling experiments have genes that exhibit little variation in the profile and are generally not of interest in the experiment. These genes are commonly removed from the data.

Mask = genevarfilter(*Data*) calculates the variance for each gene expression profile in *Data* and then identifies the expression profiles with a variance less than the 10th percentile.

Mask is a logical vector with one element for each row in *Data*. The elements of *Mask* corresponding to rows with a variance greater than the threshold have a value of 1, and those with a variance less than the threshold are 0.

`[Mask, FData] = genevarfilter(Data)` returns `FData`, a filtered data matrix. You can also create `FData` using `FData = Data(Mask,:)`.

`[Mask, FData, FNames] = genevarfilter(Data, Names)` returns `FNames`, a filtered names array, where `Names` is a cell array of the names of the genes corresponding to each row in `Data`. You can also create `FNames` using `FNames = Names(Mask)`.

Note If `Data` is a DataMatrix object with specified row names, you do not need to provide the second input `Names` to return the third output `FNames`.

`genevarfilter(..., 'PropertyName', PropertyValue, ...)` calls `genevarfilter` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:.

`genevarfilter(..., 'Percentile', PercentileValue, ...)` removes from the experimental data (`Data`) gene expression profiles with a variance less than the percentile (`PercentileValue`).

`genevarfilter(..., 'AbsValue', AbsValueValue, ...)` removes from `Data` gene expression profiles with a variance less than `AbsValueValue`.

Examples

1. Load the MAT-file, provided with the Bioinformatics Toolbox software, that contains yeast data. This MAT-file includes three variables: `yeastvalues`, a matrix of gene expression data, `genes`, a cell array of GenBank accession numbers for labeling the rows in `yeastvalues`, and `times`, a vector of time values for labeling the columns in `yeastvalues`

   ```
   load yeastdata
   ```

2. Filter genes with a small profile variance.

```
[fyeastvalues, fgenes] = genevarfilter(yeastvalues,genes);
```

References

[1] Kohane I.S., Kho A.T., Butte A.J. (2003), Microarrays for an Integrative Genomics, Cambridge, MA:MIT Press.

See Also

Bioinformatics Toolbox functions: `exprprofrange`, `exprprofvar`, `generangefilter`, `geneentropyfilter`, `genelowvalfilter`

Purpose

Read data from GenPept file

Syntax

```
GenPeptData = genpeptread('File')
```

Arguments

File	GenPept formatted file (ASCII text file). Enter a file name, a path and file name, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text of a GenPept file.

Description

`genpeptread` reads data from a GenPept formatted file into a MATLAB structure.

Note NCBI has changed the name of their protein search engine from GenPept to Entrez Protein. However, the function names in the Bioinformatics Toolbox software (`getgenpept` and `genpeptread`) are unchanged representing the still-used GenPept report format.

`GenPeptData = genpeptread('File')` reads in the GenPept formatted sequence from *File* and creates a structure `GenPeptData`, containing fields corresponding to the GenPept keywords. Each separate sequence listed in *File* is stored as a separate element of the structure. `GenPeptDATA` contains these fields:

Field
`LocusName`
`LocusSequenceLength`
`LocusMoleculeType`
`LocusGenBankDivision`
`LocusModificationDate`
`Definition`

Field
Accession
PID
Version
GI
DBSource
Keywords
Source
SourceDatabase
SourceOrganism
Reference.Number
Reference.Authors
Reference.Title
Reference.Journal
Reference.MedLine
Reference.PubMed
Reference.Remark
Comment
Features
Weight
Length
Sequence

Examples

Retrieve sequence information for the protein coded by the gene HEXA, save to a file, and then read back into the MATLAB software.

```
getgenpept('p06865', 'ToFile', 'TaySachs_Protein.txt')
genpeptread('TaySachs_Protein.txt')
```

See Also

Bioinformatics Toolbox functions: `fastaread`, `genbankread`, `getgenpept`, `pdbread`, `seqtool`

Purpose

Read Gene Expression Omnibus (GEO) Series (GSE) format data

Syntax

```
GEOData = geoseriesread(File)
```

Arguments

File

Either of the following:

- String specifying a file name, a path and file name, or a URL pointing to a file. The referenced file is a Gene Expression Omnibus (GEO) Series (GSE) format file. If you specify only a file name, that file must be on the MATLAB search path or in the current directory.
- MATLAB character array that contains the text of a GEO Series (GSE) format file.

Tip You can use the `getgeodata` function with the `'ToFile'` property to retrieve GEO Series (GSE) format data from the GEO database and create a GEO Series (GSE) format file.

Return Values

GEOData

MATLAB structure containing the following fields:

- `Header` — Header text from the GEO Series (GSE) format file, typically containing a description of the data or experiment information.
- `Data` — DataMatrix object containing the data from a GEO Series (GSE) format file. The columns and rows of the DataMatrix object correspond to the sample IDs and Ref IDs, respectively, from the GEO Series (GSE) format file.

Description

GEOData = geoseriesread(*File*) reads a Gene Expression Omnibus (GEO) Series (GSE) format file, and then creates a MATLAB structure, *GEOData*, with the following fields.

Fields	Description
Header	Header text from the GEO Series (GSE) format file, typically containing a description of the data or experiment information.
Data	DataMatrix object containing the data from a GEO Series (GSE) format file. The columns and rows of the DataMatrix object correspond to the sample IDs and Ref IDs, respectively, from the GEO Series (GSE) format file.

Examples

1. Retrieve Series (GSE) data from the GEO Web site and save it to a file.

```
geodata = getgeodata('GSE11287','ToFile','GSE11287.txt');
```

2. In a subsequent MATLAB session, you can access the Series (GSE) data from your local file, instead of retrieving it from the GEO Web site.

```
geodata = geoseriesread('GSE11287.txt')

geodata =

    Header: [1x1 struct]
      Data: [45101x6 bioma.data.DataMatrix]
```

3. Access the sample IDs using the colnames property of a DataMatrix object.

```
sampleIDs = geodata.Data.colnames

sampleIDs =
```

```
'GSM284935'  'GSM284936'  'GSM284937'  'GSM284938'  'GSM284939'  'GSM284940'
```

See Also

Bioinformatics Toolbox functions: `affyread`, `agferead`, `galread`, `geosoftread`, `getgeodata`, `gprread`, `ilmnbsread`, `sptread`

Bioinformatics Toolbox object: DataMatrix object

Purpose

Read Gene Expression Omnibus (GEO) SOFT format data

Syntax

```
GEOSOFTData = geosoftread(File)
```

Arguments

File

Either of the following:

- String specifying a file name, a path and file name, or a URL pointing to a file. The referenced file is a Gene Expression Omnibus (GEO) SOFT format Sample file (GSM), Data Set file (GDS), or Platform (GPL) file. If you specify only a file name, that file must be on the MATLAB search path or in the current directory.
- MATLAB character array that contains the text of a GEO SOFT format file.

Tip You can use the `getgeodata` function with the `'ToFile'` property to retrieve GEO SOFT format data from the GEO database and create a GEO SOFT format file.

Return Values

GEOSOFTData

MATLAB structure containing information from a GEO SOFT format file.

Description

GEOSOFTData = `geosoftread(`*File*`)` reads a Gene Expression Omnibus (GEO) SOFT format Sample file (GSM), Data Set file (GDS), or Platform (GPL) file, and then creates a MATLAB structure, *GEOSOFTData*, with the following fields.

Fields	Description
`Scope`	Type of file read (SAMPLE, DATASET, or PLATFORM)
`Accession`	Accession number for record in GEO database.
`Header`	Microarray experiment information.
`ColumnDescriptions`	Cell array containing descriptions of columns in the data.
`ColumnNames`	Cell array containing names of columns in the data.
`Data`	Array containing microarray data.
`Identifier` (GDS files only)	Cell array containing probe IDs.
`IDRef` (GDS files only)	Cell array containing indices to probes.

Note Currently, the `geosoftread` function supports Sample (GSM), Data Set (GDS), and Platform (GPL) records.

Examples

Retrieve GSM data from the GEO Web site and save it to a file.

```
geodata = getgeodata('GSM3258','ToFile','GSM3258.txt');
```

Use `geosoftread` to read a local copy of the GSM file, instead of accessing it from the GEO Web site.

```
geodata = geosoftread('GSM3258.txt')

geodata =

                Scope: 'SAMPLE'
            Accession: 'GSM3258'
```

```
                Header: [1x1 struct]
    ColumnDescriptions: {6x1 cell}
           ColumnNames: {6x1 cell}
                  Data: {5355x6 cell}
```

Read the GDS file for photosynthesis in proteobacteria.

```
gdsdata = geosoftread('GDS329.soft')

gdsdata =

                 Scope: 'DATASET'
             Accession: 'GDS329'
                Header: [1x1 struct]
    ColumnDescriptions: {6x1 cell}
           ColumnNames: {6x1 cell}
                 IDRef: {5355x1 cell}
            Identifier: {5355x1 cell}
                  Data: [5355x6 double]
```

See Also

Bioinformatics Toolbox functions: `galread`, `getgeodata`, `geoseriesread`, `gprread`, `ilmnbsread`, `sptread`

get (biograph)

Purpose

Retrieve information about biograph object

Syntax

```
get(BGobj)
BGStruct = get(BGobj)
PropertyValue = get(BGobj, 'PropertyName')
[Property1Value, Property2Value, ...] = get(BGobj,
   'Property1Name', 'Property2Name', ...)
```

Arguments

BGobj	Biograph object created with the function `biograph`.
PropertyName	Property name for a biograph object.

Return Values

BGStruct	Scalar structure, in which each field name is a property of a biograph object, and each field contains the value of that property.
PropertyValue	Value of the property specified by *PropertyName*.

Description

`get(`*BGobj*`)` displays all properties and their current values of *BGobj*, a biograph object.

BGStruct `= get(`*BGobj*`)` returns all properties of *BGobj*, a biograph object, to *BGStruct*, a scalar structure, in which each field name is a property of a biograph object, and each field contains the value of that property.

PropertyValue `= get(`*BGobj*`, '`*PropertyName*`')` returns the value of the specified property of *BGobj*, a biograph object.

`[`*Property1Value*`, `*Property2Value*`, ...] = get(`*BGobj*`, '`*Property1Name*`', '`*Property2Name*`', ...)` returns the values of the specified properties of *BGobj*, a biograph object.

Properties of a Biograph Object

Property	Description
`ID`	String to identify the biograph object. Default is `''`.
`Label`	String to label the biograph object. Default is `''`.
`Description`	String that describes the biograph object. Default is `''`.
`LayoutType`	String that specifies the algorithm for the layout engine. Choices are: • `'hierarchical'` (default) — Uses a topological order of the graph to assign levels, and then arranges the nodes from top to bottom, while minimizing crossing edges. • `'radial'` — Uses a topological order of the graph to assign levels, and then arranges the nodes from inside to outside of the circle, while minimizing crossing edges. • `'equilibrium'` — Calculates layout by minimizing the energy in a dynamic spring system.

Properties of a Biograph Object (Continued)

Property	Description
`EdgeType`	String that specifies how edges display. Choices are: • `'straight'` • `'curved'` (default) • `'segmented'` **Note** Curved or segmented edges occur only when necessary to avoid obstruction by nodes. Biograph objects with `LayoutType` equal to `'equilibrium'` or `'radial'` cannot produce curved or segmented edges.
`Scale`	Positive number that post-scales the node coordinates. Default is `1`.
`LayoutScale`	Positive number that scales the size of the nodes before calling the layout engine. Default is `1`.
`EdgeTextColor`	Three-element numeric vector of RGB values. Default is `[0, 0, 0]`, which defines black.
`EdgeFontSize`	Positive number that sets the size of the edge font in points. Default is `8`.
`ShowArrows`	Controls the display of arrows with the edges. Choices are `'on'` (default) or `'off'`.
`ArrowSize`	Positive number that sets the size of the arrows in points. Default is `8`.
`ShowWeights`	Controls the display of text indicating the weight of the edges. Choices are `'on'` (default) or `'off'`.

Properties of a Biograph Object (Continued)

Property	Description
`ShowTextInNodes`	String that specifies the node property used to label nodes when you display a biograph object using the `view` method. Choices are: • `'Label'` — Uses the `Label` property of the node object (default). • `'ID'` — Uses the `ID` property of the node object. • `'None'`
`NodeAutoSize`	Controls precalculating the node size before calling the layout engine. Choices are `'on'` (default) or `'off'`.
`NodeCallback`	User-defined callback for all nodes. Enter the name of a function, a function handle, or a cell array with multiple function handles. After using the `view` function to display the biograph object in the Biograph Viewer, you can double-click a node to activate the first callback, or right-click and select a callback to activate. Default is the anonymous function, `@(node) inspect(node)`, which displays the Property Inspector dialog box.

Properties of a Biograph Object (Continued)

Property	Description
`EdgeCallback`	User-defined callback for all edges. Enter the name of a function, a function handle, or a cell array with multiple function handles. After using the `view` function to display the biograph object in the Biograph Viewer, you can double-click an edge to activate the first callback, or right-click and select a callback to activate. Default is the anonymous function, `@(edge) inspect(edge)`, which displays the Property Inspector dialog box.
`CustomNodeDrawFcn`	Function handle to a customized function to draw nodes. Default is `[]`.
`Nodes`	Read-only column vector with handles to node objects of a biograph object. The size of the vector is the number of nodes. For properties of node objects, see Properties of a Node Object on page 3-131.
`Edges`	Read-only column vector with handles to edge objects of a biograph object. The size of the vector is the number of edges. For properties of edge objects, see Properties of an Edge Object on page 3-133.

Examples

1 Create a biograph object and assign the node IDs.

```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];
ids = {'M30931','L07625','K03454','M27323','M15390'};
bg = biograph(cm,ids);
```

2 Use the `get` function to display the node IDs.

```
get(bg.nodes,'ID')
```

```
ans =

    'M30931'
    'L07625'
    'K03454'
    'M27323'
    'M15390'
```

See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox method of a biograph object: `set`

get (clustergram)

Purpose

Retrieve information about clustergram object

Syntax

```
get(CGobj)
CGStruct = get(CGobj)
PropertyValue = get(CGobj, 'PropertyName')
[Property1Value, Property2Value, ...] = get(CGobj,
   'Property1Name', 'Property2Name', ...)
```

Arguments

CGobj	Clustergram object created with the function `clustergram`.
PropertyName	Property name for a clustergram object.

Description

`get(`*`CGobj`*`)` displays all properties and their current values of *`CGobj`*, a clustergram object.

`CGStruct` `= get(`*`CGobj`*`)` returns all properties of *`CGobj`*, a clustergram object, to *`CGStruct`*, a scalar structure, in which each field name is a property of a clustergram object, and each field contains the value of that property.

`PropertyValue` `= get(`*`CGobj`*`, '`*`PropertyName`*`')` returns the value of the specified property of *`CGobj`*, a clustergram object.

`[`*`Property1Value`*`, `*`Property2Value`*`, ...] = get(`*`CGobj`*`, '`*`Property1Name`*`', '`*`Property2Name`*`', ...)` returns the values of the specified properties of *`CGobj`*, a clustergram object.

Properties of a Clustergram Object

Property	Description
`RowLabels`	Vector of numbers or cell array of text strings to label the rows in the dendrogram and heat map. Default is a vector of values `1` through *M*, where *M* is the number of rows in *`Data`*, the matrix of data used by the `clustergram` function to create the clustergram object.
`ColumnLabels`	Vector of numbers or cell array of text strings to label the columns in the dendrogram and heat map. Default is a vector of values `1` through *N*, where *N* is the number of columns in *`Data`*, the matrix of data used by the `clustergram` function to create the clustergram object.
`RowGroupNames`	A cell array of text strings containing the names of the row groups exported to a clustergram object created using the **Export Group to Workspace** command in the Clustergram window.
`RowNodeNames`	A cell array of text strings containing the names of the row nodes exported to a clustergram object created using the **Export Group to Workspace** command in the Clustergram window.
`ColumnGroupNames`	A cell array of text strings containing the names of the column groups exported to a clustergram object created using the **Export Group to Workspace** command in the Clustergram window.

Properties of a Clustergram Object (Continued)

Property	Description
`ColumnNodeNames`	A cell array of text strings containing the names of the column nodes exported to a clustergram object created using the **Export Group to Workspace** command in the Clustergram window.
`ExprValues`	An *M*-by-*N* matrix of data, where *M* and *N* are the number of row nodes and column nodes respectively, exported to a clustergram object created using the **Export Group to Workspace** command in the Clustergram window. If the matrix contains gene expression data, typically each row corresponds to a gene and each column corresponds to a sample.
`Standardize`	Text string that specifies the dimension for standardizing the values in the data. The standardized values are transformed so that the mean is 0 and the standard deviation is 1 in the specified dimension. Possibilities are: • `'Column (1)'` — Standardized along the columns of data. • `'Row (2)'` — Standardized along the rows of data. • `'None (3)'` — Did not perform standardization.

Properties of a Clustergram Object (Continued)

Property	Description
`Cluster`	Text string that specifies the dimension for clustering the values in the data. Possibilities are: • `'Row (1)'` — Clustered rows of data only. • `'Column (2)'` — Clustered columns of data only. • `'All (3)'` — Clustered rows of data, then cluster columns of row-clustered data.
`RowPdist`	String or cell array that specifies the distance metric and optional arguments passed to the `pdist` function (Statistics Toolbox software) used to calculate the pairwise distances between rows. For information on possibilities, see the `pdist` function.
`ColumnPdist`	String or cell array that specifies the distance metric and optional arguments passed to the `pdist` function (Statistics Toolbox software) used to calculate the pairwise distances between columns. For information on possibilities, see the `pdist` function.
`Linkage`	String or two-element cell array of strings that specifies the linkage method passed to the `linkage` function (Statistics Toolbox software) used to create the hierarchical cluster tree for rows and columns. If a two-element cell array of strings, the first element is for linkage between rows, and the second element is for linkage between columns. For information on possibilities, see the `linkage` function.

Properties of a Clustergram Object (Continued)

Property	Description
`Dendrogram`	Scalar or two-element numeric vector or cell array that specifies the `'colorthreshold'` property passed to the `dendrogram` function (Statistics Toolbox software) used to create the dendrogram plot. If a two-element numeric vector or cell array, the first element is for the rows, and the second element is for the columns. For more information, see the `dendrogram` function.
`OptimalLeafOrder`	Property that enabled or disabled the optimal leaf ordering calculation, which determines the leaf order that maximizes the similarity between neighboring leaves. Possibilities are `1` (enabled) or `0` (disabled).
`LogTrans`	Controlled the $\log_2$ transform of the data from natural scale. Possibilities are `1` (true) or `0` (false).
`ColorMap`	Either of the following: • *M*-by-3 matrix of RGB values • Name or function handle of a function that returns a colormap, such as `redgreencmap` or `redbluecmap`
`DisplayRange`	Positive scalar that specifies the display range of standardized values. For example, if you specify `redgreencmap` for the `'ColorMap'` property, pure red represents values ≥ `DisplayRange`, and pure green represents values ≤ –`DisplayRange`.

Properties of a Clustergram Object (Continued)

Property	Description
`SymmetricRange`	Property to force the color scale of the heat map to be symmetric around zero. Possibilities are `1` (true) or `0` (false).
`Ratio`	Either of the following: • Scalar • Two-element vector It specifies the ratio of space that the row and column dendrograms occupy relative to the heat map. If `Ratio` is a scalar, it is the ratio for both dendrograms. If `Ratio` is a two-element vector, the first element is for the ratio of the row dendrogram width to the heat map width, and the second element is for the ratio of the column dendrogram height to the heat map height. The second element is ignored for one-dimensional clustergrams.
`Impute`	Any of the following: • Name of a function that imputes missing data. • Handle to a function that imputes missing data. • Cell array where the first element is the name of or handle to a function that imputes missing data and the remaining elements are property name/property value pairs used as inputs to the function.

Properties of a Clustergram Object (Continued)

Property	Description
`RowMarkers`	Optional structure array for annotating the groups (clusters) of rows determined by the `clustergram` function. Each structure in the array represents a group of rows and contains the following fields: • `GroupNumber` — Number to annotate the row group. • `Annotation` — String specifying text to annotate the row group. • `Color` — String or three-element vector of RGB values specifying a color, which is used to label the row group. For more information on specifying colors, see `colorspec`. If this field is empty, default is `'blue'`.
`ColumnMarkers`	Optional structure array for annotating groups (clusters) of columns determined by the `clustergram` function. Each structure in the array represents a group of rows and contains the following fields: • `GroupNumber` — Number to annotate the column group. • `Annotation` — String specifying text to annotate the column group. • `Color` — String or three-element vector of RGB values specifying a color, which is used to label the column group. For more information on specifying colors, see `colorspec`. If this field is empty, default is `'blue'`.

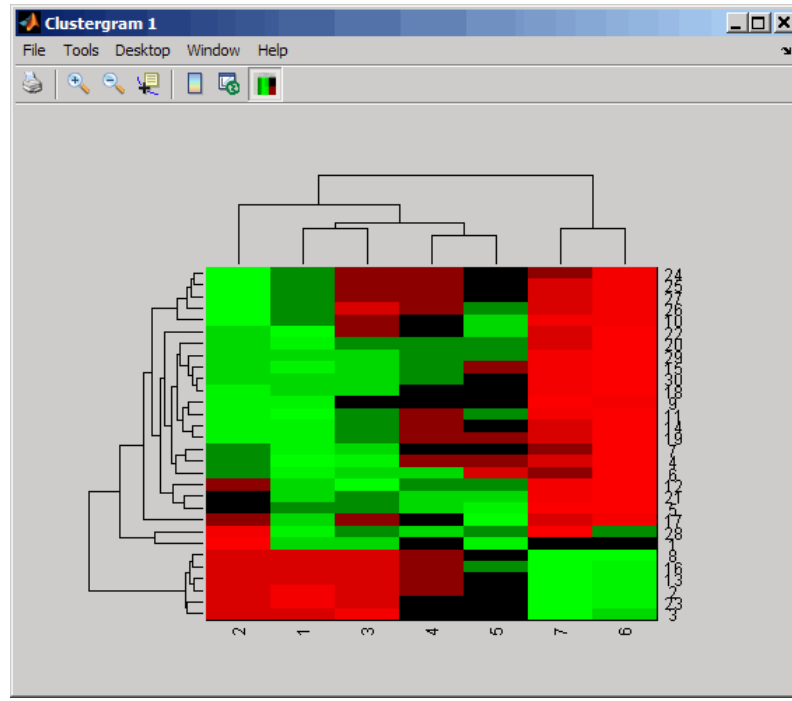
Examples

1 Load the MAT-file, provided with the Bioinformatics Toolbox software, that contains `yeastvalues`, a matrix of gene expression data.

```
load filteredyeastdata
```

2 Create a clustergram object and display the dendrograms and heat map from the gene expression data in the first 30 rows of the `yeastvalues` matrix.

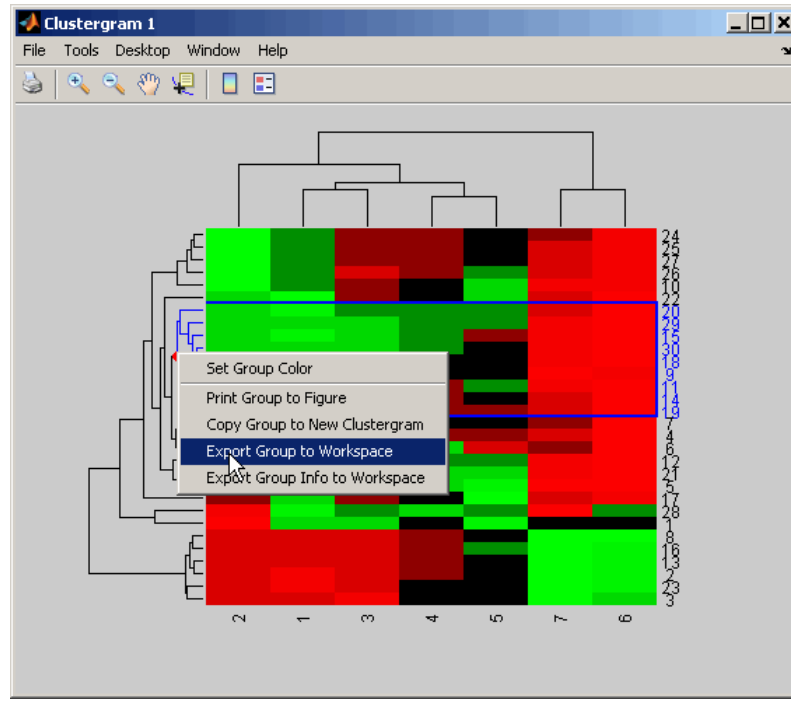
```
cgo = clustergram(yeastvalues(1:30,:))
Clustergram object with 30 rows of nodes and 7 columns of nodes.
```



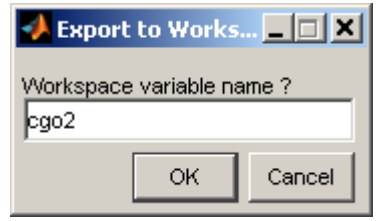
3 Use the `get` method to display the properties of the clustergram object, `cgo`.

```
get(cgo)

           RowLabels: {30x1 cell}
        ColumnLabels: {7x1 cell}
         Standardize: {'ROW (2)'}
             Cluster: {'ALL (3)'}
           RowPDist: {'Euclidean'}
         ColumnPDist: {'Euclidean'}
             Linkage: {'Average'}
          Dendrogram: {[0]}
    OptimalLeafOrder: 1
            LogTrans: 0
            Colormap: [11x3 double]
        DisplayRange: 3
      SymmetricRange: 1
               Ratio: [0.2000 0.2000]
              Impute: []
           RowMarkers: []
         ColumnMarkers: []
```

4 Export a clustergram object of a group (cluster) of rows to the MATLAB Workspace by right-clicking a node in the row dendrogram, and then selecting **Export Group to Workspace**.



5 In the Export to Workspace dialog box, type **cgo2** for the Workspace variable name for the clustergram object, and then click **OK**.



6 Use the `get` method to display the properties of `cgo2`, the clustergram object of the exported group.

```
get(cgo2)
```

```
    RowGroupNames: {8x1 cell}
     RowNodeNames: {9x1 cell}
ColumnGroupNames: {6x1 cell}
 ColumnNodeNames: {7x1 cell}
       ExprValues: [9x7 double]
      Standardize: {'ROW (2)'}
          Cluster: {'ALL (3)'}
        RowPDist: {'Euclidean'}
      ColumnPDist: {'Euclidean'}
          Linkage: {'Average'}
       Dendrogram: {[0]}
OptimalLeafOrder: 1
         LogTrans: 0
         Colormap: [11x3 double]
     DisplayRange: 3
   SymmetricRange: 1
            Ratio: [0.2000 0.2000]
           Impute: []
       RowMarkers: []
    ColumnMarkers: []
```

See Also

Bioinformatics Toolbox function: `clustergram` (object constructor)

Bioinformatics Toolbox object: clustergram object

Bioinformatics Toolbox methods of a clustergram object: `plot`, `set`, `view`

Purpose

Retrieve information about DataMatrix object

Syntax

```
get(DMObj)
DMStruct = get(DMObj)
PropertyValue = get(DMObj, 'PropertyName')
[Property1Value, Property2Value, ...] = get(DMObj,
   'Property1Name', 'Property2Name', ...)
```

Arguments

DMObj	DataMatrix object, such as created by `DataMatrix` (object constructor).
PropertyName	Property name of a DataMatrix object.

Return Values

DMStruct	Scalar structure, in which each field name is a property of a DataMatrix object, and each field contains the value of that property.
PropertyValue	Value of the property specified by *PropertyName*.

Description

`get(`*DMObj*`)` displays all properties and their current values of *DMObj*, a DataMatrix object.

DMStruct `= get(`*DMObj*`)` returns all properties of *DMObj*, a DataMatrix object, to *DMStruct*, a scalar structure, in which each field name is a property of a DataMatrix object, and each field contains the value of that property.

PropertyValue `= get(`*DMObj*`, '`*PropertyName*`')` returns the value of the specified property of *DMObj*, a DataMatrix object.

`[`*Property1Value*`, `*Property2Value*`, ...] = get(`*DMObj*`, '`*Property1Name*`', '`*Property2Name*`', ...)` returns the values of the specified properties of *DMObj*, a DataMatrix object.

Properties of a DataMatrix Object

Property	Description
`Name`	String that describes the DataMatrix object. Default is `''`.
`RowNames`	Empty array or cell array of strings that specifies the names for the rows, typically gene names or probe identifiers. The number of elements in the cell array must equal the number of rows in the matrix. Default is an empty array.
`ColNames`	Empty array or cell array of strings that specifies the names for the columns, typically sample identifiers. The number of elements in the cell array must equal the number of columns in the matrix.
`NRows`	Positive number that specifies the number of rows in the matrix.
`NCols`	Positive number that specifies the number of columns in the matrix.
`NDims`	Positive number that specifies the number of dimensions in the matrix.
`ElementClass`	String that specifies the class type, such as `single` or `double`.

Examples

1 Load the MAT-file, provided with the Bioinformatics Toolbox software, that contains yeast data. This MAT-file includes three variables: `yeastvalues`, a matrix of gene expression data, `genes`, a cell array of GenBank accession numbers for labeling the rows in `yeastvalues`, and `times`, a vector of time values for labeling the columns in `yeastvalues`.

```
load filteredyeastdata
```

2 Import the microarray object package so that the `DataMatrix` constructor function will be available.

```
import bioma.data.*
```

3 Create a DataMatrix object from the gene expression data in the first 30 rows of the `yeastvalues` matrix. Use the `genes` column vector and `times` row vector to specify the row names and column names.

```
dmo = DataMatrix(yeastvalues(1:30,:),genes(1:30,:),times);
```

4 Use the `get` method to display the properties of the DataMatrix object, `dmo`.

```
get(dmo)

           Name: ''
        RowNames: {30x1 cell}
        ColNames: {'   0'  ' 9.5'  '11.5'  '13.5'  '15.5'  '18.5'  '20.5'}
           NRows: 30
           NCols: 7
           NDims: 2
     ElementClass: 'double'
```

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: `set`

get (phytree)

Purpose

Retrieve information about phylogenetic tree object

Syntax

```
[Value1, Value2,...] = get(Tree,
'Property1','Property2',...)
get(Tree)
V = get(Tree)
```

Arguments

Tree	Phytree object created with the function `phytree`.
Name	Property name for a `phytree` object.

Description

`[Value1, Value2,...] = get(Tree, 'Property1','Property2',...)` returns the specified properties from a phytree object (`Tree`).

Properties for a `phytree` object are listed in the following table.

Property	Description
`NumLeaves`	Number of leaves
`NumBranches`	Number of branches
`NumNodes`	Number of nodes (`NumLeaves + NumBranches`)
`Pointers`	Branch to leaf/branch connectivity list
`Distances`	Edge length for every leaf/branch
`LeafNames`	Names of the leaves
`BranchNames`	Names of the branches
`NodeNames`	Names of all the nodes

`get(Tree)` displays all property names and their current values for a phytree object (*Tree*).

`V = get(Tree)` returns a structure where each field name is the name of a property of a phytree object (`Tree`) and each field contains the value of that property.

Examples

1 Read in a phylogenetic tree from a file.

```
tr = phytreeread('pf00002.tree')

Phylogenetic tree object with 33 leaves (32 branches)
```

2 Get the names of the leaves.

```
protein_names = get(tr,'LeafNames')

protein_names =

    'Q9YHC6_RANRI/126-382'
    'VIPR1_RAT/140-397'
    'VIPR_CARAU/100-359'
     ...
```

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreeread`

Bioinformatics Toolbox object: phytree object

Bioinformatics Toolbox methods of phytree object: `getbyname`, `select`

getancestors (biograph)

Purpose

Find ancestors in biograph object

Syntax

```
Nodes = getancestors(BiographNode)
Nodes = getancestors(BiographNode, NumGenerations)
```

Arguments

BiographNode	Node in a biograph object.
NumGenerations	Number of generations. Enter a positive integer.

Description

Nodes = getancestors(*BiographNode*) returns a node (BiographNode) and all of its direct ancestors.

Nodes = getancestors(*BiographNode, NumGenerations*) finds the node (*BiographNode*) and its direct ancestors up to a specified number of generations (*NumGenerations*).

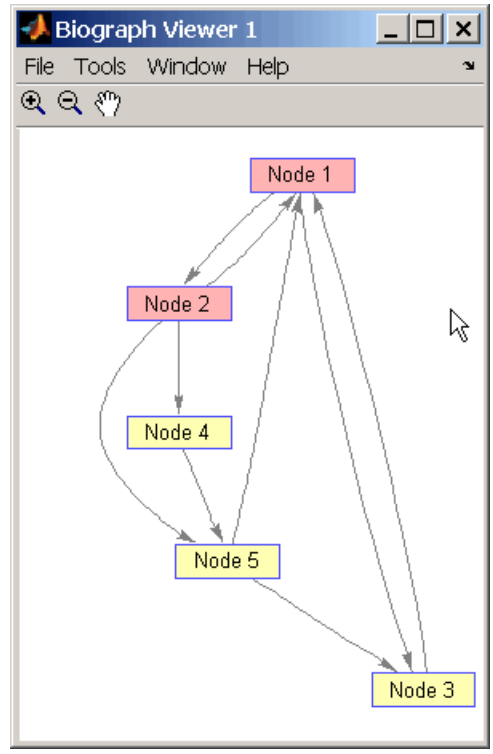
Examples

1 Create a biograph object.

```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];
bg = biograph(cm)
```

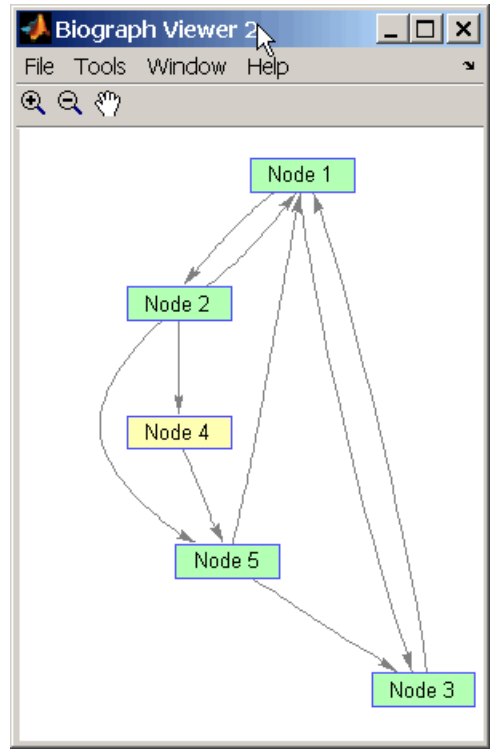
2 Find one generation of ancestors for node 2.

```
ancNodes = getancestors(bg.nodes(2));
set(ancNodes,'Color',[1 .7 .7]);
bg.view;
```



3 Find two generations of ancestors for node 2.

```
ancNodes = getancestors(bg.nodes(2),2);
set(ancNodes,'Color',[.7 1 .7]);
bg.view;
```



See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: `dolayout`, `get`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `set`, `view`

Purpose

Find terms that are ancestors of specified Gene Ontology (GO) term

Syntax

```
AncestorIDs = getancestors(GeneontObj, ID)
[AncestorIDs, Counts] = getancestors(GeneontObj, ID)
... = getancestors(..., 'Height', HeightValue, ...)
... = getancestors(..., 'Relationtype', RelationtypeValue,
   ...)
... = getancestors(..., 'Exclude', ExcludeValue, ...)
```

Description

`AncestorIDs = getancestors(GeneontObj, ID)` searches `GeneontObj`, a geneont object, for GO terms that are ancestors of the GO term(s) specified by `ID`, which is a GO term identifier or vector of identifiers. It returns `AncestorIDs`, a vector of GO term identifiers including `ID`. `ID` is a nonnegative integer or a vector containing nonnegative integers.

`[AncestorIDs, Counts] = getancestors(GeneontObj, ID)` also returns the number of times each ancestor is found. `Counts` is a column vector with the same number of elements as terms in `GeneontObj`.

Tip The `Counts` return value is useful when you tally counts in gene enrichment studies. For more information, see the Gene Ontology Enrichment in Microarray Data demo.

`... = getancestors(..., 'PropertyName', PropertyValue, ...)` calls `getancestors` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = getancestors(..., 'Height', HeightValue, ...)` searches up through a specified number of levels, `HeightValue`, in the gene ontology. `HeightValue` is a positive integer. Default is `Inf`.

`... = getancestors(..., 'Relationtype', RelationtypeValue, ...)` searches for specified relationship types, *`RelationtypeValue`*, in the gene ontology. *`RelationtypeValue`* is a string. Choices are `'is_a'`, `'part_of'`, or `'both'` (default).

`... = getancestors(..., 'Exclude', ExcludeValue, ...)` controls excluding *`ID`*, the original queried term(s), from the output *`AncestorIDs`*, unless the term was reached while searching the gene ontology. Choices are `true` or `false` (default).

Inputs

`GeneontObj`	A geneont object, such as created by the `geneont.geneont` constructor function.
`ID`	GO term identifier or vector of identifiers.
`HeightValue`	Positive integer specifying the number of levels to search upward in the gene ontology.
`RelationtypeValue`	String specifying the relationship types to search for in the gene ontology. Choices are: • `'is_a'` • `'part_of'` • `'both'` (default)
`ExcludeValue`	Controls excluding *`ID`*, the original queried term(s), from the output *`AncestorIDs`*, unless the term was reached while searching the gene ontology. Choices are `true` or `false` (default).

Outputs

`AncestorIDs`	Vector of GO term identifiers including *`ID`*.
`Counts`	Column vector with the same number of elements as terms in *`GeneontObj`*, indicating the number of times each ancestor is found.

Examples

1 Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

```
GO = geneont('LIVE', true)
```

The MATLAB software creates a geneont object and displays the number of terms in the database.

```
Gene Ontology object with 24316 Terms.
```

2 Retrieve the ancestors of the Gene Ontology term with an identifier of 46680.

```
ancestors = getancestors(GO,46680)

ancestors =
        8150
        9636
       17085
       42221
       46680
       50896
```

3 Create a subordinate Gene Ontology.

```
subontology = GO(ancestors)

Gene Ontology object with 6 Terms.
```

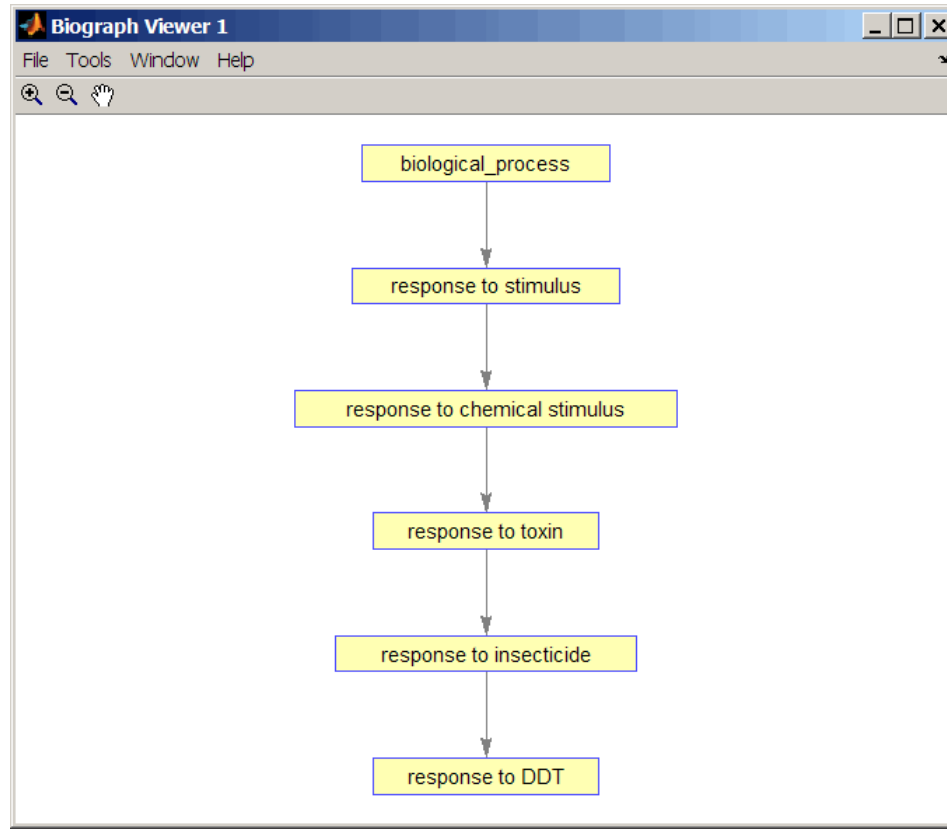
4 Create and display a report of the subordinate Gene Ontology terms, that includes the GO identifier and name.

```
rpt = get(subontology.terms,{'id','name'})

    [ 8150]    'biological_process'
    [ 9636]    'response to toxin'
    [17085]             [1x23 char]
    [42221]             [1x29 char]
    [46680]    'response to DDT'
```

```
    [50896]              [1x20 char]
```

5 View relationships of the subordinate Gene Ontology by using the `getmatrix` method to create a connection matrix to pass to the `biograph` function.

```
cm = getmatrix(subontology);
BG = biograph(cm, get(subontology.terms, 'name'));
view(BG)
```



See Also

Bioinformatics Toolbox functions: `goannotread`, `num2goid`

Bioinformatics Toolbox class: `term`

getblast

Purpose

Retrieve BLAST report from NCBI Web site

Syntax

```
Data = getblast(RID)
Data = getblast(RID, ...'Descriptions',
DescriptionsValue, ...)
Data = getblast(RID, ...'Alignments', AlignmentsValue, ...)
Data = getblast(RID, ...'ToFile', ToFileValue, ...)
Data = getblast(RID, ...'FileFormat', FileFormatValue, ...)
Data = getblast(RID, ...'WaitTime', WaitTimeValue, ...)
```

Arguments

RID	Request ID for the NCBI BLAST report, such as returned by the `blastncbi` function.
DescriptionsValue	Integer that specifies the number of descriptions in a report. Choices are any value ≥ `1` and ≤ `500`. Default is `100`.
AlignmentsValue	Integer that specifies the number of alignments to include in the report. Choices are any value ≥ `1` and ≤ `500`. Default is `50`.

Note This value must be ≤ the value you specified for the `'Alignments'` property when creating *RID* using the `blastncbi` function.

ToFileValue	String specifying a file name for saving report data.

FileFormatValue	String specifying the format of the file. Choices are `'text'` (default) or `'html'`.
WaitTimeValue	Positive value that specifies a time (in minutes) for the MATLAB software to wait for a report from the NCBI Web site to be available. If the report is still not available after the wait time, `getblast` returns an error message. Default behavior is to not wait for a report.

Tip Use the *RTOE* returned by the `blastncbi` function as the *WaitTimeValue*.

Return Values

Data	MATLAB structure or array of structures (if multiple query sequences) containing fields corresponding to BLAST keywords and data from an NCBI BLAST report.

Description

The Basic Local Alignment Search Tool (BLAST) offers a fast and powerful comparative analysis of protein and nucleotide sequences against known sequences in online databases. `getblast` parses NCBI BLAST reports, including `blastn`, `blastp`, `psiblast`, `blastx`, `tblastn`, `tblastx`, and `megablast` reports.

Data = `getblast(`*RID*`)` reads *RID*, the Request ID for the NCBI BLAST report, and returns the report data in *Data*, a MATLAB structure or array of structures. The Request ID, *RID*, must be recently generated because NCBI purges reports after 24 hours.

Data = `getblast(`*RID*`, ...'`*PropertyName*`', `*PropertyValue*`, ...)` calls `getblast` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each

PropertyName must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

Data = getblast(*RID*, ...'Descriptions', *DescriptionsValue*, ...) specifies the number of descriptions in a report. Choices are any integer ≥ 1 and ≤ 500. Default is 100.

Data = getblast(*RID*, ...'Alignments', *AlignmentsValue*, ...) specifies the number of alignments to include in the report. Choices are any integer ≥ 1 and ≤ 500. Default is 50.

Note This value must be ≤ the value you specified for the 'Alignments' property when creating *RID* using the blastncbi function.

Data = getblast(*RID*, ...'ToFile', *ToFileValue*, ...) saves the NCBI BLAST report data to a specified file. The default format for the file is 'text', but you can specify 'html' with the 'FileFormat' property.

Data = getblast(*RID*, ...'FileFormat', *FileFormatValue*, ...) specifies the format for the report. Choices are 'text' (default) or 'html'.

Data = getblast(*RID*, ...'WaitTime', *WaitTimeValue*, ...) pauses the MATLAB software and waits a specified time (in minutes) for a report from the NCBI Web site to be available. If the report is still unavailable after the wait time, getblast returns an error message. Choices are any positive value. Default behavior is to not wait for a report.

Tip Use the *RTOE* returned by the blastncbi function as the *WaitTimeValue*.

For more information about reading and interpreting BLAST reports, see:

```
http://www.ncbi.nlm.nih.gov/Education/BLASTinfo/tut1.html
```

Data contains the following fields.

Field	Description
`RID`	Request ID for retrieving results for a specific NCBI BLAST search.
`Algorithm`	NCBI algorithm used to do a BLAST search.
`Query`	Identifier of the query sequence submitted to a BLAST search.
`Database`	All databases searched.
`Hits.Name`	Name of a database sequence (subject sequence) that matched the query sequence.
`Hits.Length`	Length of a subject sequence.
`Hits.HSPs.Score`	Pairwise alignment score for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.Expect`	Expectation value for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.Identities`	Identities (match, possible, and percent) for a high-scoring sequence pair between the query sequence and a subject sequence.

Field	Description
`Hits.HSPs.Positives`	Identical or similar residues (match, possible, and percent) for a high-scoring sequence pair between the query sequence and a subject amino acid sequence. **Note** This field applies only to translated nucleotide or amino acid query sequences and/or databases.
`Hits.HSPs.Gaps`	Nonaligned residues (match, possible, and percent) for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.Frame`	Reading frame of the translated nucleotide sequence for a high-scoring sequence pair between the query sequence and a subject sequence. **Note** This field applies only when performing translated searches, that is, when using `tblastx`, `tblastn`, and `blastx`.

Field	Description
`Hits.HSPs.Strand`	Sense (`Plus` = 5' to 3' and `Minus` = 3' to 5') of the DNA strands for a high-scoring sequence pair between the query sequence and a subject sequence. **Note** This field applies only when using a nucleotide query sequence and database.
`Hits.HSPs.Alignment`	Three-row matrix showing the alignment for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.QueryIndices`	Indices of the query sequence residue positions for a high-scoring sequence pair between the query sequence and a subject sequence.
`Hits.HSPs.SubjectIndices`	Indices of the subject sequence residue positions for a high-scoring sequence pair between the query sequence and a subject sequence.
`Statistics`	Summary of statistical details about the performed search, such as lambda values, gap penalties, number of sequences searched, and number of hits.

Examples

1 Create an NCBI BLAST report request using a GenPept accession number.

```
RID = blastncbi('AAA59174','blastp','expect',1e-10)
```

```
RID =

    '1175088155-31624-126008617054.BLASTQ3'
```

2 Pass the Request ID for the report to the `getblast` function to parse the report, and return the report data in a MATLAB structure, and save the report data to a text file.

```
reportStruct = getblast(RID,'ToFile','AAA59174_BLAST.rpt')

reportStruct =

           RID: '1175093633-2786-174709873694.BLASTQ3'
     Algorithm: 'BLASTP 2.2.16 [Mar-11-2007]'
         Query: [1x63 char]
      Database: [1x96 char]
          Hits: [1x50 struct]
    Statistics: [1x1034 char]
```

Note You may need to wait for the report to become available on the NCBI Web site before you can run the preceding command.

References

[1] Altschul, S.F., Gish, W., Miller, W., Myers, E.W. and Lipman, D.J. (1990). Basic local alignment search tool. J. Mol. Biol. *215*, 403–410.

[2] Altschul, S.F., Madden, T.L., Schäffer, A.A., Zhang, J., Zhang, Z., Miller, W. and Lipman, D.J. (1997). Gapped BLAST and PSI-BLAST: a new generation of protein database search programs. Nucleic Acids Res. *25*, 3389–3402.

For more information about reading and interpreting NCBI BLAST reports, see:

```
http://www.ncbi.nlm.nih.gov/Education/BLASTinfo/Blast_output.html
```

See Also

Bioinformatics Toolbox functions: `blastformat`, `blastlocal`, `blastncbi`, `blastread`, `blastreadlocal`

getbyname (phytree)

Purpose

Branches and leaves from phytree object

Syntax

```
S = getbyname(Tree, Expression)
S = getbyname(Tree, String)
S = getbyname(Tree, String, 'Exact', ExactValue)
```

Arguments

Tree	phytree object created by `phytree` function (object constructor) or `phytreeread` function.
Expression	Regular expression or cell array of regular expressions to search for in *Tree*.
String	String or cell array of strings to search for in *Tree*.
ExactValue	Controls whether the full exact node name must match the string(s), ignoring case. Choices are `true` or `false` (default). When `true`, *S* is a numeric column vector indicating which node names match a query exactly, in full.

Description

S = `getbyname(`*Tree*`, `*Expression*`)` searches the nodes names in *Tree*, a phytree object, for the regular expression(s) specified by *Expression*. It returns *S*, a logical matrix of size `NumNodes`-by-`M`, where `M` is either `1` or the length of *Expression*. Each row in *S* corresponds to a node, and each column corresponds to a query in *Expression*. The logical matrix *S* indicates the node names that match *Expression*, ignoring case.

S = `getbyname(`*Tree*`, `*String*`)` searches the nodes names in *Tree*, a phytree object, for the string(s) specified by *String*. It returns *S*, a logical matrix of size `NumNodes`-by-`M`, where `M` is either `1` or the length of *String*. Each row in *S* corresponds to a node, and each column corresponds to a query in *String*. The logical matrix *S* indicates the node names that match *String*, ignoring case.

S = `getbyname(`*Tree*`, `*String*`, 'Exact', `*ExactValue*`)` specifies whether the full exact node name must match the string(s), ignoring case. Choices are `true` or `false` (default). When `true`, *S* is a numeric

column vector indicating which node names match a query exactly, in full.

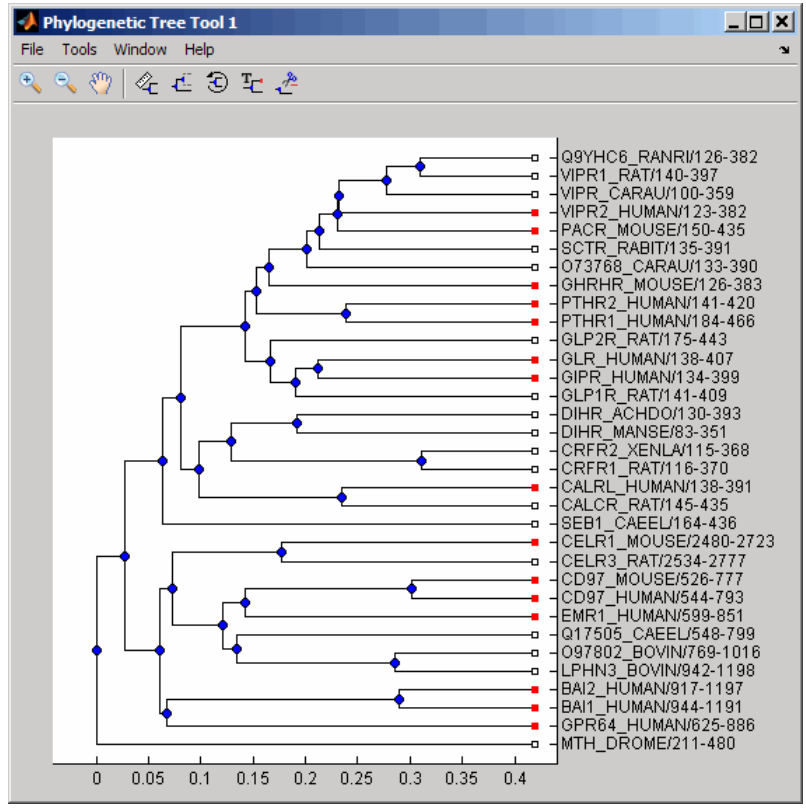
Examples

1. Read a phylogenetic tree file created from a protein family into a phytree object.

```
tr = phytreeread('pf00002.tree');
```

2. Determine all the mouse and human proteins by searching for nodes that include the strings `'mouse'` and `'human'` in their names.

```
sel = getbyname(tr,{'mouse','human'});
view(tr,any(sel,2));
```



See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreeread`

Bioinformatics Toolbox object: phytree object

Bioinformatics Toolbox methods of phytree object: `get`, `prune`, `select`

Purpose

Calculate canonical form of phylogenetic tree

Syntax

```
Pointers = getcanonical(Tree)
[Pointers, Distances, Names] = getcanonical(Tree)
```

Arguments

Tree	phytree object created by `phytree` function (object constructor).

Description

Pointers = `getcanonical(`*Tree*`)` returns the pointers for the canonical form of a phylogenetic tree (*Tree*). In a canonical tree the leaves are ordered alphabetically and the branches are ordered first by their width and then alphabetically by their first element. A canonical tree is isomorphic to all the trees with the same skeleton independently of the order of their leaves and branches.

`[`*Pointers, Distances, Names*`] = getcanonical(`*Tree*`)` returns, in addition to the pointers described above, the reordered distances (*Distances*) and node names (*Names*).

Examples

1 Create two phylogenetic trees with the same skeleton but slightly different distances.

```
b = [1 2; 3 4; 5 6; 7 8;9 10];
tr_1 = phytree(b,[.1 .2 .3 .3 .4 ]');
tr_2 = phytree(b,[.2 .1 .2 .3 .4 ]');
```

2 Plot the trees.

```
plot(tr_1)
plot(tr_2)
```

3 Check whether the trees have an isomorphic construction.

```
isequal(getcanonical(tr_1),getcanonical(tr_2))
```

```
ans =
     1
```

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreeread`

Bioinformatics Toolbox object: phytree object

Bioinformatics Toolbox methods of phytree object: `getbyname`, `select`, `subtree`

Purpose

Find descendants in biograph object

Syntax

```
Nodes = getdescendants(BiographNode)
Nodes = getdescendants(BiographNode,NumGenerations)
```

Arguments

BiographNode	Node in a biograph object.
NumGenerations	Number of generations. Enter a positive integer.

Description

Nodes = getdescendants(*BiographNode*) finds a given node (*BiographNode*) all of its direct descendants.

Nodes = getdescendants(*BiographNode,NumGenerations*) finds the node (*BiographNode*) and all of its direct descendants up to a specified number of generations (*NumGenerations*).

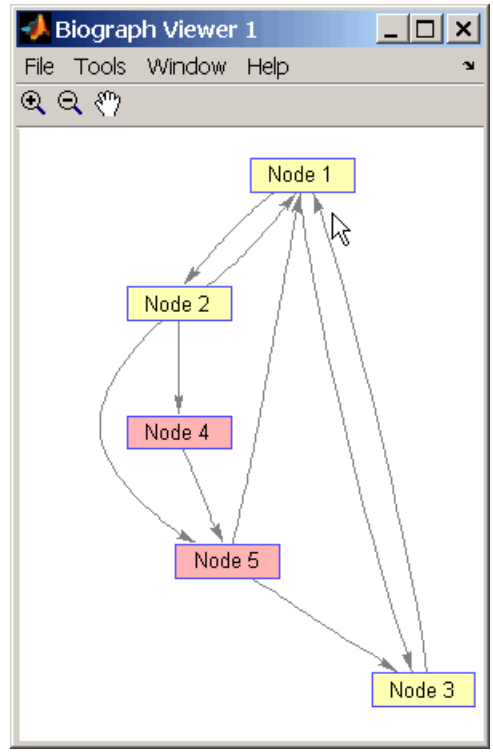
Examples

1 Create a biograph object.

```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];
bg = biograph(cm)
```

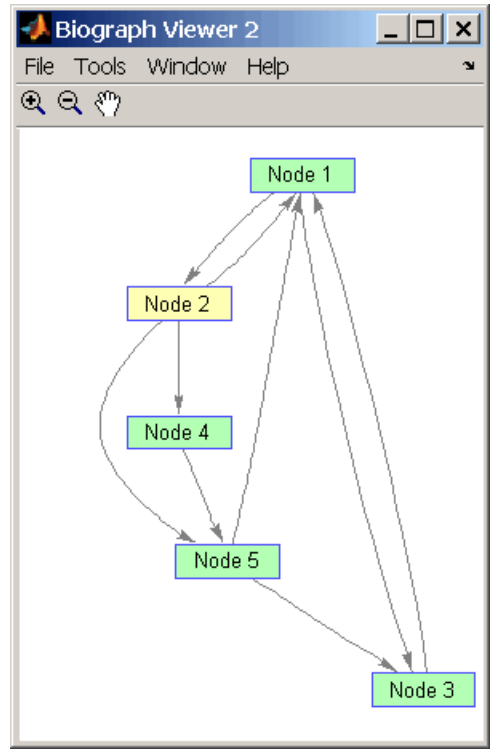
2 Find one generation of descendants for node 4.

```
desNodes = getdescendants(bg.nodes(4));
set(desNodes,'Color',[1 .7 .7]);
bg.view;
```



3 Find two generations of descendants for node 4.

```
desNodes = getdescendants(bg.nodes(4),2);
set(desNodes,'Color',[.7 1 .7]);
bg.view;
```



See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: `dolayout`, `get`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `set`, `view`

geneont.getdescendants

Purpose

Find terms that are descendants of specified Gene Ontology (GO) term

Syntax

```
DescendantIDs = getdescendants(GeneontObj, ID)
[DescendantIDs, Counts] = getdescendants(GeneontObj, ID)
... = getdescendants(..., 'Depth', DepthValue, ...)
... = getdescendants(..., 'Relationtype',
RelationtypeValue,
   ...)
... = getdescendants(..., 'Exclude', ExcludeValue, ...)
```

Description

`DescendantIDs = getdescendants(GeneontObj, ID)` searches *`GeneontObj`*, a geneont object, for GO terms that are descendants of the GO term(s) specified by *`ID`*, which is a GO term identifier or vector of identifiers. It returns *`DescendantIDs`*, a vector of GO term identifiers including *`ID`*. *`ID`* is a nonnegative integer or a vector containing nonnegative integers.

`[DescendantIDs, Counts] = getdescendants(GeneontObj, ID)` also returns the number of times each descendant is found. *`Counts`* is a column vector with the same number of elements as terms in *`GeneontObj`*.

Tip The *`Counts`* return value is useful when you tally counts in gene enrichment studies. For more information, see the Gene Ontology Enrichment in Microarray Data demo.

`... = getdescendants(..., 'PropertyName', PropertyValue, ...)` calls `getdescendants` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = getdescendants(..., 'Depth', DepthValue, ...)` searches down through a specified number of levels, *`DepthValue`*, in the gene ontology. *`DepthValue`* is a positive integer. Default is `Inf`.

`... = getdescendants(..., 'Relationtype', RelationtypeValue, ...)` searches for specified relationship types, *`RelationtypeValue`*, in the gene ontology. *`RelationtypeValue`* is a string. Choices are `'is_a'`, `'part_of'`, or `'both'` (default).

`... = getdescendants(..., 'Exclude', ExcludeValue, ...)` controls excluding *`ID`*, the original queried term(s), from the output *`DescendantIDs`*, unless the term was found while searching the gene ontology. Choices are `true` or `false` (default).

Inputs

`GeneontObj`	A geneont object, such as created by the `geneont.geneont` constructor function.
`ID`	GO term identifier or vector of identifiers.
`DepthValue`	Positive integer specifying the number of levels to search downward in the gene ontology.
`RelationtypeValue`	String specifying the relationship types to search for in the gene ontology. Choices are: • `'is_a'` • `'part_of'` • `'both'` (default)
`ExcludeValue`	Controls excluding *`ID`*, the original queried term(s), from the output *`DescendantIDs`*, unless the term was reached while searching the gene ontology. Choices are `true` or `false` (default).

Outputs

DescendantIDs	Vector of GO term identifiers including *ID*.
Counts	Column vector with the same number of elements as terms in *GeneontObj*, indicating the number of times each descendant is found.

Examples

1 Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

```
GO = geneont('LIVE', true)
```

The MATLAB software creates a geneont object and displays the number of terms in the database.

```
Gene Ontology object with 27827 Terms.
```

2 Retrieve the descendants of the "aldo-keto reductase activity" GO term with a GO identifier of 4033.

```
descendants = getdescendants(GO,4033)

descendants =

        4032
        4033
        8106
       32018
       32866
       32867
       46568
       50112
       50236
```

3 Create a subordinate Gene Ontology.

```
subontology = GO(descendants)
```

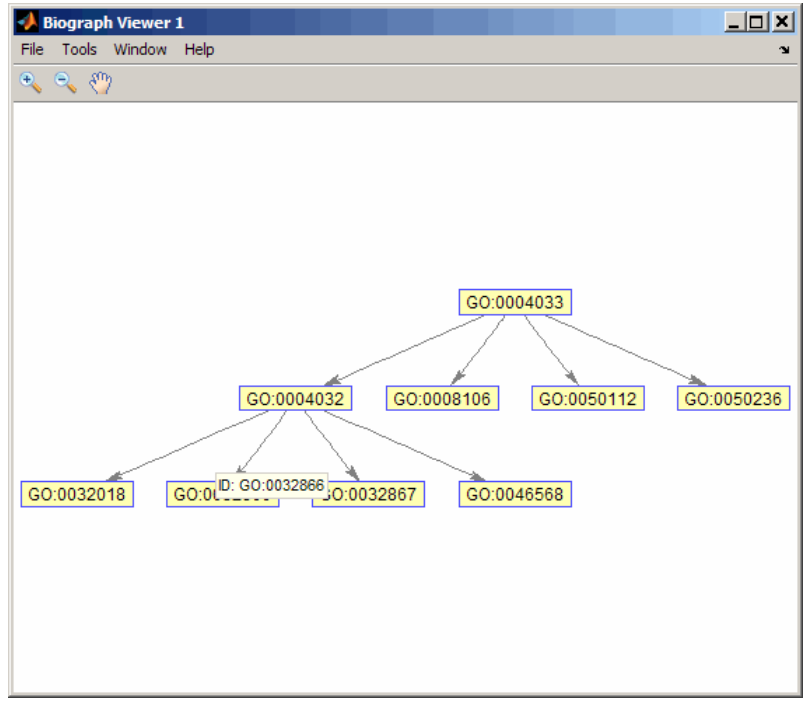
```
Gene Ontology object with 9 Terms.
```

4 Create and display a report of the subordinate Gene Ontology terms, that includes the GO identifier and name.

```
rpt = [num2goid(cell2mat(get(subontology.terms,'id')))...
       get(subontology.terms,'name')]';
disp(sprintf('%s --> %s \n',rpt{:}))

GO:0004032 --> aldehyde reductase activity
GO:0004033 --> aldo-keto reductase activity
GO:0008106 --> alcohol dehydrogenase (NADP+) activity
GO:0032018 --> 2-methylbutanal reductase activity
GO:0032866 --> xylose reductase activity
GO:0032867 --> arabinose reductase activity
GO:0046568 --> 3-methylbutanal reductase activity
GO:0050112 --> inositol 2-dehydrogenase activity
GO:0050236 --> pyridoxine 4-dehydrogenase activity
```

5 View relationships of the subordinate Gene Ontology by using the `getmatrix` method to create a connection matrix to pass to the `biograph` function.

```
cm = getmatrix(subontology);
BG = biograph(cm,rpt(1,:));
view(BG)
```



See Also

Bioinformatics Toolbox functions: `goannotread`, `num2goid`

Bioinformatics Toolbox class: `term`

Purpose

Get handles to edges in biograph object

Syntax

```
Edges = getedgesbynodeid(BGobj,SourceIDs,SinkIDs)
```

Arguments

BGobj	Biograph object.
SourceIDs, *SinkIDs*	Enter a cell string, or an empty cell array (gets all edges).

Description

Edges = getedgesbynodeid(*BGobj,SourceIDs,SinkIDs*) gets the handles to the edges that connect the specified source nodes (*SourceIDs*) to the specified sink nodes (*SinkIDs*) in a biograph object.

Example

1 Create a biograph object for the Hominidae family.

```
species = {'Homo','Pan','Gorilla','Pongo','Baboon',...
           'Macaca','Gibbon'};
cm = magic(7)>25 & 1-eye(7);
bg = biograph(cm, species);
```

2 Find all the edges that connect to the Homo node.

```
EdgesIn = getedgesbynodeid(bg,[],'Homo');
EdgesOut = getedgesbynodeid(bg,'Homo',[]);
set(EdgesIn,'LineColor',[0 1 0]);
set(EdgesOut,'LineColor',[1 0 0]);
bg.view;
```

3 Find all edges that connect members of the Cercopithecidae family to members of the Hominidae family.

```
Cercopithecidae = {'Macaca','Baboon'};
Hominidae = {'Homo','Pan','Gorilla','Pongo'};
edgesSel = getedgesbynodeid(bg,Cercopithecidae,Hominidae);
set(bg.edges,'LineColor',[.5 .5 .5]);
set(edgesSel,'LineColor',[0 0 1]);
```

```
bg.view;
```

See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: `biograph object`

Bioinformatics Toolbox methods of a biograph object: `dolayout`, `get`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `set`, `view`

Purpose

Retrieve sequence information from EMBL database

Syntax

```
EMBLData = getembl(AccessionNumber)
EMBLData = getembl(..., 'ToFile', ToFileValue, ...)
EMBLSeq = getembl(..., 'SequenceOnly', SequenceOnlyValue,
   ...)
```

Arguments

AccessionNumber	Unique identifier for a sequence record. Enter a unique combination of letters and numbers.
ToFileValue	String specifying a file name or a path and file name to which to save the data. If you specify only a file name, the file is stored in the current directory.
SequenceOnlyValue	Controls the retrieving of only the sequence without the metadata. Choices are `true` or `false` (default).

Return Values

EMBLData	MATLAB structure with fields corresponding to EMBL data.
EMBLSeq	MATLAB character string representing the sequence.

Description

`getembl` retrieves information from the European Molecular Biology Laboratory (EMBL) database for nucleotide sequences. This database is maintained by the European Bioinformatics Institute (EBI). For more details about the EMBL database, see

```
http://www.ebi.ac.uk/embl/Documentation/index.html
```

EMBLData = `getembl(`*AccessionNumber*`)` searches for the accession number in the EMBL database (`http://www.ebi.ac.uk/embl`) and returns *EMBLData*, a MATLAB structure with fields corresponding to

the EMBL two-character line type code. Each line type code is stored as a separate element in the structure.

EMBLData contains the following fields.

Field
Identification
Accession
SequenceVersion
DateCreated
DateUpdated
Description
Keyword
OrganismSpecies
OrganismClassification
Organelle
Reference
DatabaseCrossReference
Comments
Assembly
Feature
BaseCount
Sequence

EMBLData = getembl(..., '*PropertyName*', *PropertyValue*, ...) calls `getembl` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

EMBLData = getembl(..., 'ToFile', *ToFileValue*, ...) saves the information to an EMBL-formatted file. *ToFileValue* is a string specifying a file name or a path and file name to which to save the data. If you specify only a file name, the file is stored in the current directory.

Tip Read an EMBL-formatted file back into the MATLAB software using the emblread function.

EMBLSeq = getembl(..., 'SequenceOnly', *SequenceOnlyValue*, ...) controls the retrieving of only the sequence without the metadata. Choices are true or false (default).

Examples

Retrieve data for the rat liver apolipoprotein A-I.

```
emblout = getembl('X00558')
```

Retrieve data for the rat liver apolipoprotein A-I and save it to the file rat_protein. If you specify a file name without a path, the file is stored in the current directory.

```
emblout = getembl('X00558','ToFile','c:\project\rat_protein.txt')
```

Retrieve only the sequence for the rat liver apolipoprotein A-I.

```
Seq = getembl('X00558','SequenceOnly',true)
```

See Also

Bioinformatics Toolbox functions: emblread, getgenbank, getgenpept, getpdb, seqtool

getgenbank

Purpose

Retrieve sequence information from GenBank database

Syntax

```
Data = getgenbank(AccessionNumber)
getgenbank(AccessionNumber)
getgenbank(..., 'PartialSeq', PartialSeqValue, ...)
getgenbank(..., 'ToFile', ToFileValue, ...)
getgenbank(..., 'FileFormat', FileFormatValue, ...)
getgenbank(..., 'SequenceOnly', SequenceOnlyValue, ...)
```

Arguments

AccessionNumber	String specifying a unique alphanumeric identifier for a sequence record.
PartialSeqValue	Two-element array of integers containing the start and end positions of the subsequence [*StartBP*, *EndBP*] that specifies a subsequence to retrieve. *StartBP* is an integer between 1 and *EndBP*; *EndBP* is an integer between *StartBP* and the length of the sequence.
ToFileValue	String specifying either a file name or a path and file name for saving the GenBank data. If you specify only a file name, the file is saved to the MATLAB Current Directory.
FileFormatValue	String specifying the format for the file specified with the `'ToFile'` property. Choices are `'GenBank'` (default) or `'FASTA'`.
SequenceOnlyValue	Controls the return of only the sequence as a character array. Choices are `true` or `false` (default).

Description

`getgenbank` retrieves nucleotide information from the GenBank database. This database is maintained by the National Center for Biotechnology Information (NCBI). For more details about the GenBank database, see

```
http://www.ncbi.nlm.nih.gov/Genbank/
```

Data = getgenbank(*AccessionNumber*) searches for the accession number in the GenBank database and returns a MATLAB structure containing information for the sequence.

Tip If an error occurs while retrieving the GenBank-formatted information, try rerunning the query. Errors can occur due to Internet connectivity issues that are unrelated to the GenBank record.

---

getgenbank(*AccessionNumber*) displays the information in the MATLAB Command Window without returning data to a variable. The displayed information includes hyperlinks to the URLs used to search for and retrieve the data.

getgenbank(..., '*PropertyName*', *PropertyValue*, ...) calls getgenbank with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

getgenbank(..., 'PartialSeq', *PartialSeqValue*, ...) returns the specified subsequence in the Sequence field of the MATLAB structure. *PartialSeqValue* is a two-element array of integers containing the start and end positions of the subsequence [*StartBP*, *EndBP*]. *StartBP* is an integer between 1 and *EndBP*; *EndBP* is an integer between *StartBP* and the length of the sequence.

getgenbank(..., 'ToFile', *ToFileValue*, ...) saves the data returned from the GenBank database to a file. *ToFileValue* is a string specifying either a file name or a path and file name for saving the GenBank data. If you specify only a file name, the file is saved to the MATLAB Current Directory.

Tip You can read a GenBank-formatted file back into MATLAB using the `genbankread` function.

Tip To append GenBank data to an existing file, specify that file name, and the data will be added to the end of the file.

If you are using `getgenbank` in a script, you can disable the append warning message by entering the following command lines before the `getgenbank` command:

```
warnState = warning %Save the current warning state
warning('off','Bioinfo:getncbidata:AppendToFile');
```

Then enter the following command line after the `getgenbank` command:

```
warning(warnState) %Reset warning state to previous settings
```

`getgenbank(..., 'FileFormat', FileFormatValue, ...)` returns the sequence in the specified format. Choices are `'GenBank'` (default) or `'FASTA'`.

`getgenbank(..., 'SequenceOnly', SequenceOnlyValue, ...)` controls the return of only the sequence as a character array. Choices are `true` or `false` (default).

Note When the `'SequenceOnly'` and `'ToFile'` properties are used together, the output is a FASTA-formatted file.

Examples

Retrieving an RNA Sequence

To retrieve the sequence from chromosome 19 that codes for the human insulin receptor and store it in a structure, `S`, in the MATLAB Command Window, type:

```
S = getgenbank('M10051')

S =

                LocusName: 'HUMINSR'
      LocusSequenceLength: '4723'
     LocusNumberofStrands: ''
            LocusTopology: 'linear'
       LocusMoleculeType: 'mRNA'
     LocusGenBankDivision: 'PRI'
    LocusModificationDate: '06-JAN-1995'
               Definition: 'Human insulin receptor mRNA, complete cds.'
                Accession: 'M10051'
                  Version: 'M10051.1'
                       GI: '186439'
                  Project: []
                   DBLink: []
                 Keywords: 'insulin receptor; tyrosine kinase.'
                  Segment: []
                   Source: 'Homo sapiens (human)'
           SourceOrganism: [4x65 char]
                Reference: {[1x1 struct]}
                  Comment: [14x67 char]
                 Features: [51x74 char]
                      CDS: [1x1 struct]
                 Sequence: [1x4723 char]
                SearchURL: [1x67 char]
              RetrieveURL: [1x101 char]
```

Retrieving a Partial RNA Sequence

By looking at the `Features` field of the structure returned in Retrieving an RNA Sequence on page 3-627, you can determine that the coding sequence is positions 139 through 4287. To retrieve only the coding sequence from chromosome 19 that codes for the human insulin receptor and store it in a structure, `CDS`, in the MATLAB Command Window, type:

```
CDS = getgenbank('M10051','PARTIALSEQ',[139,4287]);
```

See Also

Bioinformatics Toolbox functions: `genbankread`, `getembl`, `getgenpept`, `getpdb`, `seqtool`

Purpose

Retrieve sequence information from GenPept database

Syntax

```
Data = getgenpept(AccessionNumber)
getgenpept(AccessionNumber)
getgenpept(..., 'PartialSeq', PartialSeqValue, ...)
getgenpept(..., 'ToFile', ToFileValue, ...)
getgenpept(..., 'FileFormat', FileFormatValue, ...)
getgenpept(..., 'SequenceOnly', SequenceOnlyValue, ...)
```

Arguments

AccessionNumber	String specifying a unique alphanumeric identifier for a sequence record.
PartialSeqValue	Two-element array of integers containing the start and end positions of the subsequence [*StartAA*, *EndAA*] that specifies a subsequence to retrieve. *StartAA* is an integer between 1 and *EndAA*; *EndAA* is an integer between *StartAA* and the length of the sequence.
ToFileValue	String specifying either a file name or a path and file name for saving the GenPept data. If you specify only a file name, the file is saved to the MATLAB Current Directory.
FileFormatValue	String specifying the format for the file specified with the `'ToFile'` property. Choices are `'Genpept'` (default) or `'FASTA'`.
SequenceOnlyValue	Controls the return of only the sequence as a character array. Choices are `true` or `false` (default).

Description

`getgenpept` retrieves a protein (amino acid) sequence information from the GenPept database, which is a translation of the nucleotide sequences in the GenBank database and is maintained by the National Center for Biotechnology Information (NCBI).

Note NCBI has changed the name of their protein search engine from GenPept to Entrez Protein. However, the function names in the Bioinformatics Toolbox software (`getgenpept` and `genpeptread`) are unchanged representing the still-used GenPept report format.

`Data = getgenpept(AccessionNumber)` searches for the accession number in the GenPept database and returns a MATLAB structure containing information for the sequence.

Tip If an error occurs while retrieving the GenPept-formatted information, try rerunning the query. Errors can occur due to Internet connectivity issues that are unrelated to the GenPept record.

`getgenpept(AccessionNumber)` displays the information in the MATLAB Command Window without returning data to a variable. The displayed information includes hyperlinks to the URLs used to search for and retrieve the data.

`getgenpept(..., 'PropertyName', PropertyValue, ...)` calls `getgenpept` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`getgenpept(..., 'PartialSeq', PartialSeqValue, ...)` returns the specified subsequence in the `Sequence` field of the MATLAB structure. *`PartialSeqValue`* is a two-element array of integers containing the start and end positions of the subsequence `[StartAA, EndAA]`. *`StartAA`* is an integer between 1 and *`EndAA`*; *`EndAA`* is an integer between *`StartAA`* and the length of the sequence.

`getgenpept(..., 'ToFile', ToFileValue, ...)` saves the data returned from the GenPept database to a file. *`ToFileValue`* is a string specifying either a file name or a path and file name for saving the

GenPept data. If you specify only a file name, the file is saved to the MATLAB Current Directory.

Tip You can read a GenPept-formatted file back into MATLAB using the `genpeptread` function.

Tip To append GenPept data to an existing file, specify that file name, and the data will be added to the end of the file.

If you are using `getgenpept` in a script, you can disable the append warning message by entering the following command lines before the `getgenpept` command:

```
warnState = warning %Save the current warning state
warning('off','Bioinfo:getncbidata:AppendToFile');
```

Then enter the following command line after the `getgenpept` command:

```
warning(warnState) %Reset warning state to previous settings
```

`getgenpept(..., 'FileFormat', FileFormatValue, ...)` returns the sequence in the specified format. Choices are `'GenPept'` (default) or `'FASTA'`.

`getgenpept(..., 'SequenceOnly', SequenceOnlyValue, ...)` controls the return of only the sequence as a character array. Choices are `true` or `false` (default).

Note When the `'SequenceOnly'` and `'ToFile'` properties are used together, the output is a FASTA-formatted file.

Examples

Retrieving a Peptide Sequence

To retrieve the sequence for the human insulin receptor and store it in a structure, `Seq`, in the MATLAB Command Window, type:

```
Seq = getgenpept('AAA59174')

Seq =

                LocusName: 'AAA59174'
      LocusSequenceLength: '1382'
     LocusNumberofStrands: ''
            LocusTopology: 'linear'
       LocusMoleculeType: ''
     LocusGenBankDivision: 'PRI'
    LocusModificationDate: '06-JAN-1995'
               Definition: 'insulin receptor precursor.'
                Accession: 'AAA59174'
                  Version: 'AAA59174.1'
                       GI: '307070'
                  Project: []
                 DBSource: 'locus HUMINSR accession M10051.1'
                 Keywords: ''
                   Source: 'Homo sapiens (human)'
           SourceOrganism: [4x65 char]
                Reference: {[1x1 struct]}
                  Comment: [14x67 char]
                 Features: [40x64 char]
                 Sequence: [1x1382 char]
                SearchURL: [1x104 char]
               RetrieveURL: [1x92 char]
```

Retrieving a Partial Peptide Sequence

By looking at the `Features` field of the structure returned in Retrieving a Peptide Sequence on page 3-632, you can determine that the furin-like repeats domain is positions 234 through 281. To retrieve only the furin-like repeats domain from the sequence for the human insulin

receptor and store it in a structure, `Fur`, in the MATLAB Command Window, type:

```
Fur = getgenpept('AAA59174','PARTIALSEQ',[234,281]);
```

See Also

Bioinformatics Toolbox functions: `genpeptread`, `getembl`, `getgenbank`, `getpdb`

getgeodata

Purpose

Retrieve Gene Expression Omnibus (GEO) format data

Syntax

```
GEOData = getgeodata(AccessionNumber)
getgeodata(AccessionNumber, 'ToFile', ToFileValue)
```

Arguments

AccessionNumber String specifying a unique identifier for a GEO Sample (GSM), Data Set (GDS), Platform (GPL), or Series (GSE) record in the GEO database.

Tip Recently submitted data sets may not be available for immediate download. There can be a one- to two-day delay between an experiment being submitted to the GEO database and its availability on the FTP site.

Tip If you are unable to retrieve data for an accession number, increase your Java heap space as described at:

```
http://www.mathworks.com/support/solutions/data/1-18I2C.
```

ToFileValue String specifying a file name or path and file name for saving the data. If you specify only a file name, that file will be saved in the MATLAB Current Directory.

Return Values

GEOData MATLAB structure containing information for a GEO record retrieved from the GEO database.

Description

GEOData = getgeodata(*AccessionNumber*) searches the Gene Expression Omnibus database for the specified accession number of a Sample (GSM), Data Set (GDS), Platform (GPL), or Series (GSE) record and returns a MATLAB structure containing the following fields:

Field	Description
Scope	Type of data retrieved (SAMPLE, DATASET, PLATFORM, or SERIES)
Accession	Accession number for record in GEO database.
Header	Microarray experiment information.
ColumnDescriptions	Cell array containing descriptions of columns in the data.
ColumnNames	Cell array containing names of columns in the data.
Data	Array containing microarray data.
Identifier (GDS files only)	Cell array containing probe IDs.
IDRef (GDS files only)	Cell array containing indices to probes.

Note Currently, the getgeodata function supports Sample (GSM), Data Set (GDS), Platform (GPL), and Series (GSE) records.

getgeodata(*AccessionNumber*, 'ToFile', *ToFileValue*) saves the data returned from the database to a file.

Note You can read a GEO SOFT-formatted file back into the MATLAB software using the `geosoftread` function. You can read a GEO SERIES-formatted file back into the MATLAB software using the `geoseriesread` function.

For more information, see

```
http://www.ncbi.nlm.nih.gov/About/disclaimer.html
```

Examples

```
geoStruct = getgeodata('GSM1768')
```

See Also

Bioinformatics Toolbox functions: `geoseriesread`, `geosoftread`, `getgenbank`, `getgenpept`

Purpose

Retrieve multiple sequence alignment associated with hidden Markov model (HMM) profile from PFAM database

Syntax

```
AlignStruct = gethmmalignment(PFAMName)
AlignStruct = gethmmalignment(PFAMAccessNumber)
AlignStruct = gethmmalignment(PFAMNumber)
AlignStruct = gethmmalignment(..., 'ToFile',
ToFileValue, ...)
AlignStruct = gethmmalignment(..., 'Type', TypeValue, ...)
AlignStruct = gethmmalignment(..., 'Mirror', MirrorValue,
   ...)
AlignStruct = gethmmalignment(..., 'IgnoreGaps',
IgnoreGaps,
   ...)
```

Arguments

PFAMName	String specifying a protein family name (unique identifier) of an HMM profile record in the PFAM database. For example, `7tm_2`.
PFAMAccessNumber	String specifying a protein family accession number of an HMM profile record in the PFAM database. For example, `PF00002`.
PFAMNumber	Integer specifying a protein family number of an HMM profile record in the PFAM database. For example, `2` is the protein family number for the protein family `PF0002`.
ToFileValue	String specifying a file name or a path and file name for saving the data. If you specify only a file name, that file will be saved in the MATLAB Current Directory.

TypeValue	String that specifies the set of alignments returned. Choices are: • `full` — Default. Returns all alignments that fit the HMM profile. • `seed` — Returns only the alignments used to generate the HMM profile.
MirrorValue	String that specifies a Web database. Choices are: • `Sanger` (default) • `Janelia`
IgnoreGapsValue	Controls the removal of the symbols `-` and `.` from the sequence. Choices are `true` or `false` (default).

Return Values

AlignStruct	MATLAB structure array containing the multiple sequence alignment associated with an HMM profile.

Description

AlignStruct = `gethmmalignment(`*PFAMName*`)` searches the PFAM database for the HMM profile record represented by *PFAMName*, a protein family name, retrieves the multiple sequence alignment associated with the HMM profile, and returns *AlignStruct*, a MATLAB structure array, with each structure containing the following fields:

Field	Description
`Header`	Protein name
`Sequence`	Protein sequence

AlignStruct = `gethmmalignment(`*PFAMAccessNumber*`)` searches the PFAM database for the HMM profile record represented by *PFAMAccessNumber*, a protein family accession number, retrieves the

multiple sequence alignment associated with the HMM profile, and returns *AlignStruct*, a MATLAB structure array.

AlignStruct = gethmmalignment(*PFAMNumber*) determines a protein family accession number from *PFAMNumber*, an integer, searches the PFAM database for the associated HMM profile record, retrieves the multiple sequence alignment associated with the HMM profile, and returns *AlignStruct*, a MATLAB structure array.

AlignStruct = gethmmalignment(..., '*PropertyName*', *PropertyValue*, ...) calls gethmmalignment with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

AlignStruct = gethmmalignment(..., 'ToFile', *ToFileValue*, ...) saves the data returned from the PFAM database to a file specified by *ToFileValue*.

Note You can read a FASTA-formatted file containing PFAM data back into the MATLAB software using the fastaread function.

AlignStruct = gethmmalignment(..., 'Type', *TypeValue*, ...) specifies the set of alignments returned. Choices are:

- full — Default. Returns all sequences that fit the HMM profile.
- seed — Returns only the sequences used to generate the HMM profile.

AlignStruct = gethmmalignment(..., 'Mirror', *MirrorValue*, ...) specifies a Web database. Choices are:

- Sanger (default)
- Janelia

You can reach other mirror sites by passing the complete URL to the `fastaread` function.

Note These mirror sites are maintained separately and may have slight variations.

For more information about the PFAM database, see:

```
http://pfam.sanger.ac.uk
http://pfam.janelia.org/
```

`AlignStruct` `= gethmmalignment(..., 'IgnoreGaps',` *`IgnoreGaps`*`, ...)` controls the removal of the symbols `-` and `.` from the sequence. Choices are `true` or `false` (default).

Examples

To retrieve a multiple alignment of the sequences used to train the HMM profile for global alignment to the 7-transmembrane receptor protein in the secretin family, enter either of the following:

```
pfamalign = gethmmalignment(2,'Type','seed')

pfamalign = gethmmalignment('PF00002','Type','seed')

pfamalign =

32x1 struct array with fields:
    Header
    Sequence
```

See Also

Bioinformatics Toolbox functions: `fastaread`, `gethmmprof`, `gethmmtree`, `multialignread`, `multialignwrite`, `pfamhmmread`

Purpose

Retrieve hidden Markov model (HMM) profile from PFAM database

Syntax

```
HMMStruct = gethmmprof(PFAMName)
HMMStruct = gethmmprof(PFAMNumber)
HMMStruct = gethmmprof(..., 'ToFile', ToFileValue, ...)
HMMStruct = gethmmprof(..., 'Mode', ModeValue, ...)
HMMStruct = gethmmprof(..., 'Mirror', MirrorValue, ...)
```

Arguments

PFAMName	String specifying a protein family name (unique identifier) of an HMM profile record in the PFAM database. For example, `7tm_2`.
PFAMNumber	Integer specifying a protein family number of an HMM profile record in the PFAM database. For example, `2` is the protein family number for the protein family `PF00002`.
ToFileValue	String specifying a file name or a path and file name for saving the data. If you specify only a file name, that file will be saved in the MATLAB Current Directory.
ModeValue	String that specifies the returned alignment mode. Choices are: • `ls` — Default. Global alignment mode. • `fs` — Local alignment mode.
MirrorValue	String that specifies a Web database. Choices are: • `Sanger` (default) • `Janelia`

Return Values

HMMStruct	MATLAB structure containing information for an HMM profile retrieved from the PFAM database.

Description

HMMStruct = gethmmprof(*PFAMName*) searches the PFAM database for the record represented by *PFAMName*, a protein family name, retrieves the HMM profile information, and stores it in *HMMStruct*, a MATLAB structure containing the following fields corresponding to parameters of an HMM profile.

Field	Description
Name	The protein family name (unique identifier) of the HMM profile record in the PFAM database.
PfamAccessionNumber	The protein family accession number of the HMM profile record in the PFAM database.
ModelDescription	Description of the HMM profile.
ModelLength	The length of the profile (number of MATCH states).
Alphabet	The alphabet used in the model, 'AA' or 'NT'. **Note** AlphaLength is 20 for 'AA' and 4 for 'NT'.
MatchEmission	Symbol emission probabilities in the MATCH states. The format is a matrix of size ModelLength-by-AlphaLength, where each row corresponds to the emission distribution for a specific MATCH state.
InsertEmission	Symbol emission probabilities in the INSERT state. The format is a matrix of size ModelLength-by-AlphaLength, where each row corresponds to the emission distribution for a specific INSERT state.

Field	Description
`NullEmission`	Symbol emission probabilities in the MATCH and INSERT states for the NULL model. The format is a 1-by-`AlphaLength` row vector. **Note** NULL probabilities are also known as the background probabilities.
`BeginX`	BEGIN state transition probabilities. Format is a 1-by-`(ModelLength + 1)` row vector: `[B->D1 B->M1 B->M2 B->M3 .... B->Mend]`

`MatchX`	MATCH state transition probabilities.
	Format is a 4-by-`(ModelLength - 1)` matrix:
	`[M1->M2 M2->M3 ... M[end-1]->Mend;`
	`M1->I1 M2->I2 ... M[end-1]->I[end-1];`
	`M1->D2 M2->D3 ... M[end-1]->Dend;`
	`M1->E M2->E ... M[end-1]->E ]`

`InsertX`	INSERT state transition probabilities.
	Format is a 2-by-`(ModelLength - 1)` matrix:
	`[ I1->M2 I2->M3 ... I[end-1]->Mend;`
	`I1->I1 I2->I2 ... I[end-1]->I[end-1] ]`

`DeleteX`	DELETE state transition probabilities.
	Format is a 2-by-`(ModelLength - 1)` matrix:
	`[ D1->M2 D2->M3 ... D[end-1]->Mend ;`
	`D1->D2 D2->D3 ... D[end-1]->Dend ]`

Field	Description

`FlankingInsertX`	Flanking insert states (N and C) used for LOCAL profile alignment.
	Format is a 2-by-2 matrix:
	`[N->B  C->T ;`
	` N->N  C->C]`

`LoopX`	Loop states transition probabilities used for multiple hits alignment.
	Format is a 2-by-2 matrix:
	`[E->C  J->B ;`
	` E->J  J->J]`

`NullX`	Null transition probabilities used to provide scores with log-odds values also for state transitions. Format is a 2-by-1 column vector: `[G->F ; G->G]`

`HMMStruct` = `gethmmprof(`*`PFAMNumber`*`)` determines a protein family accession number from *`PFAMNumber`*, an integer, searches the PFAM database for the associated record, retrieves the HMM profile information, and stores it in *`HMMStruct`*, a MATLAB structure.

`HMMStruct` = `gethmmprof(..., '`*`PropertyName`*`',` *`PropertyValue`*`, ...)` calls `gethmmprof` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

HMMStruct = gethmmprof(..., 'ToFile', *ToFileValue*, ...) saves the data returned from the PFAM database in a file specified by *ToFileValue*.

Note You can read an HMM-formatted file back into the MATLAB software using the pfamhmmread function.

HMMStruct = gethmmprof(..., 'Mode', *ModeValue*, ...) specifies the returned alignment mode. Choices are:

- ls (default) — Global alignment mode.
- fs — Local alignment mode.

HMMStruct = gethmmprof(..., 'Mirror', *MirrorValue*, ...) specifies a Web database. Choices are:

- Sanger (default)
- Janelia

You can reach other mirror sites by passing the complete URL to the pfamhmmread function.

Note These mirror sites are maintained separately and may have slight variations.

For more information about the PFAM database, see:

```
http://pfam.sanger.ac.uk
http://pfam.janelia.org/
```

For more information on HMM profile models, see “HMM Profile Model” on page 3-784.

Examples

To retrieve a hidden Markov model (HMM) profile for the global alignment of the 7-transmembrane receptor protein in the secretin family, enter either of the following:

```
hmm = gethmmprof(2)

hmm = gethmmprof('7tm_2')

hmm =

                    Name: '7tm_2'
    PfamAccessionNumber: 'PF00002.14'
       ModelDescription: [1x42 char]
            ModelLength: 296
               Alphabet: 'AA'
          MatchEmission: [296x20 double]
         InsertEmission: [296x20 double]
           NullEmission: [1x20 double]
                 BeginX: [297x1 double]
                 MatchX: [295x4 double]
                InsertX: [295x2 double]
                DeleteX: [295x2 double]
        FlankingInsertX: [2x2 double]
                  LoopX: [2x2 double]
                  NullX: [2x1 double]
```

See Also

Bioinformatics Toolbox functions: `gethmmalignment`, `hmmprofalign`, `hmmprofstruct`, `pfamhmmread`, `showhmmprof`

Purpose

Retrieve phylogenetic tree data from PFAM database

Syntax

```
Tree = gethmmtree(PFAMName)
Tree = gethmmtree(PFAMAccessionNumber)
Tree = gethmmtree(PFAMNumber)
Tree = gethmmtree(AccessionNumber, ...'ToFile',
ToFileValue, ...)
Tree = gethmmtree(AccessionNumber, ...'Type',
TypeValue, ...)
```

Arguments

PFAMName	String specifying a protein family name (unique identifier) of an HMM profile record in the PFAM database. For example, `7tm_2`.
PFAMAccessionNumber	String specifying a protein family accession number of an HMM profile record in the PFAM database. For example, `PF00002`.
PFAMNumber	Integer specifying a protein family number of an HMM profile record in the PFAM database. For example, `2` is the protein family number for the protein family `PF0002`.
ToFileValue	Property to specify the location and file name for saving data. Enter either a file name or a path and file name supported by your system (ASCII text file).
TypeValue	String that specifies which alignments to include in the tree. Choices are: • `'seed'` — Returns a tree with only the alignments used to generate the HMM model. • `'full'` (default) — Returns a tree with all of the alignments that match the model.

Return Values

Tree	An object containing a phylogenetic tree representative of the protein family.

Description

Tree = gethmmtree(*PFAMName*) searches the PFAM database for the record represented by *PFAMName*, a protein family name, retrieves information, and returns Tree, an object containing a phylogenetic tree representative of the protein family.

Tree = gethmmtree(*PFAMAccessionNumber*) searches the PFAM database for the record represented by *PFAMAccessionNumber*, a protein family accession number, retrieves information, and returns Tree, an object containing a phylogenetic tree representative of the protein family.

Tree = gethmmtree(*PFAMNumber*) determines a protein family accession number from *PFAMNumber*, an integer, searches the PFAM database for the associated record, retrieves information, and returns Tree, an object containing a phylogenetic tree representative of the protein family.

Tree = gethmmtree(*AccessionNumber*, ...'*PropertyName*', *PropertyValue*, ...) calls gethmmtree with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

Tree = gethmmtree(*AccessionNumber*, ...'ToFile', *ToFileValue*, ...) saves the data returned from the PFAM database in the file *ToFileValue*.

Tree = gethmmtree(*AccessionNumber*, ...'Type', *TypeValue*, ...) specifies which alignments to include in the tree. Choices for *TypeValue* are:

- 'seed' — Returns a tree with only the alignments used to generate the HMM model.

- `'full'` (default) — Returns a tree with all of the alignments that match the model.

Examples

Enter either of the following to retrieve phylogenetic tree data from the multiple-aligned sequences used to train the HMM profile model for global alignment. The PFAM accession number `PF00002` is for the 7-transmembrane receptor protein in the secretin family.

```
tree  = gethmmtree(2, 'type', 'seed')
tree  = gethmmtree('PF00002', 'type', 'seed')

  Phylogenetic tree object with 32 leaves (31 branches)
```

See Also

Bioinformatics Toolbox functions: `gethmmalignment`, `phytreeread`

getmatrix (biograph)

Purpose

Get connection matrix from biograph object

Syntax

```
[Matrix, ID, Distances] = getmatrix(BGObj)
```

Arguments

BGObj	Biograph object created by `biograph` (object constructor).

Description

`[Matrix, ID, Distances] = getmatrix(BGObj)` converts the biograph object, *`BiographObj`*, into a logical sparse matrix, *`Matrix`*, in which 1 indicates that a node (row index) is connected to another node (column index). *`ID`* is a cell array of strings listing the `ID` properties for each node, and corresponds to the rows and columns of *`Matrix`*. *`Distances`* is a column vector with one entry for every nonzero entry in *`Matrix`* traversed column-wise and representing the respective `Weight` property for each edge.

Examples

```
cm = [0 1 1 0 0;2 0 0 4 4;4 0 0 0 0;0 0 0 0 2;4 0 5 0 0];
bg = biograph(cm);
[cm, IDs, dist] = getmatrix(bg)
```

See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `view`

Purpose

Convert geneont object into relationship matrix

Syntax

```
[Matrix, ID, Relationship] = getmatrix(GeneontObj)
```

Description

`[Matrix, ID, Relationship] = getmatrix(GeneontObj)` converts a geneont object, *`GeneontObj`*, into *`Matrix`*, a matrix of relationship values between nodes (row and column indices), in which `0` indicates no relationship, `1` indicates an "is_a" relationship, and `2` indicates a "part_of" relationship. *`ID`* is a column vector listing Gene Ontology IDs that correspond to the rows and columns of *`Matrix`*. *`Relationship`* is a cell array of strings defining the types of relationships.

Inputs

`GeneontObj`	A geneont object, such as created by the `geneont.geneont` constructor function.

Outputs

`Matrix`	Matrix of relationship values between nodes (row and column indices), in which `0` indicates no relationship, `1` indicates an "is_a" relationship, and `2` indicates a "part_of" relationship.
`ID`	Column vector listing Gene Ontology IDs that correspond to the rows and columns of *`Matrix`*.
`Relationship`	Cell array of strings defining the types of relationships.

Examples

1 Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

```
GO = geneont('LIVE',true)
```

The MATLAB software creates a geneont object and displays the number of terms in the database.

```
Gene Ontology object with 27595 Terms.
```

2 Convert this geneont object into a relationship matrix.

```
[MATRIX, ID, REL] = getmatrix(GO);
```

See Also

Bioinformatics Toolbox functions: `goannotread`, `num2goid`

Bioinformatics Toolbox class: `term`

Purpose

Convert phytree object into relationship matrix

Syntax

```
[Matrix, ID, Distances] = getmatrix(PhytreeObj)
```

Arguments

PhytreeObj	phytree object created by `phytree` (object constructor).

Description

`[Matrix, ID, Distances] = getmatrix(PhytreeObj)` converts a phytree object, *PhytreeObj*, into a logical sparse matrix, *Matrix*, in which 1 indicates that a branch node (row index) is connected to its child (column index). The child can be either another branch node or a leaf node. *ID* is a column vector of strings listing the labels that correspond to the rows and columns of *Matrix*, with the labels from 1 to *Number of Leaves* being the leaf nodes, then the labels from *Number of Leaves* + 1 to *Number of Leaves* + *Number of Branches* being the branch nodes, and the label for the last branch node also being the root node. *Distances* is a column vector with one entry for every nonzero entry in *Matrix* traversed column-wise and representing the distance between the branch node and the child.

Examples

```
T = phytreeread('pf00002.tree')
[MATRIX, ID, DIST] = getmatrix(T);
```

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreetool`

Bioinformatics Toolbox object: phytree object

Bioinformatics Toolbox methods of phytree object: `get`, `pdist`, `prune`

getnewickstr (phytree)

Purpose

Create Newick-formatted string

Syntax

```
String = getnewickstr(Tree)
getnewickstr(..., 'PropertyName', PropertyValue,...)
getnewickstr(..., 'Distances', DistancesValue)
getnewickstr(..., 'BranchNames', BranchNamesValue)
```

Arguments

Tree	Phytree object created with the function `phytree`.
DistancesValue	Property to control including or excluding distances in the output. Enter either `true` (include distances) or `false` (exclude distances). Default is `true`.
BranchNamesValue	Property to control including or excluding branch names in the output. Enter either `true` (include branch names) or `false` (exclude branch names). Default is `false`.

Description

String = `getnewickstr(`*Tree*`)` returns the Newick formatted string of a phylogenetic tree object (*Tree*).

`getnewickstr(..., '`*PropertyName*`', `*PropertyValue*`,...)` defines optional properties using property name/value pairs.

`getnewickstr(..., 'Distances', `*DistancesValue*`)`, when *DistancesValue* is `false`, excludes the distances from the output.

`getnewickstr(..., 'BranchNames', `*BranchNamesValue*`)`, when *BranchNamesValue* is `true`, includes the branch names in the output.

References

Information about the Newick tree format.

`http://evolution.genetics.washington.edu/phylip/newicktree.html`

Examples

1 Create some random sequences.

```
seqs = int2nt(ceil(rand(10)*4));
```

2 Calculate pairwise distances.

```
dist = seqpdist(seqs,'alpha','nt');
```

3 Construct a phylogenetic tree.

```
tree = seqlinkage(dist);
```

4 Get the Newick string.

```
str  = getnewickstr(tree)
```

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreeread`, `phytreetool`, `phytreewrite`, `seqlinkage`

Bioinformatics Toolbox object: phytree object

Bioinformatics Toolbox methods of phytree object: `get`, `getbyname`, `getcanonical`

getnodesbyid (biograph)

Purpose

Get handles to nodes

Syntax

```
NodesHandles = getnodesbyid(BGobj,NodeIDs)
```

Arguments

BGobj	Biograph object.
NodeIDs	Enter a cell string of node identifications.

Description

NodesHandles = getnodesbyid(*BGobj,NodeIDs*) gets the handles for the specified nodes (*NodeIDs*) in a biograph object.

Example

1 Create a biograph object.

```
species = {'Homosapiens','Pan','Gorilla','Pongo','Baboon',...
           'Macaca','Gibbon'};
cm = magic(7)>25 & 1-eye(7);
bg = biograph(cm, species)
```

2 Find the handles to members of the Cercopithecidae family and members of the Hominidae family.

```
Cercopithecidae = {'Macaca','Baboon'};
Hominidae = {'Homosapiens','Pan','Gorilla','Pongo'};
CercopithecidaeNodes = getnodesbyid(bg,Cercopithecidae);
HominidaeNodes = getnodesbyid(bg,Hominidae);
```

3 Color the families differently and draw a graph.

See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: `dolayout`, `get`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `set`, `view`

Purpose

Retrieve protein structure data from Protein Data Bank (PDB) database

Syntax

```
PDBStruct = getpdb(PDBid)
PDBStruct = getpdb(PDBid,  ...'ToFile', ToFileValue, ...)
PDBStruct = getpdb(PDBid,  ...'SequenceOnly',
   SequenceOnlyValue, ...)
```

Arguments

PDBid

String specifying a unique identifier for a protein structure record in the PDB database.

Note Each structure in the PDB database is represented by a four-character alphanumeric identifier. For example, `4hhb` is the identifier for hemoglobin.

ToFileValue

String specifying a file name or a path and file name for saving the PDB-formatted data. If you specify only a file name, that file will be saved in the MATLAB Current Directory.

Tip After you save the protein structure record to a local PDB-formatted file, you can use the `pdbread` function to read the file into the MATLAB software offline or use the `molviewer` function to display and manipulate a 3-D image of the structure.

SequenceOnlyValue

Controls the return of the protein sequence only. Choices are `true` or `false` (default). If there is one sequence, it is returned as a character array. If there are multiple sequences, they are returned as a cell array.

Return Values

PDBStruct	MATLAB structure containing a field for each PDB record.

Description

The Protein Data Bank (PDB) database is an archive of experimentally determined 3-D biological macromolecular structure data. For more information about the PDB format, see:

```
http://www.wwpdb.org/documentation/format23/v2.3.html
```

`getpdb` retrieves protein structure data from the Protein Data Bank (PDB) database, which contains 3-D biological macromolecular structure data.

PDBStruct = `getpdb(`*PDBid*`)` searches the PDB database for the protein structure record specified by the identifier *PDBid* and returns the MATLAB structure *PDBStruct*, which contains a field for each PDB record. The following table summarizes the possible PDB records and the corresponding fields in the MATLAB structure *PDBStruct*:

PDB Database Record	Field in the MATLAB Structure
HEADER	Header
OBSLTE	Obsolete
TITLE	Title
CAVEAT	Caveat
COMPND	Compound
SOURCE	Source
KEYWDS	Keywords
EXPDTA	ExperimentData
AUTHOR	Authors
REVDAT	RevisionDate
SPRSDE	Superseded

PDB Database Record	Field in the MATLAB Structure
JRNL	Journal
REMARK 1	Remark1
REMARK *N* **Note** *N* equals 2 through 999.	Remark*n* **Note** *n* equals 2 through 999.
DBREF	DBReferences
SEQADV	SequenceConflicts
SEQRES	Sequence
FTNOTE	Footnote
MODRES	ModifiedResidues
HET	Heterogen
HETNAM	HeterogenName
HETSYN	HeterogenSynonym
FORMUL	Formula
HELIX	Helix
SHEET	Sheet
TURN	Turn
SSBOND	SSBond
LINK	Link
HYDBND	HydrogenBond
SLTBRG	SaltBridge
CISPEP	CISPeptides
SITE	Site

PDB Database Record	Field in the MATLAB Structure
CRYST1	Cryst1
ORIGXn	OriginX
SCALEn	Scale
MTRIXn	Matrix
TVECT	TranslationVector
MODEL	Model
ATOM	Atom
SIGATM	AtomSD
ANISOU	AnisotropicTemp
SIGUIJ	AnisotropicTempSD
TER	Terminal
HETATM	HeterogenAtom
CONECT	Connectivity

PDBStruct = getpdb(*PDBid*, ...'*PropertyName*', *PropertyValue*, ...) calls `getpdb` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

PDBStruct = getpdb(*PDBid*, ...'ToFile', *ToFileValue*, ...) saves the data returned from the database to a PDB-formatted file, *ToFileValue*.

Tip After you save the protein structure record to a local PDB-formatted file, you can use the `pdbread` function to read the file into the MATLAB software offline or use the `molviewer` function to display and manipulate a 3-D image of the structure.

PDBStruct = getpdb(*PDBid*, ...'SequenceOnly', *SequenceOnlyValue*, ...) controls the return of the protein sequence only. Choices are `true` or `false` (default). If there is one sequence, it is returned as a character array. If there are multiple sequences, they are returned as a cell array.

The Sequence Field

The `Sequence` field is also a structure containing sequence information in the following subfields:

- `NumOfResidues`
- `ChainID`
- `ResidueNames` — Contains the three-letter codes for the sequence residues.
- `Sequence` — Contains the single-letter codes for the sequence residues.

Note If the sequence has modified residues, then the `ResidueNames` subfield might not correspond to the standard three-letter amino acid codes. In this case, the `Sequence` subfield will contain the modified residue code in the position corresponding to the modified residue. The modified residue code is provided in the `ModifiedResidues` field.

The Model Field

The `Model` field is also a structure or an array of structures containing coordinate information. If the MATLAB structure contains one model, the `Model` field is a structure containing coordinate information for that model. If the MATLAB structure contains multiple models, the `Model` field is an array of structures containing coordinate information for each model. The `Model` field contains the following subfields:

- `Atom`
- `AtomSD`

- AnisotropicTemp
- AnisotropicTempSD
- Terminal
- HeterogenAtom

The Atom Field

The Atom field is also an array of structures containing the following subfields:

- AtomSerNo
- AtomName
- altLoc
- resName
- chainID
- resSeq
- iCode
- X
- Y
- Z
- occupancy
- tempFactor
- segID
- element
- charge
- AtomNameStruct — Contains three subfields: chemSymbol, remoteInd, and branch.

Examples

Retrieve the structure information for the electron transport (heme) protein that has a PDB identifier of `5CYT`, read the information into a MATLAB structure `pdbstruct`, and save the information to a PDB-formatted file `electron_transport.pdb` in the MATLAB Current Directory.

```
pdbstruct = getpdb('5CYT', 'ToFile', 'electron_transport.pdb')
```

See Also

Bioinformatics Toolbox functions: `getembl`, `getgenbank`, `getgenpept`, `molviewer`, `pdbdistplot`, `pdbread`, `pdbsuperpose`, `pdbtransform`, `pdbwrite`

getrelatives (biograph)

Purpose

Find relatives in biograph object

Syntax

```
Nodes = getrelatives(BiographNode)
Nodes = getrelatives(BiographNode,NumGenerations)
```

Arguments

BiographNode	Node in a biograph object.
NumGenerations	Number of generations. Enter a positive integer.

Description

Nodes = getrelatives(*BiographNode*) finds all the direct relatives for a given node (*BiographNode*).

Nodes = getrelatives(*BiographNode,NumGenerations*) finds the direct relatives for a given node (*BiographNode*) up to a specified number of generations (*NumGenerations*).

Examples

1 Create a biograph object.

```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];
bg = biograph(cm)
```

2 Find all nodes interacting with node 1.

```
intNodes = getrelatives(bg.nodes(1));
set(intNodes,'Color',[.7 .7 1]);
bg.view;
```

See Also

Bioinformatics Toolbox function: biograph (object constructor)

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: dolayout, get, getancestors, getdescendants, getedgesbynodeid, getnodesbyid, getrelatives, set, view

Purpose

Find terms that are relatives of specified Gene Ontology (GO) term

Syntax

```
RelativeIDs = getrelatives(GeneontObj, ID)
[RelativeIDs, Counts] = getrelatives(GeneontObj, ID)
... = getrelatives(..., 'Height', HeightValue, ...)
... = getrelatives(..., 'Depth', DepthValue, ...)
... = getrelatives(..., 'Levels', LevelsValue, ...)
... = getrelatives(..., 'Relationtype', RelationtypeValue,
   ...)
... = getrelatives(..., 'Exclude', ExcludeValue, ...)
```

Description

`RelativeIDs = getrelatives(GeneontObj, ID)` searches `GeneontObj`, a geneont object, for GO terms that are relatives of the GO term(s) specified by `ID`, which is a GO term identifier or vector of identifiers. It returns `RelativeIDs`, a vector of GO term identifiers including `ID`. `ID` is a nonnegative integer or a vector containing nonnegative integers.

`[RelativeIDs, Counts] = getrelatives(GeneontObj, ID)` also returns the number of times each relative is found. `Counts` is a column vector with the same number of elements as terms in `GeneontObj`.

Tip The `Counts` return value is useful when you tally counts in gene enrichment studies. For more information, see the Gene Ontology Enrichment in Microarray Data demo.

`... = getrelatives(..., 'PropertyName', PropertyValue, ...)` calls `getrelatives` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = getrelatives(..., 'Height', HeightValue, ...)` searches up through a specified number of levels, `HeightValue`, in the gene ontology. `HeightValue` is a positive integer. Default is `1`.

`... = getrelatives(..., 'Depth', DepthValue, ...)` searches down through a specified number of levels, *`DepthValue`*, in the gene ontology. *`DepthValue`* is a positive integer. Default is `1`.

`... = getrelatives(..., 'Levels', LevelsValue, ...)` searches up and down through a specified number of levels, *`LevelsValue`*, in the gene ontology. *`LevelsValue`* is a positive integer. When specified, it overrides *`HeightValue`* and *`DepthValue`*.

`... = getrelatives(..., 'Relationtype', RelationtypeValue, ...)` searches for specified relationship types, *`RelationtypeValue`*, in the gene ontology. *`RelationtypeValue`* is a string. Choices are `'is_a'`, `'part_of'`, or `'both'` (default).

`... = getrelatives(..., 'Exclude', ExcludeValue, ...)` controls excluding *`ID`*, the original queried term(s), from the output *`RelativeIDs`*, unless a term was found while searching the gene ontology. Choices are `true` or `false` (default).

Inputs

`GeneontObj`	A geneont object, such as created by the `geneont.geneont` constructor function.
`ID`	GO term identifier or vector of identifiers.
`HeightValue`	Positive integer specifying the number of levels to search upward in the gene ontology.
`DepthValue`	Positive integer specifying the number of levels to search downward in the gene ontology.
`LevelsValue`	Positive integer specifying the number of levels up and down to search in the gene ontology. When specified, it overrides *`HeightValue`* and *`DepthValue`*.

RelationtypeValue	String specifying the relationship types to search for in the gene ontology. Choices are: • `'is_a'` • `'part_of'` • `'both'` (default)
ExcludeValue	Controls excluding *ID*, the original queried term(s), from the output *RelativeIDs*, unless the term was reached while searching the gene ontology. Choices are `true` or `false` (default).

Outputs

RelativeIDs	Vector of GO term identifiers including *ID*.
Counts	Column vector with the same number of elements as terms in *GeneontObj*, indicating the number of times each relative is found.

Examples

1 Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

```
GO = geneont('LIVE', true)
```

The MATLAB software creates a geneont object and displays the number of terms in the database.

```
Gene Ontology object with 27769 Terms.
```

2 Retrieve the immediate relatives for the mitochondrial membrane GO term with a GO identifier of 31966.

```
relatives = getrelatives(GO,31966,'levels',1)

relatives =
```

```
  5741
  5743
 31090
 31966
 44429
```

3 Create a subordinate Gene Ontology.

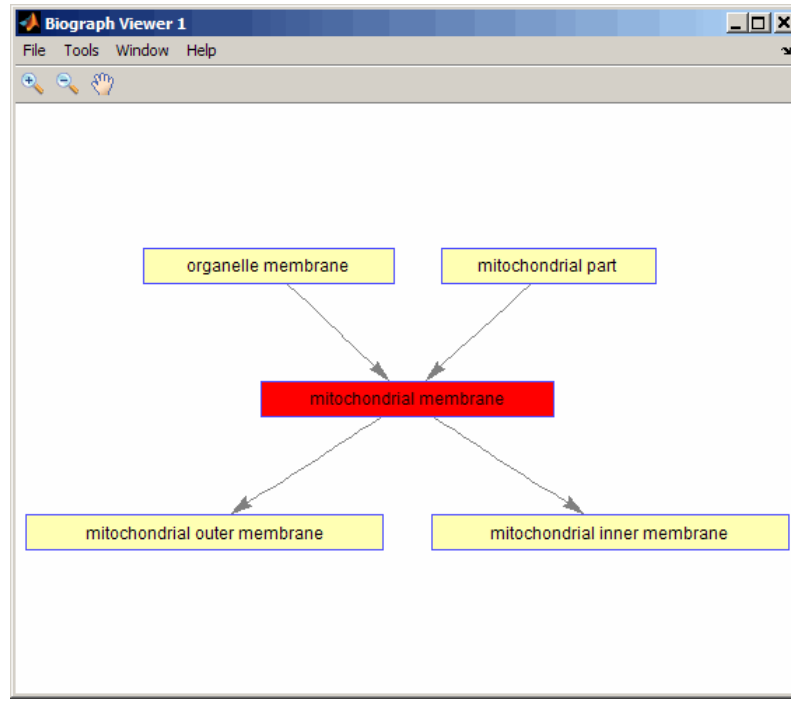
```
subontology = GO(relatives)

Gene Ontology object with 5 Terms.
```

4 Create a report of the subordinate Gene Ontology terms, that includes the GO identifier and name.

```
rpt = get(subontology.terms,{'id','name'})

rpt =

    [ 5741]             [1x28 char]
    [ 5743]             [1x28 char]
    [31090]    'organelle membrane'
    [31966]             [1x22 char]
    [44429]    'mitochondrial part'
```

5 View relationships of the subordinate Gene Ontology by using the `getmatrix` method to create a connection matrix to pass to the `biograph` function, and color the mitochondrial membrane GO term red.

```
[cm acc rels] = getmatrix(subontology);
BG = biograph(cm, get(subontology.terms, 'name'));
BG.nodes(acc==31966).Color = [1 0 0];
view(BG)
```



6 Retrieve all relatives for the mithocondrial outer membrane GO term with an identifier of `5741`.

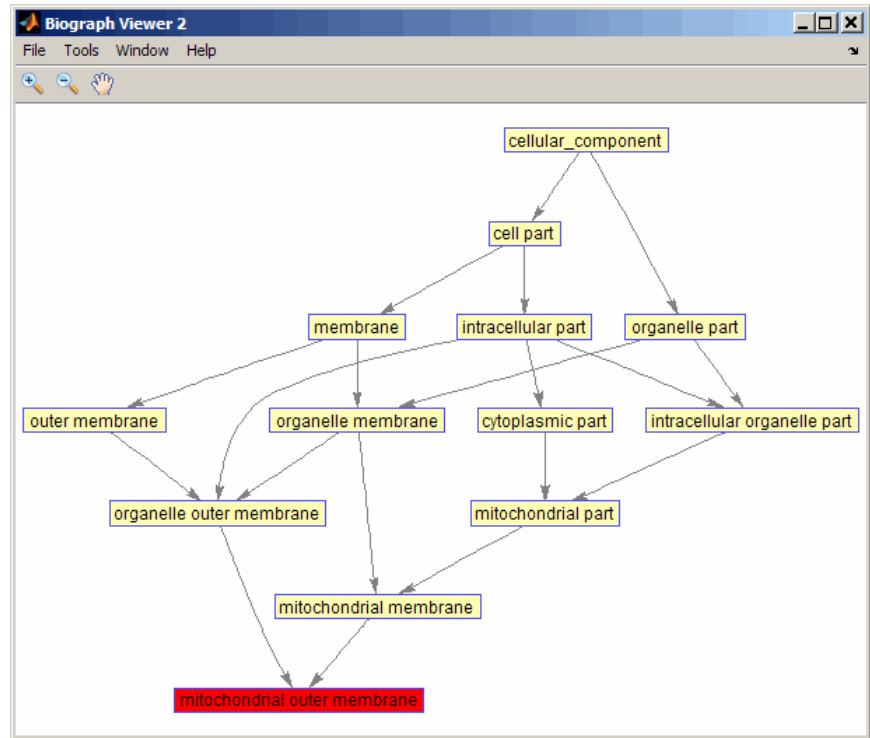
```
relatives = getrelatives(GO,5741,'levels',inf);
```

7 Create a subordinate Gene Ontology.

```
subontology = GO(relatives)

Gene Ontology object with 13 Terms.
```

8 View relationships of the subordinate Gene Ontology by using the `getmatrix` method to create a connection matrix to pass to the `biograph` function and methods, and color the mitochondrial outer membrane GO terms red.

```
[cm acc rels] = getmatrix(subontology);
BG = biograph(cm, get(subontology.terms, 'name'));
BG.nodes(acc==5741).Color = [1 0 0];
view(BG)
```



See Also

Bioinformatics Toolbox functions: `goannotread`, `num2goid`

Bioinformatics Toolbox class: `term`

Purpose

Read annotations from Gene Ontology annotated file

Syntax

```
Annotation = goannotread(File)
Annotation = goannotread(File,  ...'Fields', FieldsValue,
   ...)
Annotation = goannotread(File,  ...'Aspect', AspectValue,
   ...)
```

Arguments

File	String specifying a file name of a Gene Ontology (GO) annotated file.
FieldsValue	String or cell array of strings specifying one or more fields to read from the Gene Ontology annotated file. Default is to read all fields. Valid fields are listed below.
AspectValue	Character array specifying one or more characters. Valid aspects are: • `P` — Biological process • `F` — Molecular function • `C` — Cellular component Default is `'CFP'`, which specifies to read all aspects.

Return Values

Annotation	MATLAB array of structures containing annotations from a Gene Ontology annotated file.

Description

Annotation = `goannotread(`*File*`)` converts the contents of *File*, a Gene Ontology annotated file, into *Annotation*, an array of structures. Files should have the structure specified in:

```
http://www.geneontology.org/GO.annotation.shtml#file
```

A list with some annotated files can be found at:

```
http://www.geneontology.org/GO.current.annotations.shtml
```

Annotation = goannotread(*File*, ...'*PropertyName*', *PropertyValue*, ...) calls goannotread with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

Annotation = goannotread(*File*, ...'Fields', *FieldsValue*, ...) specifies the fields to read from the Gene Ontology annotated file. *FieldsValue* is a string or cell array of strings specifying one or more fields. Default is to read all fields. Valid fields are:

- Database
- DB_Object_ID
- DB_Object_Symbol
- Qualifier
- GOid
- DBReference
- Evidence
- WithFrom
- Aspect
- DB_Object_Name
- Synonym
- DB_Object_Type
- Taxon
- Date
- Assigned_by

For more information on these fields, see:

```
http://www.geneontology.org/GO.format.annotation.shtml
```

Annotation = goannotread(*File*, ...'Aspect', *AspectValue*, ...) specifies the aspects to read from the Gene Ontology annotated file. *AspectValue* is a character array specifying one or more characters. Valid aspects are:

- `P` — Biological process
- `F` — Molecular function
- `C` — Cellular component

Default is `'CFP'`, which specifies to read all aspects.

Examples

Reading All Annotations from a Gene Ontology Annotated File

1. Open a Web browser to

   ```
   http://www.geneontology.org/GO.current.annotations.shtml
   ```

2. Download `gene_association.sgd.gz`, the file containing `GO` annotations for the gene products of *Saccharomyces cerevisiae*, to your MATLAB Current Directory.

3. Uncompress the file using the `gunzip` function.

   ```
   gunzip('gene_association.sgd.gz')
   ```

4. Read the file into the MATLAB software.

   ```
   SGDGenes = goannotread('gene_association.sgd');
   ```

5. Create a structure with `GO` annotations and display a list of the genes.

   ```
   S = struct2cell(SGDGenes);
   genes = S(3,:)'
   ```

Reading a Subset of Annotations from a Gene Ontology Annotated File

1. Open a Web browser to

   ```
   http://www.geneontology.org/GO.current.annotations.shtml
   ```

2. Download `gene_association.goa_human.gz`, the file containing `GO` annotations for the gene products of *Homo sapiens*, to your MATLAB Current Directory.

3. Uncompress the file using the `gunzip` function.

   ```
   gunzip('gene_association.goa_human.gz')
   ```

4. Read the file into the MATLAB software, but limit the annotations to genes related to molecular function (`F`), and to the fields for the gene symbol and the associated ID, that is, `DB_Object_Symbol` and `GOid`.

   ```
   HumanStruct = goannotread('gene_association.goa_human', ...
                 'Aspect','F','Fields',{'DB_Object_Symbol','GOid'});
   ```

5. Create a list of the *Homo sapiens* genes and a list of the associated GO terms.

   ```
   Humangenes = {HumanStruct.DB_Object_Symbol};
   HumanGO = [HumanStruct.GOid];
   ```

See Also

Bioinformatics Toolbox functions: `geneont.geneont` (object constructor), `num2goid`

Bioinformatics Toolbox class: `geneont`

Bioinformatics Toolbox methods of geneont object: `geneont.getancestors`, `geneont.getdescendants`, `geneont.getmatrix`, `geneont.getrelatives`

Purpose

Return Gonnet scoring matrix

Syntax

```
gonnet
```

Description

`gonnet` returns the Gonnet matrix.

The Gonnet matrix is the recommended mutation matrix for initially aligning protein sequences. Matrix elements are ten times the logarithmic of the probability that the residues are aligned divided by the probability that the residues are aligned by chance, and then matrix elements are normalized to 250 PAM units.

Expected score = `-0.6152`, Entropy = `1.6845` bits Lowest score = `-8`, Highest score = `14.2`

Order:

```
A  R  N  D  C  Q  E  G  H  I  L  K  M  F  P  S  T  W  Y  V  B  Z  X  *
```

References

[1] Gaston, H., Gonnet, M., Cohen, A., and Benner, S. (1992). Exhaustive matching of the entire protein sequence database. Science. *256*, 1443–1445.

See Also

Bioinformatics Toolbox functions: `blosum`, `dayhoff`, `localalign`, `nuc44`, `nwalign`, `pam`, `swalign`

gprread

Purpose

Read microarray data from GenePix Results (GPR) file

Syntax

```
GPRData = gprread('File')
gprread(..., 'PropertyName', PropertyValue,...)
gprread(..., 'CleanColNames', CleanColNamesValue)
```

Arguments

File	GenePix Results (GPR) formatted file. Enter a file name or a path and file name.
CleanColNamesValue	Controls the creation of column names that can be used as variable names.

Description

GPRData = gprread('*File*') reads GenePix results data from *File* and creates a MATLAB structure (*GPRData*) with the following fields.

Field
Header
Data
Blocks
Columns
Rows
Names
IDs
ColumnNames
Indices
Shape

gprread(..., '*PropertyName*', *PropertyValue*,...) defines optional properties using property name/value pairs.

gprread(..., 'CleanColNames', *CleanColNamesValue*) controls the creation of column names that can be used as variable names. A

GPR file may contain column names with spaces and some characters that the MATLAB software cannot use in MATLAB variable names. If *CleanColNamesValue* is `true`, `gprread` returns names in the field `ColumnNames` that are valid MATLAB variable names and names that you can use in functions. By default, *CleanColNamesValue* is `false` and the field `ColumnNames` may contain characters that are invalid for MATLAB variable names.

The field `Indices` of the structure contains indices that can be used for plotting heat maps of the data.

For more details on the GPR format, see

```
http://www.moleculardevices.com/pages/software/gn_genepix_file_formats.html#gpr
```

```
http://www.moleculardevices.com/pages/software/gn_gpr_format_history.html
```

For a list of supported file format versions, see

```
http://www.moleculardevices.com/pages/software/gn_genepix_file_formats.html
```

Examples

```
% Read in a sample GPR file and plot the median foreground
% intensity for the 635 nm channel.
gprStruct = gprread('mouse_a1pd.gpr')
maimage(gprStruct,'F635 Median');

% Alternatively you can create a similar plot using
% more basic graphics commands.
F635Median = magetfield(gprStruct,'F635 Median');
imagesc(F635Median(gprStruct.Indices));
colormap bone
colorbar;
```

See Also

Bioinformatics Toolbox functions: `affyread`, `agferead`, `celintensityread`, `galread`, `geoseriesread`, `geosoftread`, `ilmnbsread`, `imageneread`, `magetfield`, `sptread`

graphallshortestpaths

Purpose

Find all shortest paths in graph

Syntax

```
[dist] = graphallshortestpaths(G)
[dist] = graphallshortestpaths(G, ...'Directed',
DirectedValue, ...)
[dist] = graphallshortestpaths(G, ...'Weights', WeightsValue,
   ...)
```

Arguments

G	N-by-N sparse matrix that represents a graph. Nonzero entries in matrix *G* represent the weights of the edges.
DirectedValue	Property that indicates whether the graph is directed or undirected. Enter `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.
WeightsValue	Column vector that specifies custom weights for the edges in matrix *G*. It must have one entry for every nonzero value (edge) in matrix *G*. The order of the custom weights in the vector must match the order of the nonzero values in matrix *G* when it is traversed column-wise. This property lets you use zero-valued weights. By default, `graphallshortestpaths` gets weight information from the nonzero entries in matrix *G*.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

`[dist] = graphallshortestpaths(G)` finds the shortest paths between every pair of nodes in the graph represented by matrix *G*, using Johnson's algorithm. Input *G* is an N-by-N sparse matrix that

represents a graph. Nonzero entries in matrix *G* represent the weights of the edges.

Output *dist* is an N-by-N matrix where *dist*(S,T) is the distance of the shortest path from source node S to target node T. Elements in the diagonal of this matrix are always 0, indicating the source node and target node are the same. A 0 not in the diagonal indicates that the distance between the source node and target node is 0. An Inf indicates there is no path between the source node and the target node.

Johnson's algorithm has a time complexity of O(N*log(N)+N*E), where N and E are the number of nodes and edges respectively.

[...] = graphallshortestpaths (*G*, '*PropertyName*', *PropertyValue*, ...) calls graphallshortestpaths with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

[*dist*] = graphallshortestpaths(*G*, ...'Directed', *DirectedValue*, ...) indicates whether the graph is directed or undirected. Set *DirectedValue* to false for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is true.

[*dist*] = graphallshortestpaths(*G*, ...'Weights', *WeightsValue*, ...) lets you specify custom weights for the edges. *WeightsValue* is a column vector having one entry for every nonzero value (edge) in matrix *G*. The order of the custom weights in the vector must match the order of the nonzero values in matrix *G* when it is traversed column-wise. This property lets you use zero-valued weights. By default, graphallshortestpaths gets weight information from the nonzero entries in matrix *G*.

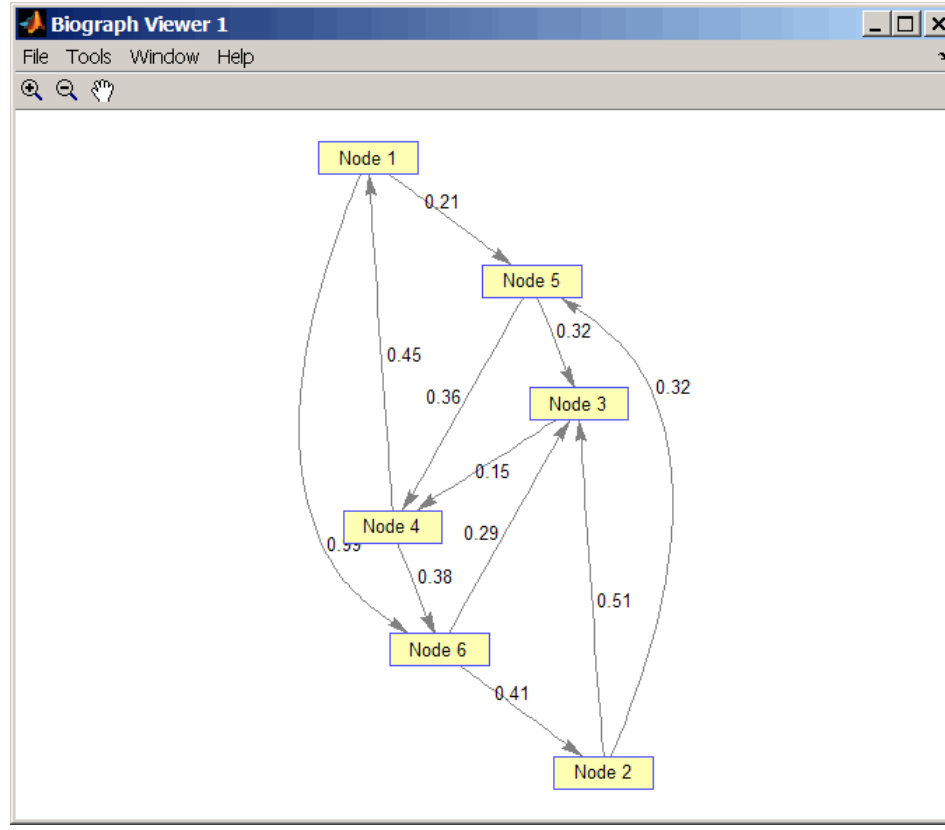
Examples

Finding All Shortest Paths in a Directed Graph

1 Create and view a directed graph with 6 nodes and 11 edges.

```
W = [.41 .99 .51 .32 .15 .45 .38 .32 .36 .29 .21];
DG = sparse([6 1 2 2 3 4 4 5 5 6 1],[2 6 3 5 4 1 6 3 4 3 5],W)
```

```
DG =

   (4,1)       0.4500
   (6,2)       0.4100
   (2,3)       0.5100
   (5,3)       0.3200
   (6,3)       0.2900
   (3,4)       0.1500
   (5,4)       0.3600
   (1,5)       0.2100
   (2,5)       0.3200
   (1,6)       0.9900
   (4,6)       0.3800

view(biograph(DG,[],'ShowWeights','on'))
```



2 Find all the shortest paths between every pair of nodes in the directed graph.

```
graphallshortestpaths(DG)

ans =

         0    1.3600    0.5300    0.5700    0.2100    0.9500
    1.1100         0    0.5100    0.6600    0.3200    1.0400
    0.6000    0.9400         0    0.1500    0.8100    0.5300
```

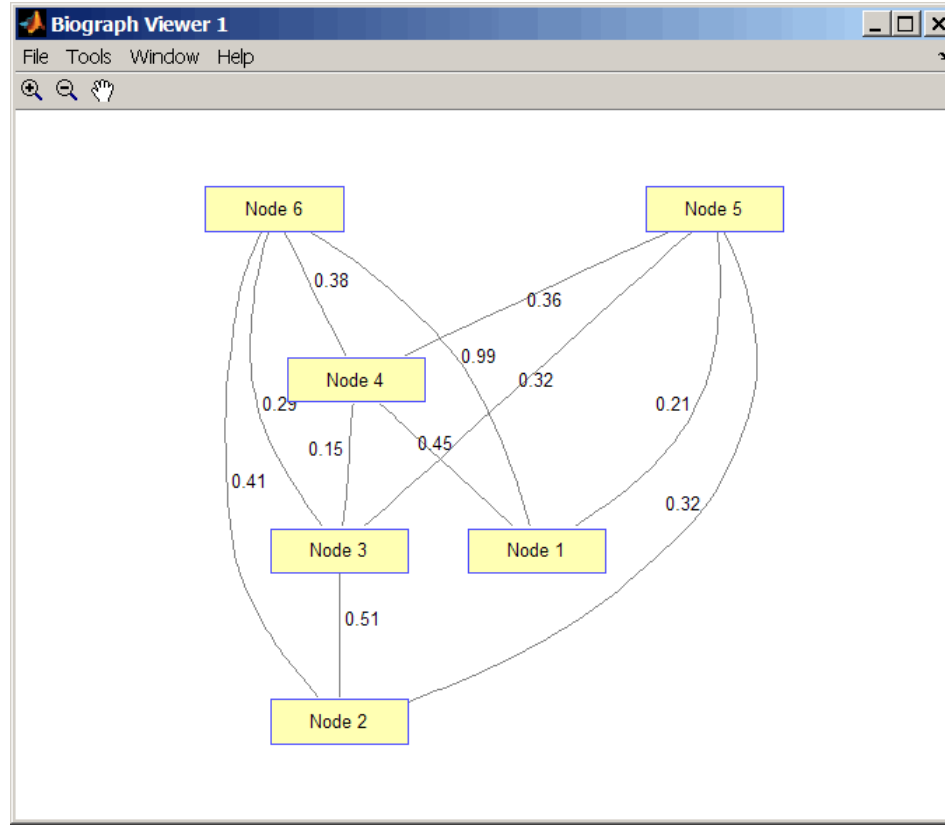
```
    0.4500    0.7900    0.6700         0    0.6600    0.3800
    0.8100    1.1500    0.3200    0.3600         0    0.7400
    0.8900    0.4100    0.2900    0.4400    0.7300         0
```

The resulting matrix shows the shortest path from node 1 (first row) to node 6 (sixth column) is 0.95. You can see this in the graph by tracing the path from node 1 to node 5 to node 4 to node 6 (0.21 + 0.36 + 0.38 = 0.95).

Finding All Shortest Paths in an Undirected Graph

1 Create and view an undirected graph with 6 nodes and 11 edges.

```
UG = tril(DG + DG')

UG =

   (4,1)       0.4500
   (5,1)       0.2100
   (6,1)       0.9900
   (3,2)       0.5100
   (5,2)       0.3200
   (6,2)       0.4100
   (4,3)       0.1500
   (5,3)       0.3200
   (6,3)       0.2900
   (5,4)       0.3600
   (6,4)       0.3800

view(biograph(UG,[],'ShowArrows','off','ShowWeights','on'))
```



2 Find all the shortest paths between every pair of nodes in the undirected graph.

```
graphallshortestpaths(UG,'directed',false)

ans =

         0    0.5300    0.5300    0.4500    0.2100    0.8300
    0.5300         0    0.5100    0.6600    0.3200    0.7000
    0.5300    0.5100         0    0.1500    0.3200    0.5300
```

```
    0.4500    0.6600    0.1500         0    0.3600    0.3800
    0.2100    0.3200    0.3200    0.3600         0    0.7400
    0.8300    0.7000    0.5300    0.3800    0.7400         0
```

The resulting matrix is symmetrical because it represents an undirected graph. It shows the shortest path from node 1 (first row) to node 6 (sixth column) is 0.83. You can see this in the graph by tracing the path from node 1 to node 4 to node 6 (0.45 + 0. 38 = 0.83). Because `UG` is an undirected graph, we can use the edge between node 1 and node 4, which we could not do in the directed graph `DG`.

References

[1] Johnson, D.B. (1977). Efficient algorithms for shortest paths in sparse networks. Journal of the ACM *24(1)*, 1-13.

[2] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphconncomp`, `graphisdag`, `graphisomorphism`, `graphisspantree`, `graphmaxflow`, `graphminspantree`, `graphpred2path`, `graphshortestpath`, `graphtopoorder`, `graphtraverse`

Bioinformatics Toolbox method of `biograph object`: `allshortestpaths`

Purpose

Find strongly or weakly connected components in graph

Syntax

```
[S, C] = graphconncomp(G)
[S, C] = graphconncomp(G, ...'Directed', DirectedValue, ...)
[S, C] = graphconncomp(G, ...'Weak', WeakValue, ...)
```

Arguments

G	N-by-N sparse matrix that represents a graph. Nonzero entries in matrix *G* indicate the presence of an edge.
DirectedValue	Property that indicates whether the graph is directed or undirected. Enter `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`. A DFS-based algorithm computes the connected components. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.
WeakValue	Property that indicates whether to find weakly connected components or strongly connected components. A weakly connected component is a maximal group of nodes that are mutually reachable by violating the edge directions. Set *WeakValue* to `true` to find weakly connected components. Default is `false`, which finds strongly connected components. The state of this parameter has no effect on undirected graphs because weakly and strongly connected components are the same in undirected graphs. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

`[S, C] = graphconncomp(G)` finds the strongly connected components of the graph represented by matrix `G` using Tarjan's algorithm. A strongly connected component is a maximal group of nodes that are mutually reachable without violating the edge directions. Input `G` is an N-by-N sparse matrix that represents a graph. Nonzero entries in matrix `G` indicate the presence of an edge.

The number of components found is returned in `S`, and `C` is a vector indicating to which component each node belongs.

Tarjan's algorithm has a time complexity of `O(N+E)`, where `N` and `E` are the number of nodes and edges respectively.

`[S, C] = graphconncomp(G, ...'PropertyName', PropertyValue, ...)` calls `graphconncomp` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[S, C] = graphconncomp(G, ...'Directed', DirectedValue, ...)` indicates whether the graph is directed or undirected. Set `directedValue` to `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`. A DFS-based algorithm computes the connected components. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.

`[S, C] = graphconncomp(G, ...'Weak', WeakValue, ...)` indicates whether to find weakly connected components or strongly connected components. A weakly connected component is a maximal group of nodes that are mutually reachable by violating the edge directions. Set `WeakValue` to `true` to find weakly connected components. Default is `false`, which finds strongly connected components. The state of this

parameter has no effect on undirected graphs because weakly and strongly connected components are the same in undirected graphs. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.

Note By definition, a single node can be a strongly connected component.

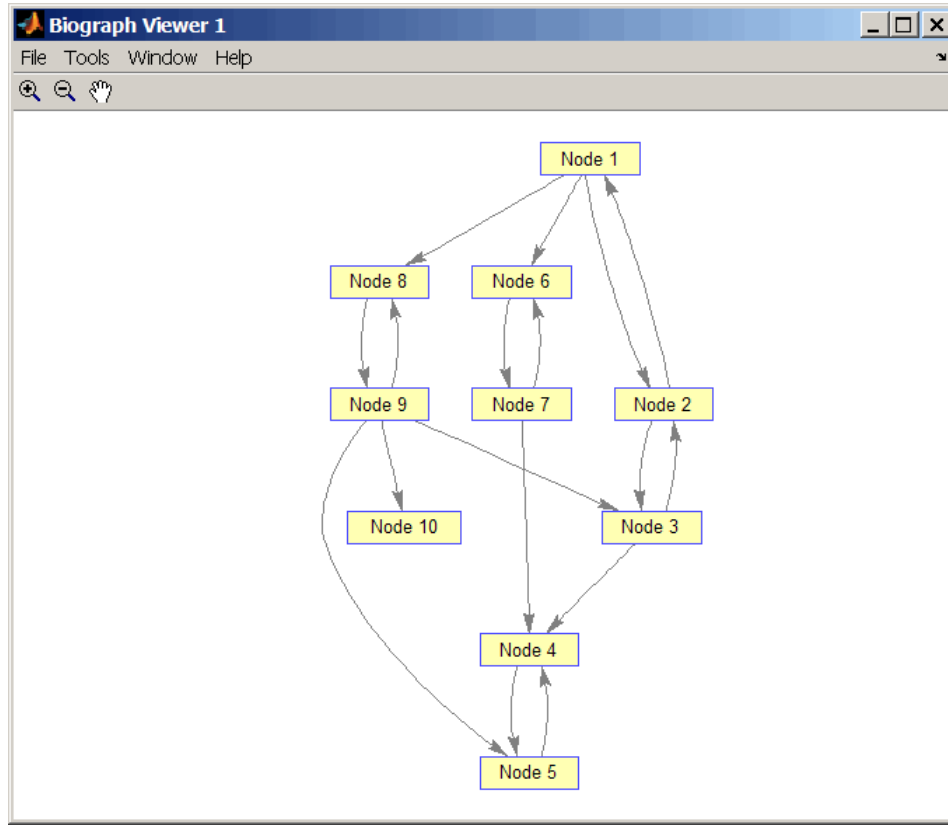
Note A directed acyclic graph (DAG) cannot have any strongly connected components larger than one.

Examples

1 Create and view a directed graph with 10 nodes and 17 edges.

```
DG = sparse([1 1 1 2 2 3 3 4 5 6 7 7 8 9 9  9 9], ...
            [2 6 8 3 1 4 2 5 4 7 6 4 9 8 10 5 3],true,10,10)

DG =

   (2,1)        1
   (1,2)        1
   (3,2)        1
   (2,3)        1
   (9,3)        1
   (3,4)        1
   (5,4)        1
   (7,4)        1
   (4,5)        1
   (9,5)        1
   (1,6)        1
   (7,6)        1
   (6,7)        1
   (1,8)        1
   (9,8)        1
```

```
    (8,9)         1
    (9,10)        1

h = view(biograph(DG));
```



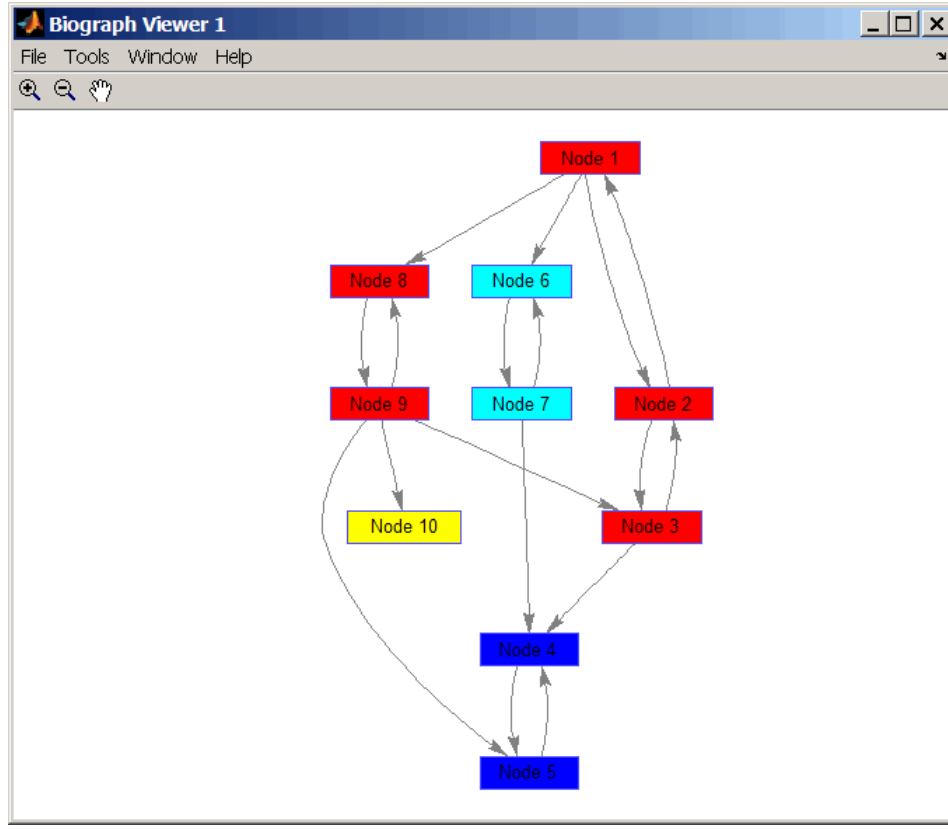
2 Find the number of strongly connected components in the directed graph and determine to which component each of the 10 nodes belongs.

```
[S,C] = graphconncomp(DG)
```

```
S =

     4


C =

     4     4     4     1     1     2     2     4     4     3
```

3 Color the nodes for each component with a different color.

```
colors = jet(S);
for i = 1:numel(h.nodes)
  h.Nodes(i).Color = colors(C(i),:);
end
```



References

[1] Tarjan, R.E., (1972). Depth first search and linear graph algorithms. SIAM Journal on Computing *1(2)*, 146–160.

[2] Sedgewick, R., (2002). Algorithms in C++, Part 5 Graph Algorithms (Addison-Wesley).

[3] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphisdag`, `graphisomorphism`, `graphisspantree`, `graphmaxflow`, `graphminspantree`, `graphpred2path`, `graphshortestpath`, `graphtopoorder`, `graphtraverse`

Bioinformatics Toolbox method of `biograph object`: `conncomp`

graphisdag

Purpose

Test for cycles in directed graph

Syntax

```
graphisdag(G)
```

Arguments

G	N-by-N sparse matrix that represents a directed graph. Nonzero entries in matrix *G* indicate the presence of an edge.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

`graphisdag(G)` returns logical 1 (`true`) if the directed graph represented by matrix *G* is a directed acyclic graph (DAG) and logical 0 (`false`) otherwise. *G* is an N-by-N sparse matrix that represents a directed graph. Nonzero entries in matrix *G* indicate the presence of an edge.

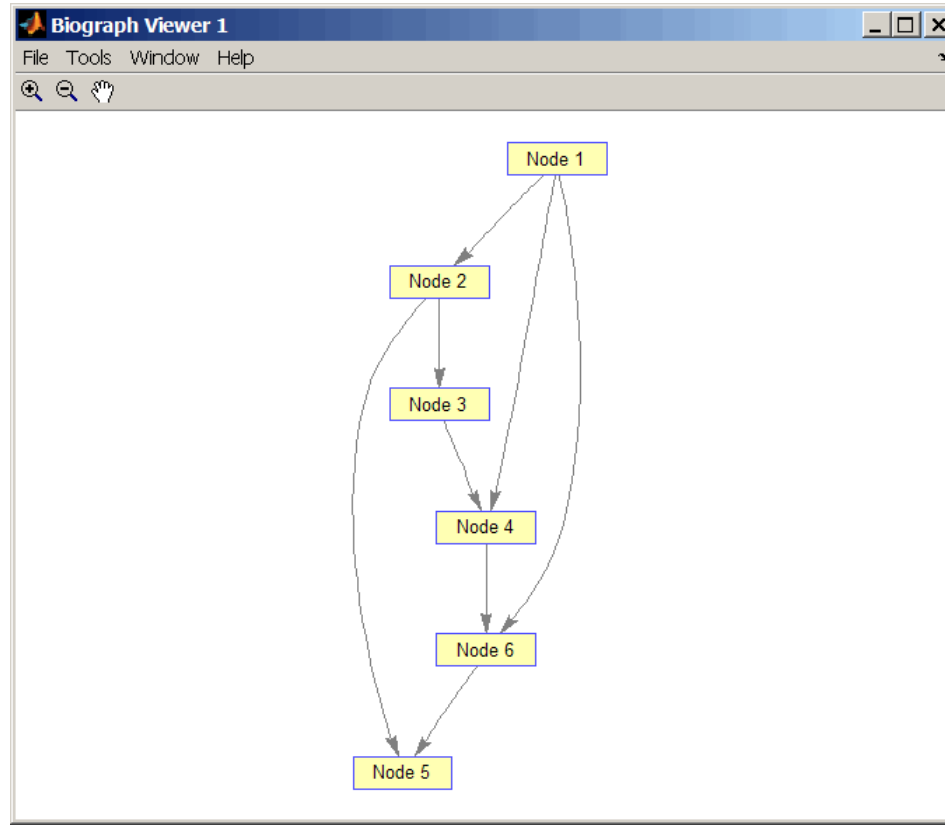
Examples

Testing for Cycles in Directed Graphs

1 Create and view a directed acyclic graph (DAG) with six nodes and eight edges.

```
DG = sparse([1 1 1 2 2 3 4 6],[2 4 6 3 5 4 6 5],true,6,6)

DG =

   (1,2)        1
   (2,3)        1
   (1,4)        1
   (3,4)        1
   (2,5)        1
   (6,5)        1
   (1,6)        1
   (4,6)        1
```

```
view(biograph(DG))
```

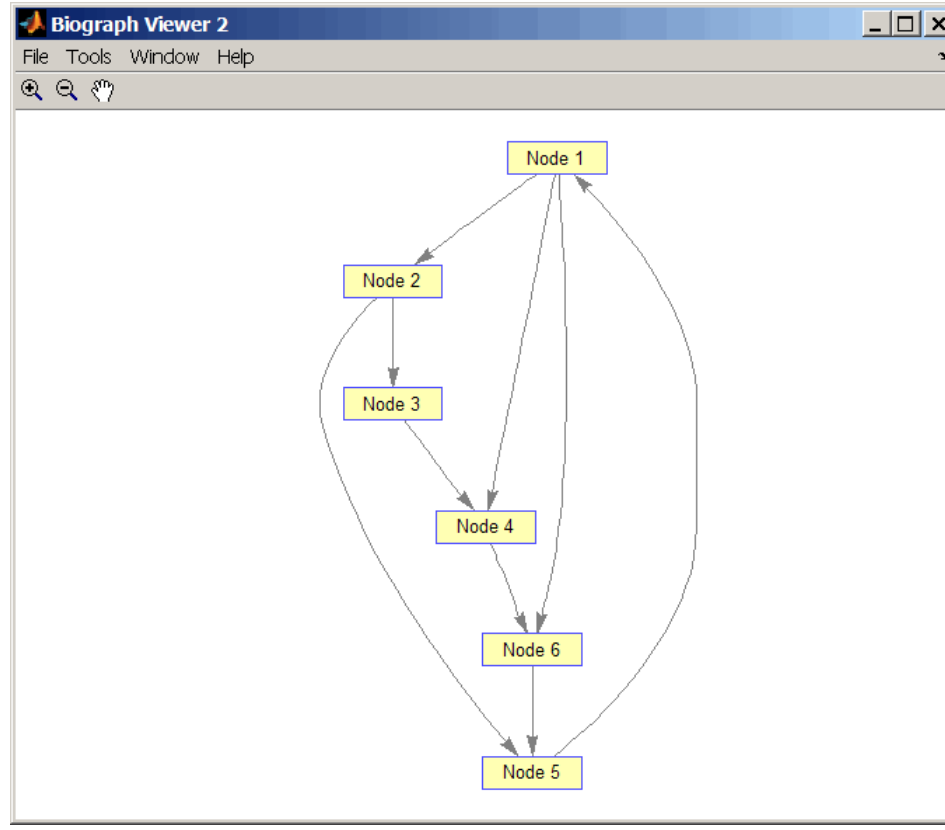


2 Test for cycles in the DAG.

```
graphisdag(DG)

ans =

     1
```

3 Add an edge to the DAG to make it cyclic, and then view the directed graph.

```
DG(5,1) = true

DG =

   (5,1)        1
   (1,2)        1
   (2,3)        1
   (1,4)        1
   (3,4)        1
   (2,5)        1
   (6,5)        1
   (1,6)        1
   (4,6)        1

view(biograph(DG))
```



4 Test for cycles in the new graph.

```
graphisdag(DG)

ans =

     0
```

Testing for Cycles in a Very Large Graph (Greater Than 20,000 Nodes and 30,000 Edges)

1 Download the Gene Ontology database to a geneont object.

```
GO = geneont('live',true);
```

2 Convert the geneont object to a matrix.

```
CM = getmatrix(GO);
```

3 Test for cycles in the graph.

```
graphisdag(CM)
```

Creating a Random DAG

1 Create and view a random directed acyclic graph (DAG) with 15 nodes and 20 edges.

```
g = sparse([],[],true,15,15);
while nnz(g) < 20
  edge = randsample(15*15,1); % get a random edge
  g(edge) = true;
  g(edge) = graphisdag(g);
end
view(biograph(g))
```

2 Test for cycles in the graph.

```
graphisdag(g)
```

References

[1] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisomorphism`, `graphisspantree`, `graphmaxflow`,

`graphminspantree`, `graphpred2path`, `graphshortestpath`, `graphtopoorder`, `graphtraverse`

Bioinformatics Toolbox method of `biograph object`: `isdag`

graphisomorphism

Purpose

Find isomorphism between two graphs

Syntax

```
[Isomorphic, Map] = graphisomorphism(G1, G2)
[Isomorphic, Map] = graphisomorphism(G1, G2,'Directed',
    DirectedValue)
```

Arguments

G1	N-by-N sparse matrix that represents a directed or undirected graph. Nonzero entries in matrix *G1* indicate the presence of an edge.
G2	N-by-N sparse matrix that represents a directed or undirected graph. *G2* must be the same (directed or undirected) as *G1*.
DirectedValue	Property that indicates whether the graphs are directed or undirected. Enter `false` when both *G1* and *G2* are undirected graphs. In this case, the upper triangles of the sparse matrices *G1* and *G2* are ignored. Default is `true`, meaning that both graphs are directed.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

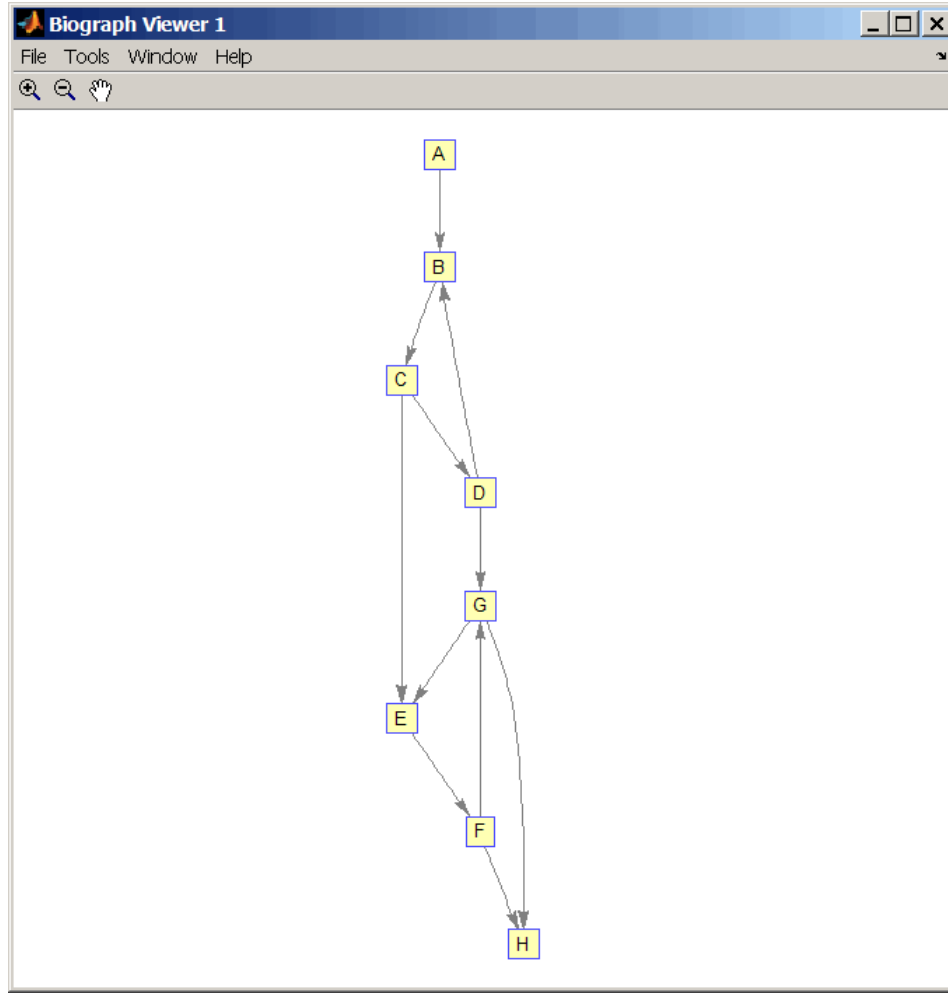
`[`*Isomorphic*`, `*Map*`] = graphisomorphism(`*G1*`, `*G2*`)` returns logical 1 (`true`) in *Isomorphic* if *G1* and *G2* are isomorphic graphs, and logical 0 (`false`) otherwise. A graph isomorphism is a 1-to-1 mapping of the nodes in the graph *G1* and the nodes in the graph *G2* such that adjacencies are preserved. *G1* and *G2* are both N-by-N sparse matrices that represent directed or undirected graphs. Return value *Isomorphic* is Boolean. When *Isomorphic* is `true`, *Map* is a row vector containing the node indices that map from *G2* to *G1*. When *Isomorphic* is `false`, the worst-case time complexity is `O(N!)`, where `N` is the number of nodes.

`[Isomorphic, Map] = graphisomorphism(G1, G2,'Directed', DirectedValue)` indicates whether the graphs are directed or undirected. Set *DirectedValue* to `false` when both *G1* and *G2* are undirected graphs. In this case, the upper triangles of the sparse matrices *G1* and *G2* are ignored. Default is `true`, meaning that both graphs are directed.

Examples

1 Create and view a directed graph with 8 nodes and 11 edges.

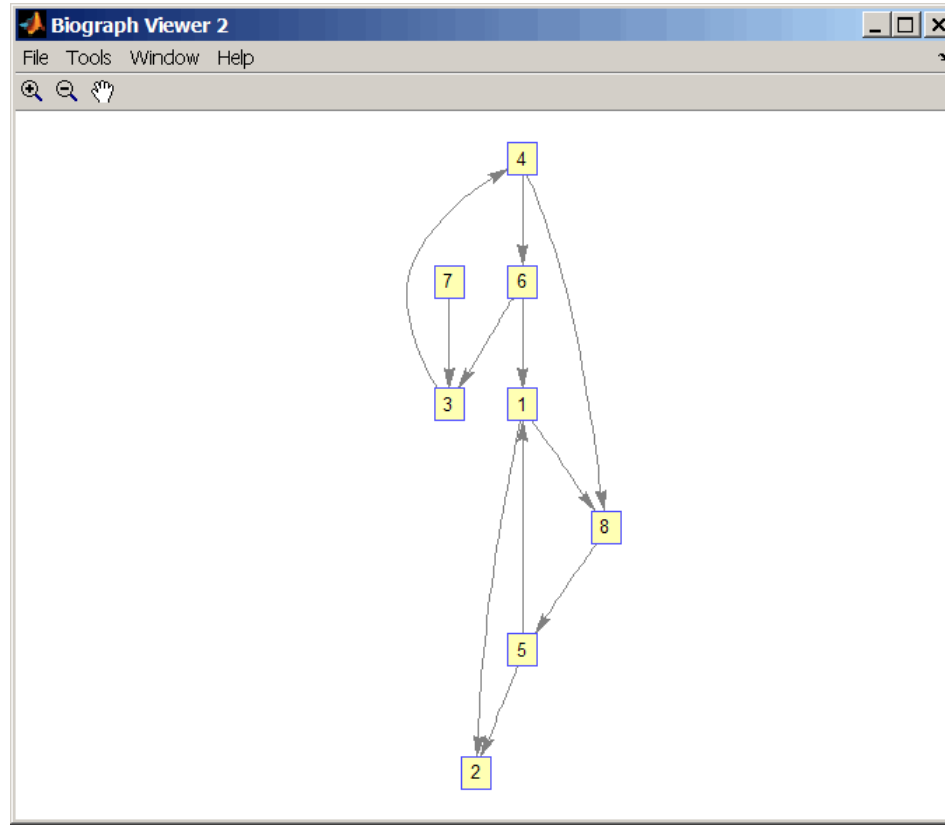
```
m('ABCDEFGH') = [1 2 3 4 5 6 7 8];
g1 = sparse(m('ABDCDCGEFFG'),m('BCBDGEEFHGH'),true,8,8)

g1 =

   (1,2)        1
   (4,2)        1
   (2,3)        1
   (3,4)        1
   (3,5)        1
   (7,5)        1
   (5,6)        1
   (4,7)        1
   (6,7)        1
   (6,8)        1
   (7,8)        1

view(biograph(g1,'ABCDEFGH'))
```



2 Set a random permutation vector and then create and view a new permuted graph.

```
p = randperm(8)
```

```
p =

     7     8     2     3     6     4     1     5

g2 = g1(p,p);
view(biograph(g2,'12345678'))
```



3 Check if the two graphs are isomorphic.

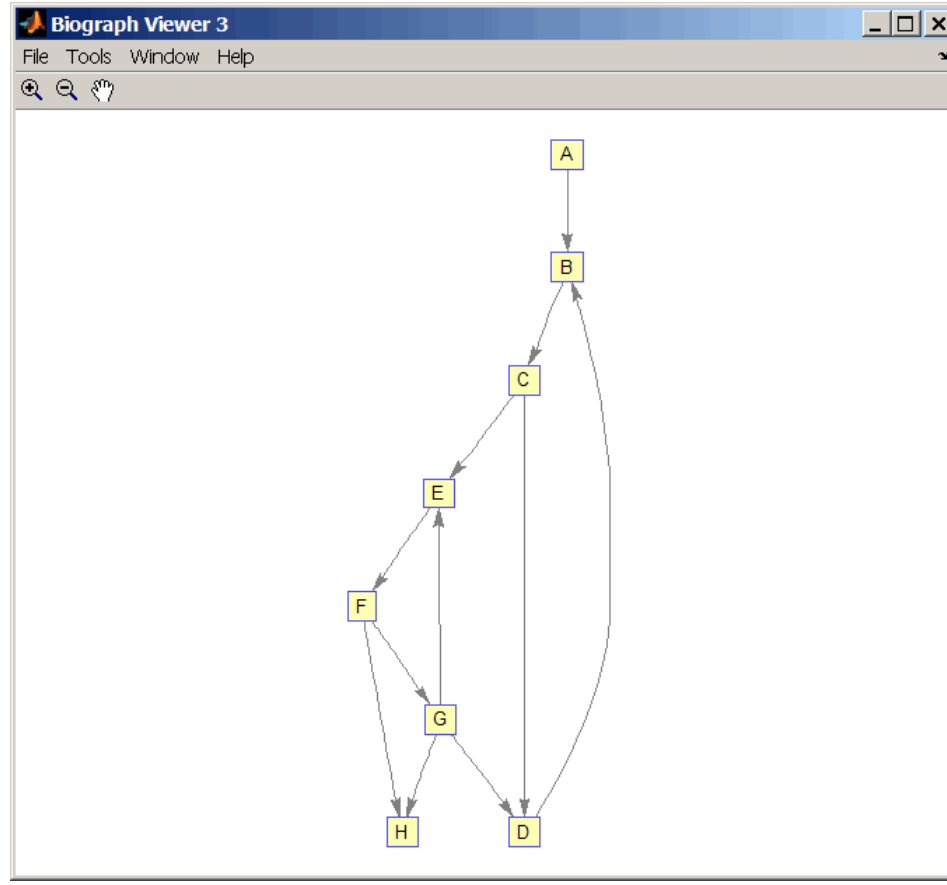
```
[F,Map] = graphisomorphism(g2,g1)
```

```
F =

     1


Map =

     7     8     2     3     6     4     1     5
```

Note that the `Map` row vector containing the node indices that map from `g2` to `g1` is the same as the permutation vector you created in step 2.

4 Reverse the direction of the D-G edge in the first graph, and then check for isomorphism again.

```
g1(m('DG'),m('GD')) = g1(m('GD'),m('DG'));
view(biograph(g1,'ABCDEFGH'))
```




```
[F,M] = graphisomorphism(g2,g1)

F =

     0


M =
```

```
     []
```

5 Convert the graphs to undirected graphs, and then check for isomorphism.

```
[F,M] = graphisomorphism(g2+g2',g1+g1','directed',false)

F =

     1


M =

     7     8     2     3     6     4     1     5
```

References

[1] Fortin, S. (1996). The Graph Isomorphism Problem. Technical Report, 96-20, Dept. of Computer Science, University of Alberta, Edomonton, Alberta, Canada.

[2] McKay, B.D. (1981). Practical Graph Isomorphism. Congressus Numerantium *30,* 45-87.

[3] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisdag`, `graphisspantree`, `graphmaxflow`, `graphminspantree`, `graphpred2path`, `graphshortestpath`, `graphtopoorder`, `graphtraverse`

Bioinformatics Toolbox methods of `biograph object`: `isomorphism`

Purpose

Determine if tree is spanning tree

Syntax

```
TF = graphisspantree(G)
```

Arguments

G	N-by-N sparse matrix whose lower triangle represents an undirected graph. Nonzero entries in matrix *G* indicate the presence of an edge.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

TF = graphisspantree(*G*) returns logical 1 (true) if *G* is a spanning tree, and logical 0 (false) otherwise. A spanning tree must touch all the nodes and must be acyclic. *G* is an N-by-N sparse matrix whose lower triangle represents an undirected graph. Nonzero entries in matrix *G* indicate the presence of an edge.

Examples

1 Create a phytree object from a phylogenetic tree file.

```
tr = phytreeread('pf00002.tree')

Phylogenetic tree object with 33 leaves (32 branches)
```

2 Create a connection matrix from the phytree object.

```
[CM,labels,dist] = getmatrix(tr);
```

3 Determine if the connection matrix is a spanning tree.

```
graphisspantree(CM)

ans =

     1
```

4 Add an edge between the root and the first leaf in the connection matrix.

```
CM(end,1) = 1;
```

5 Determine if the modified connection matrix is a spanning tree.

```
graphisspantree(CM)

ans =

     0
```

References

[1] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisdag`, `graphisomorphism`, `graphmaxflow`, `graphminspantree`, `graphpred2path`, `graphshortestpath`, `graphtopoorder`, `graphtraverse`

Bioinformatics Toolbox methods of `biograph object`: `isspantree`

Purpose

Calculate maximum flow in directed graph

Syntax

```
[MaxFlow, FlowMatrix, Cut] = graphmaxflow(G, SNode, TNode)
[...] = graphmaxflow(G, SNode, TNode, ...'Capacity',
CapacityValue, ...)
[...] = graphmaxflow(G, SNode, TNode, ...'Method', MethodValue,
    ...)
```

Arguments

G	N-by-N sparse matrix that represents a directed graph. Nonzero entries in matrix `G` represent the capacities of the edges.
SNode	Node in *G*.
TNode	Node in *G*.
CapacityValue	Column vector that specifies custom capacities for the edges in matrix *G*. It must have one entry for every nonzero value (edge) in matrix *G*. The order of the custom capacities in the vector must match the order of the nonzero values in matrix *G* when it is traversed column-wise. By default, `graphmaxflow` gets capacity information from the nonzero entries in matrix *G*.
MethodValue	String that specifies the algorithm used to find the minimal spanning tree (MST). Choices are: • `'Edmonds'` — Uses the Edmonds and Karp algorithm, the implementation of which is based on a variation called the *labeling algorithm*. Time complexity is `O(N*E^2)`, where `N` and `E` are the number of nodes and edges respectively. • `'Goldberg'` — Default algorithm. Uses the Goldberg algorithm, which uses the generic method known as *preflow-push*. Time complexity is `O(N^2*sqrt(E))`, where `N` and `E` are the number of nodes and edges respectively.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

`[MaxFlow, FlowMatrix, Cut] = graphmaxflow(G, SNode, TNode)` calculates the maximum flow of directed graph `G` from node `SNode` to node `TNode`. Input `G` is an N-by-N sparse matrix that represents a directed graph. Nonzero entries in matrix `G` represent the capacities of the edges. Output `MaxFlow` is the maximum flow, and `FlowMatrix` is a sparse matrix with all the flow values for every edge. `FlowMatrix(X,Y)` is the flow from node `X` to node `Y`. Output `Cut` is a logical row vector indicating the nodes connected to `SNode` after calculating the minimum cut between `SNode` and `TNode`. If several solutions to the minimum cut problem exist, then `Cut` is a matrix.

Tip The algorithm that determines `Cut`, all minimum cuts, has a time complexity of `O(2^N)`, where N is the number of nodes. If this information is not needed, use the `graphmaxflow` function without the third output.

`[...] = graphmaxflow(G, SNode, TNode, ...'PropertyName', PropertyValue, ...)` calls `graphmaxflow` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[...] = graphmaxflow(G, SNode, TNode, ...'Capacity', CapacityValue, ...)` lets you specify custom capacities for the edges. `CapacityValue` is a column vector having one entry for every nonzero value (edge) in matrix `G`. The order of the custom capacities in the vector must match the order of the nonzero values in matrix `G` when it is traversed column-wise. By default, `graphmaxflow` gets capacity information from the nonzero entries in matrix `G`.

`[...] = graphmaxflow(G, SNode, TNode, ...'Method', MethodValue, ...)` lets you specify the algorithm used to find the minimal spanning tree (MST). Choices are:

- `'Edmonds'` — Uses the Edmonds and Karp algorithm, the implementation of which is based on a variation called the *labeling algorithm*. Time complexity is `O(N*E^2)`, where `N` and `E` are the number of nodes and edges respectively.
- `'Goldberg'` — Default algorithm. Uses the Goldberg algorithm, which uses the generic method known as *preflow-push*. Time complexity is `O(N^2*sqrt(E))`, where `N` and `E` are the number of nodes and edges respectively.

Examples

1 Create a directed graph with six nodes and eight edges.

```
cm = sparse([1 1 2 2 3 3 4 5],[2 3 4 5 4 5 6 6],...
     [2 3 3 1 1 1 2 3],6,6)cm =

   (1,2)        2
   (1,3)        3
   (2,4)        3
   (3,4)        1
   (2,5)        1
   (3,5)        1
   (4,6)        2
   (5,6)        3
```

2 Calculate the maximum flow in the graph from node 1 to node 6.

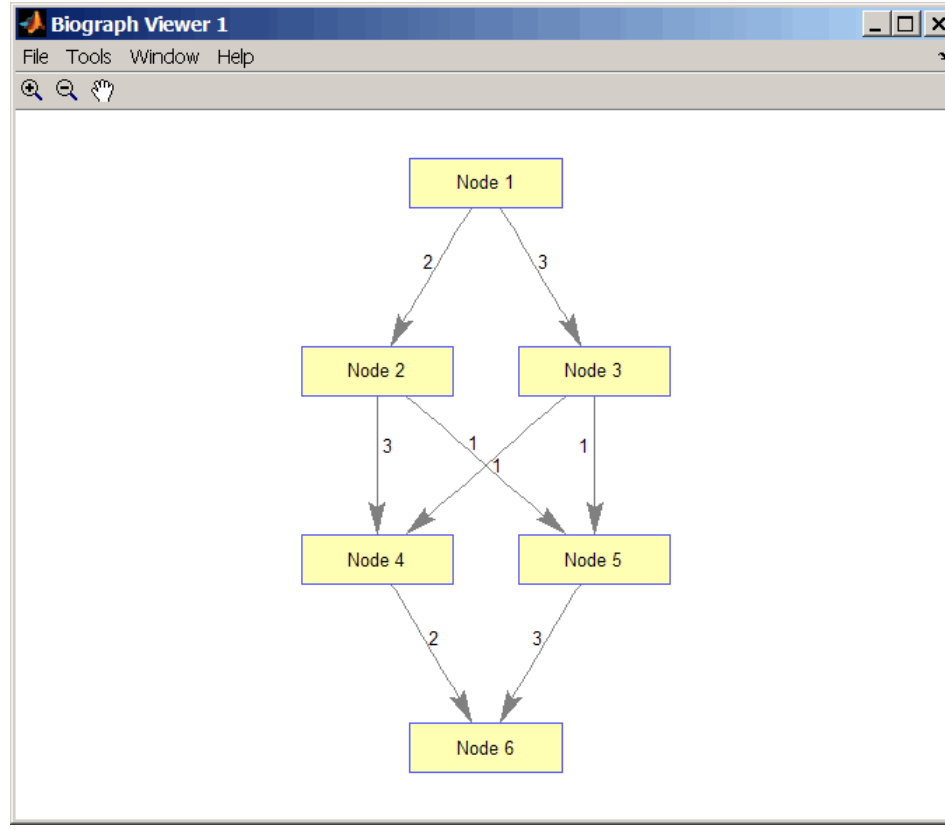
```
[M,F,K] = graphmaxflow(cm,1,6)

M =

     4


F =
```

```
    (1,2)        2
    (1,3)        2
    (2,4)        1
    (3,4)        1
    (2,5)        1
    (3,5)        1
    (4,6)        2
    (5,6)        2


K =

     1     1     1     1     0     0
     1     0     1     0     0     0
```

Notice that `K` is a two-row matrix because there are two possible solutions to the minimum cut problem.

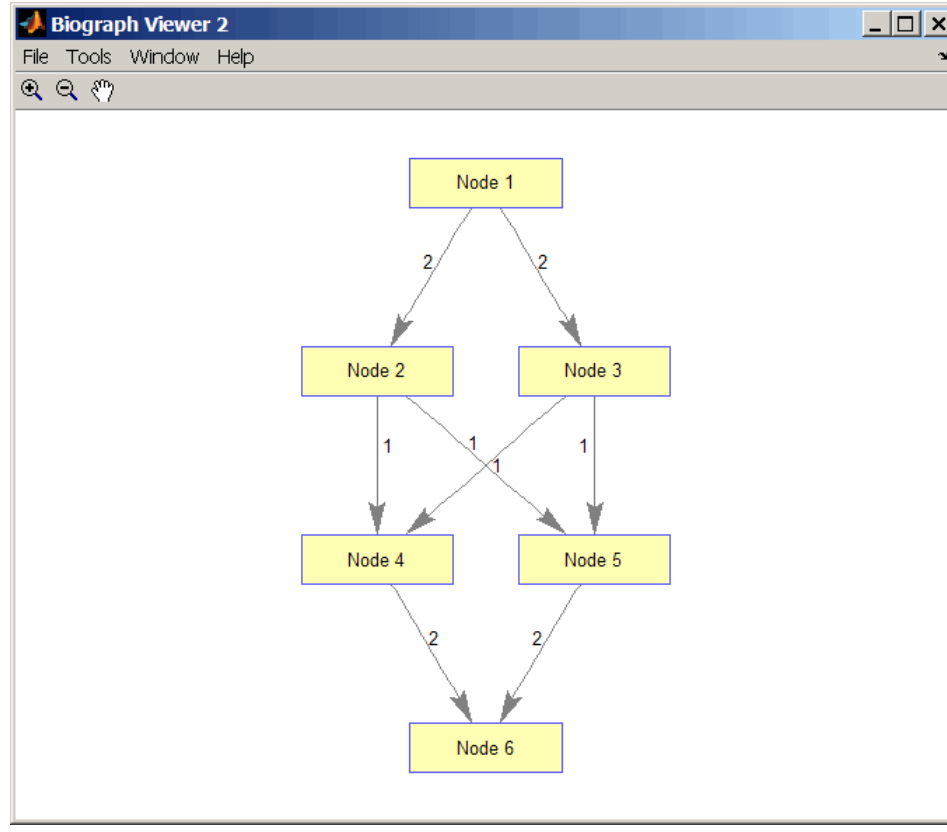
3 View the graph with the original capacities.

```
h = view(biograph(cm,[],'ShowWeights','on'))
```



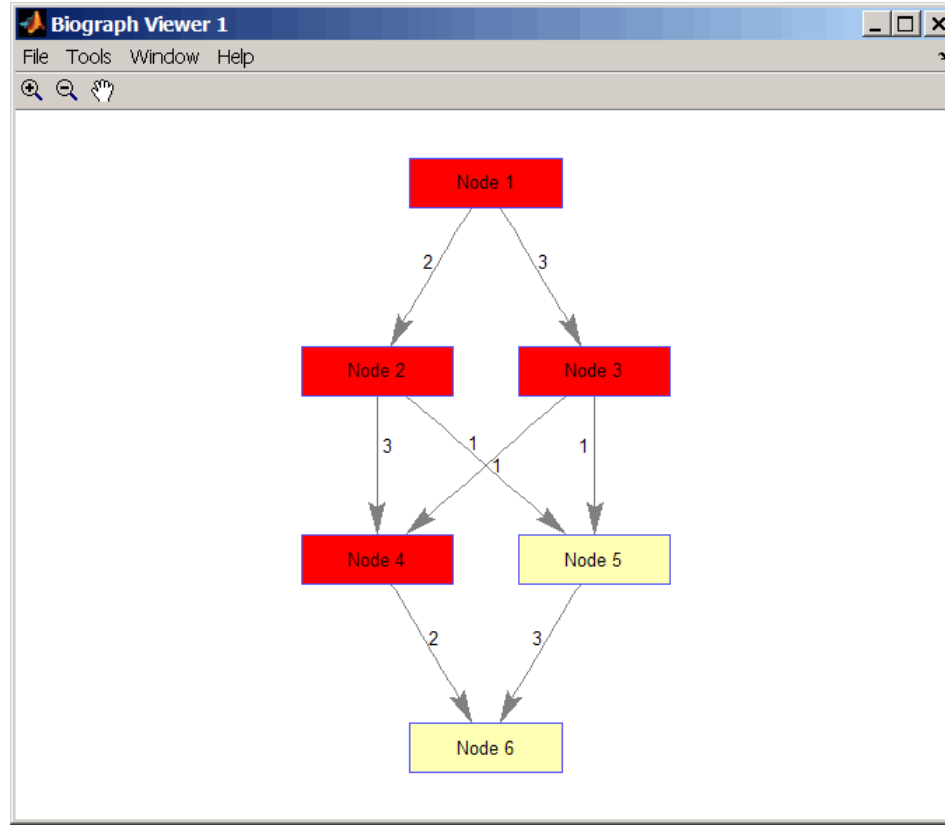
4 View the graph with the calculated maximum flows.

```
view(biograph(F,[],'ShowWeights','on'))
```



5 Show one solution to the minimum cut problem in the original graph.

```
set(h.Nodes(K(1,:)),'Color',[1 0 0])
```



Notice that in the three edges that connect the source nodes (red) to the destination nodes (yellow), the original capacities and the calculated maximum flows are the same.

References

[1] Edmonds, J. and Karp, R.M. (1972). Theoretical improvements in the algorithmic efficiency for network flow problems. Journal of the ACM *19*, 248-264.

[2] Goldberg, A.V. (1985). A New Max-Flow Algorithm. MIT Technical Report MIT/LCS/TM-291, Laboratory for Computer Science, MIT.

[3] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisdag`, `graphisomorphism`, `graphisspantree`, `graphminspantree`, `graphpred2path`, `graphshortestpath`, `graphtopoorder`, `graphtraverse`

Bioinformatics Toolbox method of `biograph object`: `maxflow`

Purpose

Find minimal spanning tree in graph

Syntax

```
[Tree, pred] = graphminspantree(G)
[Tree, pred] = graphminspantree(G, R)
[Tree, pred] = graphminspantree(..., 'Method', MethodValue, ...)
[Tree, pred] = graphminspantree(..., 'Weights', WeightsValue,
    ...)
```

Arguments

G	N-by-N sparse matrix that represents an undirected graph. Nonzero entries in matrix *G* represent the weights of the edges.
R	Scalar between 1 and the number of nodes.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

`[Tree, pred] = graphminspantree(G)` finds an acyclic subset of edges that connects all the nodes in the undirected graph *G* and for which the total weight is minimized. Weights of the edges are all nonzero entries in the lower triangle of the N-by-N sparse matrix *G*. Output *Tree* is a spanning tree represented by a sparse matrix. Output *pred* is a vector containing the predecessor nodes of the minimal spanning tree (MST), with the root node indicated by `0`. The root node defaults to the first node in the largest connected component. This computation requires an extra call to the `graphconncomp` function.

`[Tree, pred] = graphminspantree(G, R)` sets the root of the minimal spanning tree to node `R`.

`[Tree, pred] = graphminspantree(..., 'PropertyName', PropertyValue, ...)` calls `graphminspantree` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes

and is case insensitive. These property name/property value pairs are as follows:

`[Tree, pred] = graphminspantree(..., 'Method', MethodValue, ...)` lets you specify the algorithm used to find the minimal spanning tree (MST). Choices are:

- `'Kruskal'` — Grows the minimal spanning tree (MST) one edge at a time by finding an edge that connects two trees in a spreading forest of growing MSTs. Time complexity is `O(E+X*log(N))`, where `X` is the number of edges no longer than the longest edge in the MST, and `N` and `E` are the number of nodes and edges respectively.
- `'Prim'` — Default algorithm. Grows the minimal spanning tree (MST) one edge at a time by adding a minimal edge that connects a node in the growing MST with any other node. Time complexity is `O(E*log(N))`, where `N` and `E` are the number of nodes and edges respectively.

Note When the graph is unconnected, Prim's algorithm returns only the tree that contains R, while Kruskal's algorithm returns an MST for every component.

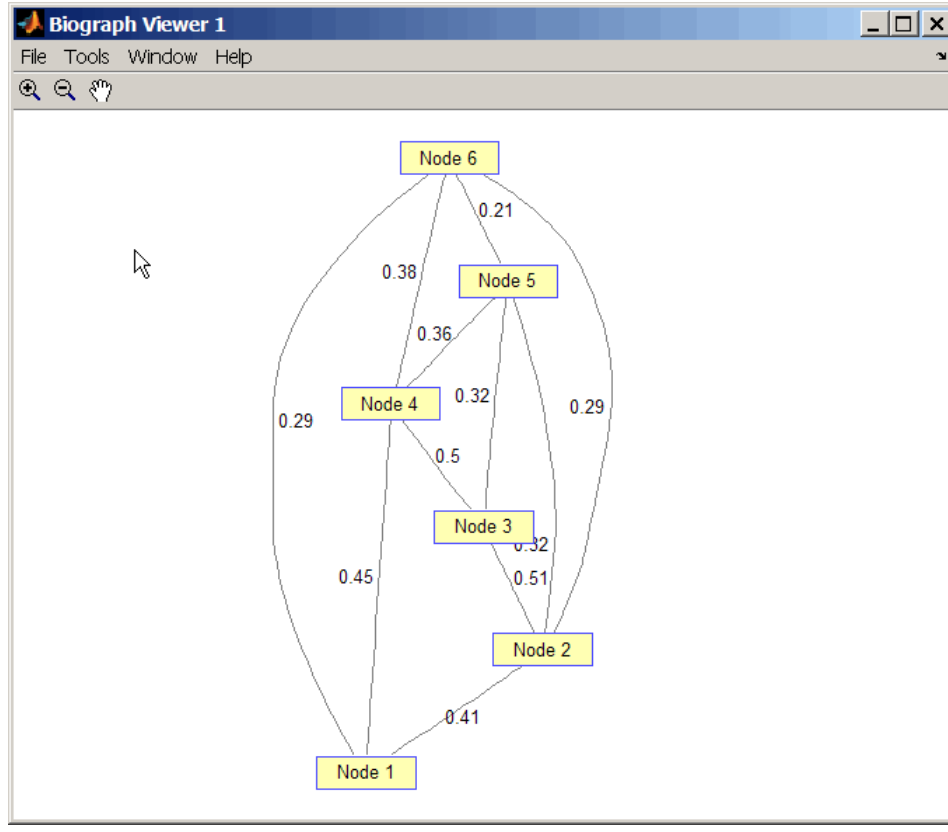
`[Tree, pred] = graphminspantree(..., 'Weights', WeightsValue, ...)` lets you specify custom weights for the edges. *`WeightsValue`* is a column vector having one entry for every nonzero value (edge) in matrix *`G`*. The order of the custom weights in the vector must match the order of the nonzero values in matrix *`G`* when it is traversed column-wise. By default, `graphminspantree` gets weight information from the nonzero entries in matrix *`G`*.

Examples

1 Create and view an undirected graph with 6 nodes and 11 edges.

```
W = [.41 .29 .51 .32 .50 .45 .38 .32 .36 .29 .21];
DG = sparse([1 1 2 2 3 4 4 5 5 6 6],[2 6 3 5 4 1 6 3 4 2 5],W);
```

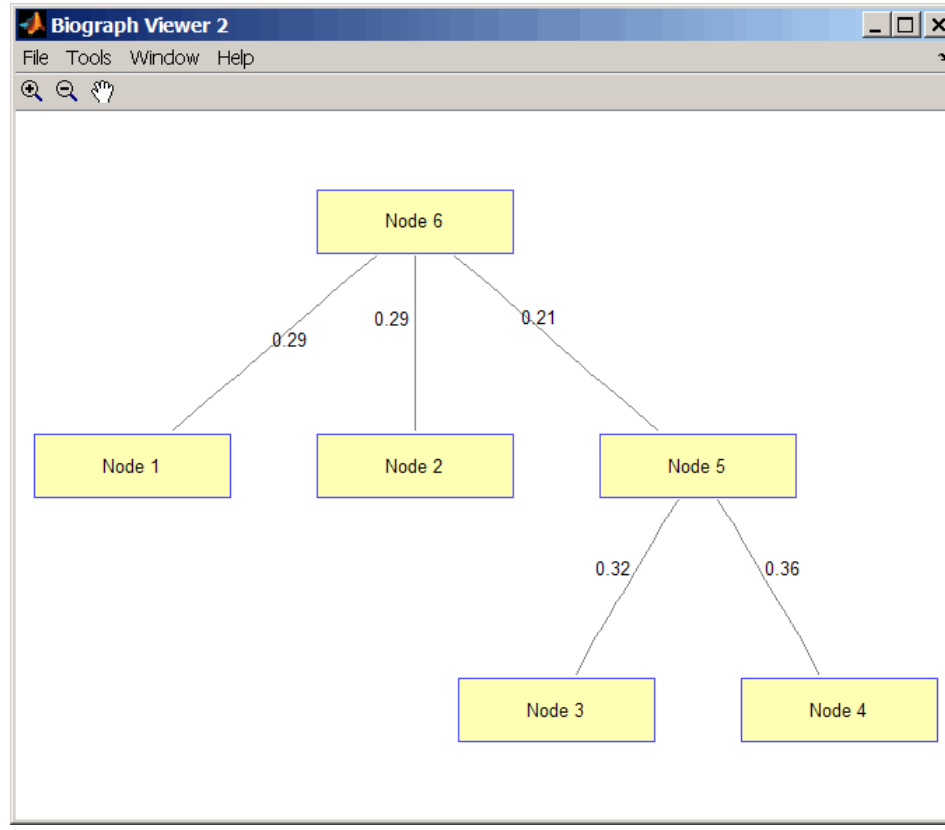
```
UG = tril(DG + DG')
UG =

   (2,1)       0.4100
   (4,1)       0.4500
   (6,1)       0.2900
   (3,2)       0.5100
   (5,2)       0.3200
   (6,2)       0.2900
   (4,3)       0.5000
   (5,3)       0.3200
   (5,4)       0.3600
   (6,4)       0.3800
   (6,5)       0.2100

view(biograph(UG,[],'ShowArrows','off','ShowWeights','on'))
```



2 Find and view the minimal spanning tree of the undirected graph.

```
[ST,pred] = graphminspantree(UG)

ST =

   (6,1)        0.2900
   (6,2)        0.2900
   (5,3)        0.3200
   (5,4)        0.3600
```

```
    (6,5)        0.2100

pred =

     0     6     5     5     6     1

view(biograph(ST,[],'ShowArrows','off','ShowWeights','on'))
```



References

[1] Kruskal, J.B. (1956). On the Shortest Spanning Subtree of a Graph and the Traveling Salesman Problem. Proceedings of the American Mathematical Society *7*, 48-50.

[2] Prim, R. (1957). Shortest Connection Networks and Some Generalizations. Bell System Technical Journal *36*, 1389-1401.

[3] Siek, J.G. Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisdag`, `graphisomorphism`, `graphisspantree`, `graphmaxflow`, `graphpred2path`, `graphshortestpath`, `graphtopoorder`, `graphtraverse`

Bioinformatics Toolbox method of `biograph object`: `minspantree`

Purpose

Convert predecessor indices to paths

Syntax

```
path = graphpred2path(pred, D)
```

Arguments

pred	Row vector or matrix of predecessor node indices. The value of the root (or source) node in *pred* must be 0.
D	Destination node in *pred*.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

path = graphpred2path(*pred*, *D*) traces back a path by following the predecessor list in *pred* starting at destination node *D*.

The value of the root (or source) node in *pred* must be 0. If a NaN is found when following the predecessor nodes, graphpred2path returns an empty path.

If *pred* is a ...	And *D* is a ...	Then *path* is a ...
row vector of predecessor node indices	scalar	row vector listing the nodes from the root (or source) to *D*.
	row vector	row cell array with every column containing the path to the destination for every element in *D*.

If *pred* is a ...	And *D* is a ...	Then *path* is a ...
matrix	scalar	column cell array with every row containing the path for every row in *pred*.
	row vector	matrix cell array with every row containing the paths for the respective row in *pred*, and every column containing the paths to the respective destination in *D*.

Note If *D* is omitted, the paths to all the destinations are calculated for every predecessor listed in *pred*.

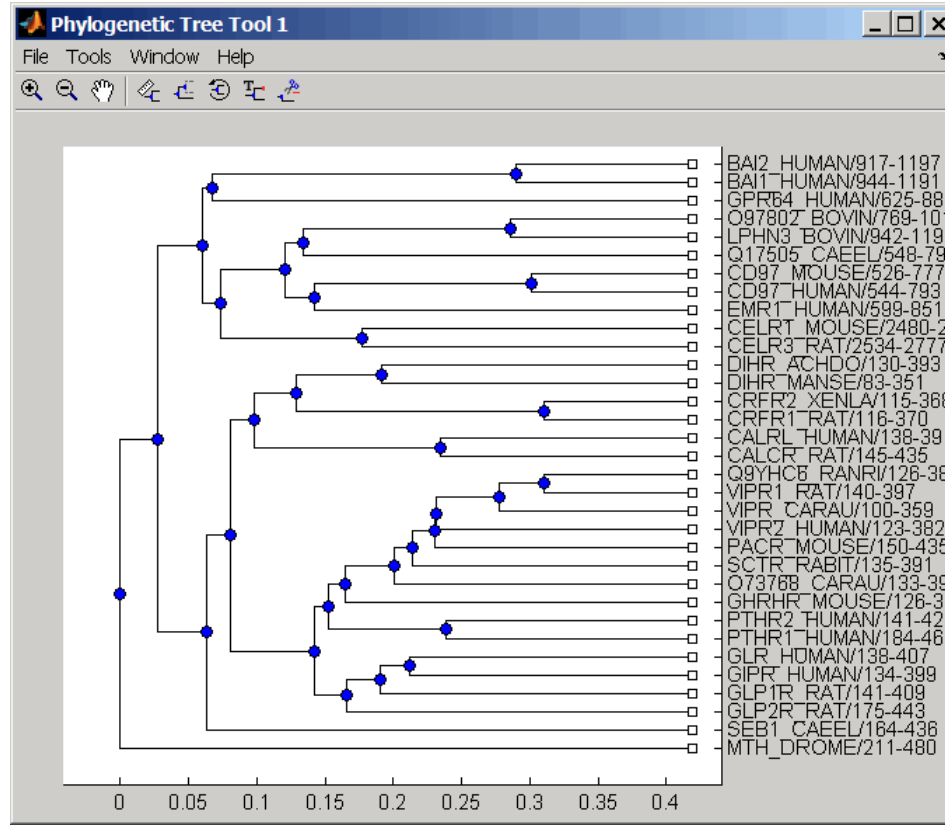
Examples

1 Create a phytree object from the phylogenetic tree file for the GLR_HUMAN protein.

```
tr = phytreeread('pf00002.tree')
    Phylogenetic tree object with 33 leaves (32 branches)
```

2 View the phytree object.

```
view(tr)
```



3 From the phytree object, create a connection matrix to represent the phylogenetic tree.

```
[CM,labels,dist] = getmatrix(tr);
```

4 Find the nodes from the root to one leaf in the phylogenetic tree created from the phylogenetic tree file for the GLR_HUMAN protein.

```
root_loc = size(CM,1)

root_loc =
```

```
    65

glr_loc = strmatch('GLR',labels)

glr_loc =

    28

[T,PRED]=graphminspantree(CM,root_loc);
PATH = graphpred2path(PRED,glr_loc)

PATH =

    65    64    53    52    46    45    44    43    28
```

References

[1] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisdag`, `graphisomorphism`, `graphisspantree`, `graphmaxflow`, `graphminspantree`, `graphshortestpath`, `graphtopoorder`, `graphtraverse`

Purpose

Solve shortest path problem in graph

Syntax

```
[dist, path, pred] = graphshortestpath(G, S)
[dist, path, pred] = graphshortestpath(G, S, T)
[...] = graphshortestpath(..., 'Directed', DirectedValue, ...)
[...] = graphshortestpath(..., 'Method', MethodValue, ...)
[...] = graphshortestpath(..., 'Weights', WeightsValue, ...)
```

Arguments

G	N-by-N sparse matrix that represents a graph. Nonzero entries in matrix *G* represent the weights of the edges.
S	Node in *G*.
T	Node in *G*.
DirectedValue	Property that indicates whether the graph is directed or undirected. Enter `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.
MethodValue	String that specifies the algorithm used to find the shortest path. Choices are: • `'Bellman-Ford'` — Assumes weights of the edges to be nonzero entries in sparse matrix `G`. Time complexity is `O(N*E)`, where `N` and `E` are the number of nodes and edges respectively. • `'BFS'` — Breadth-first search. Assumes all weights to be equal, and nonzero entries in sparse matrix `G` to represent edges. Time complexity is `O(N+E)`, where `N` and `E` are the number of nodes and edges respectively. • `'Acyclic'` — Assumes `G` to be a directed acyclic graph and that weights of the edges are nonzero entries in sparse matrix `G`. Time complexity is `O(N+E)`, where `N` and `E` are the number of nodes and edges respectively.

- `'Dijkstra'` — Default algorithm. Assumes weights of the edges to be positive values in sparse matrix `G`. Time complexity is `O(log(N)*E)`, where `N` and `E` are the number of nodes and edges respectively.

`WeightsValue` Column vector that specifies custom weights for the edges in matrix *`G`*. It must have one entry for every nonzero value (edge) in matrix *`G`*. The order of the custom weights in the vector must match the order of the nonzero values in matrix *`G`* when it is traversed column-wise. This property lets you use zero-valued weights. By default, `graphshortestpaths` gets weight information from the nonzero entries in matrix *`G`*.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

`[`*`dist`*`,` *`path`*`,` *`pred`*`] = graphshortestpath(`*`G`*`,` *`S`*`)` determines the single-source shortest paths from node *`S`* to all other nodes in the graph represented by matrix *`G`*. Input *`G`* is an N-by-N sparse matrix that represents a graph. Nonzero entries in matrix *`G`* represent the weights of the edges. *`dist`* are the `N` distances from the source to every node (using `Inf`s for nonreachable nodes and `0` for the source node). *`path`* contains the winning paths to every node. *`pred`* contains the predecessor nodes of the winning paths.

`[`*`dist`*`,` *`path`*`,` *`pred`*`] = graphshortestpath(`*`G`*`,` *`S`*`,` *`T`*`)` determines the single source-single destination shortest path from node *`S`* to node *`T`*.

`[...] = graphshortestpath(..., '`*`PropertyName`*`',` *`PropertyValue`*`, ...)` calls `graphshortestpath` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must

be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[...] = graphshortestpath(..., 'Directed', DirectedValue, ...)` indicates whether the graph is directed or undirected. Set *`DirectedValue`* to `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.

`[...] = graphshortestpath(..., 'Method', MethodValue, ...)` lets you specify the algorithm used to find the shortest path. Choices are:

- `'Bellman-Ford'` — Assumes weights of the edges to be nonzero entries in sparse matrix `G`. Time complexity is `O(N*E)`, where `N` and `E` are the number of nodes and edges respectively.
- `'BFS'` — Breadth-first search. Assumes all weights to be equal, and nonzero entries in sparse matrix `G` to represent edges. Time complexity is `O(N+E)`, where `N` and `E` are the number of nodes and edges respectively.
- `'Acyclic'` — Assumes `G` to be a directed acyclic graph and that weights of the edges are nonzero entries in sparse matrix `G`. Time complexity is `O(N+E)`, where `N` and `E` are the number of nodes and edges respectively.
- `'Dijkstra'` — Default algorithm. Assumes weights of the edges to be positive values in sparse matrix `G`. Time complexity is `O(log(N)*E)`, where `N` and `E` are the number of nodes and edges respectively.

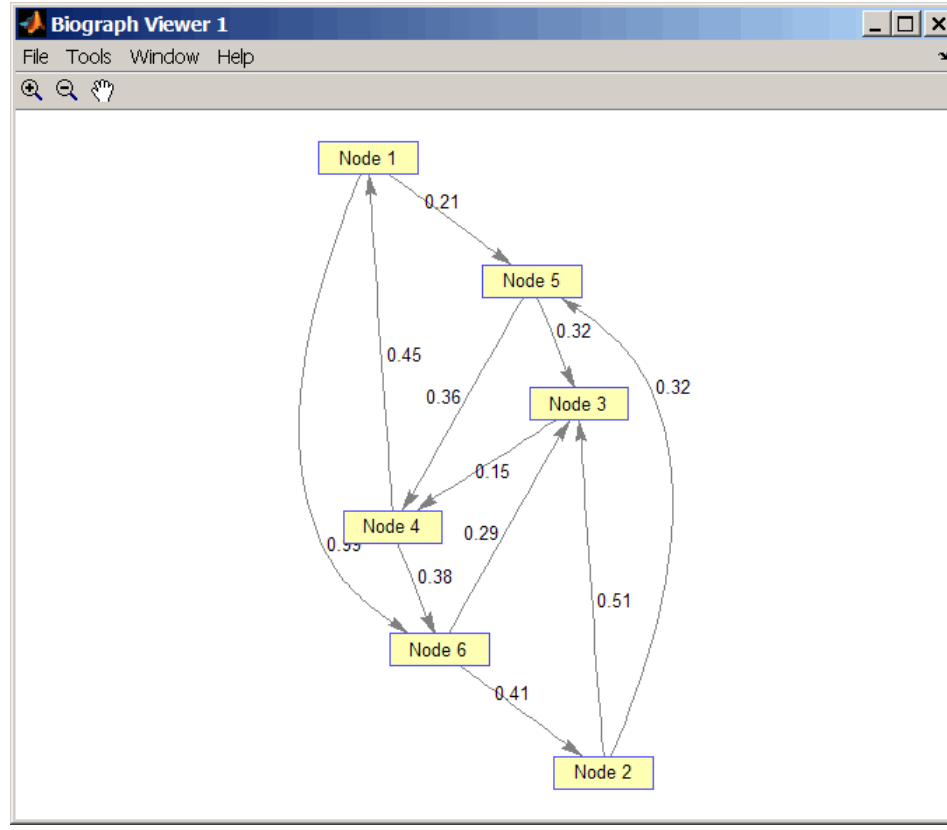
`[...] = graphshortestpath(..., 'Weights', WeightsValue, ...)` lets you specify custom weights for the edges. *`WeightsValue`* is a column vector having one entry for every nonzero value (edge) in matrix *`G`*. The order of the custom weights in the vector must match the order of the nonzero values in matrix *`G`* when it is traversed column-wise. This property lets you use zero-valued weights. By default, `graphshortestpath` gets weight information from the nonzero entries in matrix *`G`*.

Examples

Finding the Shortest Path in a Directed Graph

1 Create and view a directed graph with 6 nodes and 11 edges.

```
W = [.41 .99 .51 .32 .15 .45 .38 .32 .36 .29 .21];
DG = sparse([6 1 2 2 3 4 4 5 5 6 1],[2 6 3 5 4 1 6 3 4 3 5],W)

DG =

   (4,1)       0.4500
   (6,2)       0.4100
   (2,3)       0.5100
   (5,3)       0.3200
   (6,3)       0.2900
   (3,4)       0.1500
   (5,4)       0.3600
   (1,5)       0.2100
   (2,5)       0.3200
   (1,6)       0.9900
   (4,6)       0.3800

h = view(biograph(DG,[],'ShowWeights','on'))
Biograph object with 6 nodes and 11 edges.
```



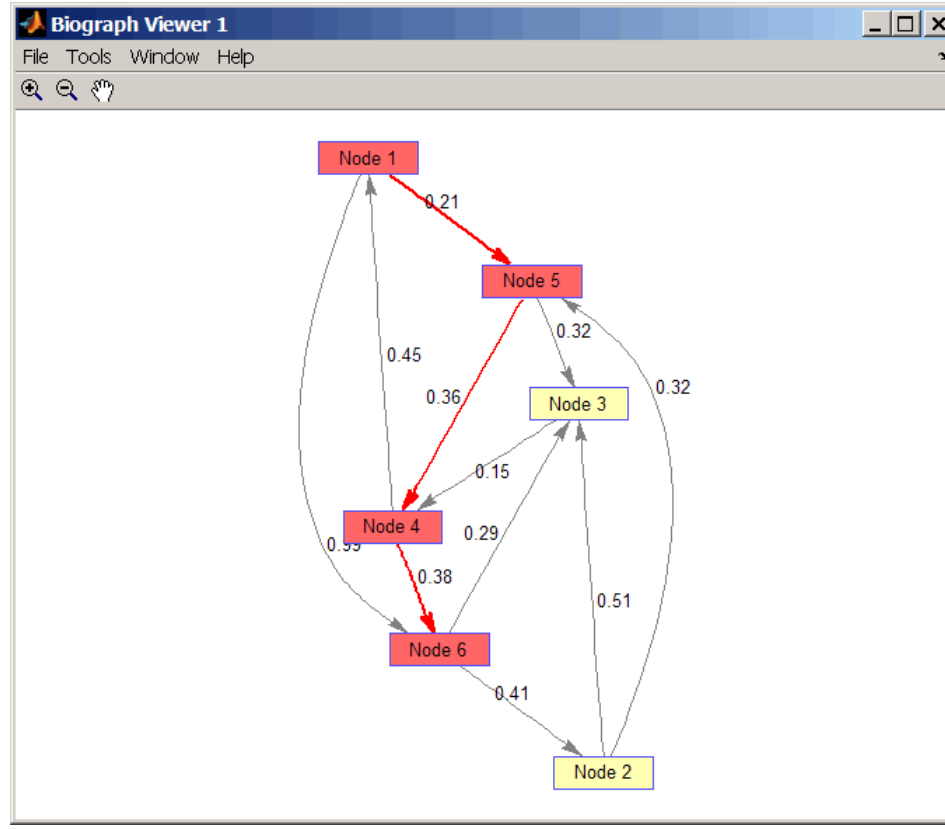
2 Find the shortest path in the graph from node 1 to node 6.

```
[dist,path,pred] = graphshortestpath(DG,1,6)

dist =

    0.9500


path =
```

```
     1     5     4     6


pred =

     0     6     5     5     1     4
```

3 Mark the nodes and edges of the shortest path by coloring them red and increasing the line width.

```
set(h.Nodes(path),'Color',[1 0.4 0.4])
edges = getedgesbynodeid(h,get(h.Nodes(path),'ID'));
set(edges,'LineColor',[1 0 0])
set(edges,'LineWidth',1.5)
```

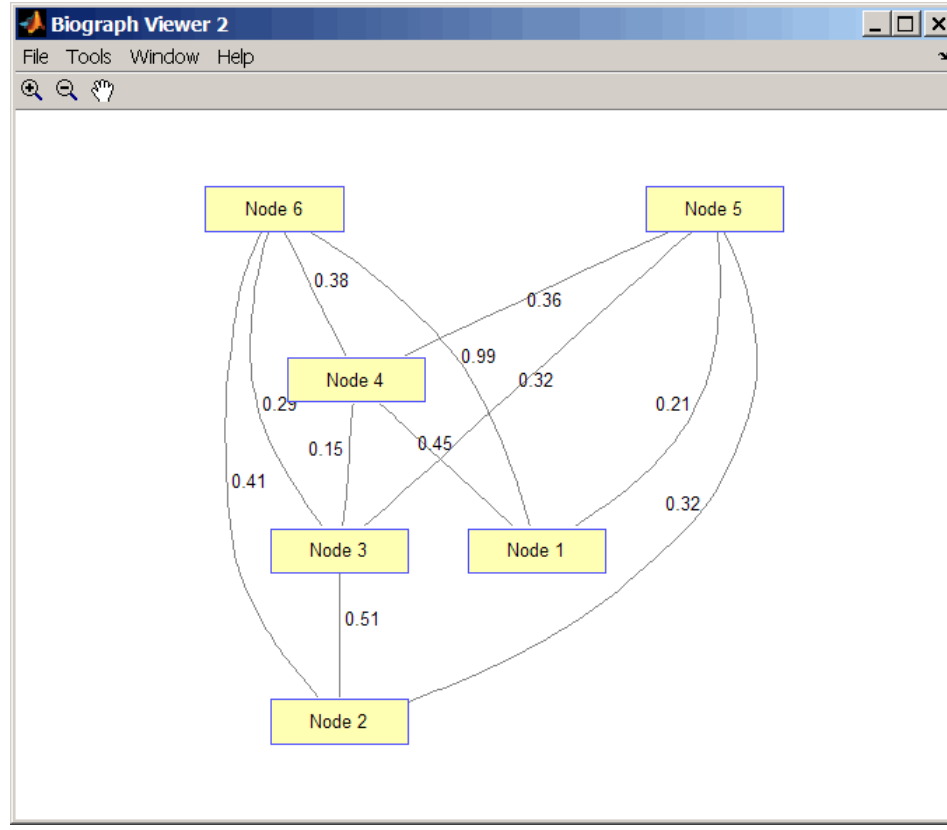


Finding the Shortest Path in an Undirected Graph

1 Create and view an undirected graph with 6 nodes and 11 edges.

```
UG = tril(DG + DG')

UG =

   (4,1)        0.4500
   (5,1)        0.2100
```

```
   (6,1)       0.9900
   (3,2)       0.5100
   (5,2)       0.3200
   (6,2)       0.4100
   (4,3)       0.1500
   (5,3)       0.3200
   (6,3)       0.2900
   (5,4)       0.3600
   (6,4)       0.3800

h = view(biograph(UG,[],'ShowArrows','off','ShowWeights','on'))
Biograph object with 6 nodes and 11 edges.
```



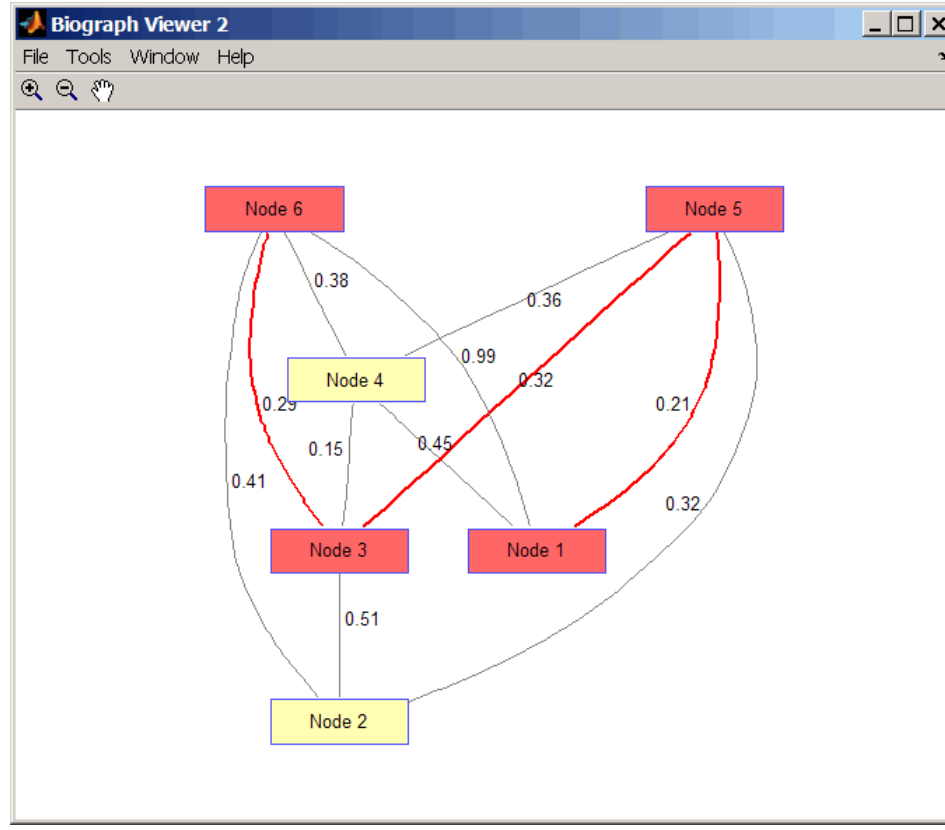
2 Find the shortest path in the graph from node 1 to node 6.

```
[dist,path,pred] = graphshortestpath(UG,1,6,'directed',false)

dist =

    0.8200


path =
```

```
     1     5     3     6


pred =

     0     5     5     1     1     3
```

3 Mark the nodes and edges of the shortest path by coloring them red and increasing the line width.

```
set(h.Nodes(path),'Color',[1 0.4 0.4])
 fowEdges = getedgesbynodeid(h,get(h.Nodes(path),'ID'));
 revEdges = getedgesbynodeid(h,get(h.Nodes(fliplr(path)),'ID'));
 edges = [fowEdges;revEdges];
 set(edges,'LineColor',[1 0 0])
 set(edges,'LineWidth',1.5)
```



References

[1] Dijkstra, E.W. (1959). A note on two problems in connexion with graphs. Numerische Mathematik *1*, 269-271.

[2] Bellman, R. (1958). On a Routing Problem. Quarterly of Applied Mathematics *16(1)*, 87-90.

[3] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisdag`, `graphisomorphism`, `graphisspantree`, `graphmaxflow`, `graphminspantree`, `graphpred2path`, `graphtopoorder`, `graphtraverse`

Bioinformatics Toolbox method of `biograph object`: `shortestpath`

Purpose

Perform topological sort of directed acyclic graph

Syntax

```
order = graphtopoorder(G)
```

Arguments

G	N-by-N sparse matrix that represents a directed acyclic graph. Nonzero entries in matrix *G* indicate the presence of an edge.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

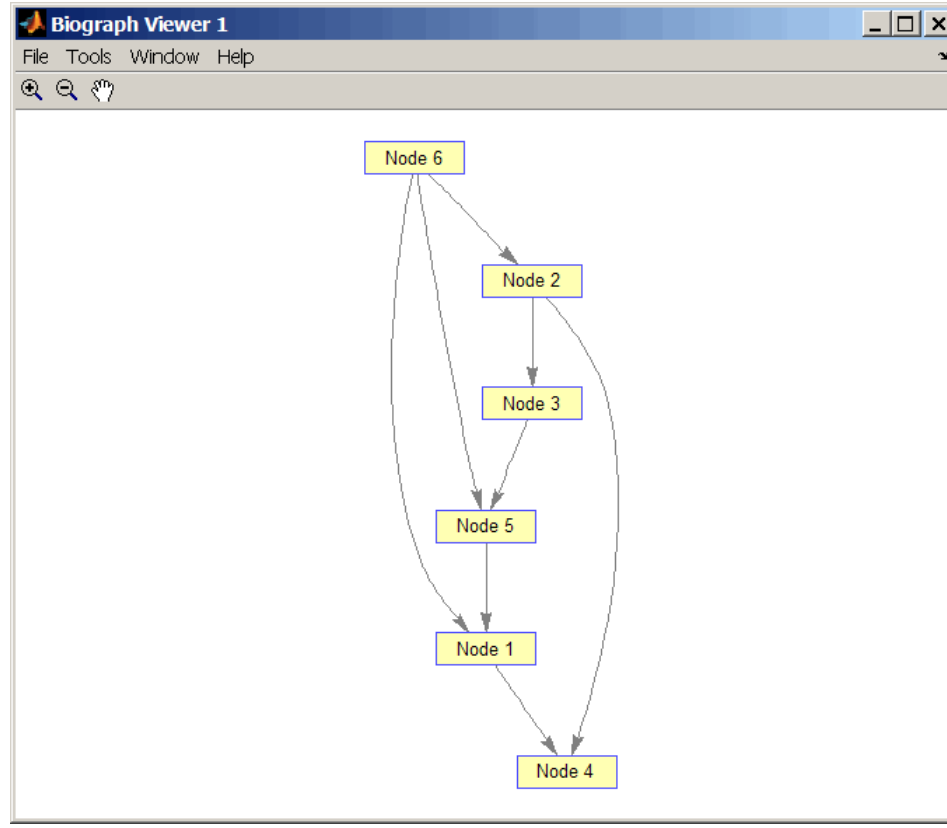
order = graphtopoorder(*G*) returns an index vector with the order of the nodes sorted topologically. In topological order, an edge can exist between a source node u and a destination node v, if and only if u appears before v in the vector *order*. *G* is an N-by-N sparse matrix that represents a directed acyclic graph (DAG). Nonzero entries in matrix *G* indicate the presence of an edge.

Examples

1 Create and view a directed acyclic graph (DAG) with six nodes and eight edges.

```
DG = sparse([6 6 6 2 2 3 5 1],[2 5 1 3 4 5 1 4],true,6,6)

DG =

   (5,1)        1
   (6,1)        1
   (6,2)        1
   (2,3)        1
   (1,4)        1
   (2,4)        1
   (3,5)        1
   (6,5)        1
```

```
view(biograph(DG))
```

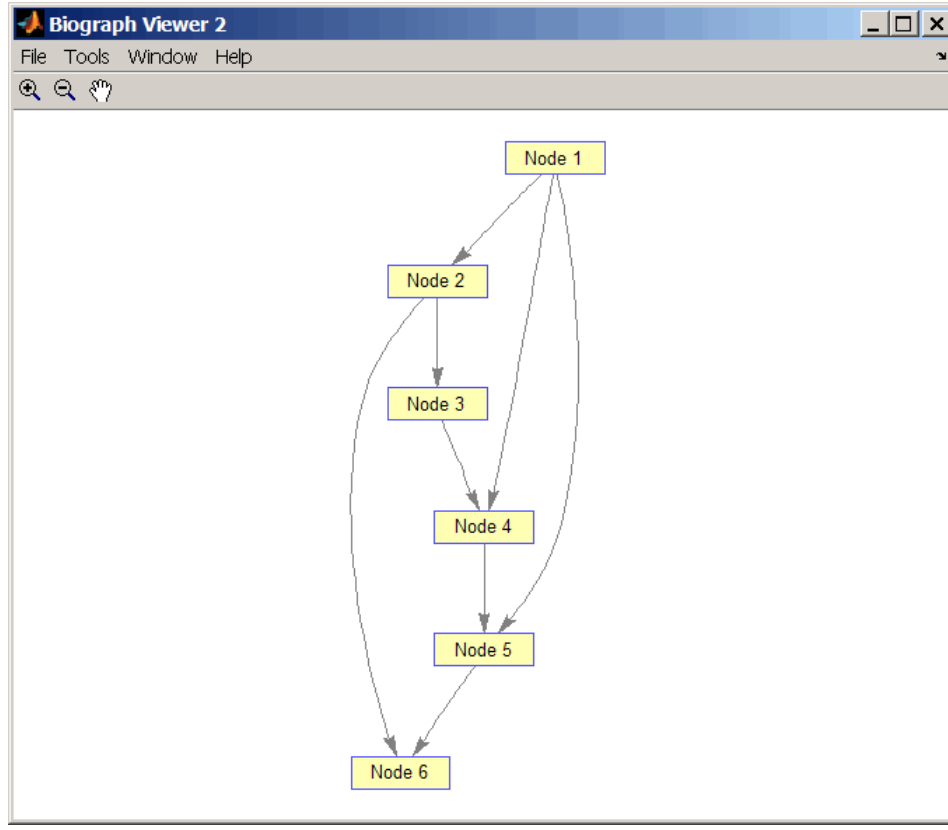


2 Find the topological order of the DAG.

```
order = graphtopoorder(DG)

order =

     6     2     3     5     1     4
```

3 Permute the nodes so that they appear ordered in the graph display.

```
DG = DG(order,order)

DG =

   (1,2)        1
   (2,3)        1
   (1,4)        1
   (3,4)        1
   (1,5)        1
   (4,5)        1
   (2,6)        1
   (5,6)        1

view(biograph(DG))
```



References

[1] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisdag`, `graphisomorphism`, `graphisspantree`, `graphmaxflow`, `graphminspantree`, `graphpred2path`, `graphshortestpath`, `graphtraverse`

Bioinformatics Toolbox method of `biograph object`: `topoorder`

Purpose

Traverse graph by following adjacent nodes

Syntax

```
[disc, pred, closed] = graphtraverse(G, S)
[...] = graphtraverse(G, S, ...'Depth', DepthValue, ...)
[...] = graphtraverse(G, S, ...'Directed', DirectedValue, ...)
[...] = graphtraverse(G, S, ...'Method', MethodValue, ...)
```

Arguments

G	N-by-N sparse matrix that represents a directed graph. Nonzero entries in matrix *G* indicate the presence of an edge.
S	Integer that indicates the source node in graph *G*.
DepthValue	Integer that indicates a node in graph *G* that specifies the depth of the search. Default is `Inf` (infinity).
DirectedValue	Property that indicates whether graph *G* is directed or undirected. Enter `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.
MethodValue	String that specifies the algorithm used to traverse the graph. Choices are: • `'BFS'` — Breadth-first search. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively. • `'DFS'` — Default algorithm. Depth-first search. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

`[disc, pred, closed] = graphtraverse(G, S)` traverses graph `G` starting from the node indicated by integer `S`. *`G`* is an N-by-N sparse matrix that represents a directed graph. Nonzero entries in matrix *`G`* indicate the presence of an edge. *`disc`* is a vector of node indices in the order in which they are discovered. *`pred`* is a vector of predecessor node indices (listed in the order of the node indices) of the resulting spanning tree. *`closed`* is a vector of node indices in the order in which they are closed.

`[...] = graphtraverse(G, S, ...'PropertyName', PropertyValue, ...)` calls `graphtraverse` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[...] = graphtraverse(G, S, ...'Depth', DepthValue, ...)` specifies the depth of the search. *`DepthValue`* is an integer indicating a node in graph *`G`*. Default is `Inf` (infinity).

`[...] = graphtraverse(G, S, ...'Directed', DirectedValue, ...)` indicates whether the graph is directed or undirected. Set *`DirectedValue`* to `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.

`[...] = graphtraverse(G, S, ...'Method', MethodValue, ...)` lets you specify the algorithm used to traverse the graph. Choices are:

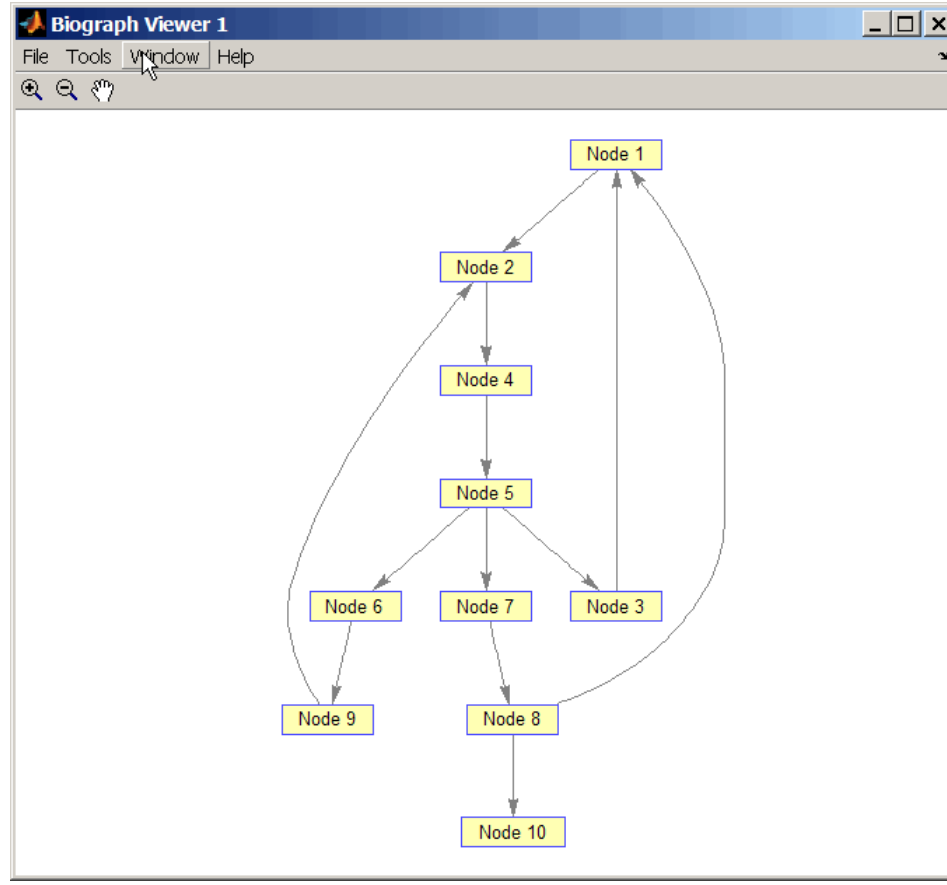
- `'BFS'` — Breadth-first search. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.
- `'DFS'` — Default algorithm. Depth-first search. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.

Examples

1 Create a directed graph with 10 nodes and 12 edges.

```
DG = sparse([1 2 3 4 5 5 5 6 7 8 8 9],...
                [2 4 1 5 3 6 7 9 8 1 10 2],true,10,10)
```

```
DG =

   (3,1)        1
   (8,1)        1
   (1,2)        1
   (9,2)        1
   (5,3)        1
   (2,4)        1
   (4,5)        1
   (5,6)        1
   (5,7)        1
   (7,8)        1
   (6,9)        1
   (8,10)       1

h = view(biograph(DG))
Biograph object with 10 nodes and 12 edges.
```

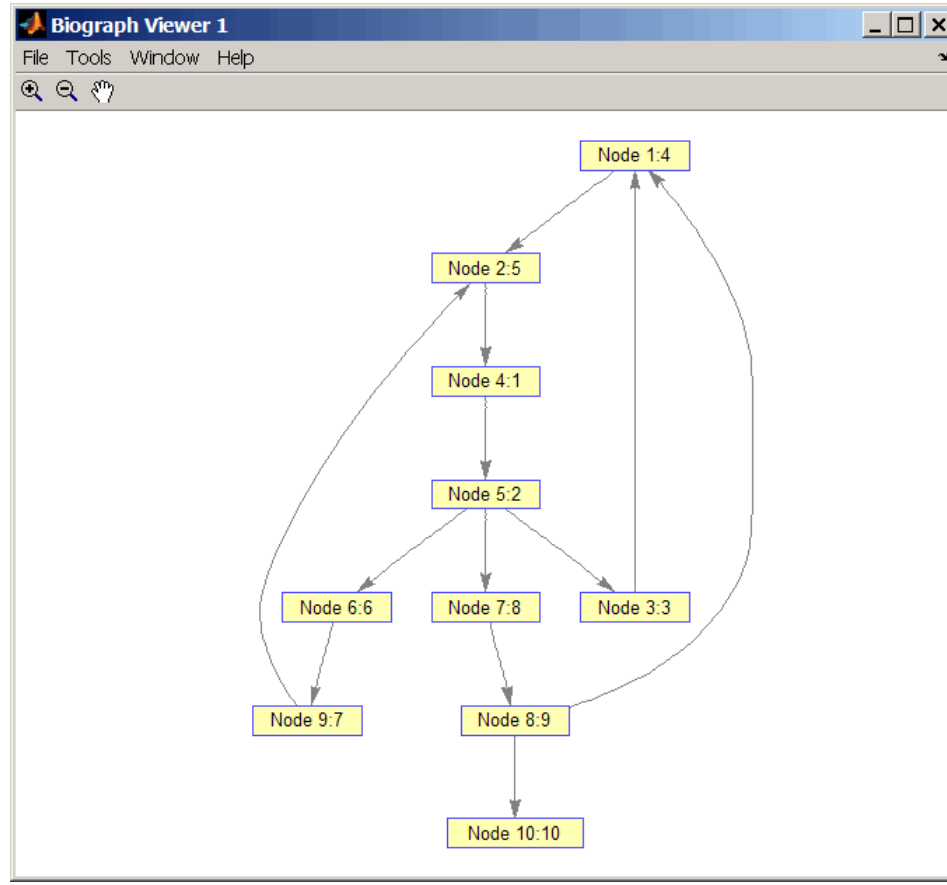


2 Traverse the graph to find the depth-first search (DFS) discovery order starting at node 4.

```
order = graphtraverse(DG,4)

order =

     4     5     3     1     2     6     9     7     8    10
```

3 Label the nodes with the DFS discovery order.

```
for i = 1:10
    h.Nodes(order(i)).Label =...
   sprintf('%s:%d',h.Nodes(order(i)).ID,i);
end
h.ShowTextInNodes = 'label'
dolayout(h)
```

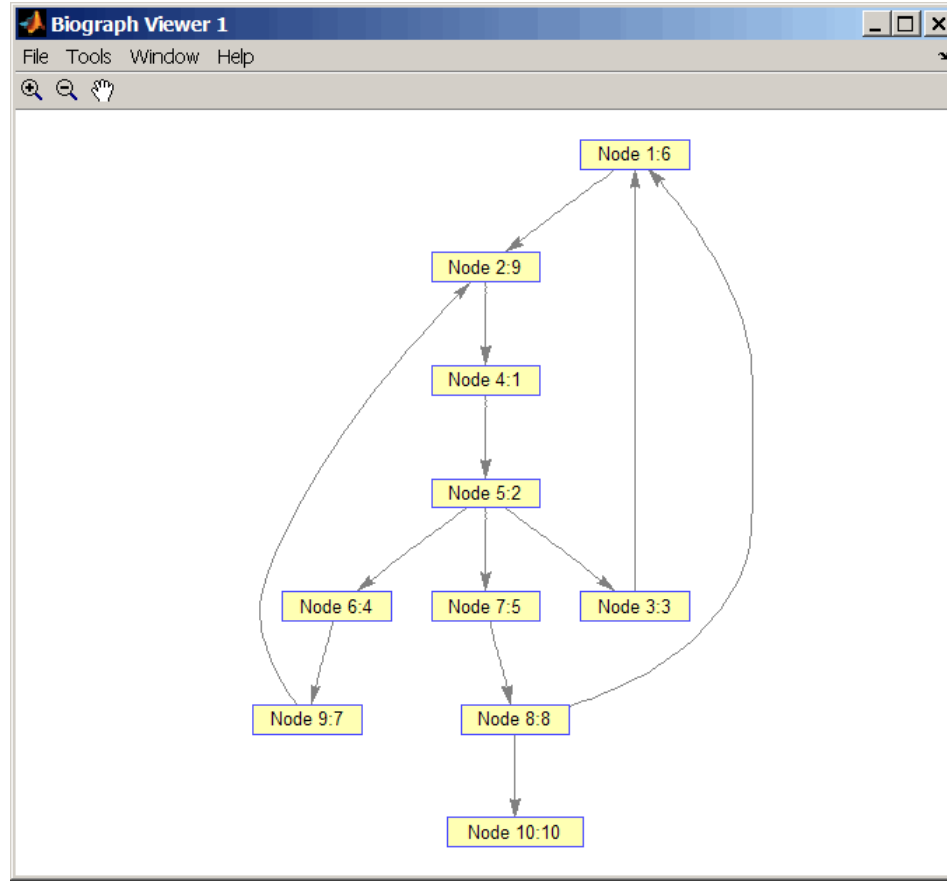


4 Traverse the graph to find the breadth-first search (BFS) discovery order starting at node 4.

```
order = graphtraverse(DG,4,'Method','BFS')

order =

     4     5     3     6     7     1     9     8     2    10
```

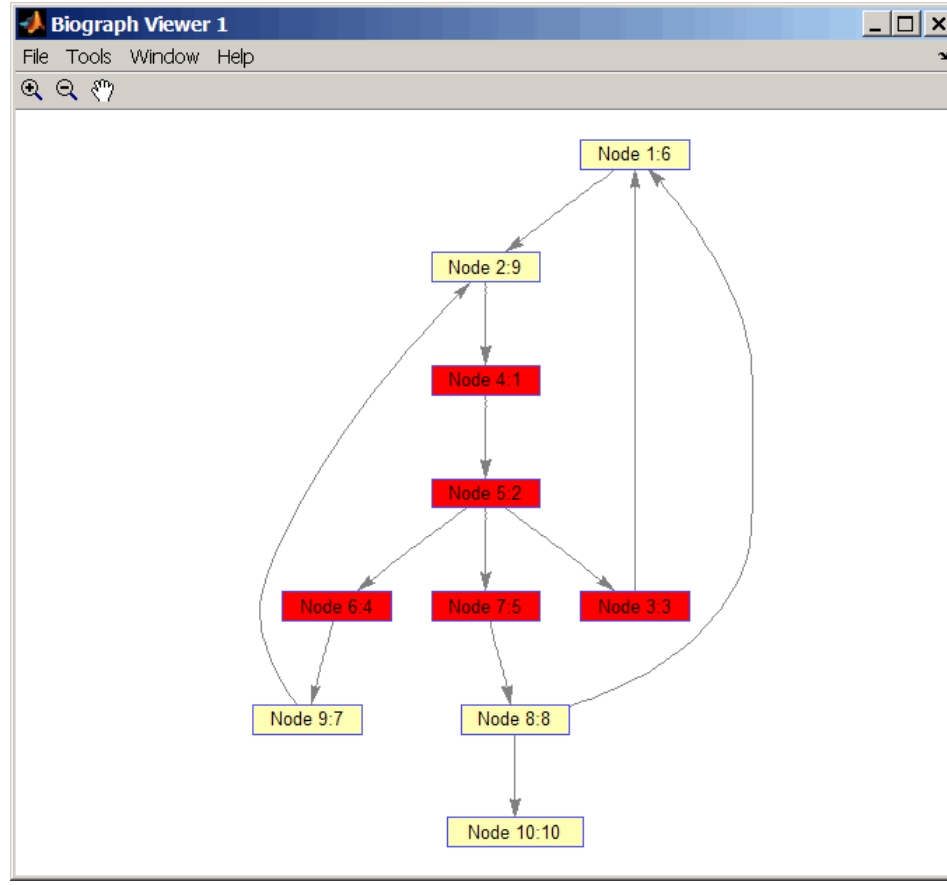
5 Label the nodes with the BFS discovery order.

```
for i = 1:10
    h.Nodes(order(i)).Label =...
   sprintf('%s:%d',h.Nodes(order(i)).ID,i);
end
h.ShowTextInNodes = 'label'
dolayout(h)
```



6 Find and color nodes that are close to (within two edges of) node 4.

```
node_idxs = graphtraverse(DG,4,'depth',2)

node_idxs =

     4     5     3     6     7

set(h.nodes(node_idxs),'Color',[1 0 0])
```



References

[1] Sedgewick, R., (2002). Algorithms in C++, Part 5 Graph Algorithms (Addison-Wesley).

[2] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `graphallshortestpaths`, `graphconncomp`, `graphisdag`, `graphisomorphism`, `graphisspantree`, `graphmaxflow`, `graphminspantree`, `graphpred2path`, `graphshortestpath`, `graphtopoorder`

Bioinformatics Toolbox method of `biograph object`: `traverse`

gt (DataMatrix)

Purpose

Test DataMatrix objects for greater than

Syntax

```
T = gt(DMObj1, DMObj2)
T = DMObj1 > DMObj2
T = gt(DMObj1, B)
T = DMObj1 > B
T = gt(B, DMObj1)
T = B > DMObj1
```

Arguments

DMObj1, *DMObj2*	DataMatrix objects, such as created by `DataMatrix` (object constructor).
B	MATLAB numeric or logical array.

Return Values

T	Logical matrix of the same size as *DMObj1* and *DMObj2* or *DMObj1* and *B*. It contains logical `1` (true) where elements in the first input are greater than the corresponding element in the second input, and logical `0` (false) otherwise.

Description

T = `gt(`*DMObj1*`, `*DMObj2*`)` or the equivalent *T* = *DMObj1* > *DMObj2* compares each element in DataMatrix object *DMObj1* to the corresponding element in DataMatrix object *DMObj2*, and returns *T*, a logical matrix of the same size as *DMObj1* and *DMObj2*, containing logical `1` (true) where elements in *DMObj1* are greater than the corresponding element in *DMObj2*, and logical `0` (false) otherwise. *DMObj1* and *DMObj2* must have the same size (number of rows and columns), unless one is a scalar (1-by-1 DataMatrix object). *DMObj1* and *DMObj2* can have different `Name` properties.

T = `gt(`*DMObj1*`, `*B*`)` or the equivalent *T* = *DMObj1* > *B* compares each element in DataMatrix object *DMObj1* to the corresponding element in *B*, a numeric or logical array, and returns *T*, a logical matrix of the same size as *DMObj1* and *B*, containing logical `1` (true) where elements

in *DMObj1* are greater than the corresponding element in *B*, and logical 0 (false) otherwise. *DMObj1* and *B* must have the same size (number of rows and columns), unless one is a scalar.

T = gt(*B*, *DMObj1*) or the equivalent *T* = *B* > *DMObj1* compares each element in *B*, a numeric or logical array, to the corresponding element in DataMatrix object *DMObj1*, and returns *T*, a logical matrix of the same size as *B* and *DMObj1*, containing logical 1 (true) where elements in *B* are greater than the corresponding element in *DMObj1*, and logical 0 (false) otherwise. *B* and *DMObj1* must have the same size (number of rows and columns), unless one is a scalar.

MATLAB calls *T* = gt(*X*, *Y*) for the syntax *T* = *X* > *Y* when *X* or *Y* is a DataMatrix object.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: lt

HeatMap object

Purpose

Object containing matrix and heat map display properties

Description

A HeatMap object contains data and display properties that you can view in a heat map (2-D color image).

Create a HeatMap object using the object constructor function `HeatMap`. View a graphical representation of the HeatMap object in a heat map using the `view` method.

The HeatMap class is a superclass of the clustergram class.

Method Summary

Following are methods of a HeatMap object:

addTitle (HeatMap)	Add title to heat map
addXLabel (HeatMap)	Label *x*-axis of heat map
addYLabel (HeatMap)	Label *y*-axis of heat map
plot (HeatMap)	Render heat map for HeatMap object
view (HeatMap)	View heat map of HeatMap object

Property Summary

Properties for Heat Map Creation

Property Name	Description
`Standardize`	String or number specifying the dimension for standardizing the data values. The standardized values are transformed so that the mean is `0` and the standard deviation is `1` in the specified dimension. Choices are: • `'column'` or `1` — Standardize along the columns of data. • `'row'` or `2` — Standardize along the rows of data. • `'none'` or `3` (default) — Do not standardize.

Properties for Heat Map Creation (Continued)

Property Name	Description
`Colormap`	Either of the following: • *M*-by-3 matrix of RGB values • Name or function handle of a function that returns a colormap, such as `redgreencmap` or `redbluecmap` Default is `redgreencmap`.
`DisplayRange`	Positive scalar specifying the display range of standardized values. Default is the maximum absolute value in the input matrix. For example, if you specify `3`, there is a color variation for values between –3 and 3, but values >3 are the same color as 3, and values < –3 are the same color as –3. For example, if you specify `redgreencmap` for the `'Colormap'` property, pure red represents values ≥ *`DisplayRangeValue`*, and pure green represents values ≤ –*`DisplayRangeValue`*.

Properties for Heat Map Creation (Continued)

Property Name	Description
`Symmetric`	Forces the color scale of the heat map to be symmetric around zero. Choices are `true` (default) or `false`.
`ImputeFun`	One of the following: • Name of a function that imputes missing data. • Handle to a function that imputes missing data. • Cell array where the first element is the name of or handle to a function that imputes missing data. The remaining elements are property name/property value pairs used as inputs to the function.

Properties for Row and Column Labels

Property Name	Description
`RowLabels`	Vector of numbers or cell array of text strings to label the rows in the heat map. Default is a vector of values `1` through *M*, where *M* is the number of rows in *`Data`*, the matrix of data used by the `HeatMap` function to create the HeatMap object.
`ColumnLabels`	Vector of numbers or cell array of text strings to label the columns in the heat map. Default is a vector of values `1` through *M*, where *M* is the number of columns in *`Data`*, the matrix of data used by the `HeatMap` function to create the HeatMap object.

Properties for Row and Column Labels (Continued)

Property Name	Description
`ColumnLabelsLocation`	String specifying the location of the column labels. Choices are `'top'` or `'bottom'` (default).
`RowLabelsLocation`	String specifying the location of the row labels. Choices are `'left'` (default) or `'right'`.
`RowLabelsColor`	Structure or structure array containing color information for labeling the rows (*y*-axis) of the heat map. If a single structure, then the fields contain a cell array of elements. If a structure array, then the fields contain one element: • `Labels` — String specifying a row label listed in the `RowLabels` vector. • `Colors` — String or three-element vector of RGB values specifying a color for the row label specified in the `Labels` field. For more information on specifying colors, see `ColorSpec`. If this field is empty, default colors are assigned to the row label.
`ColumnLabelsColor`	Structure or structure array containing color information for labeling the columns (*x*-axis) of the heat map. If a single structure, then the fields contain a cell array of elements. If a structure array, then the fields contain one element: • `Labels` — String specifying a column label listed in the `ColumnLabels` vector. • `Colors` — String or three-element vector of RGB values specifying a color for the column label specified in the `Labels` field. For more information on specifying colors,

Properties for Row and Column Labels (Continued)

Property Name	Description
	see `ColorSpec`. If this field is empty, default colors are assigned to the column label.
`LabelsWithMarkers`	Controls the display of colored markers instead of colored text for the row labels and column labels. Choices are `true` or `false` (default).
`RowLabelsRotate`	Numeric value in degrees rotation specifying the orientation of row (*y*-axis) labels. Default is `0` degrees, which is horizontal. Positive values cause counterclockwise rotation.
`ColumnLabelsRotate`	Numeric value in degrees rotation specifying the orientation of column (*x*-axis) labels. Default is `90` degrees, which is vertical. Values greater than `90` degrees cause counterclockwise rotation.

Properties for Annotating Data

Property Name	Description
`Annotate`	Controls the display of intensity values on each area of the heat map. Choices are `true` or `false` (default).
`AnnotPrecision`	Positive integer specifying the precision of the intensity values when displayed on the heat map. Default is `2`.
`AnnotColor`	String or three-element vector of RGB values specifying a color for the text of the intensity values when displayed on the heat map. Default is `'white'`. For more information on specifying colors, see `ColorSpec`.

Examples

Note The following examples use the `get` and `set` methods with property names and values of a HeatMap object. When supplying a *`PropertyName`*, be aware that it is case sensitive.

Determining Properties and Property Values of a HeatMap Object

Display all properties and their current values of a HeatMap object, *`HMobj`*:

```
get(HMobj)
```

Return all properties and their current values of *`HMobj`*, a HeatMap object, to *`CGstruct`*, a scalar structure in which each field name is a property of a HeatMap object, and each field contains the value of that property.

```
CGstruct = get(HMobj)
```

Return the value of a specific property of a HeatMap object, *`HMobj`*, using either:

```
PropertyValue = get(HMobj, 'PropertyName')
```

```
PropertyValue = HMobj.PropertyName
```

Return the value of specific properties of a HeatMap object, *`HMobj`*:

```
[Property1Value, Property2Value, ...] = get(HMobj, ...
'Property1Name', 'Property2Name', ...)
```

Determining Possible Values of HeatMap Object Properties

Display possible values for all properties that have a fixed set of property values in a HeatMap object, *`HMobj`*:

```
set(HMobj)
```

Display possible values for a specific property that has a fixed set of property values in a HeatMap object, *HMobj*:

```
set(HMobj,  'PropertyName')
```

Specifying Properties of a HeatMap Object

Set a specific property of a HeatMap object, *HMobj*, using either:

```
set(HMobj, 'PropertyName', PropertyValue)
```

```
HMobj.PropertyName = PropertyValue
```

Set multiple properties of a HeatMap object, *HMobj*:

```
set(HMobj,  'Property1Name', Property1Value, ...
    'Property2Name', Property2Value, ...)
```

See Also

Bioinformatics Toolbox function: `HeatMap` (object constructor)

Bioinformatics Toolbox methods of a HeatMap object: `addTitle`, `addXLabel`, `addYLabel`, `plot`, `view`

MATLAB function: `display`

Purpose

Display heat map of matrix data and create HeatMap object

Syntax

```
HMobj = HeatMap(Data)
HeatMap(Data, ...'RowLabels', RowLabelsValue, ...)
HeatMap(Data, ...'ColumnLabels', ColumnLabelsValue, ...)
HeatMap(Data, ...'Standardize', StandardizeValue, ...)
HeatMap(Data, ...'Colormap', ColormapValue, ...)
HeatMap(Data, ...'DisplayRange', DisplayRangeValue, ...)
HeatMap(Data, ...'Symmetric', SymmetricValue, ...)
HeatMap(Data, ...'ImputeFun', ImputeFunValue, ...)
HeatMap(Data, ...'RowLabelsColor',
RowLabelsColorValue, ...)
HeatMap(Data, ...'ColumnLabelsColor',
ColumnLabelsColorValue,
   ...)
HeatMap(Data, ...'LabelsWithMarkers',
LabelsWithMarkersValue,
   ...)
```

Arguments

Data	DataMatrix object or numeric matrix of data.
RowLabelsValue	Vector of numbers or cell array of text strings to label the rows in the heat map. Default is a vector of values 1 through *M*, where *M* is the number of rows in *Data*.
ColumnLabelsValue	Vector of numbers or cell array of text strings to label the columns in the heat map. Default is a vector of values 1 through *N*, where *N* is the number of columns in *Data*.

StandardizeValue

String or number specifying the dimension for standardizing the values in *Data*. The `HeatMap` function transforms the standardized values so that the mean is `0` and the standard deviation is `1` in the specified dimension. Choices are:

- `'column'` or `1` — Standardize along the columns of data.
- `'row'` or `2` — Standardize along the rows of data.
- `'none'` or `3` (default) — Do not standardize.

ColormapValue

Either of the following:

- *M*-by-3 matrix of RGB values
- Name of or handle to a function that returns a colormap, such as `redgreencmap` or `redbluecmap`

Default is `redgreencmap`, in which red represents values above the mean, black represents the mean, and green represents values below the mean of a row (gene) across all columns (samples).

DisplayRangeValue	Positive scalar that specifies the display range of standardized values. Default is the maximum absolute value in the input *Data*. For example, if you specify `3`, there is a color variation for values between –3 and 3, but values >3 are the same color as 3, and values < –3 are the same color as –3. For example, if you specify `redgreencmap` for the `'Colormap'` property, pure red represents values ≥ *DisplayRangeValue*, and pure green represents values ≤ –*DisplayRangeValue*.
SymmetricValue	Forces the color scale of the heat map to be symmetric around zero. Choices are `true` (default) or `false`.
ImputeFunValue	One of the following: • Name of a function that imputes missing data. • Handle to a function that imputes missing data. • Cell array where the first element is the name of or handle to a function that imputes missing data. The remaining elements are property name/property value pairs used as inputs to the function.

Tip If data points are missing, you can use the `'ImputeFun'` property to impute the missing values.

`RowLabelsColorValue` Structure or structure array containing color information for labeling the rows (*y*-axis) of the heat map. The structure or structures contain the following fields. If a single structure, then the fields contain a cell array of elements. If a structure array, then the fields contain a single element.

- `Labels` — String specifying a row label listed in the `RowLabels` vector.
- `Colors` — String or three-element vectors of RGB values specifying a color for the row label you specified in the `Labels` field. For more information on specifying colors, see `ColorSpec`. If this field is empty, default colors are assigned to the row label.

`ColumnLabelsColorValue` Structure or structure array containing color information for labeling the columns (*x*-axis) of the heat map. The structure or structures contain the following fields. If a single structure, then the fields contain a cell array of elements. If a structure array, then the fields contain a single element.

- `Labels` — String specifying a column label listed in the `ColumnLabels` vector.
- `Colors` — String or three-element vector of RGB values specifying a color for

	the column label you specified in the `Labels` field. For more information on specifying colors, see `ColorSpec`. If this field is empty, default colors are assigned to the column label.
`LabelsWithMarkersValue`	Controls the display of colored markers instead of colored text for the row labels and column labels. Choices are `true` or `false` (default).

Description

`HMobj` `= HeatMap(`*`Data`*`)` displays a heat map (2-D color image) of the data and returns an object containing the data and display properties.

`HeatMap(`*`Data`*`, ...'`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `HeatMap` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each *`PropertyName`* in single quotation marks. Each *`PropertyName`* is case insensitive. These property name/property value pairs are as follows:

`HeatMap(`*`Data`*`, ...'RowLabels', `*`RowLabelsValue`*`, ...)` uses the contents of *`RowLabelsValue`*, a vector of numbers or cell array of text strings, as labels for the rows in the heat map. Default is a vector of values `1` through *M*, where *M* is the number of rows in *`Data`*.

`HeatMap(`*`Data`*`, ...'ColumnLabels', `*`ColumnLabelsValue`*`, ...)` uses the contents of *`ColumnLabelsValue`*, a vector of numbers or cell array of text strings, as labels for the columns in the heat map. Default is a vector of values `1` through *M*, where *M* is the number of columns in *`Data`*.

`HeatMap(`*`Data`*`, ...'Standardize', `*`StandardizeValue`*`, ...)` specifies the dimension for standardizing the values in *`Data`*. The `HeatMap` function transforms the standardized values are so that the mean is `0` and the standard deviation is `1` in the specified dimension. *`StandardizeValue`* can be:

- `'column'` or `1` — Standardize along the columns of data.

- `'row'` or `2` — Standardize along the rows of data.
- `'none'` or `3` (default) — Do not standardize.

`HeatMap(`*`Data`*`, ...'Colormap', `*`ColormapValue`*`, ...)` specifies the colormap to use to create the heat map. The colormap controls the colors used to display the heat map. *`ColormapValue`* is either an *M*-by-3 matrix of RGB values or the name of or handle to a function that returns a colormap, such as `redgreencmap` or `redbluecmap`. Default is `redgreencmap`.

Note In `redgreencmap`, red represents values above the mean, black represents the mean, and green represents values below the mean of a row (gene) across all columns (samples). In `redbluecmap`, red represents values above the mean, white represents the mean, and blue represents values below the mean of a row (gene) across all columns (samples).

`HeatMap(`*`Data`*`, ...'DisplayRange', `*`DisplayRangeValue`*`, ...)` specifies the display range of standardized values. *`DisplayRangeValue`* must be a positive scalar. Default is the maximum absolute value in the input *`Data`*. For example, if you specify `3`, there is a color variation for values between –3 and 3, but values >3 are the same color as 3, and values < –3 are the same color as –3.

For example, if you specify `redgreencmap` for the `'Colormap'` property, pure red represents values ≥ *`DisplayRangeValue`*, and pure green represents values ≤ *–`DisplayRangeValue`*.

`HeatMap(`*`Data`*`, ...'Symmetric', `*`SymmetricValue`*`, ...)` controls whether the color scale of the heat map is symmetric around zero. *`SymmetricValue`* can be `true` (default) or `false`.

`HeatMap(`*`Data`*`, ...'ImputeFun', `*`ImputeFunValue`*`, ...)` specifies a function and optional inputs that impute missing data. *`ImputeFunValue`* can be any of the following:

- Name of a function that imputes missing data.

- Handle to a function that imputes missing data.
- Cell array where the first element is the name of or handle to a function that imputes missing data. The remaining elements are property name/property value pairs used as inputs to the function.

Tip If data points are missing, you can use the `'ImputeFun'` property to impute the missing values.

`HeatMap(`*`Data`*`, ...'RowLabelsColor', `*`RowLabelsColorValue`*`, ...)` specifies color information for labeling the rows (*y*-axis) of the heat map.

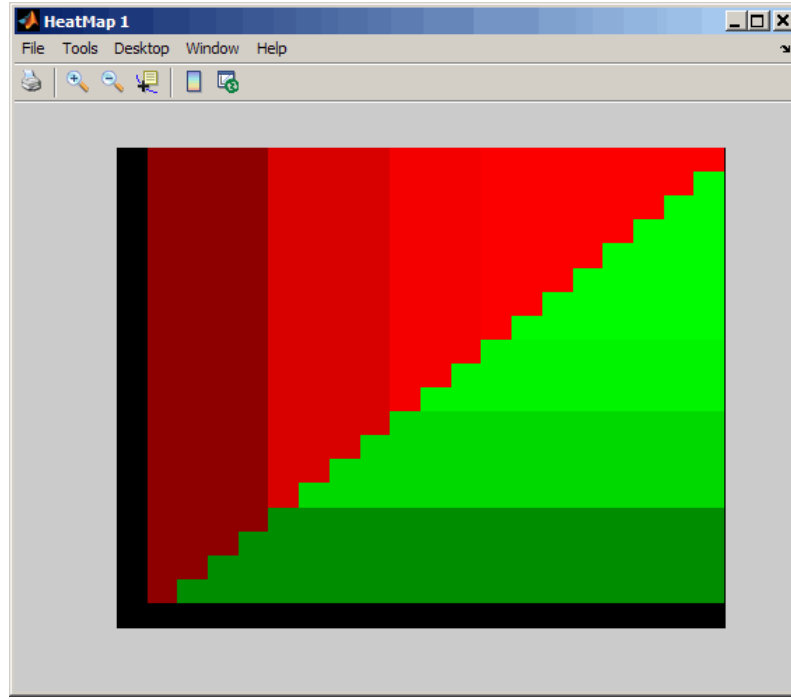
`HeatMap(`*`Data`*`, ...'ColumnLabelsColor', `*`ColumnLabelsColorValue`*`, ...)` specifies color information for labeling the columns (*x*-axis) of the heat map.

`HeatMap(`*`Data`*`, ...'LabelsWithMarkers', `*`LabelsWithMarkersValue`*`, ...)` controls the display of colored markers instead of colored text for the row labels and column labels. Choices are `true` or `false` (default).

Examples

Create a matrix of data and use the `HeatMap` function to display a 2-D color image of the data.

```
data = gallery('invhess',20);
hmo = HeatMap(data)
```



See Also

Bioinformatics Toolbox functions: `redbluecmap`, `redgreencmap`

Bioinformatics Toolbox object: HeatMap object

Bioinformatics Toolbox methods of a HeatMap object: `addTitle`, `addXLabel`, `addYLabel`, `get`, `plot`, `set`, `view`

Purpose

Align query sequence to profile using hidden Markov model alignment

Syntax

```
Score = hmmprofalign(Model, Seq)
[Score, Alignment] = hmmprofalign(Model, Seq)
[Score, Alignment, Pointer] = hmmprofalign(Model, Seq)
hmmprofalign(..., 'ShowScore', ShowScoreValue, ...)
hmmprofalign(..., 'Flanks', FlanksValue, ...)
hmmprofalign(..., 'ScoreFlanks', ScoreFlanksValue, ...)
hmmprofalign(..., 'ScoreNullTransitions',
   ScoreNullTransitionsValue, ...)
```

Arguments

Model	Hidden Markov model created with the function `hmmprofstruct`.
Seq	Amino acid or nucleotide sequence. You can also enter a structure with the field `Sequence`.
ShowScoreValue	Controls the display of the scoring space and the winning path. Choices are `true` or `false` (default).
FlanksValue	Controls the inclusion of the symbols generated by the FLANKING INSERT states in the output sequence. Choices are `true` or `false` (default).
ScoreFlanksValue	Controls the inclusion of the transition probabilities for the flanking states in the raw score. Choices are `true` or `false` (default).
ScoreNullTransitionsValue	Controls the adjustment of the raw score using the null model for transitions (`Model.NullX`). Choices are `true` or `false` (default).

Description

Score = hmmprofalign(*Model, Seq*) returns the score for the optimal alignment of the query amino acid or nucleotide sequence (Seq) to the profile hidden Markov model (*Model*). Scores are computed using log-odd ratios for emission probabilities and log probabilities for state transitions.

[*Score*, *Alignment*] = hmmprofalign(*Model, Seq*) also returns a string showing the optimal profile alignment.

Uppercase letters and dashes correspond to MATCH and DELETE states respectively (the combined count is equal to the number of states in the model). Lowercase letters are emitted by the INSERT states. For more information about the HMM profile, see hmmprofstruct.

[*Score, Alignment, Pointer*] = hmmprofalign(*Model, Seq*) also returns a vector of the same length as the profile model with indices pointing to the respective symbols of the query sequence. Null pointers (NaN) mean that such states did not emit a symbol in the aligned sequence because they represent model jumps from the BEGIN state of a MATCH state, model jumps from the from a MATCH state to the END state, or because the alignment passed through DELETE states.

hmmprofalign(..., '*PropertyName*', *PropertyValue*, ...) calls hmmprofalign with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

hmmprofalign(..., 'ShowScore', *ShowScoreValue*, ...), when *ShowScoreValue* is true, displays the scoring space and the winning path.

hmmprofalign(..., 'Flanks', *FlanksValue*, ...), when *FlanksValue* is true, includes the symbols generated by the FLANKING INSERT states in the output sequence.

hmmprofalign(..., 'ScoreFlanks', *ScoreFlanksValue*, ...), when *ScoreFlanksValue* is true, includes the transition probabilities for the flanking states in the raw score.

`hmmprofalign(..., 'ScoreNullTransitions', ScoreNullTransitionsValue, ...)`, when *`ScoreNullTransitionsValue`* is `true`, adjusts the raw score using the null model for transitions (`Model.NullX`).

Note Multiple target alignment is not supported in this implementation. All the `Model.LoopX` probabilities are ignored.

Examples

```
% load a model example
load('hmm_model_examples','model_7tm_2')
% load a sequence example
load('hmm_model_examples','sequences')
SCCR_RABIT=sequences(2).Sequence;
[a,s]=hmmprofalign(model_7tm_2,SCCR_RABIT,'showscore',true)
```

See Also

Bioinformatics Toolbox functions `gethmmprof`, `hmmprofestimate`, `hmmprofgenerate`, `hmmprofgenerate`, `hmmprofstruct`, `pfamhmmread`, `showhmmprof`, `multialign`, `profalign`

hmmprofestimate

Purpose

Estimate profile hidden Markov model (HMM) parameters using pseudocounts

Syntax

```
hmmprofestimate(Model, MultipleAlignment,
                'PropertyName', PropertyValue...)

hmmprofestimate(..., 'A', AValue)
hmmprofestimate(..., 'Ax', AxValue)
hmmprofestimate(..., 'BE', BEValue)
hmmprofestimate(..., 'BDx', BDxValue)
```

Arguments

`Model`	Hidden Markov model created with the function `hmmprofstruc`.
`MultipleAlignment`	Array of sequences. `Sequences` can also be a structured array with the aligned sequences in a field `Aligned` or `Sequences`, and the optional names in a field `Header` or `Name`.
`A`	Property to set the pseudocount weight A. Default value is `20`.
`Ax`	Property to set the pseudocount weight Ax. Default value is 20.
`BE`	Property to set the background symbol emission probabilities. Default values are taken from `Model.NullEmission`.
`BMx`	Property to set the background transition probabilities from any MATCH state ([`M->M M->I M->D`]). Default values are taken from `hmmprofstruct`.
`BDx`	Property to set the background transition probabilities from any DELETE state ([`D->M D->D`]). Default values are taken from `hmmprofstruct`.

Description

`hmmprofestimate(Model, MultipleAlignment, '`*`PropertyName`*`', `*`PropertyValue`*`...)` returns a structure with the fields containing the updated estimated parameters of a profile HMM. Symbol emission and state transition probabilities are estimated using the real counts and weighted pseudocounts obtained with the background probabilities. Default weight is `A=20`, the default background symbol emission for match and insert states is taken from `Model.NullEmission`, and the default background transition probabilities are the same as default transition probabilities returned by `hmmprofstruct`.

Model Construction: Multiple aligned sequences should contain uppercase letters and dashes indicating the model MATCH and DELETE states agreeing with `Model.ModelLength`. If model state annotation is missing, but `MultipleAlignment` is space aligned, then a "maximum entropy" criteria is used to select `Model.ModelLength` states.

Note Insert and flank insert transition probabilities are not estimated, but can be modified afterwards using `hmmprofstruct`.

`hmmprofestimate(..., 'A', `*`AValue`*`)` sets the pseudocount weight `A = Avalue` when estimating the symbol emission probabilities. Default value is `20`.

`hmmprofestimate(...,'Ax', `*`AxValue`*`)` sets the pseudocount weight `Ax = Axvalue` when estimating the transition probabilities. Default value is 20.

`hmmprofestimate(...,'BE', `*`BEValue`*`)` sets the background symbol emission probabilities. Default values are taken from `Model.NullEmission`.

`hmmprofestimate(...,'BMx', `*`BMxValue`*`)` sets the background transition probabilities from any MATCH state ([`M->M M->I M->D`]). Default values are taken from `hmmprofstruct`.

`hmmprofestimate(..., 'BDx', BDxValue)` sets the background transition probabilities from any DELETE state ([`D->M` `D->D`]). Default values are taken from `hmmprofstruct`.

See Also

Bioinformatics Toolbox functions: `hmmprofalign`, `hmmprofstruct`, `showhmmprof`

Purpose

Generate random sequence drawn from profile hidden Markov model (HMM)

Syntax

```
Sequence = hmmprofgenerate(Model)
[Sequence, Profptr] = hmmprofgenerate(Model)
... = hmmprofgenerate(Model, ...'Align', AlignValue, ...)
... = hmmprofgenerate(Model, ...'Flanks', FlanksValue, ...)
... = hmmprofgenerate(Model, ...'Signature', SignatureValue,
    ...)
```

Arguments

Model	Hidden Markov model created with the `hmmprofstruct` function.
AlignValue	Controls the use of uppercase letters for matches and lowercase letters for inserted letters. Choices are `true` or `false` (default).
FlanksValue	Controls the inclusion of the symbols generated by the FLANKING INSERT states in the output sequence. Choices are `true` or `false` (default).
SignatureValue	Controls the return of the most likely path and symbols. Choices are `true` or `false` (default).

Description

Sequence = `hmmprofgenerate(`*Model*`)` returns the string *Sequence* showing a sequence of amino acids or nucleotides drawn from the profile *Model*. The length, alphabet, and probabilities of the *Model* are stored in a structure. For more information about this structure, see `hmmprofstruct`.

`[`*Sequence*`, `*Profptr*`] = hmmprofgenerate(`*Model*`)` returns a vector of the same length as the profile model pointing to the respective states in the output sequence. Null pointers (0) mean that such states do not exist in the output sequence, either because they are never touched (i.e., jumps from the BEGIN state to MATCH states or from MATCH states to the

END state), or because DELETE states are not in the output sequence (not aligned output; see below).

`... = hmmprofgenerate(`*`Model`*`, ...'`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `hmmprofgenerate` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`... = hmmprofgenerate(`*`Model`*`, ...'Align', `*`AlignValue`*`, ...)` if `Align` is `true`, the output sequence is aligned to the model as follows: uppercase letters and dashes correspond to MATCH and DELETE states respectively (the combined count is equal to the number of states in the model). Lowercase letters are emitted by the INSERT or FLANKING INSERT states. If *`AlignValue`* is `false`, the output is a sequence of uppercase symbols. The default value is `true`.

`... = hmmprofgenerate(`*`Model`*`, ...'Flanks', `*`FlanksValue`*`, ...)` if `Flanks` is `true`, the output sequence includes the symbols generated by the FLANKING INSERT states. The default value is `false`.

`... = hmmprofgenerate(`*`Model`*`, ...'Signature', `*`SignatureValue`*`, ...)` if *`SignatureValue`* is `true`, returns the most likely path and symbols. The default value is `false`.

Examples

```
load('hmm_model_examples','model_7tm_2') % load a model example
rand_sequence = hmmprofgenerate(model_7tm_2)
```

See Also

Bioinformatics Toolbox functions: `hmmprofalign`, `hmmprofstruct`, `showhmmprof`

Purpose

Concatenate prealigned strings of several sequences to profile hidden Markov model (HMM)

Syntax

```
hmmprofmerge(Sequences)
hmmprofmerge(Sequences, Names)
hmmprofmerge(Sequences, Names, Scores)
```

Arguments

Sequences	Array of sequences. *Sequences* can also be a structured array with the aligned sequences in a field `Aligned` or `Sequences`, and the optional names in a field `Header` or `Name`.
Names	Names for the sequences. Enter a vector of names.
Scores	Pairwise alignment scores from the function `hmmprofalign`. Enter a vector of values with the same length as the number of sequences in *Sequences*.

Description

`hmmprofmerge(`*Sequences*`)` displays a set of prealigned `sequences` to an HMM model profile. The output is aligned corresponding to the HMM states.

- Match states — Uppercase letters
- Insert states — Lowercase letters or asterisks (*)
- Delete states — Dashes

Periods (.) are added at positions corresponding to inserts in other sequences. The input sequences must have the same number of profile states, that is, the joint count of capital letters and dashes must be the same.

`hmmprofmerge(`*Sequences*`, `*Names*`)` labels the sequences with `Names`.

`hmmprofmerge(`*Sequences*`, `*Names*`, `*Scores*`)` sorts the displayed sequences using `Scores`.

Examples

```
load('hmm_model_examples','model_7tm_2')  %load model
load('hmm_model_examples','sequences')  %load sequences

for ind =1:length(sequences)
    [scores(ind),sequences(ind).Aligned] =...
        hmmprofalign(model_7tm_2,sequences(ind).Sequence);
    end
hmmprofmerge(sequences, scores)
```

See Also

Bioinformatics Toolbox functions: `hmmprofalign`, `hmmprofstruct`

Purpose

Create or edit hidden Markov model (HMM) profile structure

Syntax

```
Model = hmmprofstruct(Length)
Model = hmmprofstruct(Length, Field1, Field1Value, Field2,
   Field2Value, ...)
NewModel = hmmprofstruct(Model, Field1,
Field1Value, Field2,
   Field2Value, ...)
```

Arguments

Length	Number of match states in the model.
Model	MATLAB structure containing fields for the parameters of an HMM profile created with the `hmmprofstruct` function.
Field	String containing a field name in the structure *Model*. See the table below for field names.
FieldValue	Value associated with *Field*. See the table below for descriptions.

Return Values

Model	MATLAB structure containing fields for the parameters of an HMM profile.

Description

Model = `hmmprofstruct(`*Length*`)` returns *Model*, a MATLAB structure containing fields for the parameters of an HMM profile. *Length* specifies the number of match states in the model. All other required parameters are set to the default values.

Model = `hmmprofstruct(`*Length*`, `*Field1*`, `*Field1Value*`, `*Field2*`, `*Field2Value*`, ...)` returns an HMM profile structure using the specified parameters. All other required parameters are set to default values.

NewModel = `hmmprofstruct(`*Model*`, `*Field1*`, `*Field1Value*`, `*Field2*`, `*Field2Value*`, ...)` returns an updated HMM profile

structure using the specified parameters. All other parameters are taken from the input *Model*.

HMM Profile Structure

The MATLAB structure *Model* contains the following fields, which are the required and optional parameters of an HMM profile. All probability values are in the [0 1] range.

Field	Description
ModelLength	Integer specifying the length of the profile (number of MATCH states).
Alphabet	String specifying the alphabet used in the model. Choices are 'AA' (default) or 'NT'. **Note** AlphaLength is 20 for 'AA' and 4 for 'NT'.
MatchEmission	Symbol emission probabilities in the MATCH states. Either of the following: • A matrix of size ModelLength-by-AlphaLength, where each row corresponds to the emission distribution for a specific MATCH state. Defaults to uniform distributions. • A structure containing residue counts, such as returned by aacount or basecount.

Field	Description
`InsertEmission`	Symbol emission probabilities in the INSERT state. Either of the following: • A matrix of size `ModelLength`-by-`AlphaLength`, where each row corresponds to the emission distribution for a specific INSERT state. Defaults to uniform distributions. • A structure containing residue counts, such as returned by `aacount` or `basecount`.
`NullEmission`	Symbol emission probabilities in the MATCH and INSERT states for the NULL model. Either of the following: • A 1-by-`AlphaLength` row vector. Defaults to a uniform distribution. • A structure containing residue counts, such as returned by `aacount` or `basecount`. **Note** The NULL model is used to compute the log-odds ratio at every state and avoid overflow when propagating the probabilities through the model. **Note** NULL probabilities are also known as the background probabilities.

Field	Description

BeginX	BEGIN state transition probabilities.
	Format is a 1-by-(ModelLength + 1) row vector:
	`[B->D1 B->M1 B->M2 B->M3 .... B->Mend]`
	Note If necessary, hmmprofstruct will normalize the data such that the sum of the transition probabilities from the BEGIN state equals 1:
	`sum(Model.BeginX) = 1`
	For fragment profiles:
	`sum(Model.BeginX(3:end)) = 0`
	Default is [0.01 0.99 0 0 ... 0].

MatchX	MATCH state transition probabilities.
	Format is a 4-by-(ModelLength - 1) matrix:
	`[M1->M2 M2->M3 ... M[end-1]->Mend;`
	`M1->I1 M2->I2 ... M[end-1]->I[end-1];`
	`M1->D2 M2->D3 ... M[end-1]->Dend;`
	`M1->E M2->E ... M[end-1]->E ]`

Field	Description

	Note If necessary, `hmmprofstruct` will normalize the data such that the sum of the transition probabilities from every MATCH state equals 1:
	`sum(Model.MatchX) = [ 1 1 ... 1 ]`
	For fragment profiles:
	`sum(Model.MatchX(4,:)) = 0`
	Default is `repmat([0.998 0.001 0.001 0],ModelLength-1,1)`.

`InsertX`	INSERT state transition probabilities.
	Format is a 2-by-`(ModelLength - 1)` matrix:
	`[ I1->M2 I2->M3 ... I[end-1]->Mend;`
	`I1->I1 I2->I2 ... I[end-1]->I[end-1] ]`
	Note If necessary, `hmmprofstruct` will normalize the data such that the sum of the transition probabilities from every INSERT state equals 1:
	`sum(Model.InsertX) = [ 1 1 ... 1 ]`
	Default is `repmat([0.5 0.5],ModelLength-1,1)`.

Field	Description

`DeleteX`	DELETE state transition probabilities.
	
	Format is a 2-by-`(ModelLength - 1)` matrix:
	
	`[ D1->M2 D2->M3 ... D[end-1]->Mend ;`
	`  D1->D2 D2->D3 ... D[end-1]->Dend ]`
	
	Note If necessary, `hmmprofstruct` will normalize the data such that the sum of the transition probabilities from every DELETE state equals 1:
	
	`sum(`*`Model`*`.DeleteX) = [ 1 1 ... 1 ]`
	
	Default is `repmat([0.5 0.5],ModelLength-1,1).`

`FlankingInsertX`	Flanking insert states (N and C) used for LOCAL profile alignment.
	
	Format is a 2-by-2 matrix:
	
	`[N->B  C->T ;`
	`N->N  C->C]`
	
	Note If necessary, `hmmprofstruct` will normalize the data such that the sum of the transition probabilities from Flanking Insert states equals 1:
	
	`sum(`*`Model`*`.FlankingInsertsX) = [1 1]`

Field	Description
	Note To force global alignment use: `Model.FlankingInsertsX = [1 1; 0 0]` Default is `[0.01 0.01; 0.99 0.99]`.

`LoopX`	Loop states transition probabilities used for multiple hits alignment.
	Format is a 2-by-2 matrix:
	`[E->C  J->B ;`
	`E->J  J->J]`
	Note If necessary, `hmmprofstruct` will normalize the data such that the sum of the transition probabilities from Loop states equals 1:
	`sum(Model.LoopX) = [1 1]`
	Default is `[0.5 0.01; 0.5 0.99]`.

Field	Description

`NullX`	Null transition probabilities used to provide scores with log-odds values also for state transitions.
	Format is a 2-by-1 column vector:
	`[G->F ; G->G]`
	Note If necessary, `hmmprofstruct` will normalize the data such that the sum of the transition probabilities from Null states equals 1:
	`sum(Model.NullX) = 1`
	Default is `[0.01; 0.99]`.

`IDNumber`	Optional. User-assigned identification number.
`Description`	Optional. User-assigned description of the model.

HMM Profile Model

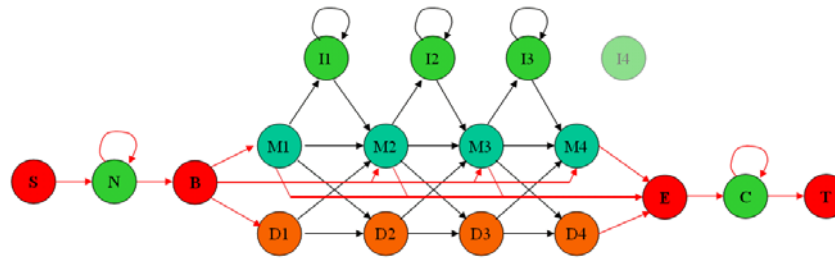
An HMM profile model is a common statistical tool for modeling structured sequences composed of symbols. These symbols include randomness in both the output (emission of symbols) and the state transitions of the process. Markov models are generally represented by state diagrams.

The following figure is a state diagram for an HMM profile of length four. INSERT, MATCH, and DELETE states are in the center section.

- INSERT state represents the excess of one or more symbols in the target sequence that are not included in the profile.

- MATCH state means that the target sequence is aligned to the profile at the specific location.
- DELETE state represents a gap or symbol absence in the target sequence (also known as a silent state because it does not emit any symbols).

Flanking states (`S`, `N`, `B`, `E`, `C`, `T`) are used for proper modeling of the ends of the sequence, either for global, local or fragment alignment of the profile. `S`, `B`, `E`, and `T` are silent, while `N` and `C` are used to insert symbols at the flanks.



Examples

Creating an HMM Profile Structure

Create an HMM profile structure with 100 MATCH states, using the amino acid alphabet.

```
hmmProfile = hmmprofstruct(100,'Alphabet','AA')

hmmProfile =

        ModelLength: 100
           Alphabet: 'AA'
      MatchEmission: [100x20 double]
    InsertEmission: [100x20 double]
      NullEmission: [1x20 double]
            BeginX: [101x1 double]
            MatchX: [99x4 double]
```

```
          InsertX: [99x2 double]
          DeleteX: [99x2 double]
 FlankingInsertX: [2x2 double]
            LoopX: [2x2 double]
            NullX: [2x1 double]
```

Editing an HMM Profile Structure

1. Use the `pfamhmmread` function to create an HMM profile structure from `pf00002.ls`, a PFAM HMM-formatted file included with the software.

   ```
   hmm02 = pfamhmmread('pf00002.ls');
   ```

2. Modify the HMM profile structure to force a global alignment by setting the looping transition probabilities in the flanking insert states to zero.

   ```
   hmm02 = hmmprofstruct(hmm02,'FlankingInsertX',[0 0;1 1]);
   hmm02.FlankingInsertX

   ans =

        0     0
        1     1
   ```

See Also

Bioinformatics Toolbox functions: `aacount`, `basecount`, `gethmmprof`, `hmmprofalign`, `hmmprofestimate`, `hmmprofgenerate`, `hmmprofmerge`, `pfamhmmread`, `showhmmprof`

Purpose

Concatenate DataMatrix objects horizontally

Syntax

```
DMObjNew = horzcat(DMObj1, DMObj2, ...)
DMObjNew = (DMObj1, DMObj2, ...)
DMObjNew = horzcat(DMObj1, B, ...)
DMObjNew = (DMObj1, B, ...)
```

Arguments

DMObj1, *DMObj2*	DataMatrix objects, such as created by `DataMatrix` (object constructor).
B	MATLAB numeric or logical array.

Return Values

DMObjNew	DataMatrix object created by horizontal concatenation.

Description

DMObjNew = `horzcat(`*DMObj1*`, `*DMObj2*`, ...)` or the equivalent *DMObjNew* = `(`*DMObj1*`, `*DMObj2*`, ...)` horizontally concatenates the DataMatrix objects *DMObj1* and *DMObj2* into *DMObjNew*, another DataMatrix object. *DMObj1* and *DMObj2* must have the same number of rows. The row names and the order of rows for *DMObjNew* are the same as *DMObj1*. The row names of *DMObj2* and any other DataMatrix object input arguments are not preserved. The columns names for *DMObjNew* are the column names of *DMObj1*, *DMObj2*, and other DataMatrix object input arguments.

DMObjNew = `horzcat(`*DMObj1*`, `*B*`, ...)` or the equivalent *DMObjNew* = `(`*DMObj1*`, `*B*`, ...)` horizontally concatenates the DataMatrix object *DMObj1* and a numeric or logical array *B* into *DMObjNew*, another DataMatrix object. *DMObj1* and *B* must have the same number of rows. The row names for *DMObjNew* are the same as *DMObj1*. The row names of *DMObj2* and any other DataMatrix object input arguments are not preserved. The column names for *DMObjNew* are the column names of *DMObj1* and empty for the columns from *B*.

MATLAB calls *DMObjNew* = horzcat(*X1*, *X2*, *X3*, ...) for the syntax *DMObjNew* = [*X1*, *X2*, *X3*, ...] when any one of *X1*, *X2*, *X3*, etc. is a DataMatrix object.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox methods of a DataMatrix object: vertcat

Purpose

Look up Illumina BeadStudio target (probe) sequence and annotation information

Syntax

```
AnnotStruct = ilmnbslookup(AnnotationFile, ID)
AnnotStruct = ilmnbslookup(AnnotationFile,
ID, 'LookUpField',
   LookUpFieldValue)
```

Arguments

AnnotationFile

String specifying a file name or a path and file name of an Illumina annotation file (CSV, BGX, or TXT format). If you specify only a file name, that file must be on the MATLAB search path or in the current directory.

Tip You can download Illumina annotation files, such as `HumanRef-8_V3_0_R0_11282963_A.bgx`, from the Illumina Web site.

ID

String or cell array of strings representing a unique identifier(s) for one or more targets (probes) on an Illumina microarray.

Tip By default, *ID* must match the `Search_key` field in *AnnotationFile*. However, you can use an identifier that corresponds to any of the fields in *AnnotationFile*, then set the `'LookUpField'` property appropriately. For example, if you want to look up annotation information for the targets (probes) on chromosome 7 only, set *ID* to `'7'`, then set *LookUpFieldValue* to `'Chromosome'`. For a list of all fields in *AnnotationFile*, see the following tables.

LookUpFieldValue

Field in *AnnotationFile* where `ilmnbslookup` looks for the specified *ID*. Default is the `Search_key` field.

Tip Set this property so that it corresponds to the *ID* you use as input.

Return Values

AnnotStruct

Structure containing the probe sequence and annotation information for one or more targets (probes) specified by *ID*, and by *AnnotationFile*, an Illumina annotation file.

AnnotStruct contains the same fields as *AnnotationFile*. The fields are described in the following two tables.

Description

AnnotStruct = ilmnbslookup(*AnnotationFile*, *ID*) returns *AnnotStruct*, a structure containing probe sequence and annotation information for one or more targets (probes) specified by *ID*, and by *AnnotationFile*, an Illumina annotation file (CSV, BGX, or TXT format).

AnnotStruct contains the same fields as *AnnotationFile*. The fields are described in the following two tables.

Structure Created from Illumina CSV Annotation File

Field	Description
Search_key	Internal identifier for the target, useful for custom design array
Target	Unique identifier for the target
ProbeId	Illumina probe identifier
Gid	GenBank identifier for the gene
Transcript	Illumina internal transcript identifier
Accession	GenBank accession number for the gene
Symbol	Typically, the gene symbol
Type	Probe type
Start	Starting position of the probe sequence in the GenBank record
Probe_Sequence	Sequence of the probe
Definition	Definition field from the GenBank record
Ontology	Gene Ontology terms associated with the gene
Synonym	Synonyms for the gene (from the GenBank record)

Structure Created from a BGX or TXT Annotation File

Field	Description
Accession	GenBank accession number for the gene
Array_Address_Id	Decoder identifier
Chromosome	Chromosome on which the gene is located
Cytoband	Cytogenetic banding region of the chromosome on which the gene associated with the target is located
Definition	Definition field from the GenBank record
Entrez_Gene_ID	Entrez Gene database identifier for the gene
GI	GenBank identifier for the gene
ILMN_Gene	Illuminainternal gene symbol
Obsolete_Probe_Id	Probe identifier before BGX annotation files
Ontology_Component	Gene Ontology cellular components associated with the gene
Ontology_Function	Gene Ontology molecular functions associated with the gene
Ontology_Process	Gene Ontology biological processes associated with the gene
Probe_Chr_Orientation	Orientation of the probe on the NCBI genome build
Probe_Coordinates	Genomic position of the probe on the NCBI genome build
Probe_Id	Illuminaprobe identifier
Probe_Sequence	Sequence of the probe

Structure Created from a BGX or TXT Annotation File (Continued)

Field	Description
Probe_Start	Start position of the probe relative to the 5' end of the source transcript sequence
Probe_Type	Information about what the probe is targeting
Protein_Product	NCBI protein accession number
RefSeq_ID	Identifier from the NCBI RefSeq database
Reporter_Composite_map	Information associated with control probes
Reporter_Group_Name	Information associated with control probes
Reporter_Group_id	Information associated with control probes
Search_Key	Internal identifier for the target, useful for custom design array
Source	Source from which the transcript sequence was obtained
Source_Reference_ID	Source's identifier
Species	Species associated with the gene
Symbol	Typically, the gene symbol
Synonyms	Synonyms for the gene (from the GenBank record)
Transcript	Illuminainternal transcript identifier
Unigene_ID	Identifier from the NCBI UniGene database

AnnotStruct = ilmnbslookup(*AnnotationFile*, *ID*, 'LookUpField', *LookUpFieldValue*) looks for *ID* in the annotation file in the field specified by *LookUpFieldValue*. Default is the Search_key field.

Examples

Note The gene expression file, TumorAdjacent-probe-raw.txt, and the annotation file, HumanRef-8_V3_0_R0_11282963_A.bgx, used in the following examples are not provided with the Bioinformatics Toolbox software.

Look Up Annotation Information for a Single Target (Probe)

1. Read the contents of a tab-delimited file exported from the Illumina BeadStudio software into a MATLAB structure.

```
ilmnStruct = ilmnbsread('TumorAdjacent-probe-raw.txt')

ilmnStruct =

             Header: [1x1 struct]
           TargetID: {22184x1 cell}
        ColumnNames: {1x37 cell}
               Data: [22184x37 double]
    TextColumnNames: {1x23 cell}
           TextData: {22184x23 cell}
```

2. Find the number of the Search_key column in the TextColumnNames cell array, which is returned in the ilmnStruct structure by the ilmnbsread function.

```
srchCol = find(strcmpi('Search_Key',ilmnStruct.TextColumnNames))

srchCol =

     1
```

3 Use the output from step 2 to look up the probe sequence and annotation information for the 10th entry in the annotation file, `HumanRef-8_V3_0_R0_11282963_A.bgx`.

```
annotation = ilmnbslookup('HumanRef-8_V3_0_R0_11282963_A.bgx',...
                          ilmnStruct.TextData{10,srchCol})
annotation =

               Accession: 'NM_144670.2'
         Array_Address_Id: '0004050154'
              Chromosome: '12'
                Cytoband: '12p13.31b'
              Definition: 'Homo sapiens alpha-2-macroglobulin-like 1 (A2ML1), mRNA.'
          Entrez_Gene_ID: '144568'
                      GI: '74271844'
               ILMN_Gene: 'A2ML1'
        Obsolete_Probe_Id: ''
       Ontology_Component: ''
        Ontology_Function: 'endopeptidase inhibitor activity [goid 4866] [evidence IEA]'
         Ontology_Process: ''
    Probe_Chr_Orientation: '+'
        Probe_Coordinates: '8920412-8920461'
                 Probe_Id: 'ILMN_2136495'
          Probe_Sequence: 'TGTAATCGCAGCCCCTTGGAAGGCCAAGGCAGGAGAATCGCCTCAACACT'
             Probe_Start: '4889'
              Probe_Type: 'S'
        Protein_Product: 'NP_653271.2'
               RefSeq_ID: 'NM_144670.2'
  Reporter_Composite_map: ''
     Reporter_Group_Name: ''
       Reporter_Group_id: ''
              Search_Key: 'ILMN_17375'
                  Source: 'RefSeq'
     Source_Reference_ID: 'NM_144670.2'
                 Species: 'Homo sapiens'
                  Symbol: 'A2ML1'
                Synonyms: [1x141 char]
```

```
    Transcript: 'ILMN_17375'
    Unigene_ID: ''
```

Look Up Annotation Information for a Subset of Targets (Probes)

Use the `ilmnbslookup` function with the `'LookUpField'` property to look up the annotation information for all targets located on chromosome 12 in the annotation file, `HumanRef-8_V3_0_R0_11282963_A.bgx`.

```
chr12annotation = ilmnbslookup('HumanRef-8_V3_0_R0_11282963_A.bgx',...
                               '12','LookUpField','Chromosome')

chr12annotation =

                 Accession: {1x1186 cell}
           Array_Address_Id: {1x1186 cell}
                 Chromosome: {1x1186 cell}
                   Cytoband: {1x1186 cell}
                 Definition: {1x1186 cell}
             Entrez_Gene_ID: {1x1186 cell}
                         GI: {1x1186 cell}
                  ILMN_Gene: {1x1186 cell}
          Obsolete_Probe_Id: {1x1186 cell}
        Ontology_Component: {1x1186 cell}
         Ontology_Function: {1x1186 cell}
          Ontology_Process: {1x1186 cell}
     Probe_Chr_Orientation: {1x1186 cell}
         Probe_Coordinates: {1x1186 cell}
                  Probe_Id: {1x1186 cell}
            Probe_Sequence: {1x1186 cell}
               Probe_Start: {1x1186 cell}
                Probe_Type: {1x1186 cell}
          Protein_Product: {1x1186 cell}
                RefSeq_ID: {1x1186 cell}
    Reporter_Composite_map: ''
       Reporter_Group_Name: ''
         Reporter_Group_id: ''
                Search_Key: {1x1186 cell}
```

```
                Source: {1x1186 cell}
Source_Reference_ID: {1x1186 cell}
            Species: {1x1186 cell}
             Symbol: {1x1186 cell}
           Synonyms: {1x1186 cell}
         Transcript: {1x1186 cell}
         Unigene_ID: {1x1186 cell}
```

The output structure indicates that there are 1,186 targets located on chromosome 12.

See Also

Bioinformatics Toolbox function: `ilmnbsread`

ilmnbsread

Purpose

Read gene expression data exported from Illumina BeadStudio software

Syntax

```
IlmnStruct = ilmnbsread(File)
IlmnStruct = ilmnbsread(File,  ...'Columns',
ColumnsValue, ...)
IlmnStruct = ilmnbsread(File,  ...'HeaderOnly',
   HeaderOnlyValue, ...)
IlmnStruct = ilmnbsread(File,  ...'CleanColNames',
   CleanColNamesValue, ...)
```

Arguments

File	String specifying a file name or a path and file name of a tab-delimited file or comma-separated expression data file exported from Illumina BeadStudio software. If you specify only a file name, that file must be on the MATLAB search path or in the current directory.
ColumnsValue	Cell array that specifies the column names to read. Default is all column names.
HeaderOnlyValue	Controls the population of only the `Header`, `ColumnNames`, and `TextColumnNames` fields in *IlmnStruct*. Choices are `true` or `false` (default).
CleanColNamesValue	Controls the conversion of any `ColumnNames` containing spaces or characters that cannot be used as MATLAB variable names, to valid MATLAB variable names. Choices are `true` or `false` (default).

Return Values

IlmnStruct	MATLAB structure containing data exported from Illumina BeadStudio software.

Description

IlmnStruct = ilmnbsread(*File*) reads *File*, a tab-delimited or comma-separated expression data file exported from the Illumina BeadStudio software, and creates *IlmnStruct*, a MATLAB structure containing the following fields.

Field	Description
Header	String containing a description of the data.
TargetID	Cell array containing unique identifiers for targets on an Illumina gene expression microarray.
ColumnNames	Cell array containing names of the columns that contain numeric data in the tab-delimited file exported from the Illumina BeadStudio software.
Data	Matrix containing numeric microarray data for each target on an Illumina gene expression microarray. **Note** ColumnNames and Data have the same number of columns.

Field	Description
TextColumnNames	Cell array containing names of the columns that contain nonnumeric data in the tab-delimited file exported from the Illumina BeadStudio software. This field can be empty.
TextData	Cell array containing nonnumeric microarray data (such as annotations) for each target on an Illumina gene expression microarray. This field can be empty. **Note** TextColumnNames and TextData have the same number of columns.

IlmnStruct = ilmnbsread(*File*, ...'*PropertyName*', *PropertyValue*, ...) calls ilmnbsread with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

IlmnStruct = ilmnbsread(*File*, ...'Columns', *ColumnsValue*, ...) reads the data only from the columns specified by *ColumnsValue*, a cell array of column names. Default behavior is to read data from all columns.

IlmnStruct = ilmnbsread(*File*, ...'HeaderOnly', *HeaderOnlyValue*, ...) controls the population of only the Header, ColumnNames, and TextColumnNames fields in *IlmnStruct*. Choices are true or false (default).

IlmnStruct = ilmnbsread(*File*, ...'CleanColNames', *CleanColNamesValue*, ...) controls the conversion of any ColumnNames containing spaces or characters that cannot be used as MATLAB variable names, to valid MATLAB variable names. Choices are true or false (default).

Tip Use the `'CleanColNames'` property if you plan to use the `ColumnNames` field as variable names.

Examples

Note The gene expression file, `TumorAdjacent-probe-raw.txt` used in the following example is not provided with the Bioinformatics Toolbox software.

Read the contents of a tab-delimited file exported from the Illumina BeadStudio software into a MATLAB structure.

```
ilmnStruct = ilmnbsread('TumorAdjacent-probe-raw.txt')

ilmnStruct =

             Header: [1x1 struct]
           TargetID: {22184x1 cell}
        ColumnNames: {1x37 cell}
               Data: [22184x37 double]
    TextColumnNames: {1x23 cell}
           TextData: {22184x23 cell}
```

See Also

Bioinformatics Toolbox functions: `affyread`, `agferead`, `celintensityread`, `galread`, `geoseriesread`, `geosoftread`, `gprread`, `ilmnbslookup`, `imageneread`, `magetfield`, `sptread`

imageneread

Purpose

Read microarray data from ImaGene Results file

Syntax

```
imagenedata = imageneread('File')
imagenedata = imageneread(..., 'CleanColNames',
CleanColNamesValue, ...)
```

Arguments

File	ImaGene Results formatted file. Enter a file name or a path and file name.
CleanColNamesValue	Controls the conversion of any `ColumnNames` containing spaces or characters that cannot be used as MATLAB variable names, to valid MATLAB variable names. Choices are `true` or `false` (default).

Description

imagenedata = imageneread('*File*') reads ImaGene results data from *File* and creates a MATLAB structure `imagedata` containing the following fields.

Field
HeaderAA
Data
Blocks
Rows
Columns
Fields
IDs
ColumnNames
Indices
Shape

imagenedata = imageneread(..., '*PropertyName*', *PropertyValue*, ...) calls imageneread with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

imagenedata = imageneread(..., 'CleanColNames', *CleanColNamesValue*, ...) controls the conversion of any ColumnNames containing spaces or characters that cannot be used as MATLAB variable names, to valid MATLAB variable names. Choices are true or false (default).

The field Indices of the structure contains indices that you can use for plotting heat maps of the data with the function image or imagesc.

For more details on the ImaGene format and example data, see the ImaGene documentation.

Examples

1. Read in a sample ImaGene Results file. Note that the example file, cy3.txt, is not provided with the Bioinformatics Toolbox software.

```
cy3Data = imageneread('cy3.txt');
```

2. Plot the signal mean.

```
maimage(cy3Data,'Signal Mean');
```

3. Read in a sample ImaGene Results file. Note that the example file, cy5.txt, is not provided with the Bioinformatics Toolbox software.

```
cy5Data = imageneread('cy5.txt');
```

4. Create a loglog plot of the signal median from two ImaGene Results files.

```
sigMedianCol = find(strcmp('Signal Median',cy3Data.ColumnNames));
cy3Median = cy3Data.Data(:,sigMedianCol);
cy5Median = cy5Data.Data(:,sigMedianCol);
maloglog(cy3Median,cy5Median,'title','Signal Median');
```

See Also

Bioinformatics Toolbox functions: `gprread`, `ilmnbsread`, `maboxplot`, `maimage`, `sptread`

Purpose

Convert amino acid sequence from integer to letter representation

Syntax

```
SeqChar = int2aa(SeqInt)
SeqChar = int2aa(SeqInt, 'Case', CaseValue)
```

Arguments

SeqInt	Row vector of integers specifying an amino acid sequence. For valid integers, see the table Mapping Amino Acid Integers to Letter Codes on page 3-805. Integers are arbitrarily assigned to IUB/IUPAC letters.
CaseValue	String specifying the case of the returned string. Choices are `'upper'` (default) or `'lower'`.

Return Values

SeqChar	Amino acid sequence specified by a string of single-letter codes.

Description

SeqChar = `int2aa(`*SeqInt*`)` converts *SeqInt*, a row vector of integers specifying an amino acid sequence, to *SeqChar*, a string of single-letter codes specifying the same amino acid sequence. For valid integers, see the table Mapping Amino Acid Integers to Letter Codes on page 3-805.

SeqChar = `int2aa(`*SeqInt*`, 'Case', `*CaseValue*`)` specifies the case of the returned string. Choices are `'upper'` (default) or `'lower'`.

Mapping Amino Acid Integers to Letter Codes

Amino Acid	Integer	Code
Alanine	1	A
Arginine	2	R
Asparagine	3	N

Mapping Amino Acid Integers to Letter Codes (Continued)

Amino Acid	Integer	Code
Aspartic acid (Aspartate)	4	D
Cysteine	5	C
Glutamine	6	Q
Glutamic acid (Glutamate)	7	E
Glycine	8	G
Histidine	9	H
Isoleucine	10	I
Leucine	11	L
Lysine	12	K
Methionine	13	M
Phenylalanine	14	F
Proline	15	P
Serine	16	S
Threonine	17	T
Tryptophan	18	W
Tyrosine	19	Y
Valine	20	V
Asparagine or Aspartic acid (Aspartate)	21	B
Glutamine or Glutamic acid (Glutamate)	22	Z
Unknown amino acid (any amino acid)	23	X
Translation stop	24	*
Gap of indeterminate length	25	-
Unknown (any integer not in table)	0 or $\geq$ 26	?

Examples

Convert an amino acid sequence from integer to letter representation.

```
s = int2aa([13 1 17 11 1 21])

s =

MATLAB
```

See Also

Bioinformatics Toolbox functions: `aa2int`, `aminolookup`, `int2nt`, `isotopicdist`, `nt2int`

Purpose

Convert nucleotide sequence from integer to letter representation

Syntax

```
SeqChar = int2nt(SeqInt)
SeqChar = int2nt(SeqInt, ...'Alphabet', AlphabetValue, ...)
SeqChar = int2nt(SeqInt, ...'Unknown', UnknownValue, ...)
SeqChar = int2nt(SeqInt, ...'Case', CaseValue, ...)
```

Arguments

SeqInt	Row vector of integers specifying a nucleotide sequence. For valid integers, see the table Mapping Nucleotide Integers to Letter Codes on page 3-809. Integers are arbitrarily assigned to IUB/IUPAC letters.
AlphabetValue	String specifying a nucleotide alphabet. Choices are: • `'DNA'` (default) — Uses the symbols `A`, `C`, `G`, and `T`. • `'RNA'` — Uses the symbols `A`, `C`, `G`, and `U`.
UnknownValue	Character to represent unknown nucleotides, that is `0` or integers ≥ `17`. Choices are any character other than the nucleotide characters `A`, `C`, `G`, `T`, and `U` and the ambiguous nucleotide characters `N`, `R`, `Y`, `K`, `M`, `S`, `W`, `B`, `D`, `H`, and `V`. Default is `*`.
CaseValue	String specifying the case of the returned character string. Choices are `'upper'` (default) or `'lower'`.

Return Values

SeqChar	Nucleotide sequence specified by a character string of codes.

Description

SeqChar = `int2nt(`*SeqInt*`)` converts *SeqInt*, a row vector of integers specifying a nucleotide sequence, to *SeqChar*, a string of codes specifying

the same nucleotide sequence. For valid codes, see the table Mapping Nucleotide Integers to Letter Codes on page 3-809.

Mapping Nucleotide Integers to Letter Codes

Nucleotide	Integer	Code
Adenosine	1	A
Cytidine	2	C
Guanine	3	G
Thymidine	4	T
Uridine (if 'Alphabet' set to 'RNA')	4	U
Purine (A or G)	5	R
Pyrimidine (T or C)	6	Y
Keto (G or T)	7	K
Amino (A or C)	8	M
Strong interaction (3 H bonds) (G or C)	9	S
Weak interaction (2 H bonds) (A or T)	10	W
Not A (C or G or T)	11	B
Not C (A or G or T)	12	D
Not G (A or C or T)	13	H
Not T or U (A or C or G)	14	V
Any nucleotide (A or C or G or T or U)	15	N
Gap of indeterminate length	16	-
Unknown (any integer not in table)	0 or ≥ 17	* (default)

SeqChar = int2nt(*SeqInt*, ...*PropertyName*', *PropertyValue*, ...) calls int2nt with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation

marks and is case insensitive. These property name/property value pairs are as follows:

SeqChar = int2nt(*SeqInt*, ...'Alphabet', *AlphabetValue*, ...) specifies a nucleotide alphabet. *AlphabetValue* can be 'DNA', which uses the symbols A, C, G, and T, or 'RNA', which uses the symbols A, C, G, and U. Default is 'DNA'.

SeqChar = int2nt(*SeqInt*, ...'Unknown', *UnknownValue*, ...) specifies the character to represent unknown nucleotides, that is 0 or integers ≥ 17. *UnknownValue* can be any character other than the nucleotide characters A, C, G, T, and U and the ambiguous nucleotide characters N, R, Y, K, M, S, W, B, D, H, and V. Default is *.

SeqChar = int2nt(*SeqInt*, ...'Case', *CaseValue*, ...) specifies the case of the returned character string. *CaseValue* can be 'upper' (default) or 'lower'.

Examples

- Convert a nucleotide sequence from integer to letter representation.

```
s = int2nt([1 2 4 3 2 4 1 3 2])

s =
ACTGCTAGC
```

- Convert a nucleotide sequence from integer to letter representation and define # as the symbol for unknown numbers 17 and greater.

```
si = [1 2 4 20 2 4 40 3 2];
s = int2nt(si, 'unknown', '#')

s =
ACT#CT#GC
```

See Also

Bioinformatics Toolbox functions: aa2int, baselookup, int2aa, nt2int

Purpose

Test for cycles in biograph object

Syntax

```
isdag(BGObj)
```

Arguments

BGObj	Biograph object created by `biograph` (object constructor).

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

`isdag(BGObj)` returns logical 1 (`true`) if an N-by-N adjacency matrix extracted from a biograph object, *`BGObj`*, is a directed acyclic graph (DAG) and logical 0 (`false`) otherwise. In the N-by-N sparse matrix, all nonzero entries indicate the presence of an edge.

References

[1] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphisdag`

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `isomorphism`, `isspantree`, `maxflow`, `minspantree`, `shortestpath`, `topoorder`, `traverse`

bioma.data.ExptData.isempty

Purpose

Determine whether ExptData object is empty

Syntax

```
TF = isempty(EDObj)
```

Description

`TF = isempty(EDObj)` returns logical `1` (`true`) if *`EDObj`* is an empty ExptData object. Otherwise, it returns logical `0` (`false`). An empty ExptData object contains no data elements.

Inputs

`EDObj`

Object of the `bioma.data.ExptData` class.

Examples

Construct an ExptData object, and then check to see if it is empty:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Determine if ExptData object is empty
isempty(EDObj)
```

See Also

`bioma.data.ExptData`

How To

- "Working with ExptData Objects"

Purpose

Determine whether MetaData object is empty

Syntax

```
TF = isempty(MDObj)
```

Description

`TF = isempty(MDObj)` returns logical `1` (`true`) if *`MDObj`* is an empty MetaData object. Otherwise, it returns logical `0` (`false`). An empty MetaData object contains no variable names, values, or descriptions.

Inputs

`MDObj`

Object of the `bioma.data.MetaData` class.

Examples

Construct a MetaData object, and then check to see if it is empty:

```
% Import bioma.data package to make constructor function
% available
import bioma.data.*
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Determine if MetaData object is empty
isempty(MDObj2)
```

See Also

`bioma.data.MetaData`

How To

- "Working with MetaData Objects"

bioma.data.MIAME.isempty

Purpose

Determine whether MIAME object is empty

Syntax

```
TF = isempty(MIAMEObj)
```

Description

`TF = isempty(MIAMEObj)` returns logical `1` (`true`) if *`MIAMEObj`* is an empty MIAME object. Otherwise, it returns logical `0` (`false`). All properties are empty in an empty MIAME object.

Inputs

`MIAMEObj`

Object of the `bioma.data.MIAME` class.

Examples

Construct a MIAME object, and then check to see if it is empty:

```
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Import bioma.data package to make constructor function
% available
import bioma.data.*
% Construct MIAME object
MIAMEObj = MIAME(geoStruct);
% Determine if MIAME object is empty
isempty(MIAMEObj)
```

See Also

`bioma.data.MIAME`

How To

- "Working with MIAME Objects"

Purpose

Test DataMatrix objects for equality

Syntax

```
TF = isequal(DMObj1, DMObj2)
TF = isequal(DMObj1, DMObj2, DMObj3, ...)
```

Arguments

DMObj1, *DMObj2*, *DMObj3*	DataMatrix objects, such as created by `DataMatrix` (object constructor).

Return Values

TF	Logical value indicating if inputs are numerically equal (have the same contents), have the same size (same `NRows` and `NCols` properties), and have the same `RowNames` and `ColNames` properties. `NaN`s are not considered equal to each other.

Description

TF = `isequal(`*DMObj1*`, `*DMObj2*`)` returns logical `1` (`true`) if the input DataMatrix objects, *DMObj1* and *DMObj2*, meet the following:

- Are numerically equal (have the same contents)
- Have the same size (same `NRows` and `NCols` properties)
- Have the same `RowNames` and `ColNames` properties

Otherwise, it returns logical `0` (`false`). *DMObj1* and *DMObj2* do not have to have the same `Name` property. `NaN`s are not considered equal to each other.

TF = `isequal(`*DMObj1*`, `*DMObj2*`, `*DMObj3*`, ...)` returns logical `1` (`true`) if all input DataMatrix objects, *DMObj1*, *DMObj2*, *DMObj3*, etc. meet the following:

- Are numerically equal (have the same contents)
- Have the same size (same `NRows` and `NCols` properties)

- Have the same `RowNames` and `ColNames` properties

Otherwise, it returns logical `0` (`false`). The input DataMatrix objects do not have to have the same `Name` property. `NaN`s are not considered equal to each other.

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox methods of a DataMatrix object: `isequalwithequalnans`

Purpose

Test DataMatrix objects for equality, treating NaNs as equal

Syntax

```
TF = isequalwithequalnans(DMObj1, DMObj2)
TF = isequalwithequalnans(DMObj1, DMObj2, DMObj3, ...)
```

Arguments

DMObj1, *DMObj2*, *DMObj3*	DataMatrix objects, such as created by `DataMatrix` (object constructor).

Return Values

TF	Logical value indicating if inputs are numerically equal (have the same contents), have the same size (same `NRows` and `NCols` properties), and have the same `RowNames` and `ColNames` properties. `NaN`s are considered equal to each other.

Description

TF = `isequalwithequalnans(`*DMObj1*`, `*DMObj2*`)` returns logical `1` (`true`) if the input DataMatrix objects, *DMObj1* and *DMObj2*, meet the following:

- Are numerically equal (have the same contents)
- Have the same size (same `NRows` and `NCols` properties)
- Have the same `RowNames` and `ColNames` properties

Otherwise, it returns logical `0` (`false`). *DMObj1* and *DMObj2* do not have to have the same `Name` property. `NaN`s are considered equal to each other.

TF = `isequalwithequalnans(`*DMObj1*`, `*DMObj2*`, `*DMObj3*`, ...)` returns logical `1` (`true`) if all input DataMatrix objects, *DMObj1*, *DMObj2*, *DMObj3*, etc. meet the following:

- Are numerically equal (have the same contents)
- Have the same size (same `NRows` and `NCols` properties)

- Have the same `RowNames` and `ColNames` properties

Otherwise, it returns logical `0` (`false`). The input DataMatrix objects do not have to have the same `Name` property. `NaN`s are considered equal to each other.

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox methods of a DataMatrix object: `isequal`

Purpose

Estimate isoelectric point for amino acid sequence

Syntax

```
pI = isoelectric(SeqAA)
[pI Charge] = isoelectric(SeqAA)
isoelectric(..., 'PropertyName', PropertyValue,...)
isoelectric(..., 'PKVals', PKValsValue)
isoelectric(..., 'Charge', ChargeValue)
isoelectric(..., 'Chart', ChartValue)
```

Arguments

SeqAA	Amino acid sequence. Enter a character string or a vector of integers from the table Mapping Amino Acid Letter Codes to Integers on page 3-2. Examples: `'ARN'` or `[1 2 3]`.
PKValsValue	Property to provide alternative pK values.
ChargeValue	Property to select a specific pH for estimating charge. Enter a number between `0` and `14`. The default value is `7.2`.
ChartValue	Property to control plotting a graph of charge versus pH. Enter `true` or `false`.

Description

`pI = isoelectric(SeqAA)` returns the estimated isoelectric point (*pI*) for an amino acid sequence. The isoelectric point is the pH at which the protein has a net charge of zero

`[pI Charge] = isoelectric(SeqAA)` returns the estimated isoelectric point (*pI*) for an amino acid sequence and the estimated charge for a given pH (default is typical intracellular pH `7.2`).

The estimates are skewed by the underlying assumptions that all amino acids are fully exposed to the solvent, that neighboring peptides have no influence on the pK of any given amino acid, and that the constitutive amino acids, as well as the N- and C-termini, are unmodified. Cysteine residues participating in disulfide bridges also affect the true pI and are not considered here. By default, `isoelectric` uses the EMBOSS amino

acid pK table, or you can substitute other values using the property `PKVals`.

- If the sequence contains ambiguous amino acid characters (b z * –), `isoelectric` ignores the characters and displays a warning message.

  ```
  Warning: Symbols other than the standard 20 amino acids
  appear in the sequence.
  ```

- If the sequence contains undefined amino acid characters (`i j o`) , `isoelectric` ignores the characters and displays a warning message.

  ```
  Warning: Sequence contains unknown characters. These will
  be ignored.
  ```

`isoelectric(..., '`*`PropertyName`*`', `*`PropertyValue`*`,...)` defines optional properties using property name/value pairs.

`isoelectric(..., 'PKVals', `*`PKValsValue`*`)` uses the alternative pK table stored in the text file *`PKValValues`*. For an example of a pK text file, see the file `Emboss.pK`.

```
N_term 8.6
K 10.8
R 12.5
H 6.5
D 3.9
E 4.1
C 8.5
Y 10.1
C_term 3.6
```

`isoelectric(..., 'Charge', `*`ChargeValue`*`)` returns the estimated charge of a sequence for a given pH (*`ChargeValue`*).

`isoelectric(..., 'Chart', `*`ChartValue`*`)` when *`ChartValue`* is `true`, returns a graph plotting the charge of the protein versus the pH of the solvent.

Example

```
% Get a sequence from PDB.
pdbSeq = getpdb('1CIV', 'SequenceOnly', true)
% Estimate its isoelectric point.
isoelectric(pdbSeq)

% Plot the charge against the pH for a short polypeptide sequence.
isoelectric('PQGGGGWGQPHGGGWGQPHGGGGWGQGGSHSQG', 'CHART', true)

% Get the Rh blood group D antigen from NCBI and calculate
% its charge at pH 7.3 (typical blood pH).
gpSeq = getgenpept('AAB39602')
[pI Charge] = isoelectric(gpSeq, 'Charge', 7.38)
```

See Also

Bioinformatics Toolbox functions: `aacount`, `molweight`

isomorphism (biograph)

Purpose

Find isomorphism between two biograph objects

Syntax

```
[Isomorphic, Map] = isomorphism(BGObj1, BGObj2)
[Isomorphic, Map] = isomorphism(BGObj1, BGObj2,'Directed',
    DirectedValue)
```

Arguments

BGObj1	Biograph object created by `biograph` (object constructor).
BGObj2	Biograph object created by `biograph` (object constructor).
DirectedValue	Property that indicates whether the graphs are directed or undirected. Enter `false` when both *BGObj1* and *BGObj2* produce undirected graphs. In this case, the upper triangles of the sparse matrices extracted from *BGObj1* and *BGObj2* are ignored. Default is `true`, meaning that both graphs are directed.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

`[`*Isomorphic*`, `*Map*`] = isomorphism(`*BGObj1*`, `*BGObj2*`)` returns logical 1 (`true`) in *Isomorphic* if two N-by-N adjacency matrices extracted from biograph objects *BGObj1* and *BGObj2* are isomorphic graphs, and logical 0 (`false`) otherwise. A graph isomorphism is a 1-to-1 mapping of the nodes in the graph from *BGObj1* and the nodes in the graph from *BGObj2* such that adjacencies are preserved. Return value *Isomorphic* is Boolean. When *Isomorphic* is `true`, *Map* is a row vector containing the node indices that map from *BGObj2* to *BGObj1*. When *Isomorphic* is `false`, the worst-case time complexity is `O(N!)`, where `N` is the number of nodes.

`[Isomorphic, Map] = isomorphism(BGObj1, BGObj2,'Directed', DirectedValue)` indicates whether the graphs are directed or undirected. Set `DirectedValue` to `false` when both `BGObj1` and `BGObj2` produce undirected graphs. In this case, the upper triangles of the sparse matrices extracted from `BGObj1` and `BGObj2` are ignored. The default is `true`, meaning that both graphs are directed.

References

[1] Fortin, S. (1996). The Graph Isomorphism Problem. Technical Report, 96-20, Dept. of Computer Science, University of Alberta, Edomonton, Alberta, Canada.

[2] McKay, B.D. (1981). Practical Graph Isomorphism. Congressus Numerantium *30*, 45-87.

[3] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphisomorphism`

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `isdag`, `isspantree`, `maxflow`, `minspantree`, `shortestpath`, `topoorder`, `traverse`

isotopicdist

Purpose

Calculate high-resolution isotope mass distribution and density function

Syntax

```
[MD, Info, DF] = isotopicdist(SeqAA)
[MD, Info, DF] = isotopicdist(Compound)
[MD, Info, DF] = isotopicdist(Formula)
isotopicdist(..., 'NTerminal', NTerminalValue, ...)
isotopicdist(..., 'CTerminal', CTerminalValue, ...)
isotopicdist(..., 'Resolution', ResolutionValue, ...)
isotopicdist(..., 'FFTResolution', FFTResolutionValue, ...)
isotopicdist(..., 'FFTRange', FFTRangeValue, ...)
isotopicdist(..., 'FFTLocation', FFTLocationValue, ...)
isotopicdist(..., 'NoiseThreshold',
NoiseThresholdValue, ...)
isotopicdist(..., 'ShowPlot', ShowPlotValue, ...)
```

Description

`[MD, Info, DF] = isotopicdist(SeqAA)` analyzes a peptide sequence and returns a matrix containing the expected mass distribution; a structure containing the monoisotopic mass, average mass, most abundant mass, nominal mass, and empirical formula; and a matrix containing the expected density function.

`[MD, Info, DF] = isotopicdist(Compound)` analyzes a compound specified by a numeric vector or matrix.

`[MD, Info, DF] = isotopicdist(Formula)` analyzes a compound specified by an empirical chemical formula represented by the structure `Formula`. The field names in `Formula` must be valid element symbols and are case sensitive. The respective values in `Formula` are the number of atoms for each element. `Formula` can also be an array of structures that specifies multiple formulas. The field names can be in any order within a structure. However, if there are multiple structures, the order must be the same in each.

`isotopicdist(..., 'PropertyName', PropertyValue, ...)` calls `isotopicdist` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each `PropertyName` in single quotation marks. Each

PropertyName is case insensitive. These property name/property value pairs are as follows:

`isotopicdist(..., 'NTerminal', NTerminalValue, ...)` modifies the N-terminal of the peptide.

`isotopicdist(..., 'CTerminal', CTerminalValue, ...)` modifies the C-terminal of the peptide.

`isotopicdist(..., 'Resolution', ResolutionValue, ...)` specifies the approximate resolution of the instrument, given as the Gaussian width (in daltons) at full width at half height (FWHH).

`isotopicdist(..., 'FFTResolution', FFTResolutionValue, ...)` specifies the number of data points per dalton, to compute the fast Fourier transform (FFT) algorithm.

`isotopicdist(..., 'FFTRange', FFTRangeValue, ...)` specifies the absolute range (window size) in daltons for the FFT algorithm and output density function.

`isotopicdist(..., 'FFTLocation', FFTLocationValue, ...)` specifies the location of the FFT range (window) defined by *FFTRangeValue*. It specifies this location by setting the location of the lower limit of the range, relative to the location of the monoisotopic peak, which is computed by `isotopicdist`.

`isotopicdist(..., 'NoiseThreshold', NoiseThresholdValue, ...)` removes points in the mass distribution that are smaller than `1/`*NoiseThresholdValue* times the most abundant mass.

`isotopicdist(..., 'ShowPlot', ShowPlotValue, ...)` controls the display of a plot of the mass distribution.

Inputs

SeqAA

Peptide sequence specified by either a:

- String of single-letter codes
- Cell array of strings that specifies multiple peptide sequences

Tip You can use the `getgenpept` and `genpeptread` functions to retrieve peptide sequences from the GenPept database or a GenPept-formatted file. You can then use the `cleave` function to perform an insilico digestion on a peptide sequence. The `cleave` function creates a cell array of strings representing peptide fragments, which you can submit to the `isotopicdist` function.

`Compound`

Compound specified by either a:

- Numeric vector of form `[C H N O S]`, where `C`, `H`, `N`, `O`, and `S` are nonnegative numbers that represent the number of atoms of carbon, hydrogen, nitrogen, oxygen, and sulfur respectively in a compound.
- M-by-5 numeric matrix that specifies multiple compounds, with each row corresponding to a compound and each column corresponding to an atom.

`Formula`

Chemical formula specified by either a:

- Structure whose field names are valid element symbols and case sensitive. Their respective values are the number of atoms for each element.
- Array of structures that specifies multiple formulas.

Note If *`Formula`* is a single structure, the order of the fields does not matter. If *`Formula`* is an array of structures, then the order of the fields must be the same in each structure.

`NTerminalValue`

Modification for the N-terminal of the peptide, specified by either:

- One of the strings `'none'`, `'amine'` (default), `'formyl'`, or `'acetyl'`
- Custom modification specified by an empirical formula, represented by a structure. The structure must have field names that are valid element symbols and case sensitive. Their respective values are the number of atoms for each element.

`CTerminalValue`

Modification for the C-terminal of the peptide, specified by either:

- One of the strings `'none'`, `'freeacid'` (default), or `'amide'`
- Custom modification specified by an empirical formula, represented by a structure. The structure must have field names that are valid element symbols and case sensitive. Their respective values are the number of atoms for each element.

`ResolutionValue`

Value in daltons specifying the approximate resolution of the instrument, given as the Gaussian width at full width half height (FWHH).

Default: `1/16` Da

`FFTResolutionValue`

Value specifying the number of data points per dalton, used to compute the FFT algorithm.

Default: `1000`

`FFTRangeValue`

Value specifying the absolute range (window size) in daltons for the FFT algorithm and output density function. By default,

this value is automatically estimated based on the weight of the molecule. The actual FFT range used internally by `isotopicdist` is further increased such that *`FFTRangeValue`* * *`FFTResolutionValue`* is a power of two.

Tip Increase the *`FFTRangeValue`* if the signal represented by the *`DF`* output appears to be truncated.

Tip Ultrahigh resolution allows you to resolve micropeaks that have the same nominal mass, but slightly different exact masses. To achieve ultrahigh resolution, increase *`FFTResolutionValue`* and reduce *`ResolutionValue`*, but ensure that *`FFTRangeValue`* * *`FFTResolutionValue`* is within the available memory.

`FFTLocationValue`

Fraction that specifies the location of the FFT range (window) defined by *`FFTRangeValue`*. It specifies this location by setting the location of the lower limit of the FFT range, relative to the location of the monoisotopic peak, which is computed by `isotopicdist`. The location of the lower limit of the FFT range is set to the mass of the monoistopic peak - (*`FFTLocationValue`* * *`FFTRangeValue`*).

Tip You may need to shift the FFT range to the left in rare cases where a compound contains an element, such as Iron or Argon, whose most abundant isotope is not the lightest one.

Default: `1/16`

`NoiseThresholdValue`

Value that removes points in the mass distribution that are smaller than `1/NoiseThresholdValue` times the most abundant mass.

Default: `1e6`

`ShowPlotValue`

Controls the display of a plot of the isotopic mass distribution. Choices are `true`, `false`, or *`I`*, which is an integer specifying a compound. If set to `true`, the first compound is plotted. Default is:

- `false` — When you specify return values.
- `true` — When you do not specify return values.

Outputs

`MD`

Mass distribution represented by a two-column matrix in which each row corresponds to an isotope. The first column lists the isotopic mass, and the second column lists the probability for that mass.

`Info`

Structure containing mass information for the peptide sequence or compound in the following fields:

- `NominalMass`
- `MonoisotopicMass`
- `ObservedAverageMass` — Estimated from the *`DF`* signal output, using instrument resolution specified by the `'Resolution'` property.
- `CalculatedAverageMass` — Calculated directly from the input formula, assuming perfect instrument resolution.
- `MostAbundantMass`

- `Formula` — Structure containing the number of atoms of each element.

DF

Density function represented by a two-column matrix in which each row corresponds to an m/z value. The first column lists the mass, and the second column lists the relative intensity of the signal at that mass.

Definitions

Average Mass

Sum of the average atomic masses of the constituent elements in a molecule.

Monoisotopic Mass

Sum of the masses of the atoms in a molecule using the unbound, ground-state, rest mass of the principle (most abundant) isotope for each element instead of the isotopic average mass.

Most Abundant Mass

Mass of the molecule with the most-highly represented isotope distribution, based on the natural abundance of the isotopes.

Nominal Mass

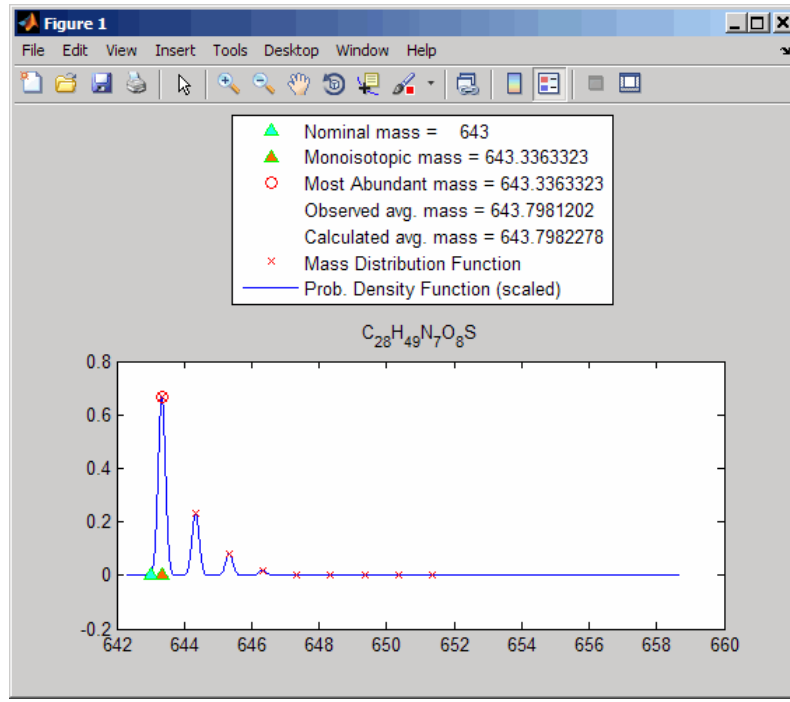
Sum of the integer masses (ignoring the mass defect) of the most abundant isotope of each element in a molecule.

Examples

Calculate and display the isotopic mass distribution of the peptide sequence `MATLAP` with an Acetyl N-terminal and an Amide C-terminal:

```
MD = isotopicdist('MATLAP','nterm','Acetyl','cterm','Amide', ...
                  'showplot',true)

MD =

  643.3363    0.6676
  644.3388    0.2306
```

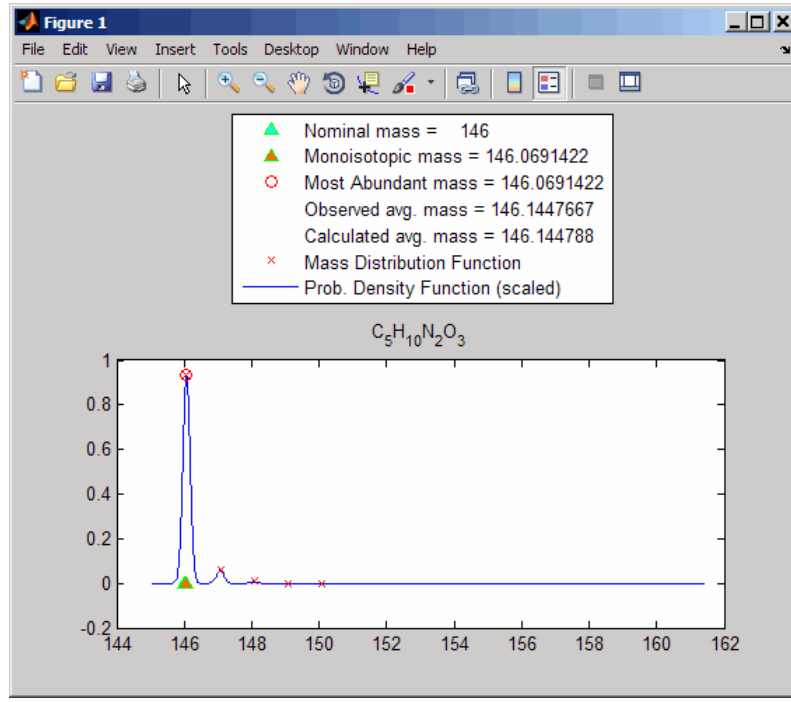
```
645.3378    0.0797
646.3386    0.0181
647.3396    0.0033
648.3409    0.0005
649.3423    0.0001
650.3439    0.0000
651.3455    0.0000
```



Calculate and display the isotopic mass distribution of Glutamine ($C_5H_{10}N_2O_3$):

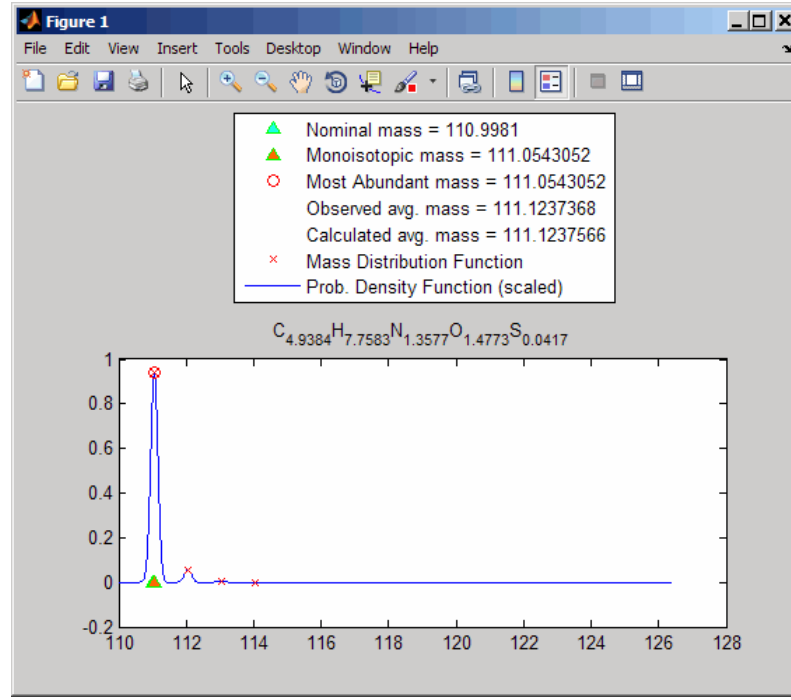
```
MD = isotopicdist([5 10 2 3 0],'showplot',true)

MD =
```

```
146.0691    0.9328
147.0715    0.0595
148.0733    0.0074
149.0755    0.0004
150.0774    0.0000
```



Display the isotopic mass distribution of the "averagine" model, whose molecular formula represents the statistical occurrences of amino acids from all known proteins:

```
isotopicdist([4.9384 7.7583 1.3577 1.4773 0.0417])
```



References

[1] Rockwood, A. L., Van Orden, S. L., and Smith, R. D. (1995). Rapid Calculation of Isotope Distributions. Anal. Chem. *67:15*, 2699–2704.

[2] Rockwood, A. L., Van Orden, S. L., and Smith, R. D. (1996). Ultrahigh Resolution Isotope Distribution Calculations. Rapid Commun. Mass Spectrum *10*, 54–59.

[3] Senko, M.W., Beu, S. C., and McLafferty, F. W. (1995). Automated assignment of charge states from resolved isotopic peaks for multiply charged ions. J. Am. Soc. Mass Spectrom. *6*, 52–56.

[4] Senko, M.W., Beu, S. C., and McLafferty, F. W. (1995). Determination of monoisotopic masses and ion populations for large

biomolecules from resolved isotopic distributions. J. Am. Soc. Mass Spectrom. *6*, 229–233.

See Also

`cleave` | `getgenpept` | `genpeptread` | `int2aa` | `nt2aa` | `aminolookup` | `cleavelookup` | `molweight`

Purpose

Determine if tree created from biograph object is spanning tree

Syntax

```
TF = isspantree(BGObj)
```

Arguments

BGObj	Biograph object created by `biograph` (object constructor).

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

TF = `isspantree(`*BGObj*`)` returns logical 1 (`true`) if the N-by-N adjacency matrix extracted from a biograph object, *BGObj*, is a spanning tree, and logical 0 (`false`) otherwise. A spanning tree must touch all the nodes and must be acyclic. The lower triangle of the N-by-N adjacency matrix represents an undirected graph, and all nonzero entries indicate the presence of an edge.

References

[1] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphisspantree`

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `isdag`, `isomorphism`, `maxflow`, `minspantree`, `shortestpath`, `topoorder`, `traverse`

jcampread

Purpose

Read JCAMP-DX-formatted files

Syntax

```
JCAMPStruct = jcampread(File)
```

Arguments

File	Either of the following: • String specifying a file name, a path and file name, or a URL pointing to a file. The referenced file is a JCAMP-DX-formatted file (ASCII text file). If you specify only a file name, that file must be on the MATLAB search path or in the current directory. • MATLAB character array that contains the text of a JCAMP-DX-formatted file.

Return Values

JCAMPStruct	MATLAB structure containing information from a JCAMP-DX-formatted file.

Description

JCAMP-DX is a file format for infrared, NMR, and mass spectrometry data from the Joint Committee on Atomic and Molecular Physical Data (JCAMP). `jcampread` supports reading data from files saved with Versions 4.24, 5, or 6 of the JCAMP-DX format. For more details, see:

```
http://www.jcamp-dx.org/
```

JCAMPStruct = `jcampread(`*File*`)` reads data from *File*, a JCAMP-DX-formatted file, and creates *JCAMPStruct*, a MATLAB structure containing the following fields.

Field
Title

Field
DataType
DataClass
Origin
Owner
Blocks
Notes

The `Blocks` field of the structure is an array of structures corresponding to each set of data in the file. These structures have the following fields.

Field
XData
YData
XUnits
YUnits
Notes

Examples

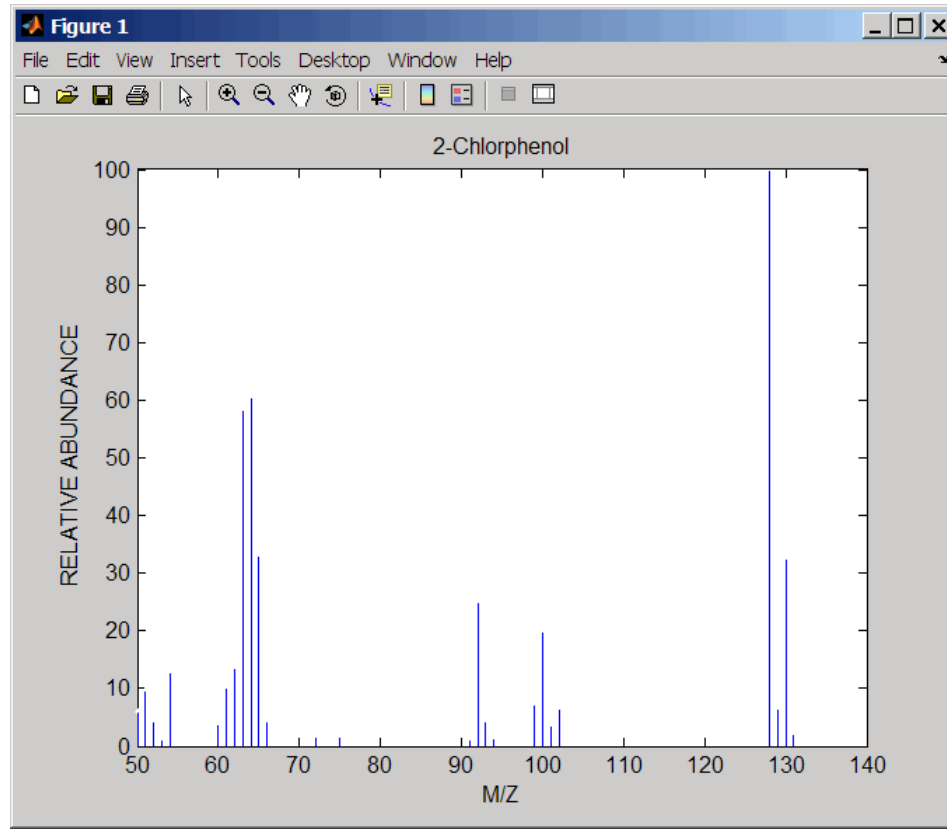
1. Download test data in the file `isa_ms1.dx` from:

   ```
   http://www.jcamp-dx.org/testdata.html
   ```

2. Read a JCAMP-DX file (`isas_ms1.dx`) into the MATLAB software and plot the mass spectrum.

   ```
   jcampStruct = jcampread('isas_ms1.dx')
   data = jcampStruct.Blocks(1);
   stem(data.XData,data.YData, '.', 'MarkerEdgeColor','w');
   title(jcampStruct.Title);
   xlabel(data.XUnits);
   ylabel(data.YUnits);
   ```

A Figure window opens with the mass spectrum.



See Also

Bioinformatics Toolbox functions: `mslowess`, `mssgolay`, `msviewer`, `mzcdfread`, `mzxmlread`, `tgspcread`

Purpose

Join two sequences to produce shortest supersequence

Syntax

```
SeqNT3 = joinseq(SeqNT1, SeqNT2)
```

Arguments

SeqNT1, *SeqNT2*	Nucleotide sequences.

Description

SeqNT3 = joinseq(*SeqNT1*, *SeqNT2*) creates a new sequence that is the shortest supersequence of *SeqNT1* and *SeqNT2*. If there is no overlap between the sequences, then *SeqNT2* is concatenated to the end of *SeqNT1*. If the length of the overlap is the same at both ends of the sequence, then the overlap at the end of *SeqNT1* and the start of *SeqNT2* is used to join the sequences.

If *SeqNT1* is a subsequence of *SeqNT2*, then *SeqNT2* is returned as the shortest supersequence and vice versa.

Examples

Join two sequences that contain an overlap.

```
seq1 = 'ACGTAAA';
seq2 = 'AAATGCA';
joined = joinseq(seq1,seq2)

joined =
    ACGTAAATGCA
```

See Also

MATLAB functions: cat, strcat, strfind

knnclassify

Purpose

Classify data using nearest neighbor method

Syntax

```
Class = knnclassify(Sample, Training, Group)
Class = knnclassify(Sample, Training, Group, k)
Class = knnclassify(Sample, Training, Group, k, distance)
Class = knnclassify(Sample, Training, Group, k, distance,
    rule)
```

Arguments

Sample	Matrix whose rows will be classified into groups. *Sample* must have the same number of columns as *Training*.
Training	Matrix used to group the rows in the matrix *Sample*. *Training* must have the same number of columns as *Sample*. Each row of *Training* belongs to the group whose value is the corresponding entry of *Group*.
Group	Vector whose distinct values define the grouping of the rows in *Training*.
k	The number of nearest neighbors used in the classification. Default is `1`.
distance	String specifying the distance metric. Choices are: • `'euclidean'` — Euclidean distance (default) • `'cityblock'` — Sum of absolute differences • `'cosine'` — One minus the cosine of the included angle between points (treated as vectors) • `'correlation'` — One minus the sample correlation between points (treated as sequences of values) • `'hamming'` — Percentage of bits that differ (suitable only for binary data)
rule	String to specify the rule used to decide how to classify the sample. Choices are:

- 'nearest' — Majority rule with nearest point tie-break (default)
- 'random' — Majority rule with random point tie-break
- 'consensus' — Consensus rule

Description

Class = knnclassify(*Sample*, *Training*, *Group*) classifies the rows of the data matrix *Sample* into groups, based on the grouping of the rows of *Training*. *Sample* and *Training* must be matrices with the same number of columns. *Group* is a vector whose distinct values define the grouping of the rows in *Training*. Each row of *Training* belongs to the group whose value is the corresponding entry of *Group*. knnclassify assigns each row of Sample to the group for the closest row of *Training*. *Group* can be a numeric vector, a string array, or a cell array of strings. *Training* and *Group* must have the same number of rows. knnclassify treats NaNs or empty strings in *Group* as missing values, and ignores the corresponding rows of *Training*. *Class* indicates which group each row of *Sample* has been assigned to, and is of the same type as *Group*.

Class = knnclassify(*Sample*, *Training*, *Group*, *k*) enables you to specify k, the number of nearest neighbors used in the classification. Default is 1.

Class = knnclassify(*Sample*, *Training*, *Group*, *k*, *distance*) enables you to specify the distance metric. Choices for *distance* are:

- 'euclidean' — Euclidean distance (default)
- 'cityblock' — Sum of absolute differences
- 'cosine' — One minus the cosine of the included angle between points (treated as vectors)
- 'correlation' — One minus the sample correlation between points (treated as sequences of values)
- 'hamming' — Percentage of bits that differ (suitable only for binary data)

Class = knnclassify(*Sample*, *Training*, *Group*, *k*, *distance*, *rule*) enables you to specify the rule used to decide how to classify the sample. Choices for *rule* are:

- 'nearest' — Majority rule with nearest point tie-break (default)
- 'random' — Majority rule with random point tie-break
- 'consensus' — Consensus rule

The default behavior is to use majority rule. That is, a sample point is assigned to the class the majority of the k nearest neighbors are from. Use 'consensus' to require a consensus, as opposed to majority rule. When using the 'consensus' option, points where not all of the k nearest neighbors are from the same class are not assigned to one of the classes. Instead the output Class for these points is NaN for numerical groups or '' for string named groups. When classifying to more than two groups or when using an even value for k, it might be necessary to break a tie in the number of nearest neighbors. Options are 'random', which selects a random tiebreaker, and 'nearest', which uses the nearest neighbor among the tied groups to break the tie. The default behavior is majority rule, with nearest tie-break.

Examples

Classifying Rows

The following example classifies the rows of the matrix sample:

```
sample = [.9 .8;.1 .3;.2 .6]

sample =
    0.9000    0.8000
    0.1000    0.3000
    0.2000    0.6000

training=[0 0;.5 .5;1 1]

training =
         0         0
    0.5000    0.5000
```

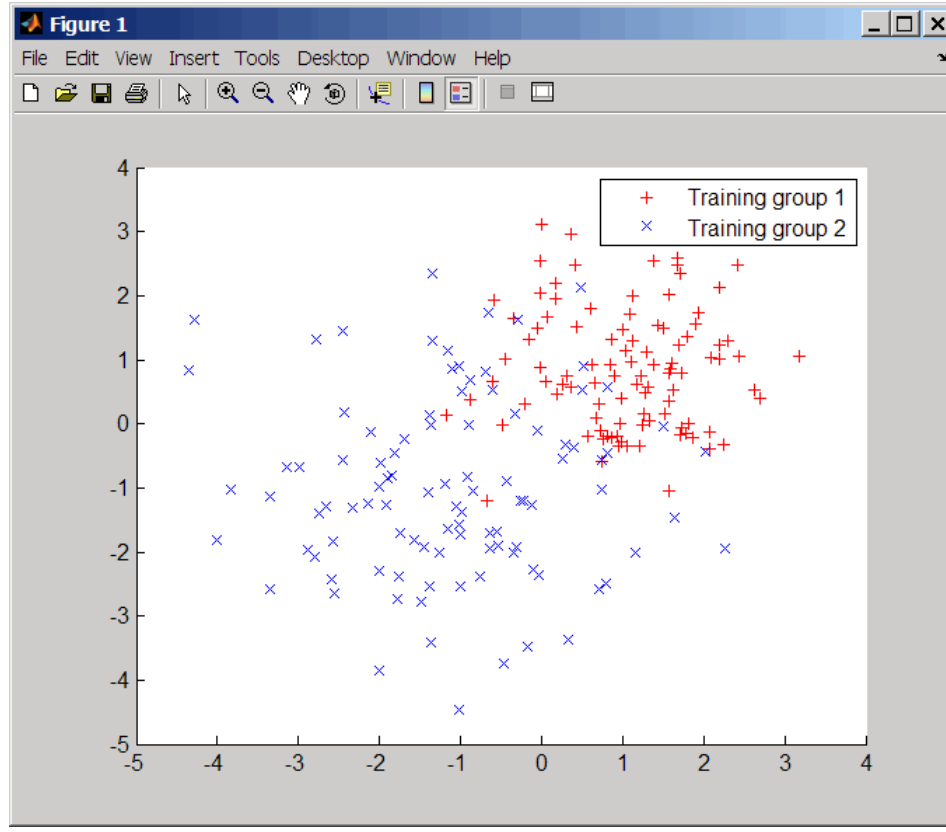
```
    1.0000    1.0000

group = [1;2;3]

group =
     1
     2
     3

class = knnclassify(sample, training, group)

class =
     3
     1
     2
```

Row 1 of `sample` is closest to row 3 of `training`, so `class(1) = 3`. Row 2 of `sample` is closest to row 1 of `training`, so `class(2) = 1`. Row 3 of `sample` is closest to row 2 of `training`, so `class(3) = 2`.

Classifying Rows into One of Two Groups

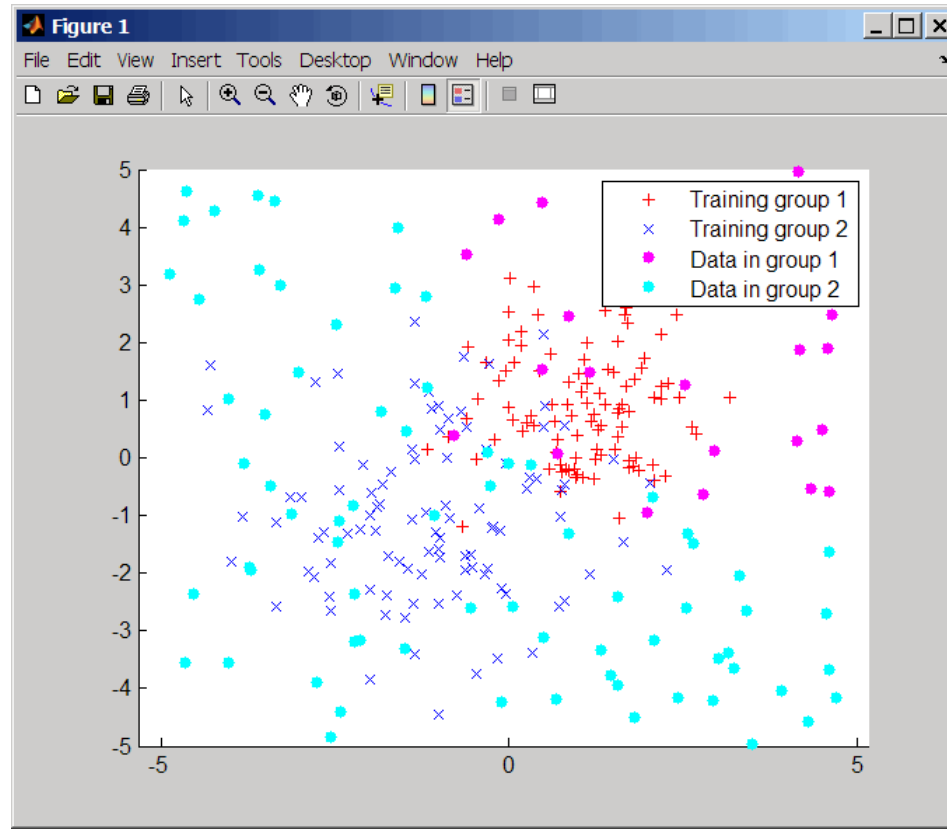
The following example classifies each row of the data in `sample` into one of the two groups in `training`. The following commands create the matrix `training` and the grouping variable `group`, and plot the rows of `training` in two groups.

```
training = [mvnrnd([ 1  1],   eye(2), 100); ...
            mvnrnd([-1 -1], 2*eye(2), 100)];
group = [repmat(1,100,1); repmat(2,100,1)];
gscatter(training(:,1),training(:,2),group,'rb','+x');
legend('Training group 1', 'Training group 2');
hold on;
```



The following commands create the matrix `sample`, classify its rows into two groups, and plot the result.

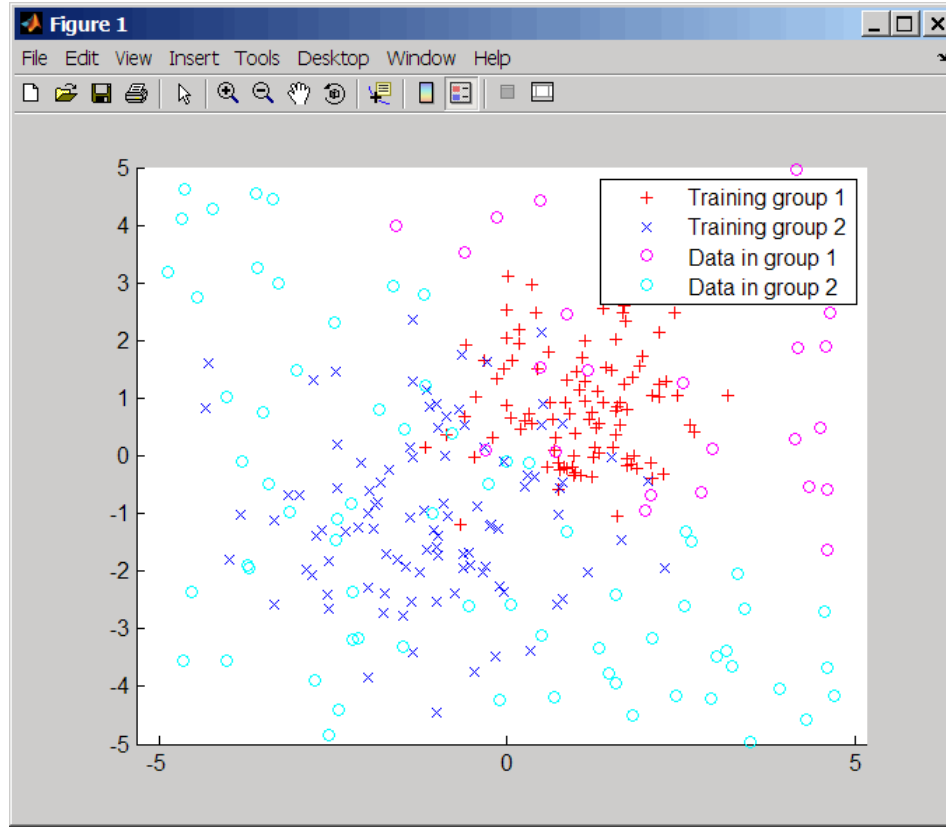
```
sample = unifrnd(-5, 5, 100, 2);
% Classify the sample using the nearest neighbor classification
c = knnclassify(sample, training, group);
gscatter(sample(:,1),sample(:,2),c,'mc'); hold on;
legend('Training group 1','Training group 2', ...
       'Data in group 1','Data in group 2');
hold off;
```



Classifying Rows Using the Three Nearest Neighbors

The following example uses the same data as in Classifying Rows into One of Two Groups on page 3-843, but classifies the rows of `sample` using three nearest neighbors instead of one.

```
gscatter(training(:,1),training(:,2),group,'rb','+x');
hold on;
c3 = knnclassify(sample, training, group, 3);
gscatter(sample(:,1),sample(:,2),c3,'mc','o');
legend('Training group 1','Training group 2','Data in group 1','Data in group 2');
```



If you compare this plot with the one in Classifying Rows into One of Two Groups on page 3-843, you see that some of the data points are classified differently using three nearest neighbors.

References

[1] Mitchell, T. (1997). Machine Learning, (McGraw-Hill).

See Also

Bioinformatics Toolbox functions: `classperf`, `crossvalind`, `knnimpute`, `svmclassify`, `svmtrain`

Statistics Toolbox function: `classify`

Purpose

Impute missing data using nearest-neighbor method

Syntax

```
knnimpute(Data)
knnimpute(Data, k)
knnimpute(..., 'Distance', DistanceValue, ...)
knnimpute(..., 'DistArgs', DistArgsValue, ...)
knnimpute(..., 'Weights', WeightsValues, ...)
knnimpute(..., 'Median', MedianValue, ...)
```

Arguments

Data

k

Description

`knnimpute(Data)` replaces `NaN`s in `Data` with the corresponding value from the nearest-neighbor column. The nearest-neighbor column is the closest column in Euclidean distance. If the corresponding value from the nearest-neighbor column is also `NaN`, the next nearest column is used.

`knnimpute(Data, k)` replaces `NaN`s in `Data` with a weighted mean of the `k` nearest-neighbor columns. The weights are inversely proportional to the distances from the neighboring columns.

`knnimpute(..., 'PropertyName', PropertyValue, ...)` calls `knnimpute` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`knnimpute(..., 'Distance', DistanceValue, ...)` computes nearest-neighbor columns using the distance metric `distfun`. The choices for *`DistanceValue`* are:

`'euclidean'`	Euclidean distance (default).
`'seuclidean'`	Standardized Euclidean distance — each coordinate in the sum of squares is inversely weighted by the sample variance of that coordinate.
`'cityblock'`	City block distance.
`'mahalanobis'`	Mahalanobis distance.
`'minkowski'`	Minkowski distance with exponent 2.
`'cosine'`	One minus the cosine of the included angle.
`'correlation'`	One minus the sample correlation between observations, treated as sequences of values.
`'hamming'`	Hamming distance — the percentage of coordinates that differ.
`'jaccard'`	One minus the Jaccard coefficient — the percentage of nonzero coordinates that differ.
`'chebychev'`	Chebychev distance (maximum coordinate difference).
function handle	A handle to a distance function, specified using `@`, for example, `@distfun`.

See `pdist` for more details.

`knnimpute(..., 'DistArgs', DistArgsValue, ...)` passes arguments (*`DistArgsValue`*) to the function `distfun`. *`DistArgsValue`* can be a single value or a cell array of values.

`knnimpute(..., 'Weights', WeightsValues, ...)` lets you specify the weights used in the weighted mean calculation. `w` should be a vector of length `k`.

`knnimpute(..., 'Median', MedianValue, ...)` when *`MedianValue`* is `true`, uses the median of the `k` nearest neighbors instead of the weighted mean.

Example 1

```
A = [1 2 5;4 5 7;NaN -1 8;7 6 0]

A =

     1     2     5
     4     5     7
   NaN    -1     8
     7     6     0
```

Note that `A(3,1) = NaN`. Because column 2 is the closest column to column 1 in Euclidean distance, `knnimpute` imputes the `(3,1)` entry of column 1 to be the corresponding entry of column 2, which is `-1`.

```
knnimpute(A)

ans =

     1     2     5
     4     5     7
    -1    -1     8
     7     6     0
```

Example 2

The following example loads the data set `yeastdata` and imputes missing values in the array `yeastvalues`:

```
load yeastdata
% Remove data for empty spots
emptySpots = strcmp('EMPTY',genes);
yeastvalues(emptySpots,:) = [];
genes(emptySpots) = [];
% Impute missing values
imputedValues = knnimpute(yeastvalues);
```

References

[1] Speed, T. (2003). Statistical Analysis of Gene Expression Microarray Data (Chapman & Hall/CRC).

[2] Hastie, T., Tibshirani, R., Sherlock, G., Eisen, M., Brown, P., and Botstein, D. (1999). “Imputing missing data for gene expression arrays”, Technical Report, Division of Biostatistics, Stanford University.

[3] Troyanskaya, O., Cantor, M., Sherlock, G., Brown, P., Hastie, T., Tibshirani, R., Botstein, D., and Altman, R. (2001). Missing value estimation methods for DNA microarrays. Bioinformatics *17(6)*, 520–525.

See Also

Statistics Toolbox function: `knnclassify`

MATLAB function: `isnan`

Statistics Toolbox functions: `nanmean`, `nanmedian`, `pdist`

Purpose

Left array divide DataMatrix objects

Syntax

```
DMObjNew = ldivide(DMObj1, DMObj2)
DMObjNew = DMObj1 .\ DMObj2
DMObjNew = ldivide(DMObj1, B)
DMObjNew = DMObj1 .\ B
DMObjNew = ldivide(B, DMObj1)
DMObjNew = B .\ DMObj1
```

Arguments

DMObj1, *DMObj2*	DataMatrix objects, such as created by `DataMatrix` (object constructor).
B	MATLAB numeric or logical array.

Return Values

DMObjNew	DataMatrix object created by left array division.

Description

DMObjNew = `ldivide(`*DMObj1*`, `*DMObj2*`)` or the equivalent *DMObjNew* = *DMObj1* `.\` *DMObj2* performs an element-by-element left array division of the DataMatrix objects *DMObj1* and *DMObj2* and places the results in *DMObjNew*, another DataMatrix object. In other words, `ldivide` divides each element in *DMObj2* by the corresponding element in *DMObj1*. *DMObj1* and *DMObj2* must have the same size (number of rows and columns), unless one is a scalar (1-by-1 DataMatrix object). The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*, unless *DMObj1* is a scalar; then they are the same as *DMObj2*.

DMObjNew = `ldivide(`*DMObj1*`, `*B*`)` or the equivalent *DMObjNew* = *DMObj1* `.\` *B* performs an element-by-element left array division of the DataMatrix object *DMObj1* and *B*, a numeric or logical array, and places the results in *DMObjNew*, another DataMatrix object. In other words, `ldivide` divides each element in *B* by the corresponding element in *DMObj1*. *DMObj1* and *B* must have the same size (number of rows and

columns), unless *B* is a scalar. The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*.

DMObjNew = ldivide(*B*, *DMObj1*) or the equivalent *DMObjNew* = *B* .\ *DMObj1* performs an element-by-element left array division of *B*, a numeric or logical array, and the DataMatrix object *DMObj1*, and places the results in *DMObjNew*, another DataMatrix object. In other words, ldivide divides each element in *DMObj1* by the corresponding element in *B*.*DMObj1* and *B* must have the same size (number of rows and columns), unless *B* is a scalar. The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*.

Note Arithmetic operations between a scalar DataMatrix object and a nonscalar array are not supported.

MATLAB calls *DMObjNew* = ldivide(*X*, *Y*) for the syntax *DMObjNew* = *X* .\ *Y* when *X* or *Y* is a DataMatrix object.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox methods of a DataMatrix object: rdivide, times

Purpose

Test DataMatrix objects for less than or equal to

Syntax

```
T = le(DMObj1, DMObj2)
T = DMObj1 <= DMObj2
T = le(DMObj1, B)
T = DMObj1 <= B
T = le(B, DMObj1)
T = B <= DMObj1
```

Arguments

DMObj1, *DMObj2*	DataMatrix objects, such as created by `DataMatrix` (object constructor).
B	MATLAB numeric or logical array.

Return Values

T	Logical matrix of the same size as *DMObj1* and *DMObj2* or *DMObj1* and *B*. It contains logical `1` (true) where elements in the first input are less than or equal to the corresponding element in the second input, and logical `0` (false) otherwise.

Description

`T = le(DMObj1, DMObj2)` or the equivalent `T = DMObj1 <= DMObj2` compares each element in DataMatrix object *DMObj1* to the corresponding element in DataMatrix object *DMObj2*, and returns *T*, a logical matrix of the same size as *DMObj1* and *DMObj2*, containing logical `1` (true) where elements in *DMObj1* are less than or equal to the corresponding element in *DMObj2*, and logical `0` (false) otherwise. *DMObj1* and *DMObj2* must have the same size (number of rows and columns), unless one is a scalar (1-by-1 DataMatrix object). *DMObj1* and *DMObj2* can have different `Name` properties.

`T = le(DMObj1, B)` or the equivalent `T = DMObj1 <= B` compares each element in DataMatrix object *DMObj1* to the corresponding element in *B*, a numeric or logical array, and returns *T*, a logical matrix of the same size as *DMObj1* and *B*, containing logical `1` (true) where elements

in *DMObj1* are less than or equal to the corresponding element in *B*, and logical 0 (false) otherwise. *DMObj1* and *B* must have the same size (number of rows and columns), unless one is a scalar.

T = le(*B*, *DMObj1*) or the equivalent *T* = *B* <= *DMObj1* compares each element in *B*, a numeric or logical array, to the corresponding element in DataMatrix object *DMObj1*, and returns *T*, a logical matrix of the same size as *B* and *DMObj1*, containing logical 1 (true) where elements in *B* are less than or equal to the corresponding element in *DMObj1*, and logical 0 (false) otherwise. *B* and *DMObj1* must have the same size (number of rows and columns), unless one is a scalar.

MATLAB calls *T* = le(*X*, *Y*) for the syntax *T* = *X* <= *Y* when *X* or *Y* is a DataMatrix object.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: ge

Purpose

Return local optimal and suboptimal alignments between two sequences

Syntax

```
AlignStruct = localalign(Seq1, Seq2)
AlignStruct = localalign(Seq1, Seq2, ...'NumAln',
   NumAlnValue, ...)
AlignStruct = localalign(Seq1, Seq2, ...'MinScore',
   MinScoreValue, ...)
AlignStruct = localalign(Seq1, Seq2, ...'Percent',
   PercentValue, ...)
AlignStruct = localalign(Seq1, Seq2, ...'DoAlignment',
   DoAlignmentValue, ...)
AlignStruct = localalign(Seq1, Seq2, ...'Alphabet',
   AlphabetValue, ...)
AlignStruct = localalign(Seq1, Seq2, ...'ScoringMatrix',
   ScoringMatrixValue, ...)
AlignStruct = localalign(Seq1, Seq2, ...'Scale',
ScaleValue,
   ...)
AlignStruct = localalign(Seq1, Seq2, ...'GapOpen',
   GapOpenValue, ...)
```

Description

`AlignStruct = localalign(Seq1, Seq2)` returns information about the first optimal (highest scoring) local alignment between two sequences in a MATLAB structure.

`AlignStruct = localalign(Seq1, Seq2, ...'PropertyName', PropertyValue, ...)` calls `localalign` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each *`PropertyName`* in single quotation marks. Each *`PropertyName`* is case insensitive. These property name/property value pairs are as follows:

`AlignStruct = localalign(Seq1, Seq2, ...'NumAln', NumAlnValue, ...)` returns information about one or more nonintersecting, local alignments (optimal and suboptimal). It limits the number of alignments to return by specifying the number of local alignments to return. It returns the alignments in decreasing order according to their score.

AlignStruct = localalign(*Seq1*, *Seq2*, ...'MinScore', *MinScoreValue*, ...) returns information about nonintersecting, local alignments (optimal and suboptimal), whose score is greater than *MinScoreValue*.

AlignStruct = localalign(*Seq1*, *Seq2*, ...'Percent', *PercentValue*, ...) returns information about one or more nonintersecting local alignments (optimal and suboptimal), whose scores are within *PercentValue* percent of the highest score. It returns the alignments in decreasing order according to their score.

AlignStruct = localalign(*Seq1*, *Seq2*, ...'DoAlignment', *DoAlignmentValue*, ...) specifies whether to include the pairwise alignments in the `Alignment` field of the output structure. Choices are `true` (default) or `false`.

AlignStruct = localalign(*Seq1*, *Seq2*, ...'Alphabet', *AlphabetValue*, ...) specifies the type of sequences. Choices are `'AA'` (default) or `'NT'`.

AlignStruct = localalign(*Seq1*, *Seq2*, ...'ScoringMatrix', *ScoringMatrixValue*, ...) specifies the scoring matrix to use for the local alignment.

AlignStruct = localalign(*Seq1*, *Seq2*, ...'Scale', *ScaleValue*, ...) specifies a scale factor applied to the output scores, thereby controlling the units of the output scores. Choices are any positive value. Default is `1`, which does not change the units of the output score.

AlignStruct = localalign(*Seq1*, *Seq2*, ...'GapOpen', *GapOpenValue*, ...) specifies the penalty for opening a gap in the alignment. Choices are any positive value. Default is `8`.

Inputs

Seq1

First amino acid or nucleotide sequence specified by any of the following:

- Character string of letters representing amino acids or nucleotides, such as returned by `int2aa` or `int2nt`
- Vector of integers representing amino acids or nucleotides, such as returned by `aa2int` or `nt2int`
- MATLAB structure containing a `Sequence` field, such as returned by `fastaread`, `fastqread`, `emblread`, `getembl`, `genbankread`, `getgenbank`, `getgenpept`, `genpeptread`, `getpdb`, `pdbread`, or `sffread`

Tip For help with letter and integer representations of amino acids and nucleotides, see Amino Acid Lookup on page 3-111 or Nucleotide Lookup on page 3-122.

`Seq2`

Second amino acid or nucleotide sequence, which `localalign` aligns with *`Seq1`*.

`NumAlnValue`

Positive scalar specifying the number of alignments to return. `localalign` returns the top *`NumAlnValue`* local, nonintersecting alignments (optimal and suboptimal). If the number of optimal alignments is greater than *`NumAlnValue`*, then `localalign` returns the first *`NumAlnValue`* alignments based on their order in the trace back matrix.

Note If you specify a *`NumAlnValue`*, you cannot specify a *`MinScoreValue`* or *`PercentValue`*.

Tip Use *NumAlnValue* to return multiple alignments when you are aligning low complexity sequences and must consider several local alignments.

Default: 1

MinScoreValue

Positive scalar specifying the minimum score of local, nonintersecting alignments (optimal and suboptimal) to return.

Note If you specify a *MinScoreValue*, you cannot specify a *NumAlnValue* or *PercentValue*.

Tip Use *MinScoreValue* to return suboptimal alignments, for example when you are interested in accounting for sequencing errors or imperfect scoring matrices.

PercentValue

Positive scalar between 0 and 100 that limits the return of local, nonintersecting alignments (optimal and suboptimal) to those alignments with a score within *PercentValue* percent of the highest score. For example, if the highest score is 10.5 and you specify 5 for *PercentValue*, then localalign determines a minimum score of 10.5 (10.5 * 0.05) = 9.975. It returns all alignments with a score of 9.975 or higher.

Note If you specify a *PercentValue*, you cannot specify a *NumAlnValue* or *MinScoreValue*.

Tip Use *PercentValue* to return optimal and suboptimal alignments when you do not know how similar the two sequences are or how well they score against a given scoring matrix.

DoAlignmentValue

Controls the inclusion of the pairwise alignments in the `Alignment` field of the output structure. Choices are `true` (default) or `false`.

AlphabetValue

String specifying the type of sequences. Choices are `'AA'` (default) or `'NT'`.

ScoringMatrixValue

Either of the following:

- String specifying the scoring matrix to use for the local alignment. Choices for amino acid sequences are:
  - `'BLOSUM62'`
  - `'BLOSUM30'` increasing by `5` up to `'BLOSUM90'`
  - `'BLOSUM100'`
  - `'PAM10'` increasing by `10` up to `'PAM500'`
  - `'DAYHOFF'`
  - `'GONNET'`

  Default is:
  - `'BLOSUM50'` — When *AlphabetValue* equals `'AA'`
  - `'NUC44'` — When *AlphabetValue* equals `'NT'`

Note The previous scoring matrices, provided with the software, also include a structure containing a scale factor that converts the units of the output score to bits. You can also use the `'Scale'` property to specify an additional scale factor to convert the output score from bits to another unit.

- Matrix representing the scoring matrix to use for the local alignment, such as returned by the `blosum`, `pam`, `dayhoff`, `gonnet`, or `nuc44` function.

Note If you use a scoring matrix that you created or was created by one of the previous functions, the matrix does not include a scale factor. The output score is returned in the same units as the scoring matrix. You can use the `'Scale'` property to specify a scale factor to convert the output score to another unit.

`ScaleValue`

Positive value that specifies a scale factor that is applied to the output scores, thereby controlling the units of the output scores.

For example, if the output score is initially determined in bits, and you enter `log(2)` for *`ScaleValue`*, then `localalign` returns *`Score`* in nats.

Default is `1`, which does not change the units of the output score.

Note If the `'ScoringMatrix'` property also specifies a scale factor, then `localalign` uses it first to scale the output score. It then applies the scale factor specified by *`ScaleValue`* to rescale the output score.

Tip Before comparing alignment scores from multiple alignments, ensure that the scores are in the same units. Use the `'Scale'` property to control the units of the output scores.

`GapOpenValue`

Positive value specifying the penalty for opening a gap in the alignment.

Default: `8`

Outputs

`AlignStruct`

MATLAB structure or array of structures containing information about the local optimal and suboptimal alignments between two sequences. Each structure represents an optimal or suboptimal alignment and contains the following fields.

Field	Description
`Score`	Score for the local optimal or suboptimal alignment.
`Start`	1-by-2 vector of indices indicating the starting point in each sequence for the alignment.
`Stop`	1-by-2 vector of indices indicating the stopping point in each sequence for the alignment.
`Alignment`	3-by-N character array showing the two sequences, *`Seq1`* and *`Seq2`*, in the first and third rows. It also shows symbols representing the optimal or suboptimal local alignment between the two sequences in the second row.

Definitions

Nonintersecting Alignments

Alignments having no matches or mismatches in common.

Optimal Alignment

An alignment with the highest score.

Suboptimal Alignment

An alignment with a score less than the highest score.

Examples

Limit the number of alignments to return between two sequences by specifying the number of alignments:

```
% Create variables containing two amino acid sequences.
Seq1 = 'VSPAGMASGYDPGKA';
Seq2 = 'IPGKATREYDVSPAG';

% Use the NumAln property to return information about the
% top three local alignments.
struct1 = localalign(Seq1, Seq2, 'numaln', 3)

struct1 =

        Score: [3x1 double]
        Start: [3x2 double]
         Stop: [3x2 double]
    Alignment: {3x1 cell}

% View the scores of the first and second alignments.
struct1.Score(1:2)

ans =

   11.0000
    9.6667

% View the first alignment.
struct1.Alignment{1}

ans =
```

```
VSPAG
|||||
VSPAG
```

Limit the number of alignments to return between two sequences by specifying a minimum score:

```
% Create variables containing two amino acid sequences.
Seq1 = 'VSPAGMASGYDPGKA';
Seq2 = 'IPGKATREYDVSPAG';

% Use the MinScore property to return information about
% only local alignments with a score greater than 8.
% Use the DoAlignment property to exclude the actual alignments.
struct2 = localalign(Seq1,Seq2,'minscore',8,'doalignment',false)

struct2 =

    Score: [2x1 double]
    Start: [2x2 double]
     Stop: [2x2 double]
```

Limit the number of alignments to return between two sequences by specifying a percentage from the maximum score:

```
% Create variables containing two amino acid sequences.
Seq1 = 'VSPAGMASGYDPGKA';
Seq2 = 'IPGKATREYDVSPAG';

% Use the Percent property to return information about only
% local alignments with a score within 15% of the maximum score.
struct3 = localalign(Seq1, Seq2, 'percent', 15)

struct3 =
```

```
         Score: [2x1 double]
         Start: [2x2 double]
          Stop: [2x2 double]
     Alignment: {2x1 cell}
```

Specify a scoring matrix and gap opening penalty when aligning two sequences:

```
% Create variables containing two nucleotide sequences.
Seq1 = 'CCAATCTACTACTGCTTGCAGTAC';
Seq2 = 'AGTCCGAGGGCTACTCTACTGAAC';

% Create a scoring matrix with a match score of 10 and a mismatch
% score of -9
sm = [10 -9 -9 -9;
      -9 10 -9 -9;
      -9 -9 10 -9;
      -9 -9 -9 10];

% Use the ScoringMatrix and GapOpen properties when returning
% information about the top three local alignments.
struct4 = localalign(Seq1, Seq2, 'alpha', 'nt', ...
         'scoringmatrix', sm, 'gapopen', 20, 'numaln', 3)

struct4 =

        Score: [3x1 double]
        Start: [3x2 double]
         Stop: [3x2 double]
    Alignment: {3x1 cell}
```

References

[1] Barton, G. (1993). An efficient algorithm to locate all locally optimal alignments between two sequences allowing for gaps. CABIOS *9*, 729–734.

[2]

See Also

`nwalign | swalign | showalignment | blosum | pam | dayhoff | gonnet | nuc44`

Tutorials

- Aligning Pairs of Sequences

How To

- "Retrieving Sequence Information from a Public Database"
- "Multiple Sequence Alignment Viewer"
- Amino Acid Lookup on page 3-111
- Nucleotide Lookup on page 3-122

Related Links

-
-
-
-

lt (DataMatrix)

Purpose

Test DataMatrix objects for less than

Syntax

```
T = lt(DMObj1, DMObj2)
T = DMObj1 < DMObj2
T = lt(DMObj1, B)
T = DMObj1 < B
T = lt(B, DMObj1)
T = B < DMObj1
```

Arguments

DMObj1, *DMObj2*	DataMatrix objects, such as created by `DataMatrix` (object constructor).
B	MATLAB numeric or logical array.

Return Values

T	Logical matrix of the same size as *DMObj1* and *DMObj2* or *DMObj1* and *B*. It contains logical `1` (true) where elements in the first input are less than the corresponding element in the second input, and logical `0` (false) otherwise.

Description

T = `lt(`*DMObj1*`, `*DMObj2*`)` or the equivalent *T* = *DMObj1* < *DMObj2* compares each element in DataMatrix object *DMObj1* to the corresponding element in DataMatrix object *DMObj2*, and returns *T*, a logical matrix of the same size as *DMObj1* and *DMObj2*, containing logical `1` (true) where elements in *DMObj1* are less than the corresponding element in *DMObj2*, and logical `0` (false) otherwise. *DMObj1* and *DMObj2* must have the same size (number of rows and columns), unless one is a scalar (1-by-1 DataMatrix object). *DMObj1* and *DMObj2* can have different `Name` properties.

T = `lt(`*DMObj1*`, `*B*`)` or the equivalent *T* = *DMObj1* < *B* compares each element in DataMatrix object *DMObj1* to the corresponding element in *B*, a numeric or logical array, and returns *T*, a logical matrix of the same size as *DMObj1* and *B*, containing logical `1` (true) where elements

in *DMObj1* are less than the corresponding element in *B*, and logical 0 (false) otherwise. *DMObj1* and *B* must have the same size (number of rows and columns), unless one is a scalar.

T = lt(*B*, *DMObj1*) or the equivalent *T* = *B* < *DMObj1* compares each element in *B*, a numeric or logical array, to the corresponding element in DataMatrix object *DMObj1*, and returns *T*, a logical matrix of the same size as *B* and *DMObj1*, containing logical 1 (true) where elements in *B* are less than the corresponding element in *DMObj1*, and logical 0 (false) otherwise. *B* and *DMObj1* must have the same size (number of rows and columns), unless one is a scalar.

MATLAB calls *T* = lt(*X*, *Y*) for the syntax *T* = *X* < *Y* when *X* or *Y* is a DataMatrix object.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: gt

maboxplot

Purpose

Create box plot for microarray data

Syntax

```
maboxplot(MAData)
maboxplot(MAData, ColumnName)
maboxplot(MAStruct, FieldName)
H = maboxplot(...)
[H, HLines] = maboxplot(...)
maboxplot(..., 'Title', TitleValue, ...)
maboxplot(..., 'Notch', NotchValue, ...)
maboxplot(..., 'Symbol', SymbolValue, ...)
maboxplot(..., 'Orientation', OrientationValue, ...)
maboxplot(..., 'WhiskerLength', WhiskerLengthValue, ...)
maboxplot(..., 'BoxPlot', BoxPlotValue, ...)
```

Arguments

MAData	DataMatrix object, numeric array, or a structure containing a field called `Data`. The values in the columns of *MAData* will be used to create box plots. If a DataMatrix object, the column names are used as labels in the box plot.
ColumnName	An array of column names corresponding to the data in *MAData* used as labels in the box plot.
MAStruct	A microarray data structure.
FieldName	A field within the microarray data structure, *MAStruct*. The values in the field *FieldName* will be used to create box plots.
TitleValue	A string to use as the title for the plot. The default title is `FieldName`.
NotchValue	Property to control the type of boxes drawn. Enter either `true` for notched boxes, or `false`, for square boxes. Default is `false`.

OrientationValue	Property to specify the orientation of the box plot. Enter `'Vertical'` or `'Horizontal'`. Default is `'Horizontal'`.
WhiskerLengthValue	Property to specify the maximum length of the whiskers as a function of the interquartile range (IQR). The whisker extends to the most extreme data value within *WhiskerLengthValue*`*IQR` of the box. Default = `1.5`. If *WhiskerLengthValue* equals `0`, then `maboxplot` displays all data values outside the box, using the plotting symbol `Symbol`.
BoxPlotValue	A cell array of property name/property value pairs to pass to the Statistics Toolbox `boxplot` function, which creates the box plot. For valid pairs, see the `boxplot` function.

Description

`maboxplot(`*MAData*`)` displays a box plot of the values in the columns of *MAData*. *MAData* can be a DataMatrix object, numeric array, or a structure containing a field called `Data`, containing microarray data.

`maboxplot(`*MAData, ColumnName*`)` labels the box plot column names.

`maboxplot(`*MAStruct, FieldName*`)` displays a box plot of the values in the field `FieldName` in the microarray data structure *MAStruct*. If *MAStruct* is block based, `maboxplot` creates a box plot of the values in the field *FieldName* for each block.

Note If you provide *MAStruct*, without providing *FieldName*, `maboxplot` uses the `Signal` element in the `ColumnNames` field of *MAStruct*, if Affymetrixdata, or the first element in the in the `ColumnNames` field of *MAStruct*, otherwise.

H `= maboxplot(...)` returns the handle of the box plot axes.

`[H, HLines] = maboxplot(...)` returns the handles of the lines used to separate the different blocks in the image.

`maboxplot(..., 'PropertyName', PropertyValue, ...)` calls `maboxplot` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`maboxplot(..., 'Title', TitleValue, ...)` allows you to specify the title of the plot. The default *`TitleValue`* is `FieldName`.

`maboxplot(..., 'Notch', NotchValue, ...)` if *`NotchValue`* is `true`, draws notched boxes. The default is `false` to show square boxes.

`maboxplot(..., 'Symbol', SymbolValue, ...)` allows you to specify the symbol used for outlier values. The default `Symbol` is `'+'`.

`maboxplot(..., 'Orientation', OrientationValue, ...)` allows you to specify the orientation of the box plot. The choices are `'Vertical'` and `'Horizontal'`. The default is `'Vertical'`.

`maboxplot(..., 'WhiskerLength', WhiskerLengthValue, ...)` allows you to specify the whisker length for the box plot. *`WhiskerLengthValue`* defines the maximum length of the whiskers as a function of the interquartile range (IQR) (default = `1.5`). The whisker extends to the most extreme data value within `WhiskerLength*IQR` of the box. If *`WhiskerLengthValue`* equals `0`, then `maboxplot` displays all data values outside the box, using the plotting symbol `Symbol`.

`maboxplot(..., 'BoxPlot', BoxPlotValue, ...)` allows you to specify arguments to pass to the `boxplot` function, which creates the box plot. *`BoxPlotValue`* is a cell array of property name/property value pairs. For valid pairs, see the `boxplot` function.

Examples

```
load yeastdata
maboxplot(yeastvalues,times);
xlabel('Sample Times');

% Using a structure
```

```
geoStruct = getgeodata('GSM1768');
maboxplot(geoStruct, 'title', 'GSM1768');

% For block-based data
madata = gprread('mouse_a1wt.gpr');
maboxplot(madata,'F635 Median','Boxplot',...
          {'Factorlabelorientation', 'horizontal'});
figure
maboxplot(madata,'F635 Median - B635','TITLE',...
          'Cy5 Channel FG - BG');
```

See Also

Bioinformatics Toolbox functions: `magetfield`, `maimage`, `mairplot`, `maloglog`, `malowess`, `manorm`, `mavolcanoplot`

Statistics Toolbox function: `boxplot`

Purpose

Estimate false discovery rate (FDR) of differentially expressed genes from two experimental conditions or phenotypes

Syntax

```
FDR = mafdr(PValues)
[FDR, Q] = mafdr(PValues)
[FDR, Q, Pi0] = mafdr(PValues)
[FDR, Q, Pi0, R2] = mafdr(PValues)
... = mafdr(PValues, ...'BHFDR', BHFDRValue, ...)
... = mafdr(PValues, ...'Lambda', LambdaValue, ...)
... = mafdr(PValues, ...'Method', MethodValue, ...)
... = mafdr(PValues, ...'Showplot', ShowplotValue, ...)
```

Arguments

PValues

Either of the following:

- Column vector of p-values for each feature (for example, gene) in a data set, such as returned by `mattest`.
- DataMatrix object containing p-values for each feature (for example, gene) in a data set, such as returned by `mattest`.

BHFDRValue

Property to control the use of the linear step-up (LSU) procedure originally introduced by Benjamini and Hochberg, 1995. Choices are `true` or `false` (default).

Note If *BHFDRValue* is set to `true`, the `Lambda` and `Method` properties are ignored.

LambdaValue Input that specifies lambda, λ, the tuning parameter used to estimate the true null hypotheses, $\hat{\pi}_0(\lambda)$. *LambdaValue* can be either:

- A single value that is `> 0` and `< 1`.
- A series of values. Each value must be `> 0` and `< 1`. There must be at least four values in the series.

> **Tip** The series of values can be expressed by a colon operator with the form `[`*`first`*`:`*`incr`*`:`*`last`*`]`, where *`first`* is the first value in the series, *`incr`* is the increment, and *`last`* is the last value in the series.

Default *LambdaValue* is the series of values `[0.01:0.01:0.95]`.

> **Note** If *LambdaValue* is set to a single value, the `Method` property is ignored.

MethodValue String that specifies a method to calculate the true null hypothesis, $\hat{\pi}_0(\lambda)$, from the tuning parameter, *LambdaValue*, when *LambdaValue* is a series of values. Choices are:

- `bootstrap` (default)

- `polynomial`

ShowplotValue Property to display two plots:

- Plot of the estimated true null hypotheses, $\hat{\pi}_0(\lambda)$, versus the tuning parameter, lambda, λ, with a cubic polynomial fitting curve
- Plot of q-values versus p-values

Choices are `true` or `false` (default).

Return Values

FDR One of the following:

- Column vector of positive FDR (pFDR) values (if *PValues* is a column vector).
- DataMatrix object containing positive FDR (pFDR) values and the same row names as *PValues* (if *PValues* is a DataMatrix object).

Q Column vector of q-values.

Pi0 Estimated true null hypothesis, $\hat{\pi}_0$.

R2 Square of the correlation coefficient.

Description

FDR = `mafdr(`*PValues*`)` computes a positive FDR (pFDR) value for each value in *PValues*, a column vector or DataMatrix object containing p-values for each gene in two microarray data sets, using a procedure introduced by Storey, 2002. *FDR* is a column vector or a DataMatrix object containing positive FDR (pFDR) values.

`[`*FDR, Q*`] = mafdr(`*PValues*`)` also returns a q-value for each p-value in *PValues*. *Q* is a column vector.

`[FDR, Q, Pi0] = mafdr(PValues)` also returns *Pi0*, the estimated true null hypothesis, $\hat{\pi}_0$, if using the procedure introduced by Storey, 2002.

`[FDR, Q, Pi0, R2] = mafdr(PValues)` also returns *R2*, the square of the correlation coefficient, if using the procedure introduced by Storey, 2002, and the `polynomial` method to calculate the true null hypothesis, $\hat{\pi}_0$, from the tuning parameter, lambda, λ.

`... = mafdr(PValues, ...'PropertyName', PropertyValue, ...)` calls `mafdr` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = mafdr(PValues, ...'BHFDR', BHFDRValue, ...)` controls the use of the linear step-up (LSU) procedure originally introduced by Benjamini and Hochberg, 1995, to computes an FDR-adjusted p-value for each value in *PValues*. Choices are `true` or `false` (default).

Note If *BHFDRValue* is set to `true`, the `Lambda` and `Method` properties are ignored.

`... = mafdr(PValues, ...'Lambda', LambdaValue, ...)` specifies lambda, λ, the tuning parameter used to estimate the true null hypotheses, $\hat{\pi}_0(\lambda)$. *LambdaValue* can be either:

- A single value that is `> 0` and `< 1`.
- A series of values. Each value must be `> 0` and `< 1`. There must be at least four values in the series.

Tip The series of values can be expressed by a colon operator with the form `[first:incr:last]`, where *`first`* is the first value in the series, *`incr`* is the increment, and *`last`* is the last value in the series.

Default *`LambdaValue`* is the series of values `[0.01:0.01:0.95]`.

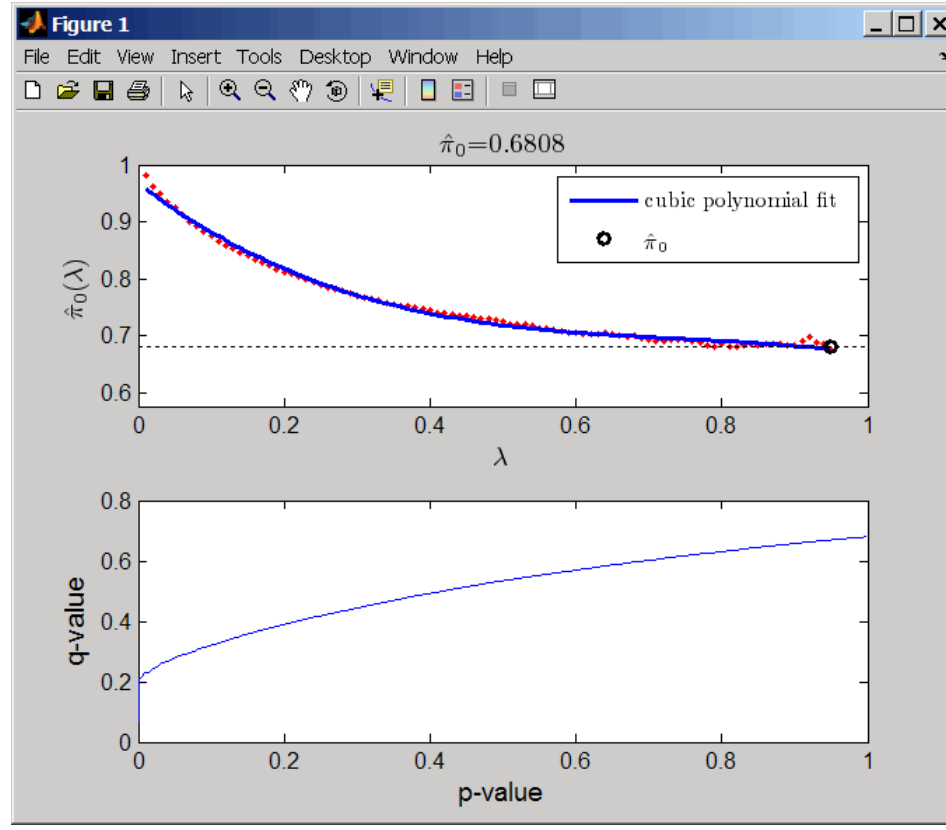
Note If *`LambdaValue`* is set to a single value, the `Method` property is ignored.

`... = mafdr(`*`PValues`*`, ...'Method', `*`MethodValue`*`, ...)` specifies a method to calculate the true null hypothesis, $\hat{\pi}_0$, from the tuning parameter, *`LambdaValue`*, when *`LambdaValue`* is a series of values. Choices are `bootstrap` (default) or `polynomial`.

`... = mafdr(`*`PValues`*`, ...'Showplot', `*`ShowplotValue`*`, ...)` controls the display of two plots:

- Plot of the estimated true null hypotheses, $\hat{\pi}_0(\lambda)$, versus the tuning parameter, lambda, with a cubic polynomial fitting curve
- Plot of q-values versus p-values

Choices are `true` or `false` (default).



Examples

1 Load the MAT-file, included with the Bioinformatics Toolbox software, that contains Affymetrix data from a prostate cancer study, specifically probe intensity data from Affymetrix HG-U133A GeneChip arrays. The two variables in the MAT-file, `dependentData` and `independentData`, are two matrices of gene expression values from two experimental conditions.

```
load prostatecancerexpdata
```

2 Use the `mattest` function to calculate p-values for the gene expression values in the two matrices.

```
pvalues = mattest(dependentData, independentData, 'permute', true);
```

3 Use the `mafdr` function to calculate positive FDR values and q-values for the gene expression values in the two matrices and plot the data.

```
[fdr, q] = mafdr(pvalues, 'showplot', true);
```

The `prostatecancerexpdata.mat` file used in this example contains data from Best et al., 2005.

References

[1] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L., Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan, W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823–6834.

[2] Storey, J.D. (2002). A direct approach to false discovery rates. Journal of the Royal Statistical Society *64(3)*, 479–498.

[3] Storey, J.D., and Tibshirani, R. (2003). Statistical significance for genomewide studies. Proc Nat Acad Sci *100(16)*, 9440–9445.

[4] Storey, J.D., Taylor, J.E., and Siegmund, D. (2004). Strong control conservative point estimation and simultaneous conservative consistency of false discovery rates: A unified approach. Journal of the Royal Statistical Society *66*, 187–205.

[5] Benjamini, Y., and Hochberg, Y. (1995). Controlling the false discovery rate: A practical and powerful approach to multiple testing. Journal of the Royal Statistical Society *57*, 289–300.

See Also

Bioinformatics Toolbox functions: `affygcrma`, `affyrma`, `gcrma`, `mairplot`, `maloglog`, `mapcaplot`, `mattest`, `mavolcanoplot`, `rmasummary`

magetfield

Purpose

Extract data from microarray structure

Syntax

```
magetfield(MAStruct, FieldName)
```

Arguments

MAStruct	Microarray structure.
FieldName	A column in *MAStruct*.

Description

`magetfield(MAStruct, FieldName)` extracts data for *FieldName*, a column in *MAStruct*, microarray structure.

The benefit of this function is to hide the details of extracting a column of data from a structure created with one of the microarray reader functions (`gprread`, `agferead`, `sptread`, `imageneread`).

Examples

```
maStruct = gprread('mouse_a1wt.gpr');
cy3data = magetfield(maStruct,'F635 Median');
cy5data = magetfield(maStruct,'F532 Median');
mairplot(cy3data,cy5data,'title','R vs G IR plot');
```

See Also

Bioinformatics Toolbox functions: `agferead`, `gprread`, `ilmnbsread`, `imageneread`, `maboxplot`, `mairplot`, `maloglog`, `malowess`, `sptread`

Purpose

Spatial image for microarray data

Syntax

```
maimage(X, FieldName)
H = maimage(...)
[H, HLines] = maimage(...)
maimage(..., 'PropertyName', PropertyValue,...)
maimage(..., 'Title', TitleValue)
maimage(..., 'ColorBar', ColorBarValue)
maimage(..., 'HandleGraphicsPropertyName' PropertyValue)
```

Arguments

X	A microarray data structure.
FieldName	A field in the microarray data structure *X*.
TitleValue	A string to use as the title for the plot. The default title is `FieldName`.
ColorBarValue	Property to control displaying a color bar in the Figure window. Enter either `true` or `false`. The default value is `false`.

Description

`maimage(X, FieldName)` displays an image of field *FieldName* from microarray data structure *X*. Microarray data can be GenPix Results (GPR) format. After creating the image, click a data point to display the value and ID, if known.

`H = maimage(...)` returns the handle of the image.

`[H, HLines] = maimage(...)` returns the handles of the lines used to separate the different blocks in the image.

`maimage(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`maimage(..., 'Title', TitleValue)` allows you to specify the title of the plot. The default title is `FieldName`.

`maimage(..., 'ColorBar', ColorBarValue)`, when *`ColorBarValue`* is `true`, a color bar is shown. If *`ColorBarValue`* is `false`, no color bar is shown. The default is for the color bar to be shown.

`maimage(..., 'HandleGraphicsPropertyName' PropertyValue)` allows you to pass optional Handle Graphics® property name/value pairs to the function. For example, a name/value pair for color could be `maimage(..., 'color' 'r')`.

Examples

```
madata = gprread('mouse_a1wt.gpr');
maimage(madata,'F635 Median');
figure;
maimage(madata,'F635 Median - B635',...
        'Title','Cy5 Channel FG - BG');
colormap hot
```

See Also

Bioinformatics Toolbox functions: `maboxplot`, `magetfield`, `mairplot`, `maloglog`, `malowess`

MATLAB function: `imagesc`

Purpose

Perform rank invariant set normalization on gene expression values from two experimental conditions or phenotypes

Syntax

```
NormDataY = mainvarsetnorm(DataX, DataY)
NormDataY = mainvarsetnorm(..., 'Thresholds',
ThresholdsValue, ...)
NormDataY = mainvarsetnorm(..., 'Exclude',
ExcludeValue, ...)
NormDataY = mainvarsetnorm(..., 'Percentile',
   PercentileValue, ...)
NormDataY = mainvarsetnorm(..., 'Iterate',
IterateValue, ...)
NormDataY = mainvarsetnorm(..., 'Method', MethodValue, ...)
NormDataY = mainvarsetnorm(..., 'Span', SpanValue, ...)
NormDataY = mainvarsetnorm(..., 'Showplot', ShowplotValue,
   ...)
```

Arguments

DataX	Vector of gene expression values from a single experimental condition or phenotype, where each row corresponds to a gene. These data points are used as the baseline.
DataY	Vector of gene expression values from a single experimental condition or phenotype, where each row corresponds to a gene. These data points will be normalized using the baseline.

ThresholdsValue Vector that sets the thresholds for the lowest average rank and the highest average rank between the two data sets. The average rank for each data point is determined by first converting the values in *DataX* and *DataY* to ranks, then averaging the two ranks for each data point. Then, the threshold for each data point is determined by interpolating between the threshold for the lowest average rank and the threshold for the highest average rank.

Note These individual thresholds are used to determine the rank invariant set, which is a set of data points, each having a proportional rank difference (prd) smaller than its predetermined threshold. For more information on the rank invariant set, see "Description" on page 3-886.

ThresholdsValue is a 1-by-2 vector [*LT, HT*], where *LT* is the threshold for the lowest average rank and *HT* is threshold for the highest average rank. Select these two thresholds empirically to limit the spread of the invariant set, but allow enough data points to determine the normalization relationship. Values must be between `0` and `1`. Default is [`0.03, 0.07`].

ExcludeValue Property to filter the invariant set of data points, by excluding the data points whose average rank (between *DataX* and *DataY*) is in the highest *N* ranked averages or lowest *N* ranked averages.

PercentileValue Property to stop the iteration process when the number of data points in the invariant set reaches *N* percent of the total number of input data points. Default is `1`.

Note If you do not use this property, the iteration process continues until no more data points are eliminated.

IterateValue Property to control the iteration process for determining the invariant set of data points. Enter `true` to repeat the process until either no more data points are eliminated, or a predetermined percentage of data points (*PercentileValue*) is reached. Enter `false` to perform only one iteration of the process. Default is `true`.

Tip Select `false` for smaller data sets, typically less than 200 data points.

MethodValue Property to select the smoothing method used to normalize the data. Enter `'lowess'` or `'runmedian'`. Default is `'lowess'`.

SpanValue	Property to set the window size for the smoothing method. If *SpanValue* is less than 1, the window size is that percentage of the number of data points. If *SpanValue* is equal to or greater than 1, the window size is of size *SpanValue*. Default is `0.05`, which corresponds to a window size equal to 5% of the total number of data points in the invariant set.
ShowplotValue	Property to control the plotting of a pair of M-A scatter plots (before and after normalization). M is the ratio between *DataX* and *DataY*. A is the average of *DataX* and *DataY*. Enter `true` to create the pair of M-A scatter plots. Default is `false`.

Description

NormDataY = `mainvarsetnorm(`*DataX, DataY*`)` normalizes the values in *DataY*, a vector of gene expression values, to a reference vector, *DataX*, using the invariant set method. *NormDataY* is a vector of normalized gene expression values from *DataY*.

Specifically, `mainvarsetnorm`:

- Determines the proportional rank difference (*prd*) for each pair of ranks, *RankX* and *RankY*, from the two vectors of gene expression values, *DataX* and *DataY*.

  prd = abs(*RankX* - *RankY*)

- Determines the invariant set of data points by selecting data points whose proportional rank differences (*prd*) are below *threshold*, which is a predetermined threshold for a given data point (defined by the *ThresholdsValue* property). It optionally repeats the process until either no more data points are eliminated, or a predetermined percentage of data points is reached.

  The invariant set is data points with a *prd* < *threshold*.

- Uses the invariant set of data points to calculate the lowess or running median smoothing curve, which is used to normalize the data in *DataY*.

Note If *DataX* or *DataY* contains NaN values, then *NormDataY* will also contain NaN values at the corresponding positions.

Tip `mainvarsetnorm` is useful for correcting for dye bias in two-color microarray data.

NormDataY = `mainvarsetnorm(..., '`*PropertyName*`',` *PropertyValue*`, ...)` calls `mainvarsetnorm` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

NormDataY = `mainvarsetnorm(..., 'Thresholds',` *ThresholdsValue*`, ...)` sets the thresholds for the lowest average rank and the highest average rank between the two data sets. The average rank for each data point is determined by first converting the values in *DataX* and *DataY* to ranks, then averaging the two ranks for each data point. Then, the threshold for each data point is determined by interpolating between the threshold for the lowest average rank and the threshold for the highest average rank.

Note These individual thresholds are used to determine the rank invariant set, which is a set of data points, each having a proportional rank difference (prd) smaller than its predetermined threshold. For more information on the rank invariant set, see “Description” on page 3-886.

ThresholdsValue is a 1-by-2 vector [*LT, HT*], where *LT* is the threshold for the lowest average rank and *HT* is threshold for the highest average rank. Select these two thresholds empirically to limit the spread of the invariant set, but allow enough data points to determine the normalization relationship. Values must be between `0` and `1`. Default is [`0.03, 0.07`].

NormDataY = `mainvarsetnorm(..., 'Exclude', ` *ExcludeValue*`, ...)` filters the invariant set of data points, by excluding the data points whose average rank (between *DataX* and *DataY*) is in the highest *N* ranked averages or lowest *N* ranked averages.

NormDataY = `mainvarsetnorm(..., 'Percentile',` *PercentileValue*`, ...)` stops the iteration process when the number of data points in the invariant set reaches *N* percent of the total number of input data points. Default is `1`.

Note If you do not use this property, the iteration process continues until no more data points are eliminated.

NormDataY = `mainvarsetnorm(..., 'Iterate',` *IterateValue*`, ...)` controls the iteration process for determining the invariant set of data points. When *IterateValue* is `true`, `mainvarsetnorm` repeats the process until either no more data points are eliminated, or a predetermined percentage of data points (*PercentileValue*) is reached. When *IterateValue* is `false`, performs only one iteration of the process. Default is `true`.

Tip Select `false` for smaller data sets, typically less than 200 data points.

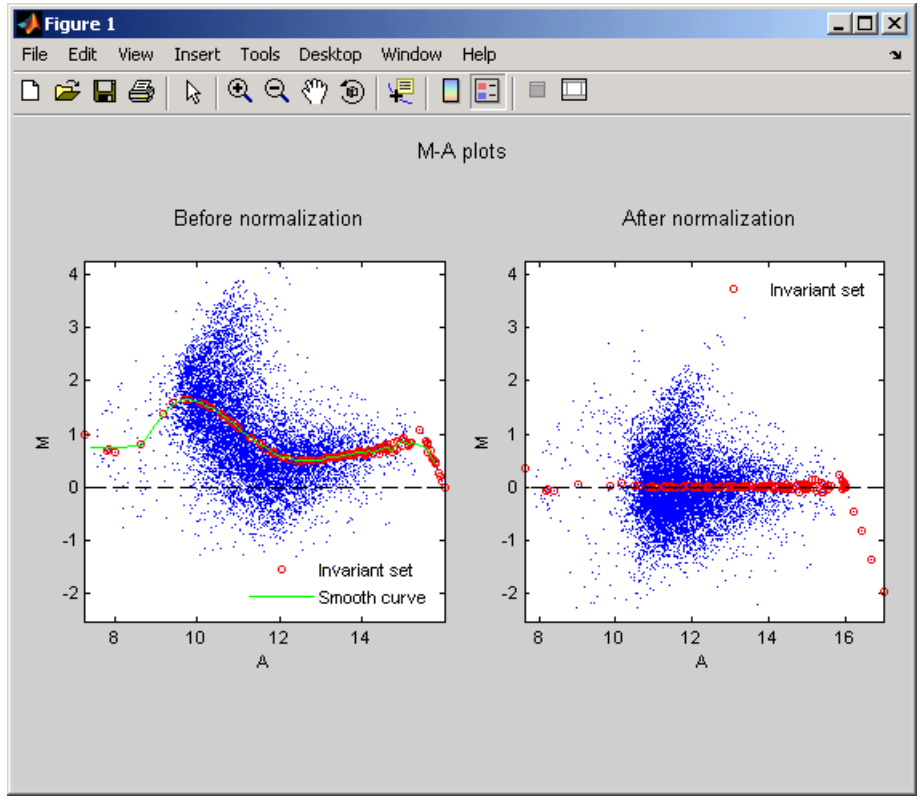
NormDataY = `mainvarsetnorm(..., 'Method',` *MethodValue*`, ...)` selects the smoothing method for normalizing the data. When *MethodValue* is `'lowess'`, `mainvarsetnorm` uses the lowess method.

When *MethodValue* is 'runmedian', mainvarsetnorm uses the running median method. Default is 'lowess'.

NormDataY = mainvarsetnorm(..., 'Span', *SpanValue*, ...) sets the window size for the smoothing method. If *SpanValue* is less than 1, the window size is that percentage of the number of data points. If *SpanValue* is equal to or greater than 1, the window size is of size *SpanValue*. Default is 0.05, which corresponds to a window size equal to 5% of the total number of data points in the invariant set.

NormDataY = mainvarsetnorm(..., 'Showplot', *ShowplotValue*, ...) determines whether to plot a pair of M-A scatter plots (before and after normalization). M is the ratio between *DataX* and *DataY*. A is the average of *DataX* and *DataY*. When *ShowplotValue* is true, mainvarsetnorm plots the M-A scatter plots. Default is false.

The following example illustrates how mainvarsetnorm can correct for dye bias or scanning differences between two channels of data from a two-color microarray experiment. Under perfect experimental conditions, data points with equal expression values would fall along the M = 0 line, which represents a gene expression ratio of 1. However, dye bias caused the measured values in one channel to be higher than the other channel, as seen in the Before Normalization plot. Normalization corrected the variance, as seen in the After Normalization plot.



Examples

The following example extracts data from a GPR file and creates two column vectors of gene expression values from different experimental conditions. It then normalizes one of the data sets.

```
maStruct = gprread('mouse_a1wt.gpr');
cy3data = magetfield(maStruct, 'F635 Median');
cy5data = magetfield(maStruct, 'F532 Median');
Normcy5data = mainvarsetnorm(cy3data, cy5data);
```

References

[1] Tseng, G.C., Oh, Min-Kyu, Rohlin, L., Liao, J.C., and Wong, W.H. (2001) Issues in cDNA microarray analysis: quality filtering, channel

normalization, models of variations and assessment of gene effects. Nucleic Acids Research. *29*, 2549-2557.

[2] Hoffmann, R., Seidl, T., and Dugas, M. (2002) Profound effect of normalization on detection of differentially expressed genes in oligonucleotide microarray data analysis. Genome Biology. *3(7)*: research 0033.1-0033.11.

See Also

`affyinvarsetnorm`, `malowess`, `manorm`, `quantilenorm`

mairplot

Purpose

Create intensity versus ratio scatter plot of microarray data

Syntax

```
mairplot(DataX, DataY)
[Intensity, Ratio] = mairplot(DataX, DataY)
[Intensity, Ratio, H] = mairplot(DataX, DataY)
... = mairplot(..., 'Type', TypeValue, ...)
... = mairplot(..., 'LogTrans', LogTransValue, ...)
... = mairplot(..., 'FactorLines', FactorLinesValue, ...)
... = mairplot(..., 'Title', TitleValue, ...)
... = mairplot(..., 'Labels', LabelsValue, ...)
... = mairplot(..., 'Normalize', NormalizeValue, ...)
... = mairplot(..., 'LowessOptions', LowessOptionsValue, ...)
... = mairplot(..., 'Showplot', ShowplotValue, ...)
... = mairplot(..., 'PlotOnly', PlotOnlyValue, ...)
```

Arguments

DataX, *DataY*	DataMatrix object or vector of gene expression values where each row corresponds to a gene. For example, in a two-color microarray experiment, *DataX* could be cy3 intensity values and *DataY* could be cy5 intensity values.
TypeValue	String that specifies the plot type. Choices are `'IR'` (plots $\log_{10}$ of the product of the *DataX* and *DataY* intensities versus $\log_2$ of the intensity ratios) or `'MA'` (plots (1/2)$\log_2$ of the product of the *DataX* and *DataY* intensities versus $\log_2$ of the intensity ratios). Default is `'IR'`.
LogTransValue	Controls the conversion of data in *X* and *Y* from natural scale to $\log_2$ scale. Set *LogTransValue* to `false`, when the data is already $\log_2$ scale. Default is `true`, which assumes the data is natural scale.

FactorLinesValue Adds lines to the plot showing a factor of *N* change. Default is 2, which corresponds to a level of 1 and -1 on a $\log_2$ scale.

Tip You can also change the factor lines interactively, after creating the plot.

TitleValue String that specifies a title for the plot.

LabelsValue Cell array of labels for the data. If labels are defined, then clicking a point on the plot shows the label corresponding to that point.

NormalizeValue Controls the display of lowess normalized ratio values. Enter `true` to display to lowess normalized ratio values. Default is `false`.

Tip You can also normalize the data from the MAIR Plot window, after creating the plot.

LowessOptionsValue Cell array of one, two, or three property name/value pairs in any order that affect the lowess normalization. Choices for property name/value pairs are:

- `'Order'`, *OrderValue*
- `'Robust'`, *RobustValue*
- `'Span'`, *SpanValue*

For more information on the preceding property name/value pairs, see `malowess`.

ShowplotValue Controls the display of the scatter plot. Choices are `true` (default) or `false`.

PlotOnlyValue Controls the display of the scatter plot without user interface components. Choices are `true` or `false` (default).

Note If you set the `'PlotOnly'` property to `true`, you can still display labels for data points by clicking a data point, and you can still adjust the horizontal fold change lines by click-dragging the lines.

Return Values

Intensity DataMatrix object or vector containing intensity values for the microarray gene expression data, calculated as:

- $\log_{10}$ of the product of the *DataX* and *DataY* intensities (when `Type` is `'IR'`)
- $(1/2)\log_2$ of the product of the *DataX* and *DataY* intensities (when `Type` is `'MA'`)

Note If *DataX* or *DataY* is a DataMatrix object, then *Intensity* is also a DataMatrix object with the same properties.

Ratio DataMatrix object or vector containing ratios of the microarray gene expression data, calculated as `log2(`*DataX*`./`*DataY*`)`.

Note If *DataX* or *DataY* is a DataMatrix object, then *Ratio* is also a DataMatrix object with the same properties.

H	Handle of the plot.

Description

`mairplot(`*DataX*`, `*DataY*`)` creates a scatter plot that plots $\log_{10}$ of the product of the *DataX* and *DataY* intensities versus $\log_2$ of the intensity ratios.

`[`*Intensity*`, `*Ratio*`] = mairplot(`*DataX*`, `*DataY*`)` returns the intensity and ratio values. If you set `'Normalize'` to `true`, the returned ratio values are normalized.

`[`*Intensity*`, `*Ratio*`, `*H*`] = mairplot(`*DataX*`, `*DataY*`)` returns the handle of the plot.

... `= mairplot(..., '`*PropertyName*`', `*PropertyValue*`, ...)` calls `mairplot` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

... `= mairplot(..., 'Type', `*TypeValue*`, ...)` specifies the plot type. Choices are `'IR'` (plots $\log_{10}$ of the product of the *DataX* and *DataY* intensities versus $\log_2$ of the intensity ratios) or `'MA'` (plots $(1/2)\log_2$ of the product of the *DataX* and *DataY* intensities versus $\log_2$ of the intensity ratios). Default is `'IR'`.

... `= mairplot(..., 'LogTrans', `*LogTransValue*`, ...)` controls the conversion of data in *X* and *Y* from natural to log $_2$ scale. Set *LogTransValue* to `false`, when the data is already log $_2$ scale. Default is `true`, which assumes the data is natural scale.

... `= mairplot(..., 'FactorLines', `*FactorLinesValue*`, ...)` adds lines to the plot showing a factor of *N* change. Default is 2, which corresponds to a level of 1 and -1 on a $\log_2$ scale.

Tip You can also change the factor lines interactively, after creating the plot.

`... = mairplot(..., 'Title', TitleValue, ...)` specifies a title for the plot.

`... = mairplot(..., 'Labels', LabelsValue, ...)` specifies a cell array of labels for the data. If labels are defined, then clicking a point on the plot shows the label corresponding to that point.

`... = mairplot(..., 'Normalize', NormalizeValue, ...)` controls the display of lowess normalized ratio values. Enter `true` to display to lowess normalized ratio values. Default is `false`.

Tip You can also normalize the data from the MAIR Plot window, after creating the plot.

`... = mairplot(..., 'LowessOptions', LowessOptionsValue, ...)` lets you specify up to three property name/value pairs (in any order) that affect the lowess normalization. Choices for property name/value pairs are:

- `'Order', OrderValue`
- `'Robust', RobustValue`
- `'Span', SpanValue`

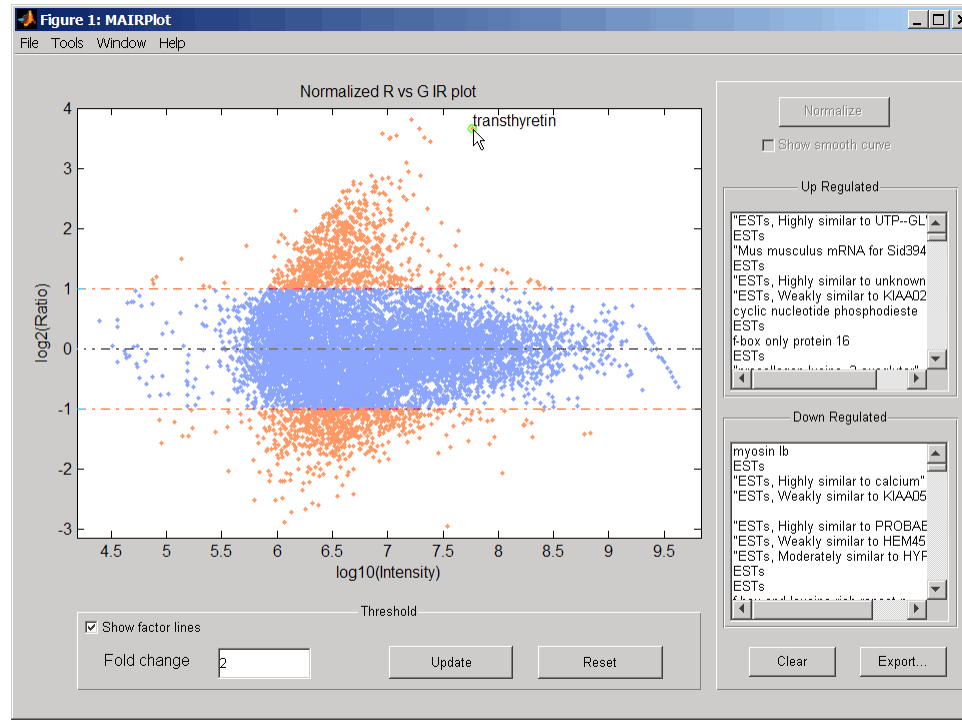
For more information on the previous three property name/value pairs, see the `malowess` function.

`... = mairplot(..., 'Showplot', ShowplotValue, ...)` controls the display of the scatter plot. Choices are `true` (default) or `false`.

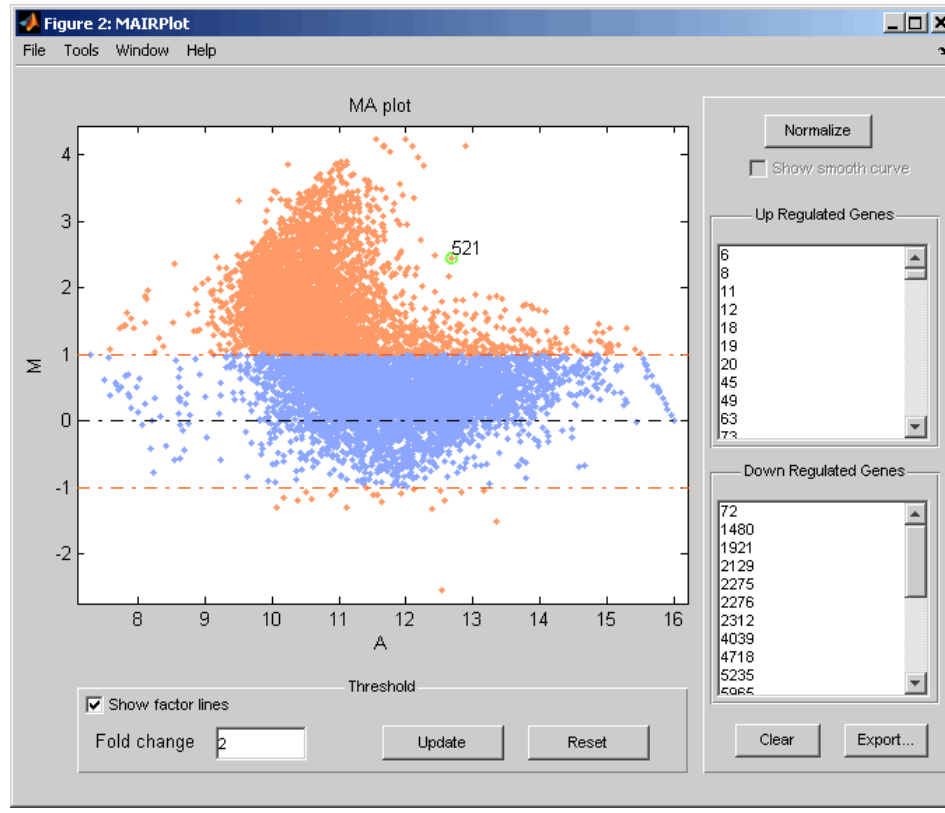
`...  = mairplot(..., 'PlotOnly', PlotOnlyValue, ...)` controls the display of the scatter plot without user interface components. Choices are `true` or `false` (default).

Note If you set the `'PlotOnly'` property to `true`, you can still display labels for data points by clicking a data point, and you can still adjust the horizontal fold change lines by click-dragging the lines.

Following is an IR plot of normalized data.



Following is an MA plot of unnormalized data.



The intensity versus ratio scatter plot displays the following:

- $\log_{10}$ (Intensity) versus $\log_2$ (Ratio) scatter plot of genes.
- Two horizontal fold change lines at a fold change level of 2, which corresponds to a ratio of 1 and –1 on a $\log_2$ (Ratio) scale. (Lines will be at different fold change levels, if you used the `'FactorLines'` property.)
- Data points for genes that are considered differentially expressed (outside of the fold change lines) appear in orange.

After you display the intensity versus ratio scatter plot, you can interactively do the following:

- Adjust the horizontal fold change lines by click-dragging one line or entering a value in the **Fold Change** text box, then clicking **Update**.
- Display labels for data points by clicking a data point.
- Select a gene from the **Up Regulated** or **Down Regulated** list to highlight the corresponding data point in the plot. Press and hold **Ctrl** or **Shift** to select multiple genes.
- Zoom the plot by selecting **Tools > Zoom In** or **Tools > Zoom Out**.
- View lists of significantly up-regulated and down-regulated genes, and optionally, export the gene labels and indices to a structure in the MATLAB Workspace by clicking **Export**.
- Normalize the data by clicking the **Normalize** button, then selecting whether to show the normalized plot in a separate window. If you show the normalized plot in a separate window, the **Show smooth curve** check box becomes available in the original (unnormalized) plot.

Tip To select different lowess normalization options before normalizing, select **Tools > Set LOWESS Normalization Options**, then enter options in the Options for LOWESS dialog box.

Examples

1 Use the `gprread` function to create a structure containing microarray data.

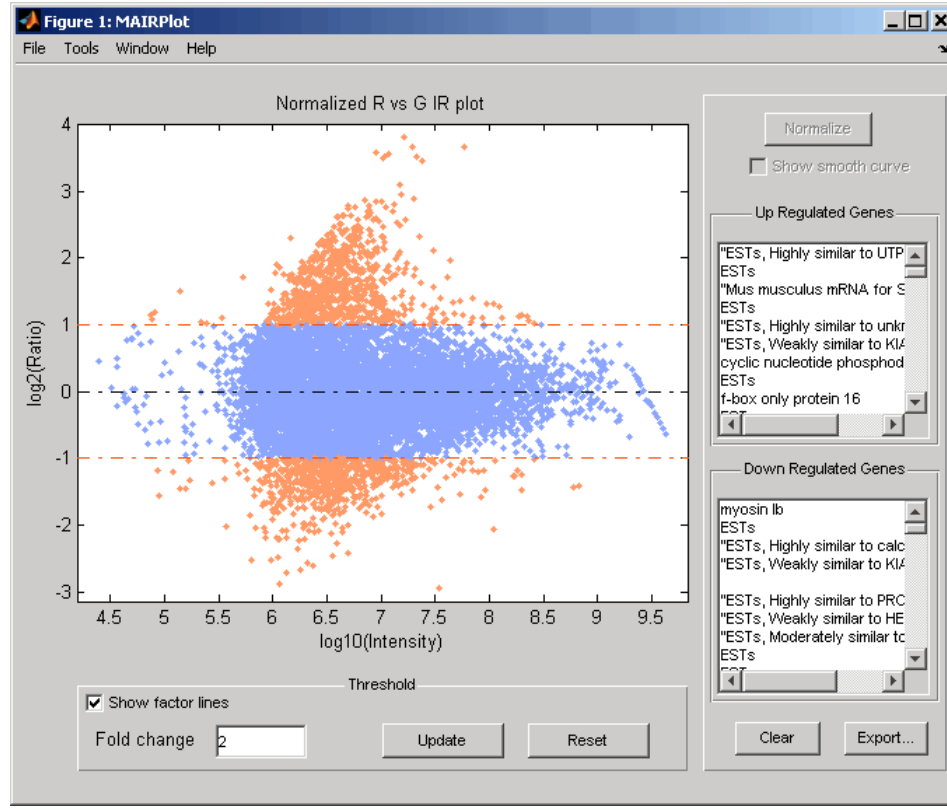
```
maStruct = gprread('mouse_a1wt.gpr');
```

2 Use the `magetfield` function to extract the green (cy3) and red (cy5) signals from the structure.

```
cy3data = magetfield(maStruct,'F635 Median');
cy5data = magetfield(maStruct,'F532 Median');
```

3 Create an intensity versus ratio scatter plot of the cy3 and cy5 data. Normalize the data and add a title and labels:

```
mairplot(cy3data, cy5data, 'Normalize', true, ...
    'Title','Normalized R vs G IR plot', ...
    'Labels', maStruct.Names)
```

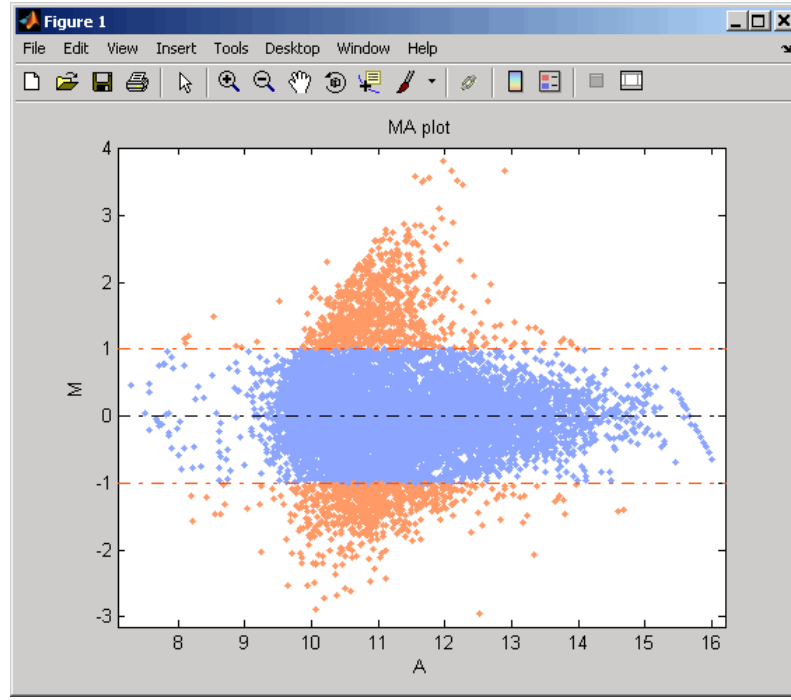


4 Return intensity values and ratios without displaying the plot.

```
[intensities, ratios] = mairplot(cy3data, cy5data, 'Showplot', false);
```

5 Create a normalized MA plot of the cy3 and cy5 data without the user interface components.

```
mairplot(cy3data, cy5data, 'Normalize', true, ...
    'Type','MA','PlotOnly',true)
```



References

[1] Quackenbush, J. (2002). Microarray Data Normalization and Transformation. Nature Genetics *Suppl. 32*, 496–501.

[2] Dudoit, S., Yang, Y.H., Callow, M.J., and Speed, T.P. (2002). Statistical Methods for Identifying Differentially Expressed Genes in Replicated cDNA Microarray Experiments. Statistica Sinica *12*, 111–139.

See Also

Bioinformatics Toolbox functions: `maboxplot`, `magetfield`, `maimage`, `mainvarsetnorm`, `maloglog`, `malowess`, `manorm`, `mattest`, `mavolcanoplot`

Purpose

Create loglog plot of microarray data

Syntax

```
maloglog(X, Y)
maloglog(X, Y, ...'FactorLines', N, ...)
maloglog(X, Y, ...'Title', TitleValue, ...)
maloglog(X, Y, ...'Labels', LabelsValues, ...)
maloglog(X, Y, ...'HandleGraphicsName', HGValue, ...)
H = maloglog(...)
```

Arguments

X, *Y*	DataMatrix object or numeric array of microarray expression values from a single experimental condition.
N	Property to add two lines to the plot showing a factor of *N* change.
TitleValue	A string to use as the title for the plot.
LabelsValue	A cell array of labels for the data in *X* and *Y*. If you specify *LabelsValue*, then clicking a data point in the plot shows the label corresponding to that point.

Description

`maloglog(X, Y)` creates a loglog scatter plot of *X* versus *Y*. *X* and *Y* are DataMatrix objects or numeric arrays of microarray expression values from two different experimental conditions.

`maloglog(X, Y, ...'PropertyName', PropertyValue, ...)` calls `maloglog` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`maloglog(X, Y, ...'FactorLines', N, ...)` adds two lines to the plot showing a factor of *N* change.

`maloglog(X, Y, ...'Title', TitleValue, ...)` allows you to specify a title for the plot.

`maloglog(X, Y, ...'Labels', LabelsValues, ...)` allows you to specify a cell array of labels for the data. If `LabelsValues` is defined, then clicking a data point in the plot shows the label corresponding to that point.

`maloglog(X, Y, ...'HandleGraphicsName', HGValue, ...)` allows you to pass optional Handle Graphics property name/property value pairs to the function.

`H = maloglog(...)` returns the handle to the plot.

Examples

```
maStruct = gprread('mouse_a1wt.gpr');
Red = magetfield(maStruct,'F635 Median');
Green = magetfield(maStruct,'F532 Median');
maloglog(Red,Green,'title','Red vs Green');
% Add factorlines and labels
figure
maloglog(Red,Green,'title','Red vs Green',...
                'FactorLines',2,'LABELS',maStruct.Names);
% Now create a normalized plot
figure
maloglog(manorm(Red),manorm(Green),'title',...
                'Normalized Red vs Green','FactorLines',2,...
                'LABELS',maStruct.Names);
```

See Also

Bioinformatics Toolbox functions: `maboxplot`, `magetfield`, `mainvarsetnorm`, `maimage`, `mairplot`, `malowess`, `manorm`, `mattest`, `mavolcanoplot`

MATLAB function: `loglog`

Purpose

Smooth microarray data using Lowess method

Syntax

```
YSmooth = malowess(X, Y)
YSmooth = malowess(X, Y, ...'Order', OrderValue, ...)
YSmooth = malowess(X, Y, ...'Robust', RobustValue, ...)
YSmooth = malowess(X, Y, ...'Span', SpanValue, ...)
```

Arguments

X, *Y*	DataMatrix object or numeric vector containing scatter data.
OrderValue	Property to select the order of the algorithm. Enter either `1` (linear fit) or `2` (quadratic fit). The default order is `1`.
RobustValue	Property to select a robust fit. Enter either `true` or `false`.
SpanValue	Property to specify the window size. The default value is `0.05` (5% of total points in *X*)

Description

YSmooth = `malowess(`*X*`, `*Y*`)` smooths scatter data in *X* and *Y* using the Lowess smoothing method. The default window size is 5% of the length of *X*. *YSmooth* is a numeric vector or, if *Y* is a DataMatrix object, also a DataMatrix object with the same properties as *Y*.

YSmooth = `malowess(`*X*`, `*Y*`, ...'`*PropertyName*`', `*PropertyValue*`, ...)` calls `malowess` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

YSmooth = `malowess(`*X*`, `*Y*`, ...'Order', `*OrderValue*`, ...)` chooses the order of the algorithm. Note that the Curve Fitting Toolbox™ software refers to Lowess smoothing of order `2` as Loess smoothing.

YSmooth = malowess(*X*, *Y*, ...'Robust', *RobustValue*, ...) uses a robust fit when *RobustValue* is set to true. This option can take a long time to calculate.

YSmooth = malowess(*X*, *Y*, ...'Span', *SpanValue*, ...) modifies the window size for the smoothing function. If *SpanValue* is less than 1, the window size is taken to be a fraction of the number of points in the data. If *SpanValue* is greater than 1, the window is of size *SpanValue*.

Examples

```
maStruct = gprread('mouse_a1wt.gpr');
cy3data = magetfield(maStruct, 'F635 Median');
cy5data = magetfield(maStruct, 'F532 Median');
[x,y] = mairplot(cy3data, cy5data);
drawnow
ysmooth = malowess(x,y);
hold on;
plot(x, ysmooth, 'rx')
ynorm = y - ysmooth;
```

See Also

Bioinformatics Toolbox functions: affyinvarsetnorm, maboxplot, magetfield, maimage, mainvarsetnorm, mairplot, maloglog, manorm, quantilenorm

Statistics Toolbox function: robustfit

Purpose

Normalize microarray data

Syntax

```
XNorm = manorm(X)
XNorm = manorm(MAStruct, FieldName)
[XNorm, ColVal] = manorm(...)
manorm(..., 'Method', MethodValue, ...)
manorm(..., 'Extra_Args', Extra_ArgsValue, ...)
manorm(..., 'LogData', LogDataValue, ...)
manorm(..., 'Percentile', PercentileValue, ...)
manorm(..., 'Global', GlobalValue, ...)
manorm(..., 'StructureOutput', StructureOutputValue, ...)
manorm(..., 'NewColumnName', NewColumnNameValue, ...)
```

Arguments

X	Numeric array or DataMatrix object of microarray data.
MAStruct	Microarray structure.
FieldName	Field.

Description

XNorm = manorm(*X*) scales the values in each column of *X*, a numeric array or DataMatrix object of microarray data, by dividing by the mean column intensity. *XNorm* is a vector, matrix, or DataMatrix object of normalized microarray data.

XNorm = manorm(*MAStruct*, *FieldName*) scales the data in *MAStruct*, a microarray structure, for a field specified by *FieldName*, for each block or print-tip by dividing each block by the mean column intensity. The output is a matrix with each column corresponding to the normalized data for each block.

[*XNorm*, *ColVal*] = manorm(...) returns the values used to normalize the data.

manorm(..., '*PropertyName*', *PropertyValue*, ...) calls manorm with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`manorm(..., 'Method', MethodValue, ...)` allows you to choose the method for scaling or centering the data. *`MethodValue`* can be `'Mean'`(default), `'Median'`, `'STD'` (standard deviation), `'MAD'` (median absolute deviation), or a function handle. If you pass a function handle, then the function should ignore NaNs and must return a single value per column of the input data.

`manorm(..., 'Extra_Args', Extra_ArgsValue, ...)` allows you to pass extra arguments to the function *`MethodValue`*. *`Extra_ArgsValue`* must be a cell array.

`manorm(..., 'LogData', LogDataValue, ...)`, when *`LogDataValue`* is `true`, works with log ratio data in which case the mean (or *`MethodValue`*) of each column is subtracted from the values in the columns, instead of dividing the column by the normalizing value.

`manorm(..., 'Percentile', PercentileValue, ...)` only uses the percentile (*`PercentileValue`*) of the data preventing large outliers from skewing the normalization. If *`PercentileValue`* is a vector containing two values, then the range from the *`PercentileValue(1)`* percentile to the *`PercentileValue(2)`* percentile is used. The default value is `100`, that is to use all the data in the data set.

`manorm(..., 'Global', GlobalValue, ...)` when *`GlobalValue`* is `true`, normalizes the values in the data set by the global mean (or *`MethodValue`*) of the data, as opposed to normalizing each column or block of the data independently.

`manorm(..., 'StructureOutput', StructureOutputValue, ...)`, when *`StructureOutputValue`* is `true`, the input data is a structure returns the input structure with an additional data field for the normalized data.

`manorm(..., 'NewColumnName', NewColumnNameValue, ...)`, when using `StructureOutput`, allows you to specify the name of the column that is appended to the list of `ColumnNames` in the structure. The default behavior is to prefix `'Block Normalized'` to the `FieldName` string.

Examples

```
maStruct = gprread('mouse_a1wt.gpr');
% Extract some data of interest.
```

```
Red = magetfield(maStruct,'F635 Median');
Green = magetfield(maStruct,'F532 Median');
% Create a log-log plot.
maloglog(Red,Green,'factorlines',true)
% Center the data.
normRed = manorm(Red);
normGreen = manorm(Green);
% Create a log-log plot of the centered data.
figure
maloglog(normRed,normGreen,'title','Normalized','factorlines',true)

% Alternatively, you can work directly with the structure
normRedBs = manorm(maStruct,'F635 Median - B635');
normGreenBs = manorm(maStruct,'F532 Median - B532');
% Create a log-log plot of the centered data. This includes some
% zero values so turn off the warning.
figure
w = warning('off','Bioinfo:maloglog:ZeroValues');
warning('off','Bioinfo:maloglog:NegativeValues');
maloglog(normRedBs,normGreenBs,'title',...
                'Normalized Background-Subtracted Median Values',...
                'factorlines',true)
        warning(w);
```

See Also

Bioinformatics Toolbox functions: affyinvarsetnorm, maboxplot, magetfield, mainvarsetnorm, mairplot, maloglog, malowess, quantilenorm, rmasummary

mapcaplot

Purpose

Create Principal Component Analysis (PCA) plot of microarray data

Syntax

```
mapcaplot(Data)
mapcaplot(Data, Label)
```

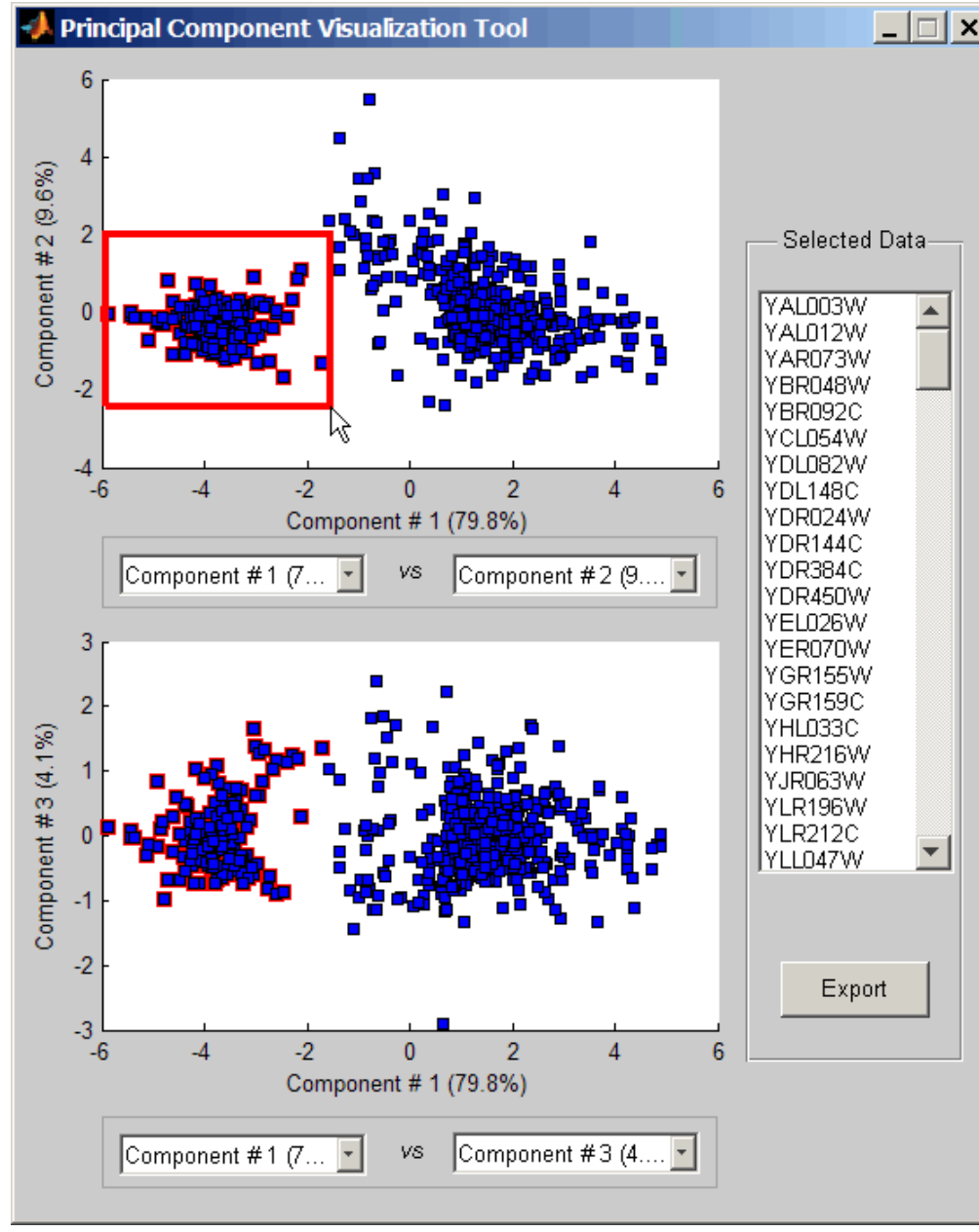
Arguments

Data	DataMatrix object or numeric array containing microarray expression profile data. If a DataMatrix object, the row names are used as labels in the plot, unless you provide labels with the second input *Label*.
Label	Cell array of strings representing labels for the data points in the plot.

Description

`mapcaplot(Data)` creates 2-D scatter plots of principal components of *Data*, a DataMatrix object or numeric array containing microarray expression profile data.

`mapcaplot(Data, Label)` uses the elements of the cell array of strings *Label*, instead of the row numbers, to label the data points in the PCA plots.


Principal Component Visualization Tool
Component # 2 (9.6%)
Component # 1 (79.8%)
Component #1 (7...
vs
Component #2 (9....
Component # 3 (4.1%)
Component # 1 (79.8%)
Component #1 (7...
vs
Component #3 (4....
Selected Data
YAL003W
YAL012W
YAR073W
YBR048W
YBR092C
YCL054W
YDL082W
YDL148C
YDR024W
YDR144C
YDR384C
YDR450W
YEL026W
YER070W
YGR155W
YGR159C
YHL033C
YHR216W
YJR063W
YLR196W
YLR212C
YLL047W
Export

Once you plot the principal components, you can:

- Select principal components for the `x` and `y` axes from the drop-down list boxes below each scatter plot.
- Click a data point to display its label.
- Select a subset of data points by click-dragging a box around them. This will highlight the points in the selected region and the corresponding points in the other axes. The labels of the selected data points appear in the list box.
- Select a label in the list box to highlight the corresponding data point in the plot. Press and hold **Ctrl** or **Shift** to select multiple data points.
- Export the gene labels and indices to a structure in the MATLAB workspace by clicking **Export**.

Examples

```
load filteredyeastdata
mapcaplot(yeastvalues, genes)
```

See Also

Bioinformatics Toolbox functions: `clustergram`, `mattest`, `mavolcanoplot`

Statistics Toolbox function: `princomp`

Purpose

Perform two-sample t-test to evaluate differential expression of genes from two experimental conditions or phenotypes

Syntax

```
PValues = mattest(DataX, DataY)
[PValues, TScores] = mattest(DataX, DataY)
[PValues, TScores, DFs] = mattest(DataX, DataY)
... = mattest(..., 'VarType', VarTypeValue, ...)
... = mattest(..., 'Permute', PermuteValue, ...)
... = mattest(..., 'Bootstrap', BootstrapValue, ...)
... = mattest(..., 'Showhist', ShowhistValue, ...)
... = mattest(..., 'Showplot', ShowplotValue, ...)
... = mattest(..., 'Labels', LabelsValue, ...)
```

Arguments

DataX, *DataY*

DataMatrix object or a matrix of gene expression values where each row corresponds to a gene and each column corresponds to a replicate. *DataX* and *DataY* must have the same number of rows and are assumed to be normally distributed in each class with equal variances.

DataX contains data from one experimental condition and *DataY* contains data from a different experimental condition. For example, *DataX* could be expression values from cancer cells, and *DataY* could be expression values from normal cells.

VarTypeValue

String that specifies the variance type of the test. *VarTypeValue* can be `'equal'` or `'unequal'` (default). If set to `'equal'`, `mattest` performs the test assuming the two samples have equal variances. If set to `'unequal'`, `mattest` performs the test assuming the two samples have unknown and unequal variances.

PermuteValue	Controls whether permutation tests are run, and if so, how many. Choices are `true`, `false` (default), or any integer greater than `2`. If set to `true`, the number of permutations is `1000`.
BootstrapValue	Controls whether bootstrap tests are run, and if so, how many. Choices are `true`, `false` (default), or any integer greater than `2`. If set to `true`, the number of bootstrap tests is `1000`.
ShowhistValue	Controls the display of histograms of t-score distributions and p-value distributions. Choices are `true` or `false` (default).
ShowplotValue	Controls the display of a normal t-score quantile plot. Choices are `true` or `false` (default). In the t-score quantile plot, data points with t-scores `> (1 - 1/(2N))` or `< 1/(2N)` display with red circles. `N` is the total number of genes.
LabelsValue	Cell array of labels (typically gene names or probe set IDs) for each row in *DataX* and *DataY*. The labels display if you click a data point in the t-score quantile plot.

Return Values

PValues One of the following:

- Column vector of p-values for each gene in *DataX* and *DataY* (if both inputs are matrices).
- DataMatrix object with row names the same as the first input DataMatrix object and a column

	name of `p-values` (if at least one input is a DataMatrix object).
TScores	Column vector of t-scores for each gene in *DataX* and *DataY*.
DFs	Column vector containing the degree of freedom for each gene in *DataX* and *DataY*.

Description

PValues = mattest(*DataX, DataY*) performs an unpaired t-test for differential expression with a standard two-tailed and two-sample t-test on every gene in *DataX* and *DataY* and returns a p-value for each gene. *DataX* and *DataY* are either a DataMatrix object or a matrix of gene expression values, in which each row corresponds to a gene, and each column corresponds to a replicate. *DataX* contains data from one experimental condition and *DataY* contains data from another experimental condition. *DataX* and *DataY* must have the same number of rows and are assumed to be normally distributed in each class. *PValues* is a column vector of p-values for each gene, or, if at least one of the inputs is a DataMatrix object, a DataMatrix object with row names the same as the first input DataMatrix object and a column name of `p-values`.

[*PValues, TScores*] = mattest(*DataX, DataY*) also returns a t-score for each gene in *DataX* and *DataY*. *TScores* is a column vector of t-scores for each gene.

[*PValues, TScores, DFs*] = mattest(*DataX, DataY*) also returns *DFs*, a column vector containing the degree of freedom for each gene across both data sets, *DataX* and *DataY*.

... = mattest(..., '*PropertyName*', *PropertyValue*, ...) calls `mattest` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

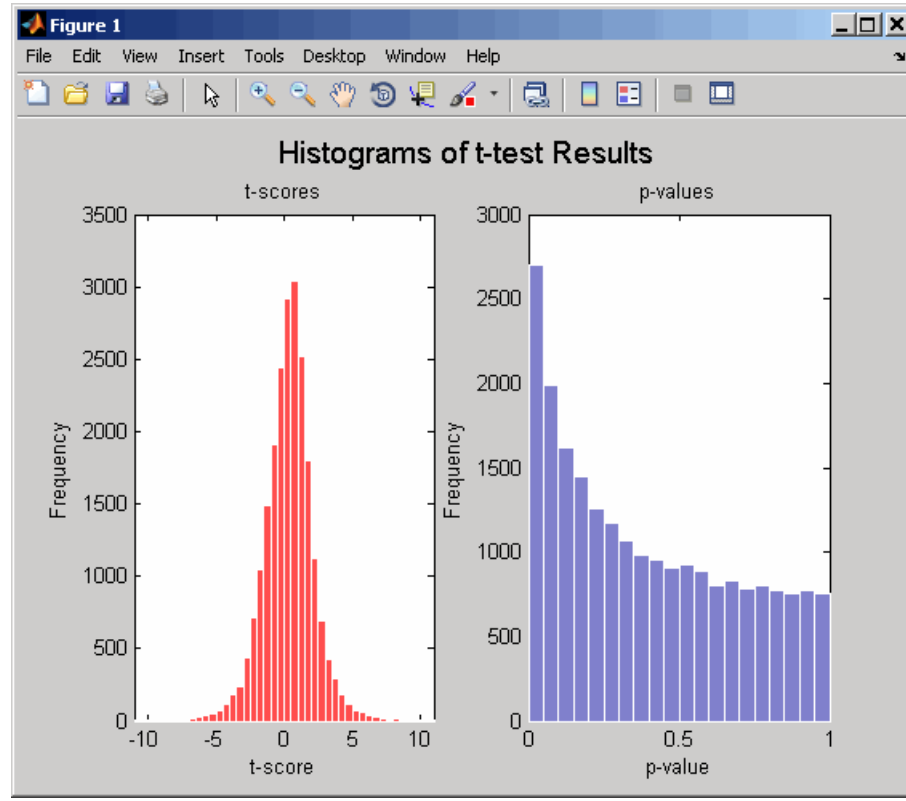
... = mattest(..., 'VarType', *VarTypeValue*, ...) specifies the variance type of the test. *VarTypeValue* can be `'equal'` or `'unequal'`

(default). If set to `'equal'`, `mattest` performs the test assuming the two samples have equal variances. If set to `'unequal'`, `mattest` performs the test assuming the two samples have unknown and unequal variances.

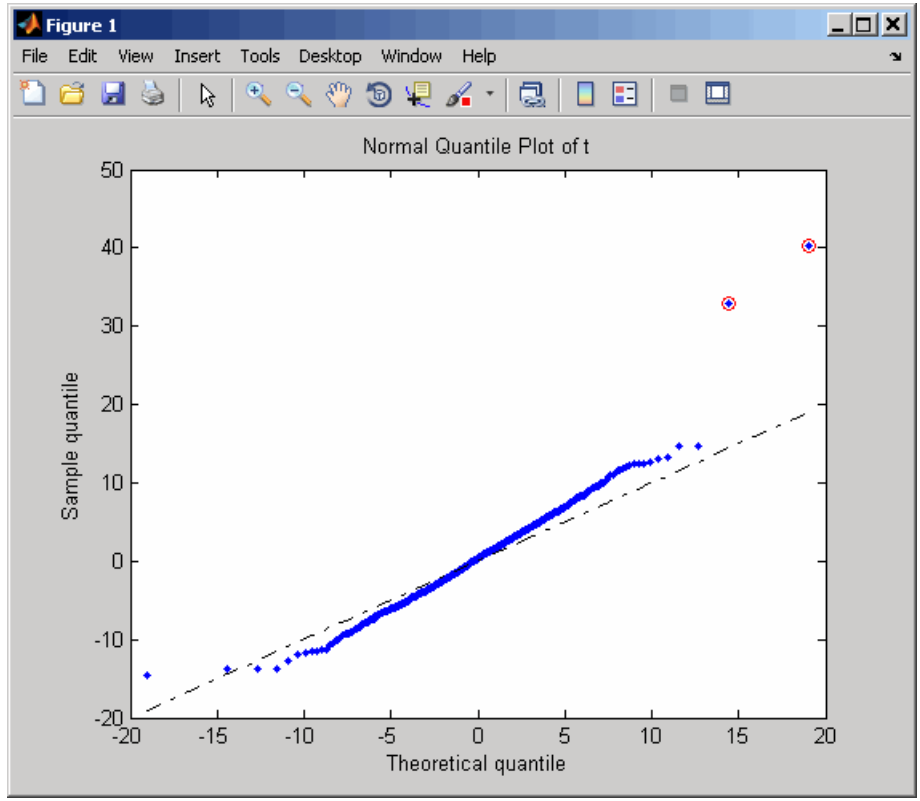
`... = mattest(..., 'Permute', PermuteValue, ...)` controls whether permutation tests are run, and if so, how many. *`PermuteValue`* can be `true`, `false` (default), or any integer greater than `2`. If set to `true`, the number of permutations is `1000`.

`... = mattest(..., 'Bootstrap', BootstrapValue, ...)` controls whether bootstrap tests are run, and if so, how many. *`BootstrapValue`* can be `true`, `false` (default), or any integer greater than `2`. If set to `true`, the number of bootstrap tests is `1000`.

`... = mattest(..., 'Showhist', ShowhistValue, ...)` controls the display of histograms of t-score distributions and p-value distributions. When *`ShowhistValue`* is `true`, `mattest` displays histograms. Default is `false`.



`...  = mattest(..., 'Showplot', ShowplotValue, ...)` controls the display of a normal t-score quantile plot. When *`ShowplotValue`* is `true`, `mattest` displays a quantile-quantile plot. Default is `false`. In the t-score quantile plot, the black diagonal line represents the sample quantile being equal to the theoretical quantile. Data points of genes considered to be differentially expressed lie farther away from this line. Specifically, data points with t-scores > `(1 - 1/(2N))` or < `1/(2N)` display with red circles. `N` is the total number of genes.



`... = mattest(..., 'Labels', LabelsValue, ...)` controls the display of labels when you click a data point in the t-score quantile plot. *`LabelsValue`* is a cell array of labels (typically gene names or probe set IDs) for each row in *`DataX`* and *`DataY`*.

Examples

1. Load the MAT-file, included with the Bioinformatics Toolbox software, that contains Affymetrix data from a prostate cancer study, specifically probe intensity data from Affymetrix HG-U133A GeneChip arrays. The two variables in the MAT-file, `dependentData` and `independentData`, are two matrices of gene expression values from two experimental conditions.

```
load prostatecancerexpdata
```

2 Calculate the p-values and t-scores for the gene expression values in the two matrices and display a normal t-score quantile plot.

```
[pvalues,tscores] = mattest(dependentData, independentData,...
                    'showplot',true);
```

3 Calculate the p-values and t-scores again using permutation tests (1000 permutations) and displaying histograms of t-score distributions and p-value distributions.

```
[pvalues,tscores] = mattest(dependentData,independentData,...
                    'permute',true,'showhist',true,...
                    'showplot',true);
```

4 Calculate the p-values and t-scores again using bootstrap tests (2000 tests) and displaying histograms of t-score distributions and p-value distributions.

```
[pvalues,tscores] = mattest(dependentData,independentData,...
                    'bootstrap',2000,'showhist',true,...
                    'showplot',true);
```

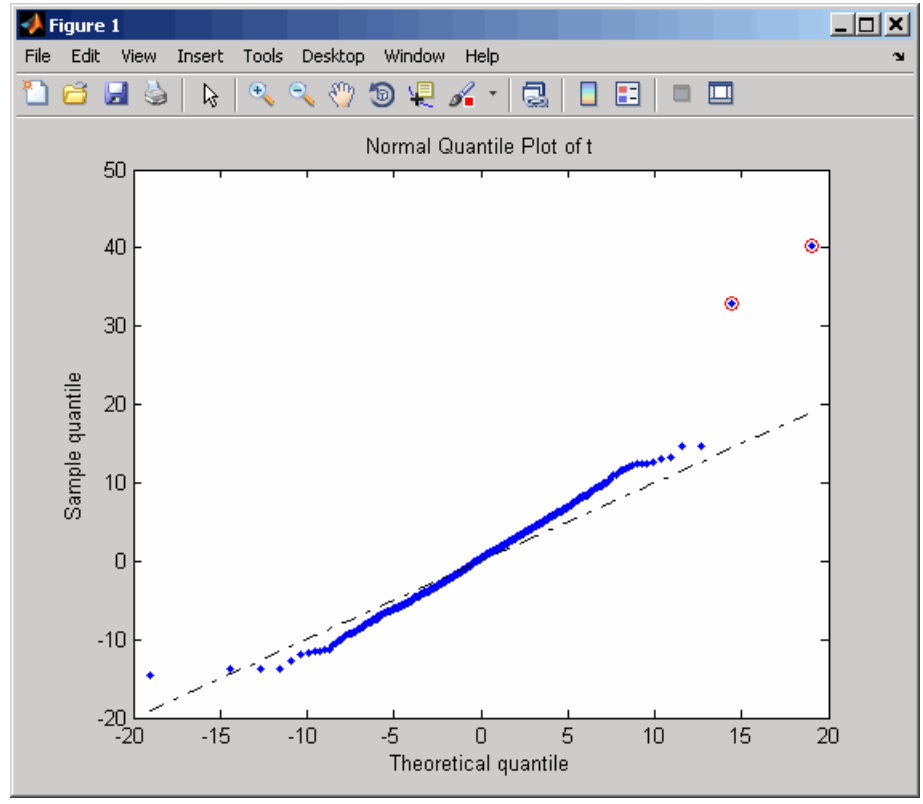
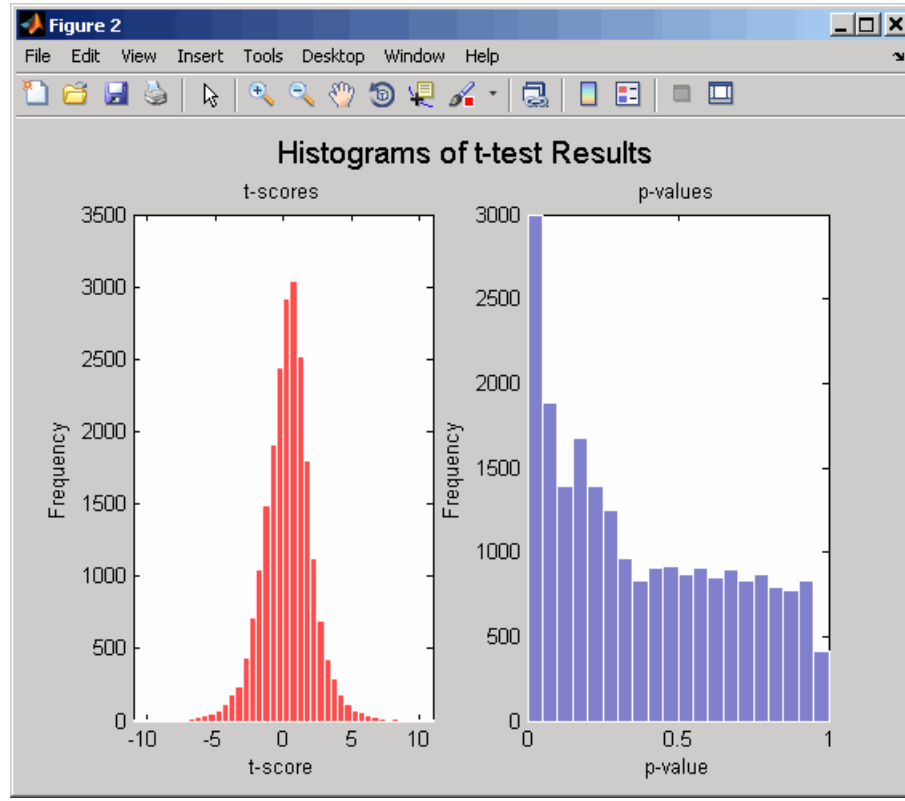


Figure 1
File Edit View Insert Tools Desktop Window Help
Normal Quantile Plot of t
Sample quantile
Theoretical quantile
50
40
30
20
10
0
-10
-20
-20 -15 -10 -5 0 5 10 15 20



The `prostatecancerexpdata.mat` file used in this example contains data from Best et al., 2005.

References

[1] Huber, W., von Heydebreck, A., Sültmann, H., Poustka, A., and Vingron, M. (2002). Variance stabilization applied to microarray data calibration and to the quantification of differential expression. Bioinformatics *18 (Suppl. 1)*, S96–S104.

[2] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L., Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan,

W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823–6834.

See Also

Bioinformatics Toolbox functions: `affygcrma`, `affyrma`, `maboxplot`, `mafdr`, `mainvarsetnorm`, `mairplot`, `maloglog`, `malowess`, `manorm`, `mavolcanoplot`, `rmasummary`

Purpose

Create significance versus gene expression ratio (fold change) scatter plot of microarray data

Syntax

```
mavolcanoplot(DataX, DataY, PValues)
SigStructure = mavolcanoplot(DataX, DataY, PValues)
... mavolcanoplot(..., 'Labels', LabelsValue, ...)
... mavolcanoplot(..., 'LogTrans', LogTransValue, ...)
... mavolcanoplot(..., 'PCutoff', PCutoffValue, ...)
... mavolcanoplot(..., 'Foldchange', FoldchangeValue, ...)
... mavolcanoplot(..., 'PlotOnly', PlotOnlyValue, ...)
```

Arguments

DataX, *DataY*

DataMatrix object, matrix, or vector of gene expression values from a single experimental condition. If a DataMatrix object or a matrix, each row is a gene, each column is a sample, and an average expression value is calculated for each gene.

Note If the values in *DataX* or *DataY* are natural scale, use the `LogTrans` property to convert them to $\log_2$ scale.

PValues

Either of the following:

- Column vector of p-values for each feature (for example, gene) in a data set, such as returned by `mattest`.
- DataMatrix object containing p-values for each feature (for example, gene) in a data set, such as returned by `mattest`.

LabelsValue — Cell array of labels (typically gene names or probe set IDs) for the data. After creating the plot, you can click a data point to display the label associated with it. If you do not provide a *LabelsValue*, data points are labeled with row numbers from *DataX* and *DataY*.

LogTransValue — Property to control the conversion of data in *DataX* and *DataY* from natural scale to $\log_2$ scale. Enter `true` to convert data to $\log_2$ scale, or `false`. Default is `false`, which assumes data is already $\log_2$ scale.

PCutoffValue — Lets you specify a cutoff p-value to define data points that are statistically significant. This value is displayed graphically as a horizontal line on the plot. Default is `0.05`, which is equivalent to 1.3010 on the $-\log_{10}$ (p-value) scale.

Note You can also change the p-value cutoff interactively after creating the plot.

FoldchangeValue — Lets you specify a ratio fold change to define data points that are differentially expressed. Default is `2`, which corresponds to a ratio of 1 and –1 on a $\log_2$ (ratio) scale.

Note You can also change the fold change interactively after creating the plot.

PlotOnlyValue — Controls the display of the volcano plot without user interface components. Choices are `true` or `false` (default).

Note If you set the `'PlotOnly'` property to `true`, you can still display labels for data points by clicking a data point, and you can still adjust vertical fold change lines and the horizontal p-value cutoff line by click-dragging the lines.

Return Values

SigStructure	Structure containing information for genes that are considered to be both statistically significant (above the p-value cutoff) and significantly differentially expressed (outside of the fold change values). The fields are listed below.

Description

`mavolcanoplot(`*DataX, DataY, PValues*`)` creates a scatter plot of gene expression data, plotting significance versus fold change of gene expression ratios of two data sets, *DataX* and *DataY*. It plots significance as the $-\log_{10}$ (p-value) from the input, *PValues*. *DataX* and *DataY* can be vectors, matrices, or DataMatrix objects. *PValues* is a clumn vector or DataMatrix object.

SigStructure `= mavolcanoplot(`*DataX, DataY, PValues*`)` returns a structure containing information for genes that are considered to be both statistically significant (above the p-value cutoff) and significantly differentially expressed (outside of the fold change values). The fields within *SigStructure* are sorted by p-value and include:

- `Name`
- `PCutoff`
- `FCThreshold`
- `GeneLabels`
- `PValues`

- `FoldChanges`

Note The fields `PValues` and `FoldChanges` will be either vectors or DataMatrix objects depending on the type of input *`PValues`*.

`... mavolcanoplot(..., '`*`PropertyName`*`', `*`PropertyValue`*`, ...)` defines optional properties that use property name/value pairs in any order. These property name/value pairs are as follows:

`... mavolcanoplot(..., 'Labels', `*`LabelsValue`*`, ...)` lets you provide a cell array of labels (typically gene names or probe set IDs) for the data. After creating the plot, you can click a data point to display the label associated with it. If you do not provide a *`LabelsValue`*, data points are labeled with row numbers from *`DataX`* and *`DataY`*.

`... mavolcanoplot(..., 'LogTrans', `*`LogTransValue`*`, ...)` controls the conversion of data from *`DataX`* and *`DataY`* to $\log_2$ scale. When *`LogTransValue`* is `true`, `mavolcanoplot` converts data from natural to $\log_2$ scale. Default is `false`, which assumes the data is already $\log_2$ scale.

`... mavolcanoplot(..., 'PCutoff', `*`PCutoffValue`*`, ...)` lets you specify a p-value cutoff to define data points that are statistically significant. This value displays graphically as a horizontal line on the plot. Default is `0.05`, which is equivalent to 1.3010 on the $-\log_{10}$ (p-value) scale.

Note You can also change the p-value cutoff interactively after creating the plot.

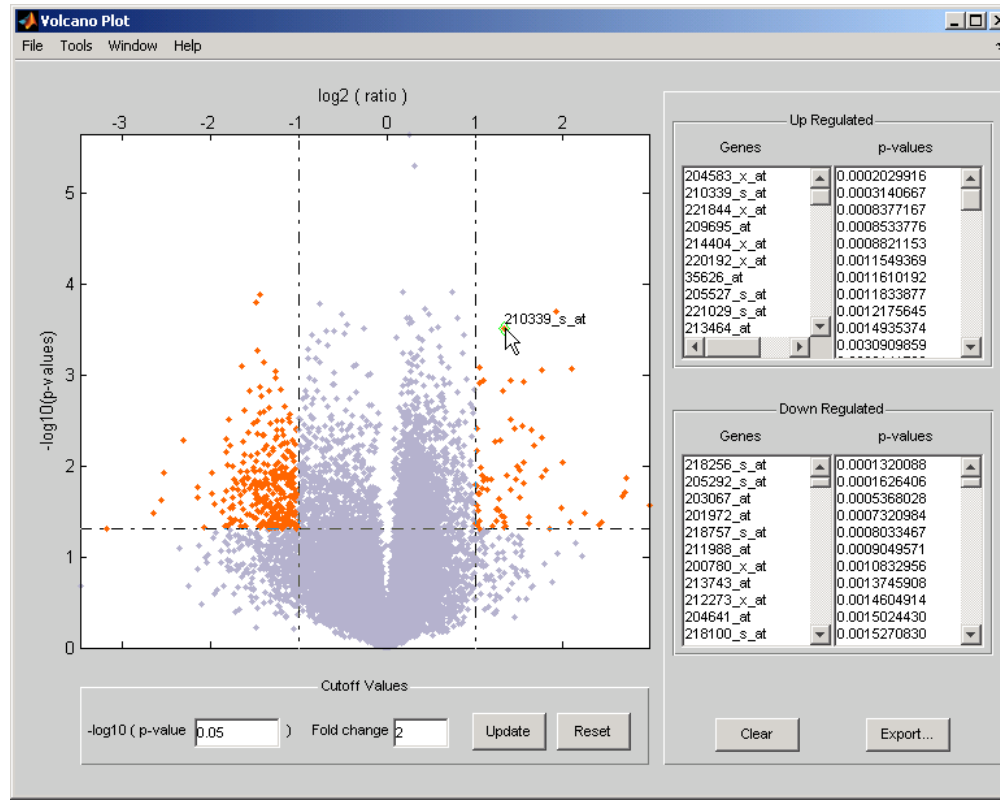
`... mavolcanoplot(..., 'Foldchange', `*`FoldchangeValue`*`, ...)` lets you specify a ratio fold change to define data points that are differentially expressed. Fold changes display graphically as two

vertical lines on the plot. Default is `2`, which corresponds to a ratio of 1 and –1 on a $\log_2$ (ratio) scale.

Note You can also change the fold change interactively after creating the plot.

`... mavolcanoplot(..., 'PlotOnly', PlotOnlyValue, ...)` controls the display of the volcano plot without user interface components. Choices are `true` or `false` (default).

Note If you set the `'PlotOnly'` property to `true`, you can still display labels for data points by clicking a data point, and you can still adjust vertical fold change lines and the horizontal p-value cutoff line by click-dragging the lines.



The volcano plot displays the following:

- $-\log_{10}$ (p-value) versus $\log_2$ (ratio) scatter plot of genes
- Two vertical fold change lines at a fold change level of 2, which corresponds to a ratio of 1 and –1 on a $\log_2$ (ratio) scale. (Lines will be at different fold change levels, if you used the `'Foldchange'` property.)
- One horizontal line at the 0.05 p-value level, which is equivalent to 1.3010 on the $-\log_{10}$ (p-value) scale. (The line will be at a different p-value level, if you used the `'PCutoff'` property.)

- Data points for genes that are considered both statistically significant (above the p-value line) and differentially expressed (outside of the fold changes lines) appear in orange.

After you display the volcano scatter plot, you can interactively:

- Adjust the vertical fold change lines by click-dragging one line or entering a value in the **Fold Change** text box.
- Adjust the horizontal p-value cutoff line by click-dragging or entering a value in the **p-value Cutoff** text box.
- Display labels for data points by clicking a data point.
- Select a gene from the **Up Regulated** or **Down Regulated** list to highlight the corresponding data point in the plot. Press and hold **Ctrl** or **Shift** to select multiple genes.
- Zoom the plot by selecting **Tools > Zoom In** or **Tools > Zoom Out**.
- View lists of significantly up-regulated and down-regulated genes and their associated p-values, and optionally, export the labels, p-values, and fold changes to a structure in the MATLAB Workspace by clicking **Export**.

Examples

1. Load a MAT-file, included with the Bioinformatics Toolbox software, which contains Affymetrix data variables, including `dependentData` and `independentData`, two matrices of gene expression values from two experimental conditions.

   ```
   load prostatecancerexpdata
   ```

2. Use the `mattest` function to calculate p-values for the gene expression values in the two matrices.

   ```
   pvalues = mattest(dependentData, independentData);
   ```

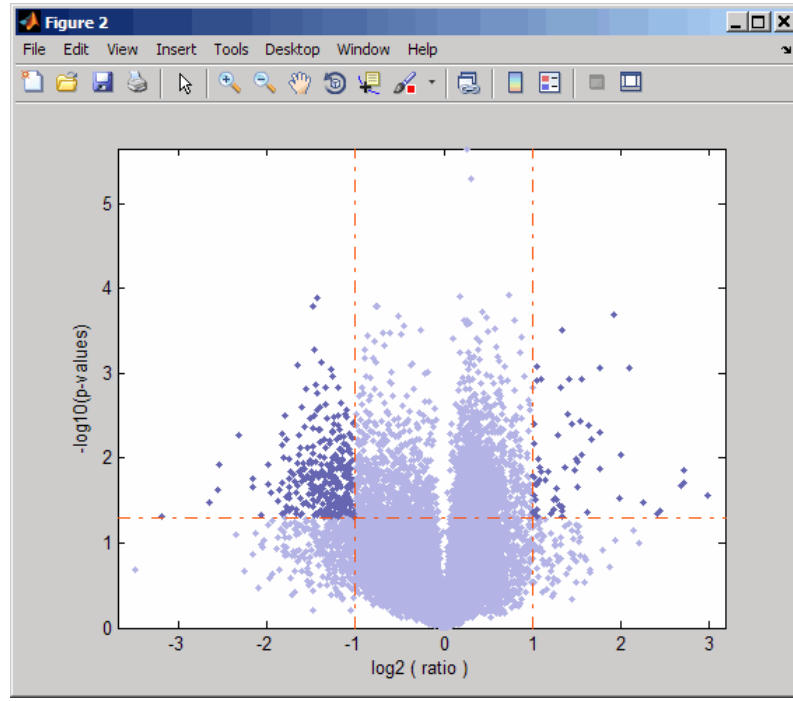
3. Using the two matrices, the `pvalues` calculated by `mattest`, and the `probesetIDs` column vector of labels provided, use `mavolcanoplot` to

create a significance versus gene expression ratio scatter plot of the microarray data from the two experimental conditions.

```
mavolcanoplot(dependentData, independentData, pvalues,...
'Labels', probesetIDs)
```

4 View the volcano plot without the user interface components.

```
mavolcanoplot(dependentData, independentData, pvalues,...
'Labels', probesetIDs,'Plotonly', true)
```



The `prostatecancerexpdata.mat` file used in the previous example contains data from Best et al., 2005.

References

[1] Cui, X., Churchill, G.A. (2003). Statistical tests for differential expression in cDNA microarray experiments. Genome Biology *4*, 210.

[2] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L., Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan, W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823–6834.

See Also

Bioinformatics Toolbox functions: `maboxplot`, `maimage`, `mainvarsetnorm`, `mairplot`, `maloglog`, `malowess`, `manorm`, `mapcaplot`, `mattest`

max (DataMatrix)

Purpose

Return maximum values in DataMatrix object

Syntax

```
M = max(DMObj1)
[M, Indices] = max(DMObj1)
[M, Indices, Names] = max(DMObj1)
... = max(DMObj1, [], Dim)
MA = max(DMObj1, DMObj2)
```

Arguments

DMObj1, *DMObj2*

DataMatrix objects, such as created by `DataMatrix` (object constructor).

Note *DMObj1* and *DMObj2* must be the same size, unless one is a scalar.

Dim

Scalar specifying the dimension of *DMObj* to return the maximum values. Choices are:

- `1` — Default. Returns a row vector containing a maximum value for each column.
- `2` — Returns a column vector containing a maximum value for each row.

Return Values

M

One of the following:

- Scalar specifying the maximum value in *DMObj* when it contains vector of data
- Row vector containing the maximum value for each column in *DMObj* (when *Dim* = 1)

- Column vector containing the maximum value for each row in *DMObj* (when *Dim* = 2)

Indices Either of the following:

- Positive integer specifying the index of the maximum value in a DataMatrix object containing a vector of data
- Vector containing the indices for the maximum value in each column (if *Dim* = 1) or row (if *Dim* = 2) in a DataMatrix object containing a matrix of data

Names Vector of the row names (if *Dim* = 1) or column names (if *Dim* = 2) corresponding to the maximum value in each column or each row of a DataMatrix object.

MA Numeric array created from the maximum elements in either of the following:

- Two DataMatrix objects
- A DataMatrix object and a numeric array

Description

M = max(*DMObj1*) returns the maximum value(s) in *DMObj1*, a DataMatrix object. If *DMObj1* contains a vector of data, *M* is a scalar. If *DMObj1* contains a matrix of data, *M* is a row vector containing a maximum value in each column.

[*M*, *Indices*] = max(*DMObj1*) returns *Indices*, the indices of the maximum value(s) in *DMObj1*, a DataMatrix object. If *DMObj1* contains a vector of data, *Indices* is a positive integer. If *DMObj1* contains a matrix of data, *Indices* is a vector containing the indices for the maximum value in each column (if *Dim* = 1) or row (if *Dim* = 2). If there are multiple maximum values in a column or row, the index for the first value is returned.

[*M*, *Indices*, *Names*] = max(*DMObj1*) returns *Names*, a vector of the row names (if *Dim* = 1) or column names (if *Dim* = 2) corresponding to the

maximum value in each column or each row of*DMObj1*, a DataMatrix object. If there are multiple maximum values in a column or row, the row or column name for the first value is returned.

`... = max(`*`DMObj1`*`, [], `*`Dim`*`)` specifies which dimension to return the maximum values for, that is each column or each row in a DataMatrix object. If *`Dim`* = 1, returns *`M`*, a row vector containing the maximum value in each column. If *`Dim`* = 2, returns *`M`*, a column vector containing the maximum value in each row. Default *`Dim`* = 1.

`MA` `= max(`*`DMObj1`*`, `*`DMObj2`*`)` returns *`MA`*, a numeric array containing the larger of the two values from each position of *`DMObj1`* and *`DMObj2`*. *`DMObj1`* and *`DMObj2`* can both be DataMatrix objects, or one can be a DataMatrix object and the other a numeric array. They must be the same size, unless one is a scalar. *`MA`* has the same size (number of rows and columns) as the first nonscalar input.

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox methods of a DataMatrix object: `min`, `sum`

Purpose

Calculate maximum flow in biograph object

Syntax

```
[MaxFlow, FlowMatrix, Cut] = maxflow(BGObj, SNode, TNode)
[...] = maxflow(BGObj, SNode, TNode, ...'Capacity',
CapacityValue, ...)
[...] = maxflow(BGObj, SNode, TNode, ...'Method', MethodValue,
    ...)
```

Arguments

BGObj	Biograph object created by `biograph` (object constructor).
SNode	Node in a directed graph represented by an N-by-N adjacency matrix extracted from biograph object, *BGObj*.
TNode	Node in a directed graph represented by an N-by-N adjacency matrix extracted from biograph object, *BGObj*.
CapacityValue	Column vector that specifies custom capacities for the edges in the N-by-N adjacency matrix. It must have one entry for every nonzero value (edge) in the N-by-N adjacency matrix. The order of the custom capacities in the vector must match the order of the nonzero values in the N-by-N adjacency matrix when it is traversed column-wise. By default, `maxflow` gets capacity information from the nonzero entries in the N-by-N adjacency matrix.
MethodValue	String that specifies the algorithm used to find the minimal spanning tree (MST). Choices are: • `'Edmonds'` — Uses the Edmonds and Karp algorithm, the implementation of which is based on a variation called the *labeling algorithm*. Time complexity is `O(N*E^2)`, where `N` and `E` are the number of nodes and edges respectively.

- `'Goldberg'` — Default algorithm. Uses the Goldberg algorithm, which uses the generic method known as *preflow-push*. Time complexity is `O(N^2*sqrt(E))`, where `N` and `E` are the number of nodes and edges respectively.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

`[MaxFlow, FlowMatrix, Cut] = maxflow(BGObj, SNode, TNode)` calculates the maximum flow of a directed graph represented by an N-by-N adjacency matrix extracted from a biograph object, `BGObj`, from node `SNode` to node `TNode`. Nonzero entries in the matrix determine the capacity of the edges. Output `MaxFlow` is the maximum flow, and `FlowMatrix` is a sparse matrix with all the flow values for every edge. `FlowMatrix(X,Y)` is the flow from node `X` to node `Y`. Output `Cut` is a logical row vector indicating the nodes connected to `SNode` after calculating the minimum cut between `SNode` and `TNode`. If several solutions to the minimum cut problem exist, then `Cut` is a matrix.

Tip The algorithm that determines `Cut`, all minimum cuts, has a time complexity of `O(2^N)`, where N is the number of nodes. If this information is not needed, use the `maxflow` method without the third output.

`[...] = maxflow(BGObj, SNode, TNode, ...'PropertyName', PropertyValue, ...)` calls `maxflow` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[...] = maxflow(BGObj, SNode, TNode, ...'Capacity', CapacityValue, ...)` lets you specify custom capacities for the edges. *`CapacityValue`* is a column vector having one entry for every nonzero value (edge) in the N-by-N adjacency matrix. The order of the custom capacities in the vector must match the order of the nonzero values in the matrix when it is traversed column-wise. By default, `graphmaxflow` gets capacity information from the nonzero entries in the matrix.

`[...] = maxflow(BGObj, SNode, TNode, ...'Method', MethodValue, ...)` lets you specify the algorithm used to find the minimal spanning tree (MST). Choices are:

- `'Edmonds'` — Uses the Edmonds and Karp algorithm, the implementation of which is based on a variation called the *labeling algorithm*. Time complexity is `O(N*E^2)`, where `N` and `E` are the number of nodes and edges respectively.
- `'Goldberg'` — Default algorithm. Uses the Goldberg algorithm, which uses the generic method known as *preflow-push*. Time complexity is `O(N^2*sqrt(E))`, where `N` and `E` are the number of nodes and edges respectively.

References

[1] Edmonds, J. and Karp, R.M. (1972). Theoretical improvements in the algorithmic efficiency for network flow problems. Journal of the ACM *19*, 248-264.

[2] Goldberg, A.V. (1985). A New Max-Flow Algorithm. MIT Technical Report MIT/LCS/TM-291, Laboratory for Computer Science, MIT.

[3] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphmaxflow`

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object:
`allshortestpaths`, `conncomp`, `isdag`, `isomorphism`, `isspantree`, `minspantree`, `shortestpath`, `topoorder`, `traverse`

Purpose

Return average or mean values in DataMatrix object

Syntax

```
M = mean(DMObj)
M = mean(DMObj, Dim)
M = mean(DMObj, Dim, IgnoreNaN)
```

Arguments

DMObj	DataMatrix object, such as created by `DataMatrix` (object constructor).
Dim	Scalar specifying the dimension of *DMObj* to calculate the means. Choices are: • `1` — Default. Returns mean values for elements in each column. • `2` — Returns mean values for elements in each row.
IgnoreNaN	Specifies if NaNs should be ignored. Choices are `true` (default) or `false`.

Return Values

M	Either of the following: • Row vector containing the mean values from elements in each column in *DMObj* (when *Dim* = 1) • Column vector containing the mean values from elements in each row in *DMObj* (when *Dim* = 2)

Description

M = `mean(`*DMObj*`)` returns the mean values of the elements in the columns of a DataMatrix object, treating NaNs as missing values. *M* is a row vector containing the mean values for elements in each column in *DMObj*.

M = `mean(`*DMObj*`, `*Dim*`)` returns the mean values of the elements in the columns or rows of a DataMatrix object, as specified by *Dim*. If *Dim* = 1,

returns *M*, a row vector containing the mean values for elements in each column in *DMObj*. If *Dim* = 2, returns *M*, a column vector containing the mean values for elements in each row in *DMObj*. Default *Dim* = 1.

M = mean(*DMObj*, *Dim*, *IgnoreNaN*) specifies if NaNs should be ignored. *IgnoreNaN* can be true (default) or false.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox methods of a DataMatrix object: max, median, min, sum

Purpose

Return median values in DataMatrix object

Syntax

```
Med = median(DMObj)
Med = median(DMObj, Dim)
Med = median(DMObj, Dim, IgnoreNaN)
```

Arguments

DMObj	DataMatrix object, such as created by `DataMatrix` (object constructor).
Dim	Scalar specifying the dimension of *DMObj* to calculate the medians. Choices are: • `1` — Default. Returns median values for elements in each column. • `2` — Returns median values for elements in each row.
IgnoreNaN	Specifies if NaNs should be ignored. Choices are `true` (default) or `false`.

Return Values

Med	Either of the following: • Row vector containing the median values from elements in each column in *DMObj* (when *Dim* = 1) • Column vector containing the median values from elements in each row in *DMObj* (when *Dim* = 2)

Description

Med = median(*DMObj*) returns the median values of the elements in the columns of a DataMatrix object, treating NaNs as missing values. *Med* is a row vector containing the median values for elements in each column in *DMObj*.

Med = median(*DMObj*, *Dim*) returns the median values of the elements in the columns or rows of a DataMatrix object, as specified by *Dim*. If *Dim* = 1, returns *Med*, a row vector containing the median values for elements in each column in *DMObj*. If *Dim* = 2, returns *Med*, a column vector containing the median values for elements in each row in *DMObj*. Default *Dim* = 1.

Med = median(*DMObj*, *Dim*, *IgnoreNaN*) specifies if NaNs should be ignored. *IgnoreNaN* can be `true` (default) or `false`.

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox methods of a DataMatrix object: `max`, `mean`, `min`, `sum`

Purpose

Display visualization of microtiter plate

Syntax

```
microplateplot(Data)
Handle = microplateplot(...)
microplateplot(Data, ...'RowLabels', RowLabelsValue, ...)
microplateplot(Data, ...'ColumnLabels', ColumnLabelsValue,
   ...)
microplateplot(Data, ...'TextLabels', TextLabelsValue, ...)
microplateplot(Data, ...'TextFontSize', TextFontSizeValue,
   ...)
microplateplot(Data, ...'MissingValueColor',
   MissingValueColorValue, ...)
microplateplot(Data, ...'ToolTipFormat',
ToolTipFormatValue,
   ...)
```

Description

`microplateplot(Data)` displays an image of a microtiter plate with each well colored according to intensity values, such as from a plate reader.

`Handle = microplateplot(...)` returns the handle to the axes of the plot.

`microplateplot(..., 'PropertyName', PropertyValue, ...)` calls `microplateplot` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each *`PropertyName`* in single quotation marks. Each *`PropertyName`* is case insensitive. These property name/property value pairs are as follows:

`microplateplot(Data, ...'RowLabels', RowLabelsValue, ...)` lets you specify labels for the rows of data.

`microplateplot(Data, ...'ColumnLabels', ColumnLabelsValue, ...)` lets you specify labels for the columns of data.

`microplateplot(Data, ...'TextLabels', TextLabelsValue, ...)` lets you specify text to overlay of the wells in the image.

`microplateplot(`*`Data`*`, ...'TextFontSize', `*`TextFontSizeValue`*`, ...)` lets you specify the font size of the text you specify with the `'TextLabels'` property.

`microplateplot(`*`Data`*`, ...'MissingValueColor', `*`MissingValueColorValue`*`, ...)` lets you specify the color of wells with missing values (NaN values).

`microplateplot(`*`Data`*`, ...'ToolTipFormat', `*`ToolTipFormatValue`*`, ...)` lets you specify the format of the text used in the well tooltips. The well tooltips display the actual value from the input matrix when you click a well. *`ToolTipFormatValue`* is a format string, such as used by the `sprintf` function. Default is `'Value: %.3f'`, which specifies including three digits to the right of the decimal in fixed-point notation.

Inputs

`Data`

DataMatrix object or matrix containing intensity values, such as from a plate reader.

Tip For help importing data from a spreadsheet or data file into a MATLAB matrix, see "Importing Text Data Files".

Note The `microplateplot` function converts any nonnumeric symbols or characters in the matrix to NaN values.

`RowLabelsValue`

Cell array of strings that specifies labels for the rows of data. Default is the first *`N`*letters of the alphabet, where *`N`* is the number of rows in *`Data`*. If there are more than 26 rows in *`Data`*, then the default is `AA, AB, ..., ZZ`. If *`Data`* is a DataMatrix object, then the default is the row labels of *`Data`*.

ColumnLabelsValue

Cell array of strings that specifies labels for the columns of data. Default is `1, 2, ..., M`, where *M* is the number of columns in *Data*. If *Data* is a DataMatrix object, then the default is the column labels of *Data*.

TextLabelsValue

Cell array of strings the same size as *Data* that specifies text to overlay on the wells of the image.

TextFontSizeValue

Positive integer specifying the font size of the text you specify with the `'TextLabels'` property. Default font size is determined automatically based on the size of the Figure window.

MissingValueColorValue

Three-element numeric vector of RGB values that specifies the color of wells with missing values (NaN values). Default is `[0, 0, 0]`, which defines black.

ToolTipFormatValue

Format string, such as used by the `sprintf` function, that specifies the format of the text used in the well tooltips. The well tooltips display the actual value from the input matrix when you click a well.

Default: `'Value:  %.3f'`, which specifies including three digits to the right of the decimal in fixed-point notation.

Outputs

Handle

Handle to the axes of the plot.

Tip Use the *Handle* output with the `set` function and the `'YDir'` or `'XDir'` property to reverse the order of the `A` through `H` labels or `1` through `12` labels respectively. Note that in the microplate plot, the default order for the `A` through `H` labels, or `'YDir'` property, is `'reverse'` (top to bottom), and the default order for the `1` through `12` labels, or `'XDir'` property, is `'normal'` (left to right). For more information on the `'XDir'` and `'YDir'` properties, see "Properties That Control the X-, Y-, or Z-Axis".

Examples

Creating a Plot of a Microplate, Changing the Colormap, Viewing Well Values, and Adding Text Labels

1. Load a MAT-file, included with the Bioinformatics Toolbox software, which contains two variables: `assaydata`, an 8-by-12 matrix of data values from a microtiter plate, and `whiteToRed`, a 64-by-3 matrix that defines a colormap.

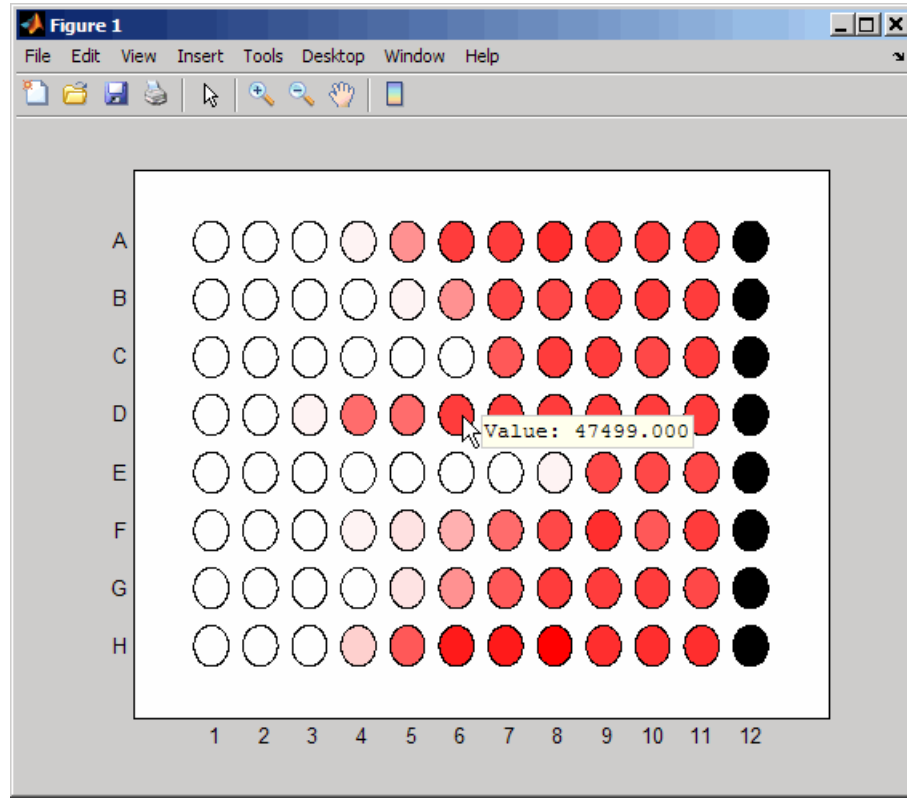
   ```
   load microPlateAssay
   ```

2. Create a visualization of the data from the microtiter plate.

   ```
   microplateplot(assaydata)
   ```

3. Change the visualization to use a white-to-red colormap, and then view a tooltip displaying the value of well D6 by clicking the well.

   ```
   colormap(whiteToRed)
   ```



Notice that all wells in column 12 are black, indicating missing data.

4 Overlay an `X` on well E8.

a Create an empty cell array.

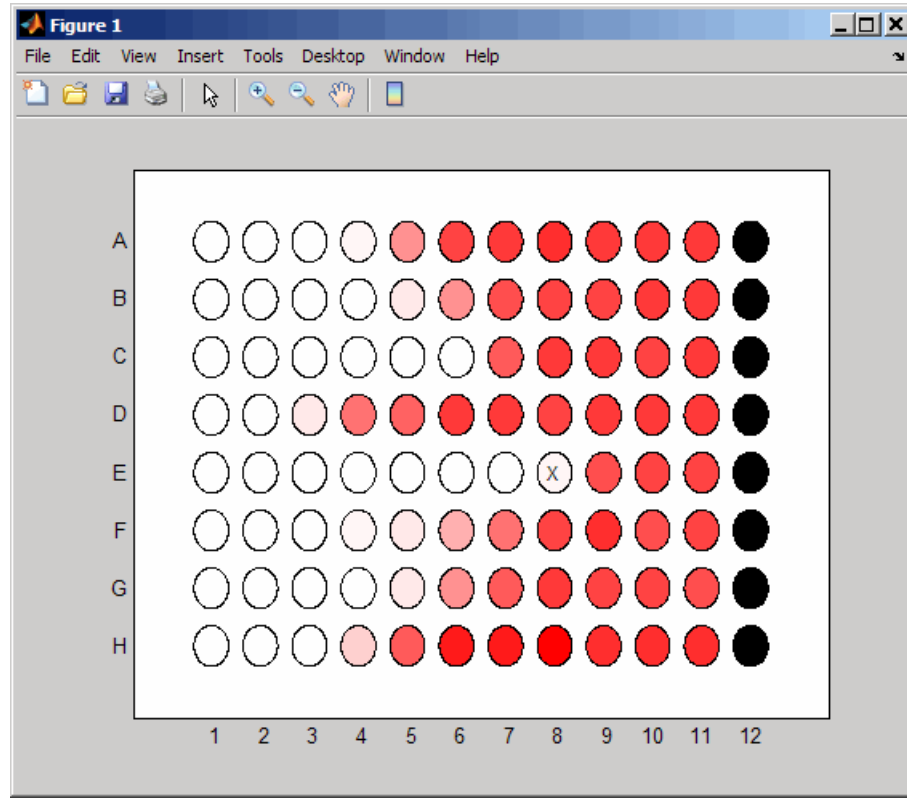
```
mask = cell(8,12);
```

b Add the string `'X'` to the cell in the fifth row and eighth column of the array.

```
mask{5,8} = 'X';
```

c Pass the cell array to the `microplateplot` function using the `'TextLabels'` property.

```
microplateplot(assaydata,'TEXTLABELS',mask);
```



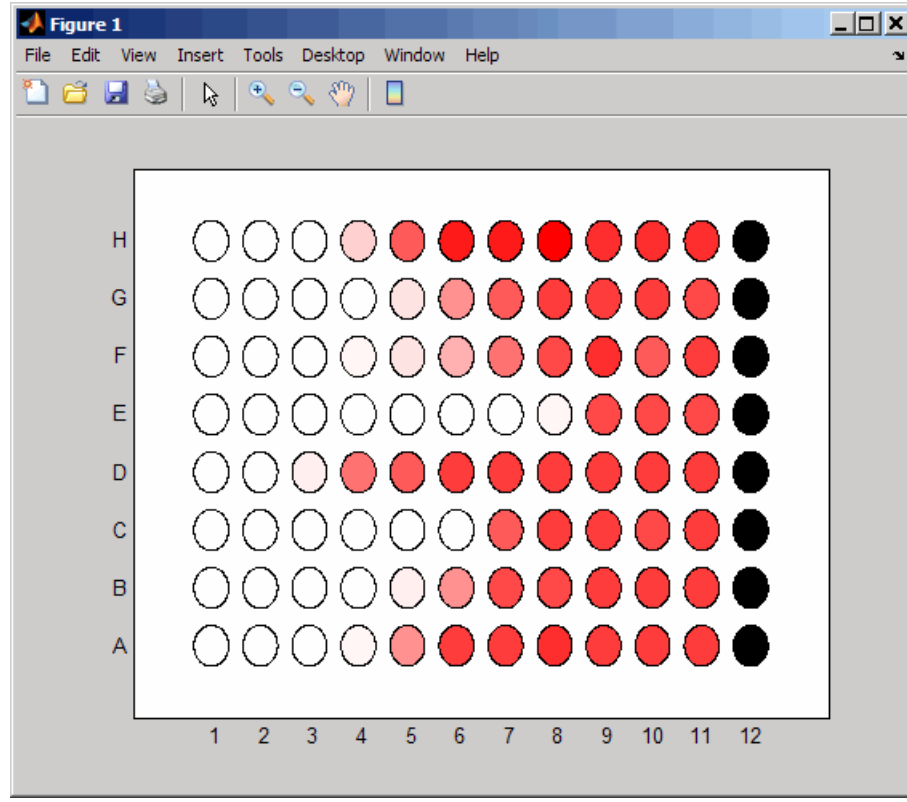
Changing the Order of Row Labels in the Plot

1 If you have not already done so, create a plot of a microplate by completing steps 1 through 3 in Creating a Plot of a Microplate,

Changing the Colormap, Viewing Well Values, and Adding Text Labels on page 3-946.

2 Return a handle to the axes of the plot, and then reverse the order of the row letter labels.

```
h = microplateplot(assaydata);
set(h,'YDir','normal')
```



Adding a Title and Axis Labels to the Plot

For information on adding a title and *x*-axis and *y*-axis labels to your plot, see "Annotating Graphs".

Printing and Exporting the Plot

For information on printing or exporting your plot, see "Printing and Exporting".

See Also

`imagesc` | `sprintf` | `set`

How To

- "Importing Text Data Files"
- "Properties That Control the X-, Y-, or Z-Axis"
- "Annotating Graphs"
- "Printing and Exporting"

Purpose

Return minimum values in DataMatrix object

Syntax

```
M = min(DMObj1)
[M, Indices] = min(DMObj1)
[M, Indices, Names] = min(DMObj1)
... = min(DMObj1, [], Dim)
MA = min(DMObj1, DMObj2)
```

Arguments

DMObj1, *DMObj2*

DataMatrix objects, such as created by `DataMatrix` (object constructor).

Note *DMObj1* and *DMObj2* must be the same size, unless one is a scalar.

Dim

Scalar specifying the dimension of *DMObj* to return the minimum values. Choices are:

- `1` — Default. Returns a row vector containing a minimum value for each column.
- `2` — Returns a column vector containing a minimum value for each row.

Return Values

M

One of the following:

- Scalar specifying the minimum value in *DMObj* when it contains vector of data
- Row vector containing the minimum value for each column in *DMObj* (when *Dim* = `1`)

- Column vector containing the minimum value for each row in *DMObj* (when *Dim* = 2)

Indices Either of the following:

- Positive integer specifying the index of the minimum value in a DataMatrix object containing a vector of data
- Vector containing the indices for the minimum value in each column (if *Dim* = 1) or row (if *Dim* = 2) in a DataMatrix object containing a matrix of data

Names Vector of the row names (if *Dim* = 1) or column names (if *Dim* = 2) corresponding to the minimum value in each column or each row of a DataMatrix object.

MA Numeric array created from the minimum elements in either of the following:

- Two DataMatrix objects
- A DataMatrix object and a numeric array

Description

M = min(*DMObj1*) returns the minimum value(s) in *DMObj1*, a DataMatrix object. If *DMObj1* contains a vector of data, *M* is a scalar. If *DMObj1* contains a matrix of data, *M* is a row vector containing a minimum value in each column.

[*M*, *Indices*] = min(*DMObj1*) returns *Indices*, the indices of the minimum value(s) in *DMObj1*, a DataMatrix object. If *DMObj1* contains a vector of data, *Indices* is a positive integer. If *DMObj1* contains a matrix of data, *Indices* is a vector containing the indices for the minimum value in each column (if *Dim* = 1) or row (if *Dim* = 2). If there are multiple minimum values in a column or row, the index for the first value is returned.

[*M*, *Indices*, *Names*] = min(*DMObj1*) returns *Names*, a vector of the row names (if *Dim* = 1) or column names (if *Dim* = 2) corresponding to

the minimum value in each column or each row of*DMObj1*, a DataMatrix object. If there is more than one minimum value in a column or row, the row or column name for the first value is returned.

`... = min(`*`DMObj1`*`, [], `*`Dim`*`)` specifies which dimension to return the minimum values for, that is each column or each row in a DataMatrix object. If *`Dim`* = 1, returns *`M`*, a row vector containing the minimum value in each column. If *`Dim`* = 2, returns *`M`*, a column vector containing the minimum value in each row. Default *`Dim`* = 1.

`MA` `= min(`*`DMObj1`*`, `*`DMObj2`*`)` returns *`MA`*, a numeric array containing the smaller of the two values from each position of *`DMObj1`* and *`DMObj2`*. *`DMObj1`* and *`DMObj2`* can both be DataMatrix objects, or one can be a DataMatrix object and the other a numeric array. They must be the same size, unless one is a scalar. *`MA`* has the same size (number of rows and columns) as the first nonscalar input.

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox methods of a DataMatrix object: `max`, `sum`

minspantree (biograph)

Purpose

Find minimal spanning tree in biograph object

Syntax

```
[Tree, pred] = minspantree(BGObj)
[Tree, pred] = minspantree(BGObj, R)
[Tree, pred] = minspantree(..., 'Method', MethodValue, ...)
[Tree, pred] = minspantree(..., 'Weights', WeightsValue, ...)
```

Arguments

BGObj	Biograph object created by `biograph` (object constructor).
R	Scalar between 1 and the number of nodes.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

`[Tree, pred] = minspantree(BGObj)` finds an acyclic subset of edges that connects all the nodes in the undirected graph represented by an N-by-N adjacency matrix extracted from a biograph object, *BGObj*, and for which the total weight is minimized. Weights of the edges are all nonzero entries in the lower triangle of the N-by-N sparse matrix. Output *Tree* is a spanning tree represented by a sparse matrix. Output *pred* is a vector containing the predecessor nodes of the minimal spanning tree (MST), with the root node indicated by `0`. The root node defaults to the first node in the largest connected component. This computation requires an extra call to the `graphconncomp` function.

`[Tree, pred] = minspantree(BGObj, R)` sets the root of the minimal spanning tree to node `R`.

`[Tree, pred] = minspantree(..., 'PropertyName', PropertyValue, ...)` calls `minspantree` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[Tree, pred] = minspantree(..., 'Method', MethodValue, ...)` lets you specify the algorithm used to find the minimal spanning tree (MST). Choices are:

- `'Kruskal'` — Grows the minimal spanning tree (MST) one edge at a time by finding an edge that connects two trees in a spreading forest of growing MSTs. Time complexity is `O(E+X*log(N))`, where `X` is the number of edges no longer than the longest edge in the MST, and `N` and `E` are the number of nodes and edges respectively.
- `'Prim'` — Default algorithm. Grows the minimal spanning tree (MST) one edge at a time by adding a minimal edge that connects a node in the growing MST with any other node. Time complexity is `O(E*log(N))`, where `N` and `E` are the number of nodes and edges respectively.

Note When the graph is unconnected, Prim's algorithm returns only the tree that contains R, while Kruskal's algorithm returns an MST for every component.

`[Tree, pred] = minspantree(..., 'Weights', WeightsValue, ...)` lets you specify custom weights for the edges. *`WeightsValue`* is a column vector having one entry for every nonzero value (edge) in the N-by-N sparse matrix. The order of the custom weights in the vector must match the order of the nonzero values in the N-by-N sparse matrix when it is traversed column-wise. By default, `minspantree` gets weight information from the nonzero entries in the N-by-N sparse matrix.

References

[1] Kruskal, J.B. (1956). On the Shortest Spanning Subtree of a Graph and the Traveling Salesman Problem. Proceedings of the American Mathematical Society *7*, 48-50.

[2] Prim, R. (1957). Shortest Connection Networks and Some Generalizations. Bell System Technical Journal *36*, 1389-1401.

[3] Siek, J.G. Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphminspantree`

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `isdag`, `isomorphism`, `isspantree`, `maxflow`, `shortestpath`, `topoorder`, `traverse`

Purpose

Subtract DataMatrix objects

Syntax

```
DMObjNew = minus(DMObj1, DMObj2)
DMObjNew = DMObj1 - DMObj2
DMObjNew = minus(DMObj1, B)
DMObjNew = DMObj1 - B
DMObjNew = minus(B, DMObj1)
DMObjNew = B - DMObj1
```

Arguments

DMObj1, *DMObj2*	DataMatrix objects, such as created by `DataMatrix` (object constructor).
B	MATLAB numeric or logical array.

Return Values

DMObjNew	DataMatrix object created by subtraction.

Description

DMObjNew = `minus(`*DMObj1*`, `*DMObj2*`)` or the equivalent *DMObjNew* = *DMObj1* - *DMObj2* performs an element-by-element subtraction of the DataMatrix object *DMObj2* from the DataMatrix object *DMObj1* and places the results in *DMObjNew*, another DataMatrix object. *DMObj1* and *DMObj2* must have the same size (number of rows and columns), unless one is a scalar (1-by-1 DataMatrix object). The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*, unless *DMObj1* is a scalar; then they are the same as *DMObj2*.

DMObjNew = `minus(`*DMObj1*`, `*B*`)` or the equivalent *DMObjNew* = *DMObj1* - *B* performs an element-by-element subtraction of *B*, a numeric or logical array, from the DataMatrix object *DMObj1*, and places the results in *DMObjNew*, another DataMatrix object. *DMObj1* and *B* must have the same size (number of rows and columns), unless *B* is a scalar. The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*.

DMObjNew = minus(*B*, *DMObj1*) or the equivalent *DMObjNew* = *B* - *DMObj1* performs an element-by-element subtraction of the DataMatrix object *DMObj1* from *B*, a numeric or logical array, and places the results in *DMObjNew*, another DataMatrix object. *DMObj1* and *B* must have the same size (number of rows and columns), unless *B* is a scalar. The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*.

Note Arithmetic operations between a scalar DataMatrix object and a nonscalar array are not supported.

MATLAB calls *DMObjNew* = minus(*X*, *Y*) for the syntax *DMObjNew* = *X* - *Y* when *X* or *Y* is a DataMatrix object.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: plus

Purpose

Calculate molecular weight of amino acid sequence

Syntax

```
molweight(SeqAA)
```

Arguments

SeqAA	Amino acid sequence. Enter a character string or a vector of integers from the tableAmino Acid Lookup on page 3-111. Examples: `'ARN'`, `[1 2 3]`. You can also enter a structure with the field `Sequence`.

Description

`molweight(SeqAA)` calculates the molecular weight for the amino acid sequence *SeqAA*.

Examples

1 Retrieve an amino acid sequence from the NCBI GenPept database.

```
rhodopsin = getgenpept('NP_000530');
```

2 Calculate the molecular weight of the sequence.

```
rhodopsinMW = molweight(rhodopsin)

rhodopsinMW =

  3.8892e+004
```

See Also

Bioinformatics Toolbox functions: `aacount`, `atomiccomp`, `isoelectric`, `isotopicdist`, `proteinplot`

molviewer

Purpose

Display and manipulate 3-D molecule structure

Syntax

```
molviewer
molviewer(File)
molviewer(pdbID)
molviewer(pdbStruct)
FigureHandle = molviewer(...)
```

Arguments

File

String specifying one of the following:

- File name of a file on the MATLAB search path or in the MATLAB Current Directory
- Path and file name
- URL pointing to a file (URL must begin with a protocol such as http://, ftp://, or file://)

The referenced file is a molecule model file, such as a Protein Data Bank (PDB)-formatted file (ASCII text file). Valid file types include:

- PDB
- MOL (MDL)
- SDF
- XYZ
- SMOL
- JVXL
- CIF/mmCIF

pdbID

String specifying a unique identifier for a protein structure record in the PDB database.

Note Each structure in the PDB database is represented by a four-character alphanumeric identifier. For example, `4hhb` is the identifier for hemoglobin.

`pdbStruct` A structure containing a field for each PDB record, such as returned by the `getpdb` or `pdbread` function.

Return Values

`FigureHandle` Figure handle to a Molecule Viewer window.

Description

`molviewer` opens a blank Molecule Viewer window. You can display 3-D molecular structures by selecting **File > Open**, **File > Load PDB ID**, or **File > Open URL**.

`molviewer(`*`File`*`)` reads the data in a molecule model file, *`File`*, and opens a Molecule Viewer window displaying the 3-D molecular structure for viewing and manipulation.

`molviewer(`*`pdbID`*`)` retrieves the data for a protein structure record, *`pdbID`*, from the PDB database and opens a Molecule Viewer window displaying the 3-D molecular structure for viewing and manipulation.

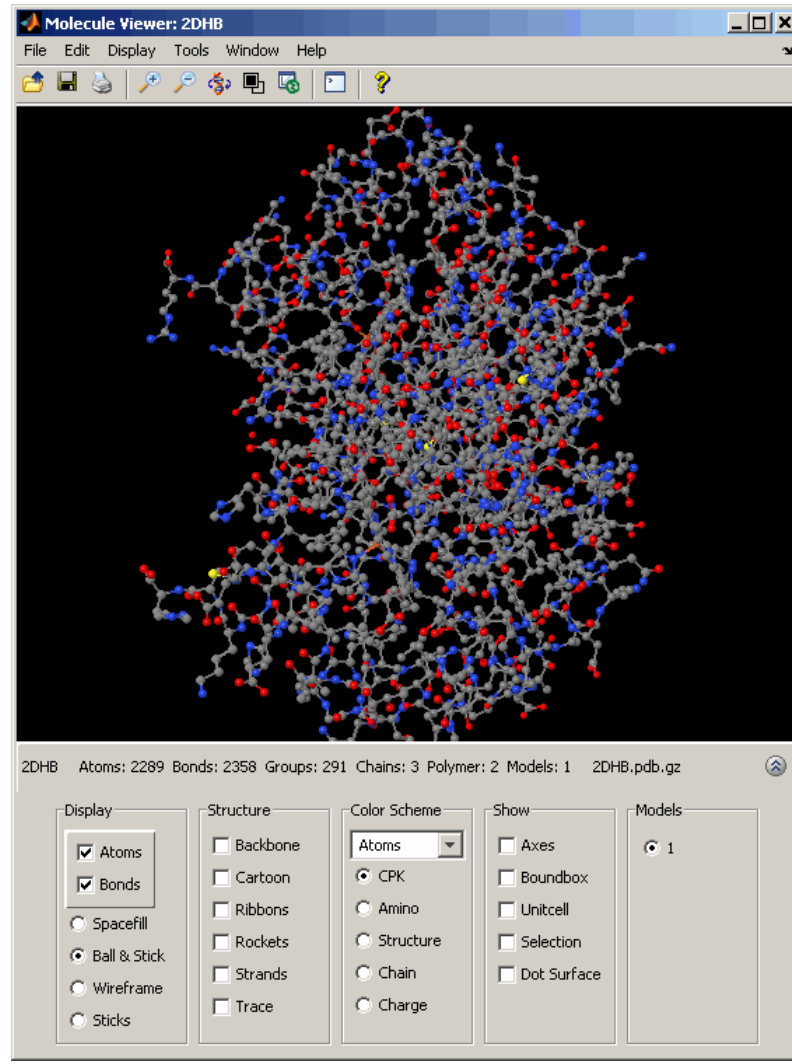
`molviewer(`*`pdbStruct`*`)` reads the data from *`pdbStruct`*, a structure containing a field for each PDB record, and opens a Molecule Viewer window displaying a 3-D molecular structure for viewing and manipulation.

`FigureHandle` `= molviewer(...)` returns the figure handle to the Molecule Viewer window.

Tip You can pass the *`FigureHandle`* to the `evalrasmolscript` function, which sends RasMol script commands to the Molecule Viewer window.

Tip If you receive any errors related to memory or Java™ heap space, try increasing your Java heap space as described at:

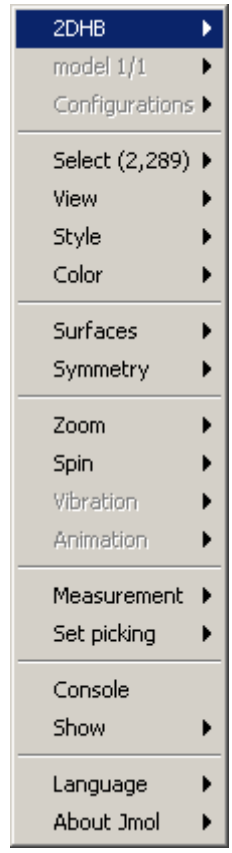
```
http://www.mathworks.com/support/solutions/data/1-18I2C.html
```



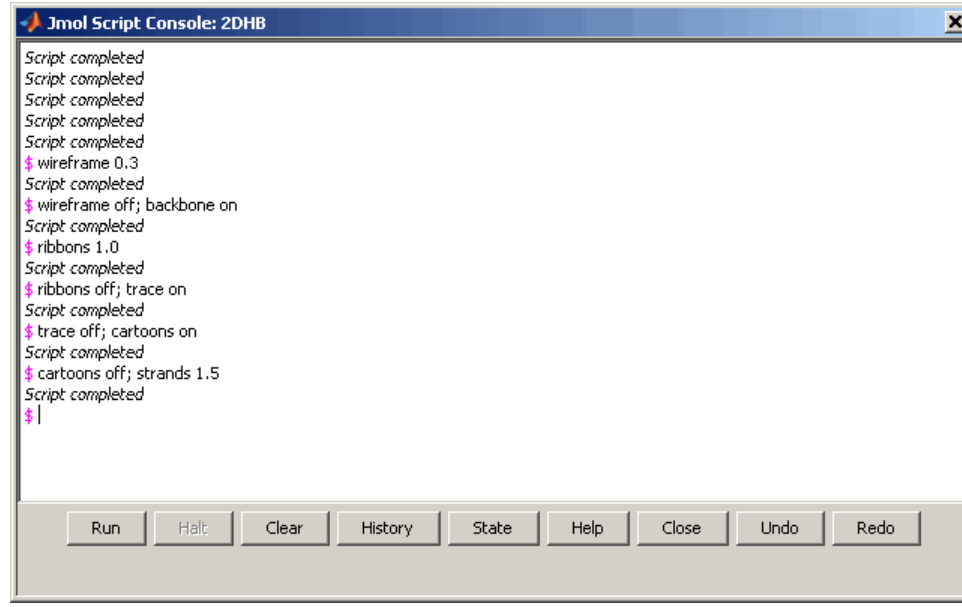
After displaying the 3-D molecule structure, you can:

- Click-drag the molecule to spin, rotate, and view it from different angles.
- Hover the mouse over a subcomponent of the molecule to display an identification label for it.
- Zoom the plot by turning the mouse scroll wheel or clicking the following buttons:

   or 
- Spin the molecule by clicking  .
- Change the background color between black and white by clicking  .
- Reset the molecule position by clicking  .
- Show or hide the Control Panel by clicking  .
- Manipulate and annotate the 3-D structure by selecting options in the Control Panel or, for a complete list of options, by right-clicking the Molecule Viewer window to select commands:



- Display the Jmol Script Console by clicking  .



Examples

View the acetylsalicylic acid (aspirin) molecule, whose structural information is contained in the Elsevier MDL molecule file `aspirin.mol`.

```
molviewer('aspirin.mol')
```

View the H5N1 influenza virus hemagglutinin molecule, whose structural information is located at `www.rcsb.org/pdb/files/2FK0.pdb.gz`.

```
molviewer('http://www.rcsb.org/pdb/files/2FK0.pdb.gz')
```

View the molecule with a PDB identifier of `2DHB`.

```
molviewer('2DHB')
```

View the molecule with a PDB identifier of `4hhb`, and create a figure handle for the molecule viewer.

```
FH = molviewer('4hhb')
```

Use the `getpdb` function to retrieve protein structure data from the PDB database and create a MATLAB structure. Then view the protein molecule.

```
pdbstruct = getpdb('1vqx')
molviewer(pdbstruct)
```

See Also

Bioinformatics Toolbox functions: `evalrasmolscript`, `getpdb`, `pdbread`, `pdbsuperpose`, `pdbtransform`, `pdbwrite`

Purpose

Align peaks in signal to reference peaks

Syntax

```
IntensitiesOut = msalign(X, Intensities, RefX)
... = msalign(..., 'Rescaling', RescalingValue, ...)
... = msalign(..., 'Weights', WeightsValue, ...)
... = msalign(..., 'MaxShift', MaxShiftValue, ...)
... = msalign(..., 'WidthOfPulses',
WidthOfPulsesValue, ...)
... = msalign(..., 'WindowSizeRatio', WindowSizeRatioValue,
   ...)
... = msalign(..., 'Iterations', IterationsValue, ...)
... = msalign(..., 'GridSteps', GridStepsValue, ...)
... = msalign(..., 'SearchSpace', SearchSpaceValue, ...)
... = msalign(..., 'ShowPlot', ShowPlotValue, ...)
[IntensitiesOut, RefXOut] = msalign(...,
'Group', GroupValue,
   ...)
```

Arguments

X	Vector of separation-unit values for a set of signals with peaks. The number of elements in the vector equals the number of rows in the matrix *Intensities*. The separation unit can quantify wavelength, frequency, distance, time, or m/z depending on the instrument that generates the signal data.
Intensities	Matrix of intensity values for a set of peaks that share the same separation-unit range. Each row corresponds to a separation-unit value, and each column corresponds to either a set of signals with peaks or a retention time. The number of rows equals the number of elements in vector *X*.

RefX	Vector of separation-unit values of known reference masses in a sample signal.
	Tip For reference peaks, select compounds that are not expected to have significant shifts among the different signals. For example, in mass spectrometry, select compounds that do not undergo structural transformation, such as phosphorylation. Doing so increases the accuracy of your alignment and lets you detect compounds that exhibit structural transformations among the sample signal.
RescalingValue	Controls the rescaling of *X*. Choices are `true` (default) or `false`. When `false`, the output signal is aligned only to the reference peaks by using constant shifts. By default, `msalign` estimates a rescaling factor, unless *RefX* contains only one reference peak.
WeightsValue	Vector of positive values, with the same number of elements as *RefX*. The default vector is `ones(size(`*RefX*`))`.
MaxShiftValue	Two-element vector, in which the first element is negative and the second element is positive, that specifies the lower and upper limits of a range, in separation units, relative to each peak. No peak shifts beyond these limits. Default is `[-100 100]`.

WidthOfPulsesValue	Positive value that specifies the width, in separation units, for all the Gaussian pulses used to build the correlating synthetic signal. The point of the peak where the Gaussian pulse reaches 60.65% of its maximum is set to the width specified by *WidthOfPulsesValue*. Default is 10.
WindowSizeRatioValue	Positive value that specifies a scaling factor that determines the size of the window around every alignment peak. The synthetic signal is compared to the input signal only within these regions, which saves computation time. The size of the window is given in separation-units by *WidthOfPulsesValue* * *WindowSizeRatioValue*. Default is 2.5, which means at the limits of the window, the Gaussian pulses have a value of 4.39% of their maximum.
IterationsValue	Positive integer that specifies the number of refining iterations. At every iteration, the search grid is scaled down to improve the estimates. Default is 5.
GridStepsValue	Positive integer that specifies the number of steps for the search grid. At every iteration, the search area is divided by *GridStepsValue*^2. Default is 20.
SearchSpaceValue	String that specifies the type of search space. Choices are: • 'regular' — Default. Evenly spaced lattice. • 'latin' — Random Latin hypercube with *GridStepsValue*^2 samples.

ShowPlotValue

Controls the display of a plot of an original and aligned signal over the reference masses specified by *RefX*. Choices are `true`, `false`, or *I*, an integer specifying the index of a signal in *Intensities*. If you set to `true`, the first signal in *Intensities* is plotted. Default is:

- `false` — When return values are specified.
- `true` — When return values are not specified.

GroupValue

Controls the creation of *RefXOut*, a new vector of separation-unit values to be used as reference masses for aligning the peaks. This vector is created by adjusting the values in *RefX*, based on the sample data from multiple signals in *Intensities*, such that the overall shifting and scaling of the peaks is minimized. Choices are `true` or `false` (default).

Tip Set *GroupValue* to `true` only if *Intensities* contains data for a large number of signals, and you are not confident of the separation-unit values used for your reference peaks in *RefX*. Leave *GroupValue* set to `false` if you are confident of the separation-unit values used for your reference peaks in *RefX*.

Return Values

IntensitiesOut	Matrix of intensity values for a set of peaks that share the same separation-unit range. Each row corresponds to a separation-unit value, and each column corresponds to either a set of signals with peaks or a retention time. The intensity values represent a shifting and scaling of the data.
RefXOut	Vector of separation-unit values of reference masses, calculated from *RefX* and the sample data from multiple signals in *Intensities*, when you set *GroupValue* to `true`.

Description

Tip Use the following syntaxes with data from any separation technique that produces signal data, such as spectroscopy, NMR, electrophoresis, chromatography, or mass spectrometry.

IntensitiesOut = `msalign(`*X*`,` *Intensities*`,` *RefX*`)` aligns the peaks in raw, noisy signal data, represented by *Intensities* and *X*, to reference peaks, provided by *RefX*. First, it creates a synthetic signal from the reference peaks using Gaussian pulses centered at the separation-unit values specified by *RefX*. Then, it shifts and scales the separation-unit scale to find the maximum alignment between the input signals and the synthetic signal. (It uses an iterative multiresolution grid search until it finds the best scale and shift factors for each signal.) Once the new separation-unit scale is determined, the corrected signals are created by resampling their intensities at the original separation-unit values, creating *IntensitiesOut*, a vector or matrix of corrected intensity values. The resampling method preserves the shape of the peaks.

Tip The `msalign` function works best with three to five reference peaks that you know will appear in the signal. If you use a single reference peak (internal standard), there is a possibility of aligning sample peaks to the incorrect reference peaks as `msalign` both scales and shifts the *`X`* vector. If using a single reference peak, you might need to only shift the *`X`* vector. To do this, use *`IntensitiesOut`* `= interp1(`*`X`*`,` *`Intensities`*`,` *`X`*`-(`*`ReferencePeak-ExperimentalPeak`*`)`. For more information, see Aligning a Mass Spectrum with One Reference Peak on page 3-978.

`...  = msalign(...,` '*`PropertyName`*'`,` *`PropertyValue`*`, ...)` calls `msalign` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`...  = msalign(..., 'Rescaling',` *`RescalingValue`*`, ...)` controls the rescaling of *`X`*. Choices are `true` (default) or `false`. When `false`, the output signal is aligned only to the reference peaks by using constant shifts. By default, `msalign` estimates a rescaling factor, unless *`RefX`* contains only one reference peak.

`...  = msalign(..., 'Weights',` *`WeightsValue`*`, ...)` specifies the relative weight for each mass in *`RefX`*, the vector of reference separation-unit values. *`WeightsValue`* is a vector of positive values, with the same number of elements as *`RefX`*. The default vector is `ones(size(`*`RefX`*`))`, which means each reference peak is weighted equally, so that more intense reference peaks have a greater effect in the alignment algorithm. If you have a less intense reference peak, you can increase its weight to emphasize it more in the alignment algorithm.

`...  = msalign(..., 'MaxShift',` *`MaxShiftValue`*`, ...)` specifies the lower and upper limits of the range, in separation units, relative to each peak. No peak shifts beyond these limits. *`MaxShiftValue`* is a two-element vector, in which the first element is negative and the second element is positive. Default is `[-100 100]`.

Note Use these values to tune the robustness of the algorithm. Ideally, you should keep the range within the maximum expected shift. If you try to correct larger shifts by increasing the limits, you increase the possibility of picking incorrect peaks to align to the reference masses.

`...  = msalign(..., 'WidthOfPulses', WidthOfPulsesValue, ...)` specifies the width, in separation units, for all the Gaussian pulses used to build the correlating synthetic signal. The point of the peak where the Gaussian pulse reaches `60.65`% of its maximum is set to the width you specify with *`WidthOfPulsesValue`*. Choices are any positive value. Default is `10`. *`WidthOfPulsesValue`* may also be a function handle. The function is evaluated at the respective separation-unit values and returns a variable width for the pulses. Its evaluation should give reasonable values from `0` to `max(abs(Range))`; otherwise, the function returns an error.

Note Tuning the spread of the Gaussian pulses controls a tradeoff between robustness (wider pulses) and precision (narrower pulses). However, the spread of the pulses is unrelated to the shape of the observed peaks in the signal. The purpose of the pulse spread is to drive the optimization algorithm.

`...  = msalign(..., 'WindowSizeRatio', WindowSizeRatioValue, ...)` specifies a scaling factor that determines the size of the window around every alignment peak. The synthetic signal is compared to the sample signal only within these regions, which saves computation time. The size of the window is given in separation units by *`WidthOfPulsesValue`* `*` *`WindowSizeRatioValue`*. Choices are any positive value. Default is `2.5`, which means at the limits of the window, the Gaussian pulses have a value of `4.39`% of their maximum.

`... = msalign(..., 'Iterations', IterationsValue, ...)` specifies the number of refining iterations. At every iteration, the search grid is scaled down to improve the estimates. Choices are any positive integer. Default is `5`.

`... = msalign(..., 'GridSteps', GridStepsValue, ...)` specifies the number of steps for the search grid. At every iteration, the search area is divided by `GridStepsValue^2`. Choices are any positive integer. Default is `20`.

`... = msalign(..., 'SearchSpace', SearchSpaceValue, ...)` specifies the type of search space. Choices are:

- `'regular'` — Default. Evenly spaced lattice.
- `'latin'` — Random Latin hypercube with `GridStepsValue^2` samples.

`... = msalign(..., 'ShowPlot', ShowPlotValue, ...)` controls the display of a plot of an original and aligned signal over the reference masses specified by `RefX`. Choices are `true`, `false`, or `I`, an integer specifying the index of a signal in `Intensities`. If set to `true`, the first signal in `Intensities` is plotted. Default is:

- `false` — When return values are specified.
- `true` — When return values are not specified.

`[IntensitiesOut, RefXOut] = msalign(..., 'Group', GroupValue, ...)` controls the creation of `RefXOut`, a new vector of separation-unit values to use as reference masses for aligning the peaks. This vector is created by adjusting the values in `RefX`, based on the sample data from multiple signals in `Intensities`, such that the overall shifting and scaling of the peaks is minimized. Choices are `true` or `false` (default).

Tip Set *GroupValue* to `true` only if *Intensities* contains data for a large number of signals, and you are not confident of the separation-unit values used for your reference peaks in *RefX*. Leave *GroupValue* set to `false` if you are confident of the separation-unit values used for your reference peaks in *RefX*.

Examples

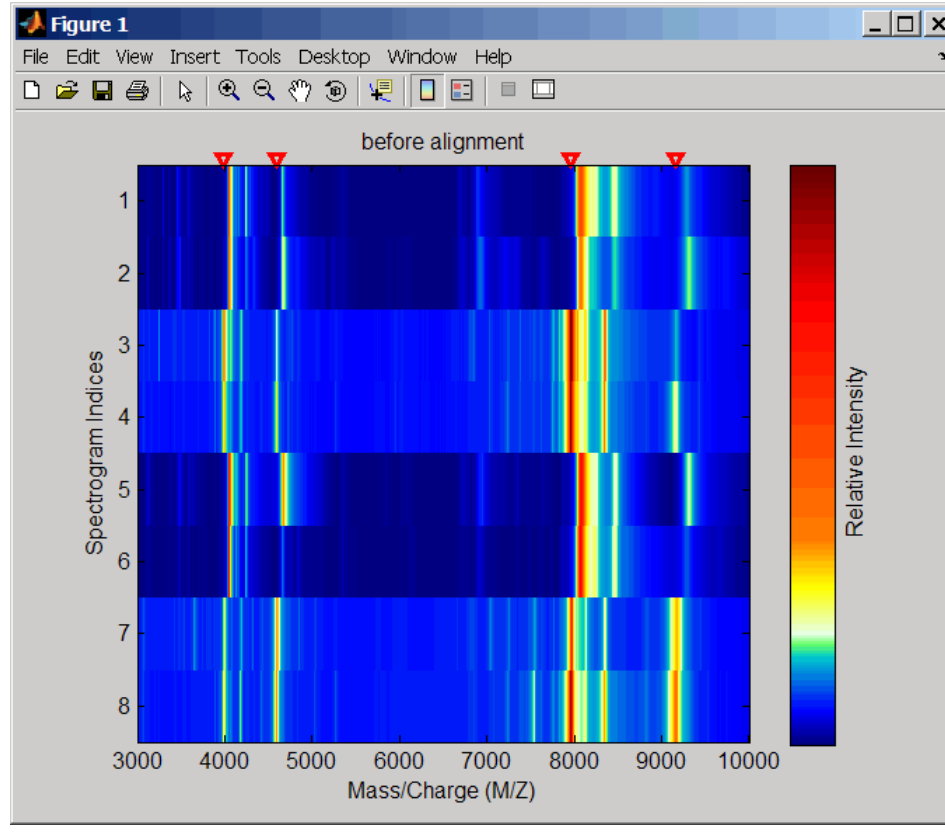
Aligning a Mass Spectrum with Three or More Reference Peaks

1. Load a MAT-file, included with the Bioinformatics Toolbox software, that contains sample data, reference masses, and parameter data for synthetic peak width.

```
load sample_lo_res
R = [3991.4 4598 7964 9160];
W = [60 100 60 100];
```

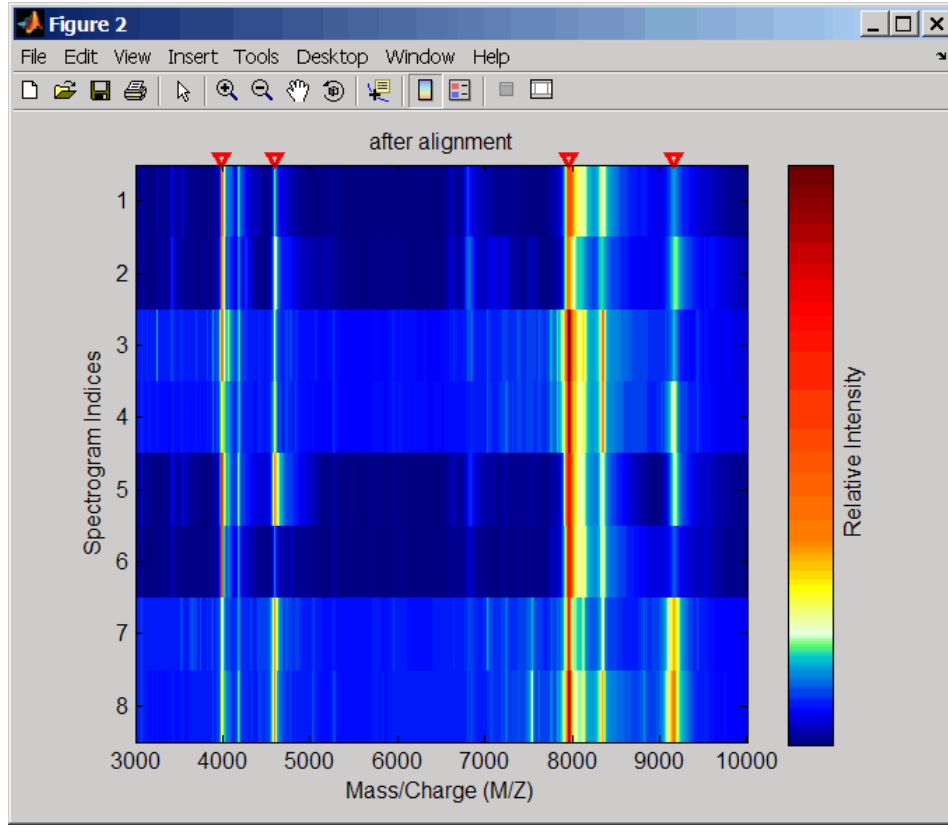
2. Display a color image of the mass spectra before alignment.

```
msheatmap(MZ_lo_res,Y_lo_res,'markers',R,'range',[3000 10000])
title('before alignment')
```



3 Align spectra with reference masses and display a color image of mass spectra after alignment.

```
YA = msalign(MZ_lo_res,Y_lo_res,R,'weights',W);
msheatmap(MZ_lo_res,YA,'markers',R,'range',[3000 10000])
title('after alignment')
```



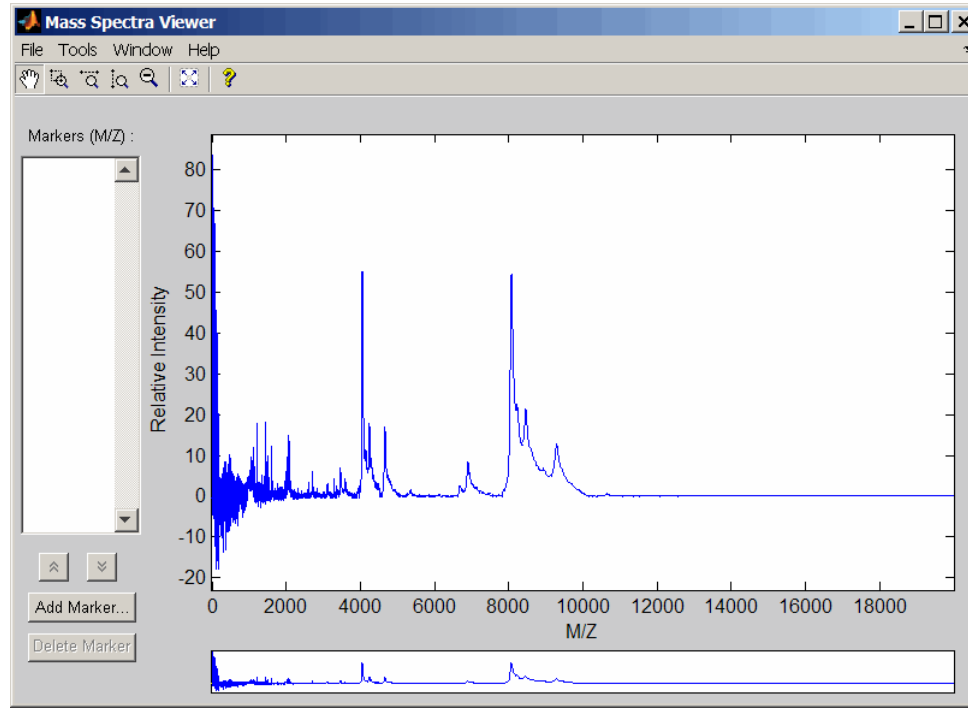
Aligning a Mass Spectrum with One Reference Peak

It is not recommended to use the `msalign` function if you have only one reference peak. Instead, use the following procedure, which shifts the `X` input vector, but does not scale it.

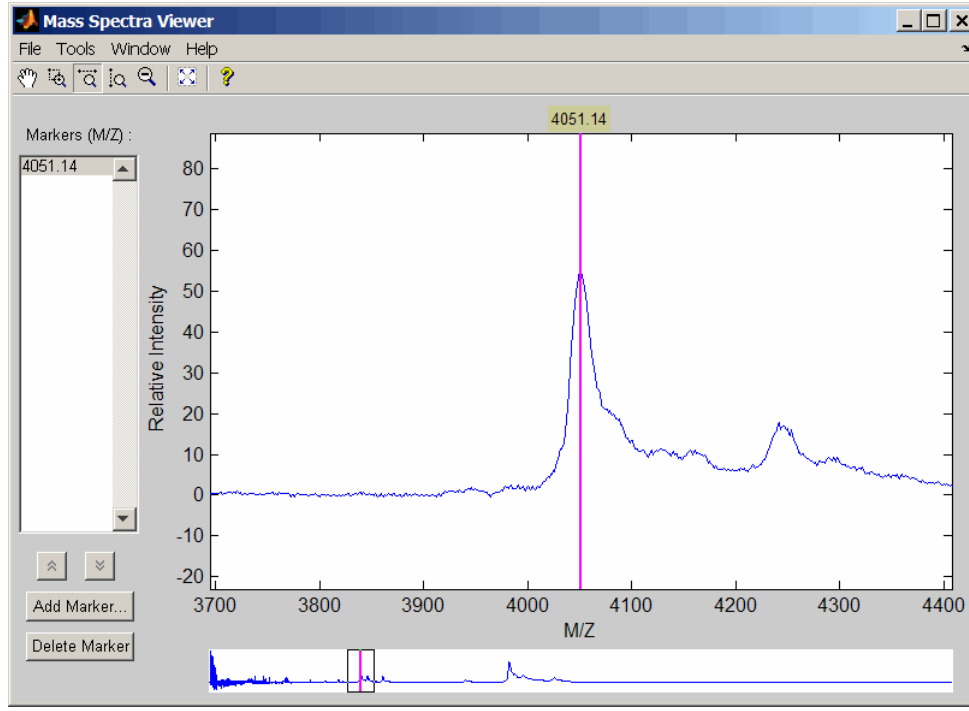
1 Load sample data and view the first sample spectrum.

```
load sample_lo_res
MZ = MZ_lo_res;
Y = Y_lo_res(:,1);
```

```
msviewer(MZ, Y)
```



2 Use the tall peak around 4000 m/z as the reference peak. To determine the reference peak's m/z value, click  , and then click-drag to zoom in on the peak. Right-click in the center of the peak, and then click **Add Marker** to label the peak with its m/z value.



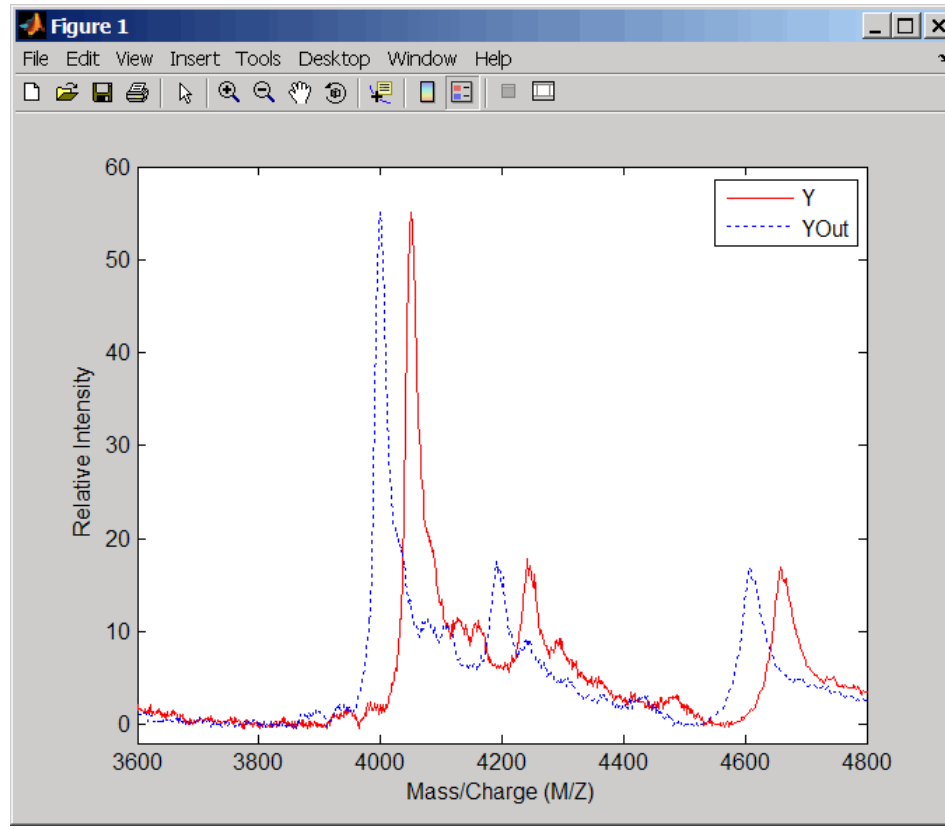
3 Shift a spectrum by the difference between `RP`, the known reference mass of 4000 m/z, and `SP`, the experimental mass of 4051.14 m/z.

```
RP = 4000;
SP = 4051.14;
YOut = interp1(MZ, Y, MZ-(RP-SP));
```

4 Plot the original spectrum in red and the shifted spectrum in blue and zoom in on the reference peak.

```
plot(MZ,Y,'r',MZ,YOut,'b:')
xlabel('Mass/Charge (M/Z)')
ylabel('Relative Intensity')
```

```
legend('Y','YOut')
axis([3600 4800 -2 60])
```



References

[1] Monchamp, P., Andrade-Cetto, L., Zhang, J.Y., and Henson, R. (2007) Signal Processing Methods for Mass Spectrometry. In Systems Bioinformatics: An Engineering Case-Based Approach, G. Alterovitz and M.F. Ramoni, eds. (Artech House Publishers).

See Also

Bioinformatics Toolbox functions: `msbackadj`, `msheatmap`, `mspalign`, `mspeaks`, `msresample`, `msviewer`

Bioinformatics Toolbox demo:

Preprocessing Raw Mass Spectrometry Data

Purpose

Correct baseline of signal with peaks

Syntax

```
Yout = msbackadj(X, Intensities)
Yout = msbackadj(X, Intensities, ...'WindowSize',
WindowSizeValue, ...)
Yout = msbackadj(X, Intensities, ...'StepSize',
   StepSizeValue, ...)
Yout = msbackadj(X, Intensities, ...'RegressionMethod',
   RegressionMethodValue, ...)
Yout = msbackadj(X, Intensities, ...'EstimationMethod',
   EstimationMethodValue, ...)
Yout = msbackadj(X, Intensities, ...'SmoothMethod',
   SmoothMethodValue, ...)
Yout = msbackadj(X, Intensities, ...'QuantileValue',
   QuantileValueValue, ...)
Yout = msbackadj(X, Intensities, ...'PreserveHeights',
   PreserveHeightsValue, ...)
Yout = msbackadj(X, Intensities, ...'ShowPlot',
   ShowPlotValue, ...)
```

Arguments

X	Vector of separation-unit values for a set of signals with peaks. The number of elements in the vector equals the number of rows in the matrix *Intensities*. The separation unit can quantify wavelength, frequency, distance, time, or m/z depending on the instrument that generates the signal data.
Intensities	Matrix of intensity values for a set of peaks that share the same separation-unit range. Each row corresponds to a separation-unit value, and each column corresponds to either a set of signals with peaks or a retention time. The number of rows equals the number of elements in vector *X*.

Description

Tip Use the following syntaxes with data from any separation technique that produces signal data, such as spectroscopy, NMR, electrophoresis, chromatography, or mass spectrometry.

`Yout = msbackadj(X, Intensities)` adjusts the variable baseline of a raw signal with peaks by following steps:

1. Estimates the baseline within multiple shifted windows of width `200` separation units
2. Regresses the varying baseline to the window points using a spline approximation
3. Adjusts the baseline of the peak signals supplied by *`Intensities`*

`Yout = msbackadj(X, Intensities, ...'PropertyName', PropertyValue, ...)` calls `msbackadj` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`Yout = msbackadj(X, Intensities, ...'WindowSize', WindowSizeValue, ...)` specifies the width for the shifting window. *`WindowSizeValue`* can also be a function handle. The function is evaluated at the respective *`X`* values and returns a variable width for the windows. This option is useful for cases where the resolution of the signal is dissimilar at different regions. The default value is `200` (baseline point estimated for windows with a width of `200` separation units).

Note The result of this algorithm depends on carefully choosing the window size and the step size. Consider the width of your peaks in the signal and the presence of possible drifts. If you have wider peaks toward the end of the signal, you may want to use variable parameters.

Yout = msbackadj(*X*, *Intensities*, ...'StepSize', *StepSizeValue*, ...) specifies the steps for the shifting window. The default value is 200 separation units (baseline point is estimated for windows placed every 200 separation units). *StepSizeValue* can also be a function handle. The function is evaluated at the respective separation-unit values and returns the distance between adjacent windows.

Yout = msbackadj(*X*, *Intensities*, ...'RegressionMethod', *RegressionMethodValue*, ...) specifies the method to regress the window estimated points to a soft curve. Enter 'pchip' (shape-preserving piecewise cubic interpolation), 'linear' (linear interpolation), or 'spline' (spline interpolation). The default value is 'pchip'.

Yout = msbackadj(*X*, *Intensities*, ...'EstimationMethod', *EstimationMethodValue*, ...) specifies the method for finding the likely baseline value in every window. Enter 'quantile' (quantile value is set to 10%) or 'em' (assumes a doubly stochastic model). With em, every sample is the independent and identically distributed (i.i.d.) draw of any of two normal distributed classes (background or peaks). Because the class label is hidden, the distributions are estimated with an Expectation-Maximization algorithm. The ultimate baseline value is the mean of the background class.

Yout = msbackadj(*X*, *Intensities*, ...'SmoothMethod', *SmoothMethodValue*, ...) specifies the method for smoothing the curve of estimated points and eliminating the effects of possible outliers. Enter 'none', 'lowess' (linear fit), 'loess' (quadratic fit), 'rlowess' (robust linear), or 'rloess' (robust quadratic fit). Default is 'none'.

Yout = msbackadj(*X*, *Intensities*, ...'QuantileValue', *QuantileValueValue*, ...) specifies the quantile value. The default value is 0.10.

Yout = msbackadj(*X*, *Intensities*, ...'PreserveHeights', *PreserveHeightsValue*, ...), when *PreserveHeightsValue* is true, sets the baseline subtraction mode to preserve the height of the tallest peak in the signal. The default value is false and peak heights are not preserved.

Yout = msbackadj(*X*, *Intensities*, ...'ShowPlot', *ShowPlotValue*, ...) plots the baseline-estimated points, the regressed baseline, and the original signal. When you call msbackadj without output arguments, the signal is plotted unless *ShowPlotValue* is false. When *ShowPlotValue* is true, only the first signal in *Intensities* is plotted. *ShowPlotValue* can also contain an index to one of the signals in *Intensities*.

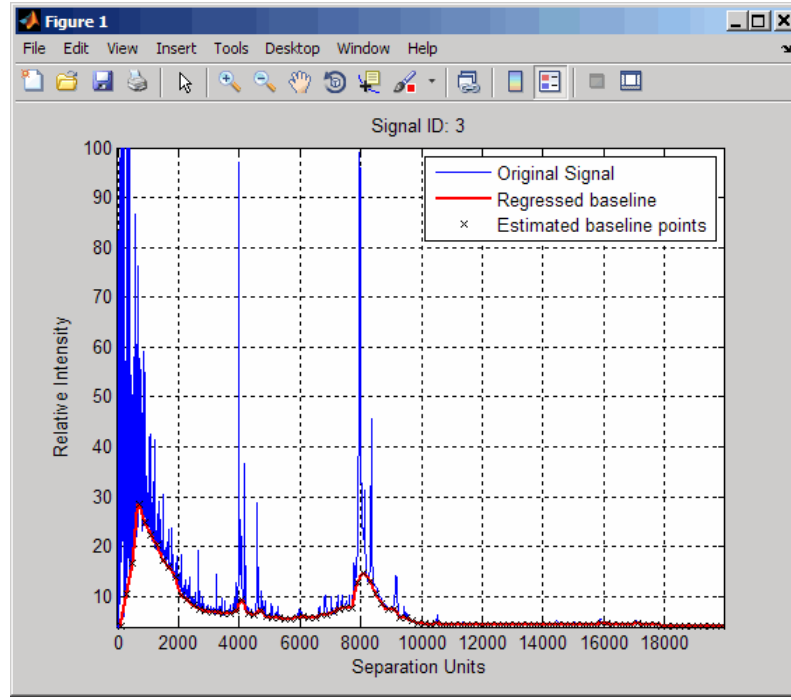
Examples

1. Load a MAT-file, included with the Bioinformatics Toolbox software, that contains some sample data.

```
load sample_lo_res
```

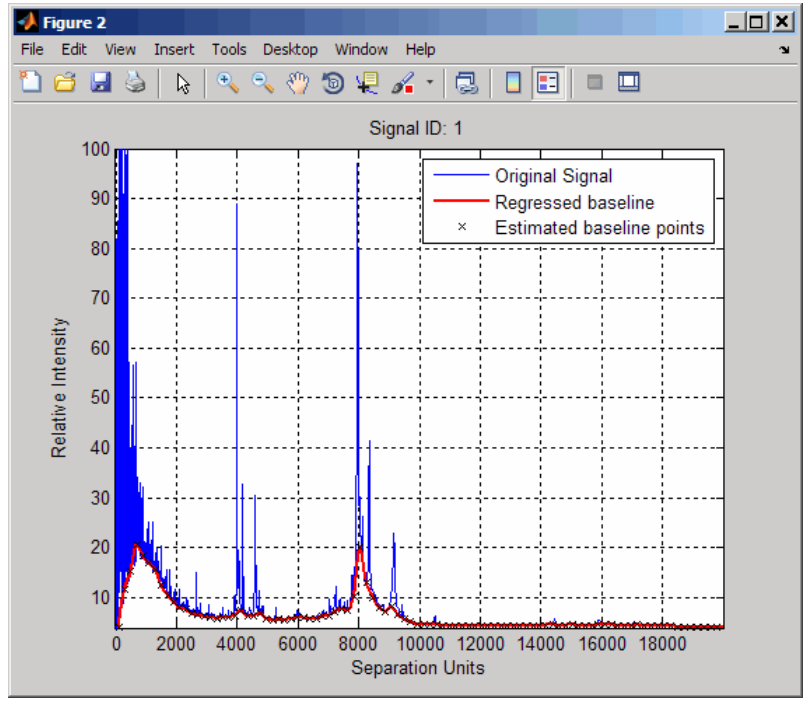
2. Adjust the baseline for a group of spectra and show only the third spectrum and its estimated background.

```
YB = msbackadj(MZ_lo_res,Y_lo_res,'SHOWPLOT',3);
```



3 Plot the estimated baseline for the fourth spectrum in `Y_lo_res` using an anonymous function to describe an m/z dependent parameter.

```
wf = @(mz) 200 + .001 .* mz;
msbackadj(MZ_lo_res,Y_lo_res(:,4),'STEPSIZE',wf);
```



See Also

Bioinformatics Toolbox functions: `msalign`, `msheatmap`, `mslowess`, `msnorm`, `mspeaks`, `msresample`, `mssgolay`, `msviewer`

Purpose

Plot set of peak lists from LC/MS or GC/MS data set

Syntax

```
msdotplot(Peaks, Times)
msdotplot(FigHandle, Peaks, Times)
msdotplot(..., 'Quantile', QuantileValue)
PlotHandle = msdotplot(...)
```

Arguments

Peaks

Cell array of peak lists, where each element is a two-column matrix with m/z values in the first column and ion intensity values in the second column. Each element corresponds to a spectrum or retention time.

Tip You can use the `mzxml2peaks` function to create the *Peaks* cell array.

Times

Vector of retention times associated with an LC/MS or GC/MS data set. The number of elements in *Times* equals the number of elements in the cell array *Peaks*.

Tip You can use the `mzxml2peaks` function to create the *Times* vector.

FigHandle

Handle to an open Figure window such as one created by the `msheatmap` function.

QuantileValue

Value that specifies a percentage. When peaks are ranked by intensity, only those that rank above this percentage are plotted. Choices are any value $\geq$ `0` and $\leq$ `1`. Default is `0`. For example, setting *QuantileValue* = `0` plots all peaks, and setting *QuantileValue* = `0.8` plots only the 20% most intense peaks.

Return Values

PlotHandle	Handle to the line series object (figure plot).

Description

`msdotplot(`*`Peaks`*`, `*`Times`*`)` plots a set of peak lists from a liquid chromatography/mass spectrometry (LC/MS) or gas chromatography/mass spectrometry (GC/MS) data set represented by *`Peaks`*, a cell array of peak lists, where each element is a two-column matrix with m/z values in the first column and ion intensity values in the second column, and *`Times`*, a vector of retention times associated with the spectra. *`Peaks`* and *`Times`* have the same number of elements. The data is plotted into any existing figure generated by the `msheatmap` function; otherwise, the data is plotted into a new Figure window.

`msdotplot(`*`FigHandle`*`, `*`Peaks`*`, `*`Times`*`)` plots the set of peak lists into the axes contained in an open Figure window with the handle *`FigHandle`*.

Tip This syntax is useful to overlay a dot plot on top of a heat map of mass spectrometry data created with the `msheatmap` function.

`msdotplot(..., 'Quantile', `*`QuantileValue`*`)` plots only the most intense peaks, specifically those in the percentage above the specified *`QuantileValue`*. Choices are any value ≥ `0` and ≤ `1`. Default is `0`. For example, setting *`QuantileValue`* = `0` plots all peaks, and setting *`QuantileValue`* = `0.8` plots only the 20% most intense peaks.

`PlotHandle` = `msdotplot(...)` returns a handle to the line series object (figure plot). You can use this handle as input to the `get` function to display a list of the plot's properties. You can use this handle as input to the `set` function to change the plot's properties, including showing and hiding points.

Examples

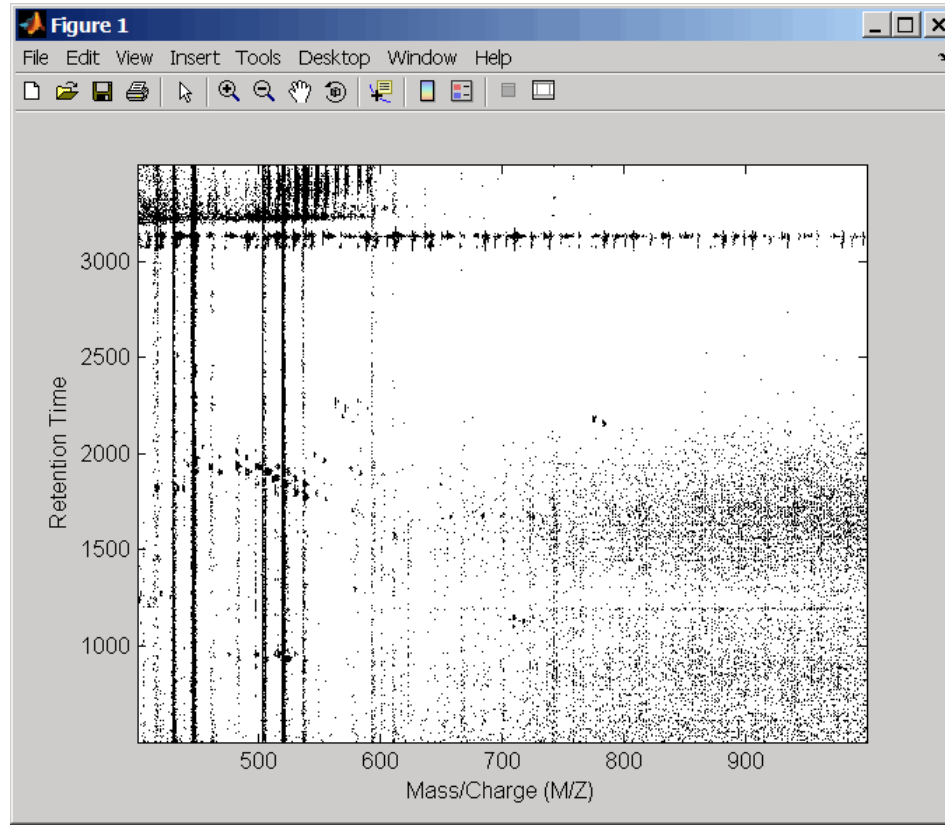
1. Load a MAT-file, included with the Bioinformatics Toolbox software, which contains LC/MS data variables, including `peaks` and `ret_time`. `peaks` is a cell array of peak lists, where each element is a two-column

matrix of m/z values and ion intensity values, and each element corresponds to a spectrum or retention time. `ret_time` is a column vector of retention times associated with the LC/MS data set.

```
load lcmsdata
```

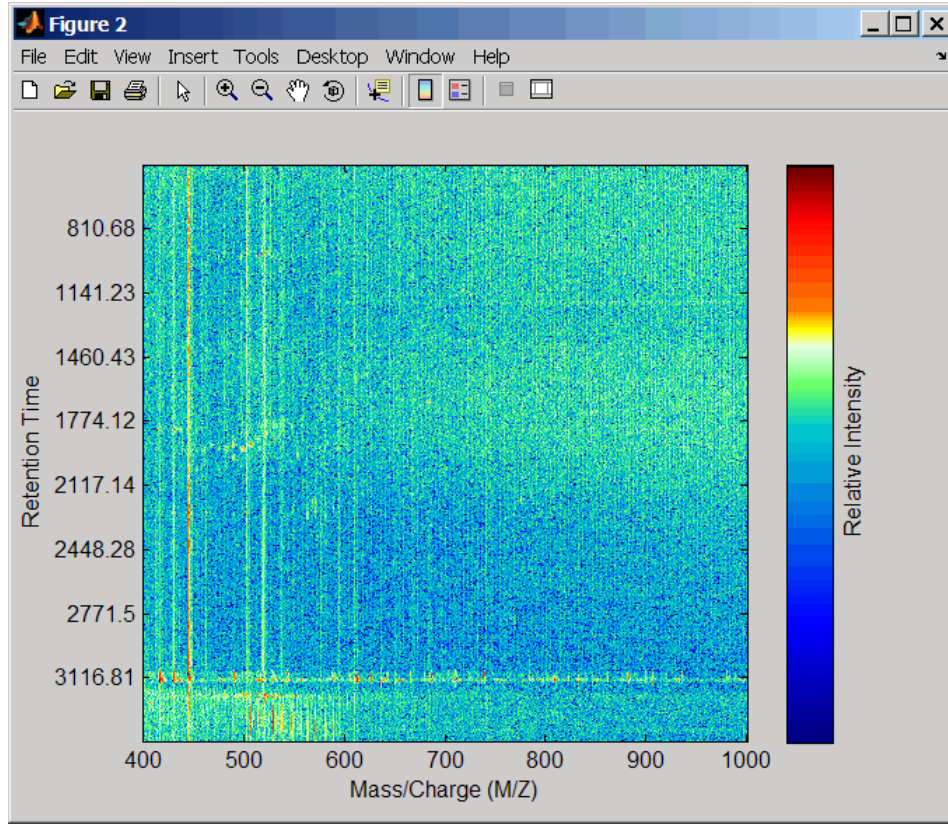
2 Create a dot plot with only the 5% most intense peaks.

```
msdotplot(peaks,ret_time,'Quantile',0.95)
```



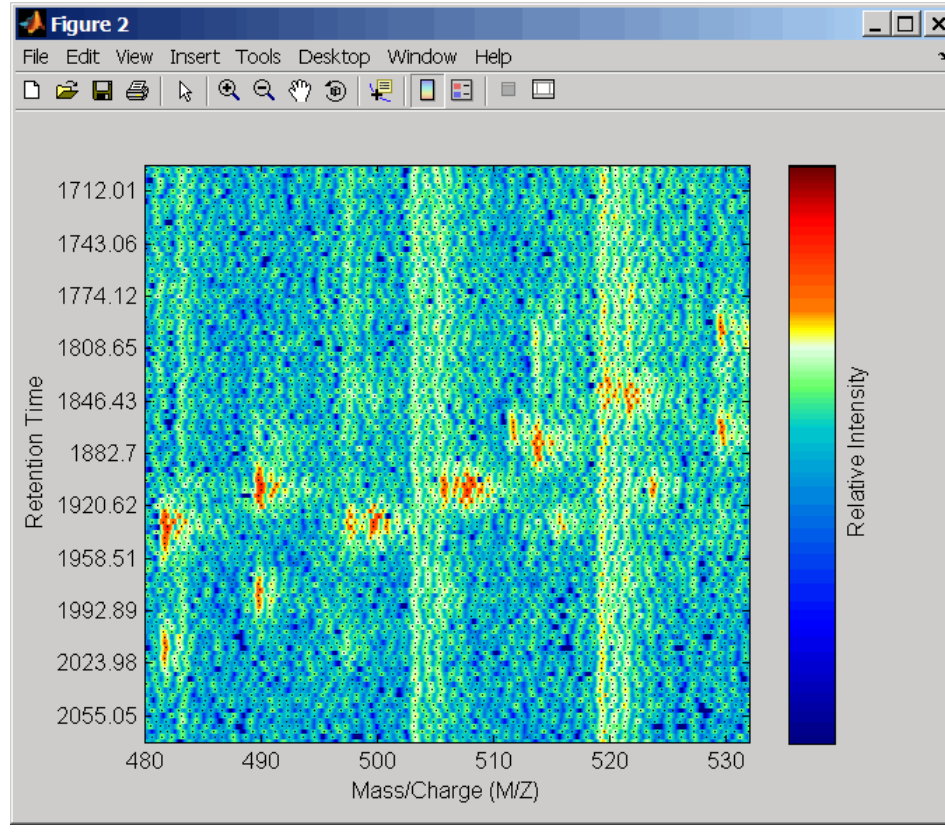
3 Resample the data, then create a heat map of the LC/MS data.

```
[MZ,Y] = msppresample(peaks,5000);
msheatmap(MZ,ret_time,log(Y))
```



4 Overlay the dot plot on the heat map, and then zoom in to see the detail.

```
msdotplot(peaks,ret_time)
axis([480 532 375 485])
```



See Also

Bioinformatics Toolbox functions: `msheatmap`, `mspalign`, `mspeaks`, `msppresample`, `mzcdf2peaks`, `mzcdfread`, `mzxml2peaks`, `mzxmlread`

msheatmap

Purpose

Create pseudocolor image of set of mass spectra

Syntax

```
msheatmap(MZ, Intensities)
msheatmap(MZ, Times, Intensities)
msheatmap(..., 'Midpoint', MidpointValue, ...)
msheatmap(..., 'Range', RangeValue, ...)
msheatmap(..., 'Markers', MarkersValue, ...)
msheatmap(..., 'SpecIdx', SpecIdxValue, ...)
msheatmap(..., 'Group', GroupValue, ...)
msheatmap(..., 'Resolution', ResolutionValue, ...)
```

Arguments

MZ

Column vector of common mass/charge (m/z) values for a set of spectra. The number of elements in the vector equals the number of rows in the matrix *Intensities*.

Note You can use the `msppresample` function to create the *MZ* vector.

Times

Column vector of retention times associated with a liquid chromatography/mass spectrometry (LC/MS) or gas chromatography/mass spectrometry (GC/MS) data set. The number of elements in the vector equals the number of columns in the matrix *Intensities*. The retention times are used to label the *y*-axis of the heat map.

Tip You can use the `mzxml2peaks` function to create the *Times* vector.

Intensities Matrix of intensity values for a set of mass spectra that share the same m/z range. Each row corresponds to an m/z value, and each column corresponds to a spectrum or retention time. The number of rows equals the number of elements in vector *MZ*. The number of columns equals the number of elements in vector *Times*.

Note You can use the `msppresample` function to create the *Intensities* matrix.

MidpointValue Value specifying a quantile of the ion intensity values to fall below the midpoint of the colormap, meaning they do not represent peaks. `msheatmap` uses a custom colormap where cool colors represent nonpeak regions, white represents the midpoint, and warm colors represent peaks. Choices are any value ≥ `0` and ≤ `1`. Default is:

- `0.99` — For LC/MS or GC/MS data or when input *T* is provided. This means that 1% of the pixels are warm colors and represent peaks.
- `0.95` — For non-LC/MS or non-GC/MS data or when input *T* is not provided. This means that 5% of the pixels are warm colors and represent peaks.

Tip You can also change the midpoint interactively after creating the heat map by right-clicking the color bar, selecting **Interactive Colormap Shift**, and then click-dragging the cursor vertically on the color bar. This technique is useful when comparing multiple heat maps.

RangeValue — 1-by-2 vector specifying the m/z range for the *x*-axis of the heat map. *RangeValue* must be within `[min(MZ) max(MZ)]`. Default is the full range `[min(MZ) max(MZ)]`.

MarkersValue — Vector of m/z values to mark on the top horizontal axis of the heat map. Default is `[]`.

SpecIdxValue — Either of the following:

- Vector of values with the same number of elements as columns (spectra) in the matrix *Intensities*.
- Cell array of strings with the same number of elements as columns (spectra) in the matrix *Intensities*.

Each value or string specifies a label for the corresponding spectrum. These values or strings are used to label the *y*-axis of the heat map.

Note If input *Times* is provided, it is assumed that *Intensities* contains LC/MS or GC/MS data, and *SpecIdxValue* is ignored.

GroupValue Either of the following:

- Vector of values with the same number of elements as rows in the matrix *Intensities*
- Cell array of strings with the same number of elements as rows (spectra) in the matrix *Intensities*

Each value or string specifies a group to which the corresponding spectrum belongs. The spectra are sorted and combined into groups along the *y*-axis in the heat map.

Note If input *Times* is provided, it is assumed that *Intensities* contains LC/MS or GC/MS data, and *GroupValue* is ignored.

ResolutionValue Value specifying the horizontal resolution of the heat map image. Increase this value to enhance details. Decrease this value to reduce memory usage. Default is:

- `0.5` — When *MZ* contains > 2,500 elements.
- `0.05` — When *MZ* contains <= 2,500 elements.

Description

`msheatmap(`*MZ*`, `*Intensities*`)` displays a pseudocolor heat map image of the intensities for the spectra in matrix *Intensities*.

`msheatmap(`*MZ*`, `*Times*`, `*Intensities*`)` displays a pseudocolor heat map image of the intensities for the spectra in matrix *Intensities*, using the retention times in vector *Times* to label the *y*-axis.

`msheatmap(..., '`*PropertyName*`', `*PropertyValue*`, ...)` calls `msheatmap` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`msheatmap(..., 'Midpoint', MidpointValue, ...)` specifies a quantile of the ion intensity values to fall below the midpoint of the colormap, meaning they do not represent peaks. `msheatmap` uses a custom colormap where cool colors represent nonpeak regions, white represents the midpoint, and warm colors represent peaks. Choices are any value between `0` and `1`. Default is:

- `0.99` — For LC/MS or GC/MS data or when input `T` is provided. This means that 1% of the pixels are warm colors and represent peaks.
- `0.95` — For non-LC/MS or non-GC/MS data or when input `T` is not provided. This means that 5% of the pixels are warm colors and represent peaks.

Tip You can also change the midpoint interactively after creating the heat map by right-clicking the color bar, selecting **Interactive Colormap Shift**, then click-dragging the cursor vertically on the color bar. This technique is useful when comparing multiple heat maps.

`msheatmap(..., 'Range', RangeValue, ...)` specifies the m/z range for the `x`-axis of the heat map. `RangeValue` is a 1-by-2 vector that must be within `[min(MZ) max(MZ)]`. Default is the full range `[min(MZ) max(MZ)]`.

`msheatmap(..., 'Markers', MarkersValue, ...)` places markers along the top horizontal axis of the heat map for the m/z values specified in the vector `MarkersValue`. Default is `[]`.

`msheatmap(..., 'SpecIdx', SpecIdxValue, ...)` labels the spectra along the `y`-axis in the heat map. The labels are specified by `SpecIdxValue`, a vector of values or cell array of strings. The number of values or strings is the same as the number of columns (spectra) in the matrix `Intensities`. Each value or string specifies a label for the corresponding spectrum.

`msheatmap(..., 'Group', GroupValue, ...)` sorts and combines spectra into groups along the `y`-axis in the heat map. The groups are

specified by *GroupValue*, a vector of values or cell array of strings. The number of values or strings is the same as the number of rows in the matrix *Intensities*. Each value or string specifies a group to which the corresponding spectrum belongs.

`msheatmap(..., 'Resolution', ResolutionValue, ...)` specifies the horizontal resolution of the heat map image. Increase this value to enhance details. Decrease this value to reduce memory usage. Default is:

- 0.5 — When *MZ* contains > 2,500 elements.
- 0.05 — When *MZ* contains <= 2,500 elements.

Examples

SELDI-TOF Data

1 Load SELDI-TOF sample data.

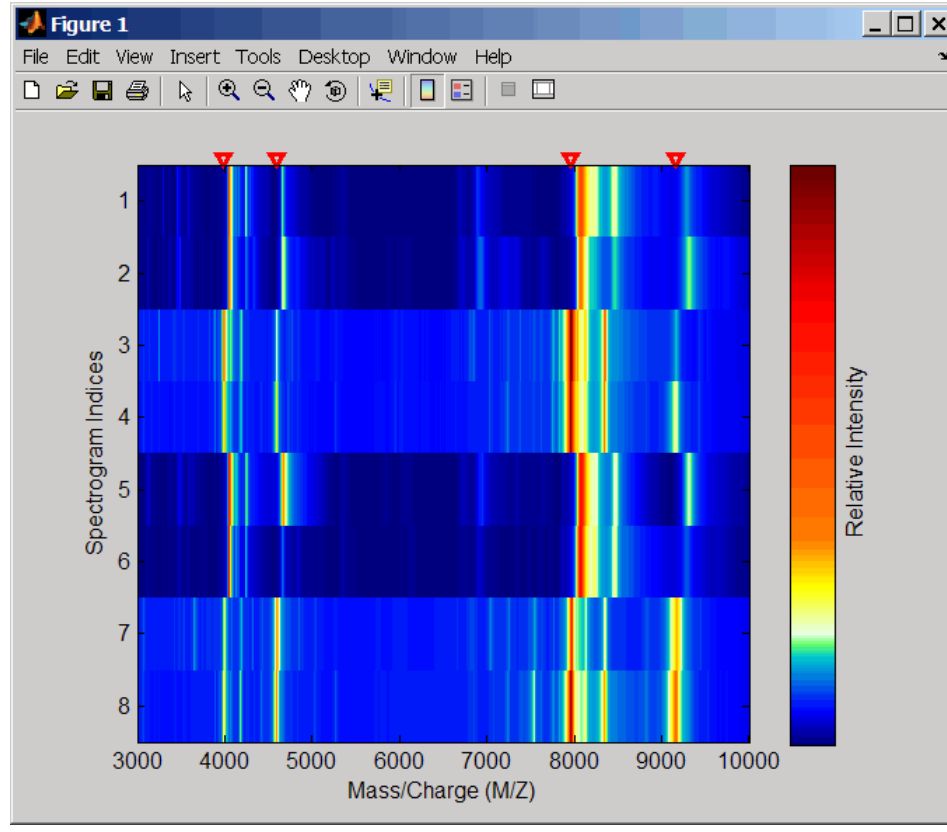
```
load sample_lo_res
```

2 Create a vector of four m/z values to mark along the top horizontal axis of the heat map.

```
M = [3991.4 4598 7964 9160];
```

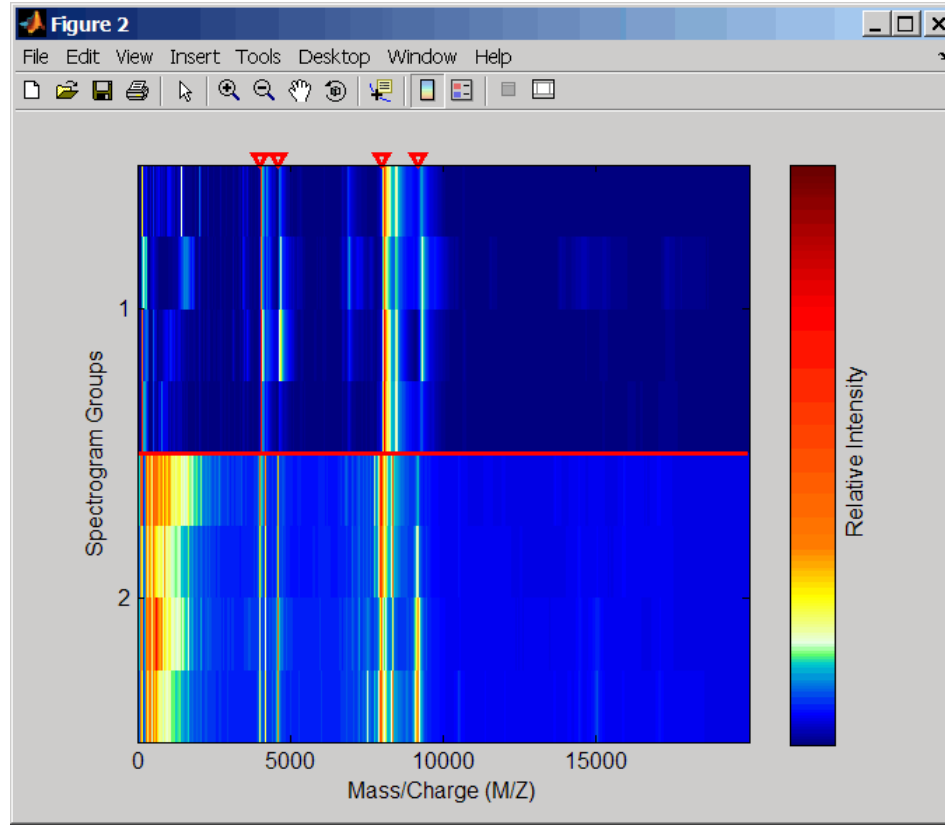
3 Display the heat map with m/z markers and a limited m/z range.

```
msheatmap(MZ_lo_res,Y_lo_res,'markers',M,'range',[3000 10000])
```



4 Display the heat map again grouping each spectrum into one of two groups.

```
TwoGroups = [1 1 2 2 1 1 2 2];
msheatmap(MZ_lo_res,Y_lo_res,'markers',M,'group',TwoGroups)
```



Liquid Chromatography/Mass Spectrometry (LC/MS) Data

1 Load LC/MS sample data.

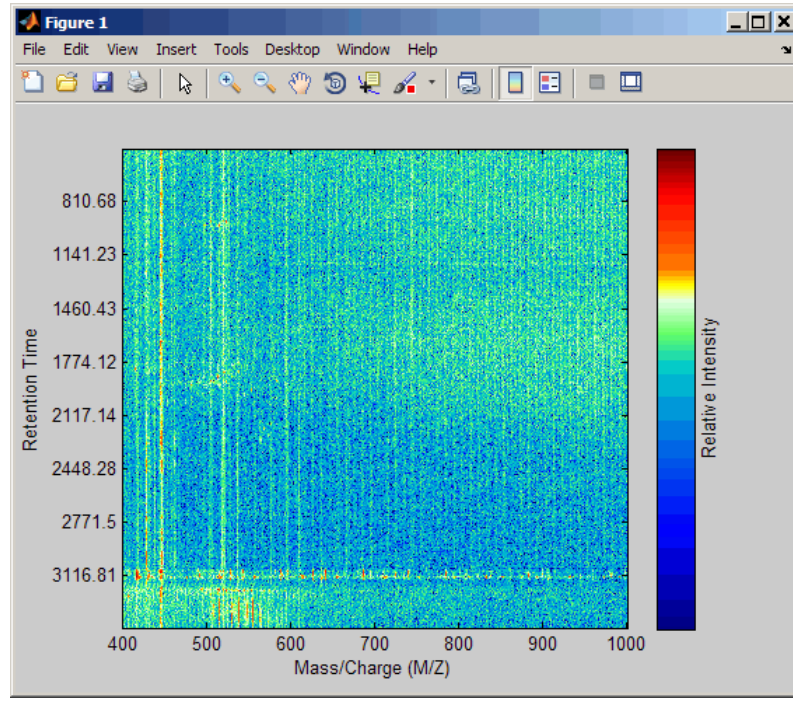
```
load lcmsdata
```

2 Resample the peak lists to create a vector of m/z values and a matrix of intensity values.

```
[MZ, Intensities] = msppresample(peaks, 5000);
```

3 Display the heat map showing mass spectra at different retention times.

```
msheatmap(MZ, ret_time, log(Intensities))
```



See Also

Bioinformatics Toolbox functions: `msalign`, `msbackadj`, `msdotplot`, `mslowess`, `msnorm`, `mspalign`, `msresample`, `mssgolay`, `msviewer`

Purpose

Smooth signal with peaks using nonparametric method

Syntax

```
Yout = mslowess(X, Intensities)
mslowess(..., 'Order', OrderValue, ...)
mslowess(..., 'Span', SpanValue, ...)
mslowess(..., 'Kernel', KernelValue, ...)
mslowess(..., 'RobustIterations',
RobustIterationsValue, ...)
mslowess(..., 'ShowPlot', ShowPlotValue, ...)
```

Arguments

X	Vector of separation-unit values for a set of signals with peaks. The number of elements in the vector equals the number of rows in the matrix *Intensities*. The separation unit can quantify wavelength, frequency, distance, time, or m/z depending on the instrument that generates the signal data.
Intensities	Matrix of intensity values for a set of peaks that share the same separation-unit range. Each row corresponds to a separation-unit value, and each column corresponds to either a set of signals with peaks or a retention time. The number of rows equals the number of elements in vector *X*.

Description

Tip Use the following syntaxes with data from any separation technique that produces signal data, such as spectroscopy, NMR, electrophoresis, chromatography, or mass spectrometry.

Yout = mslowess(*X*, *Intensities*) smooths raw noisy signal data, *Intensities*, using a locally weighted linear regression (Lowess) method with a default span of 10 samples.

Note `mslowess` assumes the input vector, *`X`*, may not have uniformly spaced separation units. Therefore, the sliding window for smoothing is centered using the closest samples in terms of the *`X`* value and not in terms of the *`X`* index.

Note When the input vector, *`X`*, does not have repeated values or NaN values, the algorithm is approximately twice as fast.

`mslowess(`*`X`*`,` *`Intensities`*`, ...'`*`PropertyName`*`',` *`PropertyValue`*`, ...)` calls `mslowess` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`mslowess(..., 'Order',` *`OrderValue`*`, ...)` specifies the order (*`OrderValue`*) of the Lowess smoother. Enter `1` (linear polynomial fit or Lowess), `2` (quadratic polynomial fit or Loess), or `0` (equivalent to a weighted local mean estimator and presumably faster because only a mean computation is performed instead of a least-squares regression). The default value is `1`.

Note Curve Fitting Toolbox software also refers to Lowess smoothing of order `2` as Loess smoothing.

`mslowess(..., 'Span',` *`SpanValue`*`, ...)` specifies the window size for the smoothing kernel. If *`SpanValue`* is greater than `1`, the window is equal to *`SpanValue`* number of samples independent of the separation-unit vector, *`X`*. The default value is `10` samples. Higher values will smooth the signal more at the expense of computation time. If *`SpanValue`* is less than `1`, the window size is taken to be a fraction

of the number of points in the data. For example, when *SpanValue* is 0.005, the window size is equal to 0.50% of the number of points in *X*.

mslowess(..., 'Kernel', *KernelValue*, ...) selects the function specified by *KernelValue* for weighting the observed intensities. Samples close to the separation-unit location being smoothed have the most weight in determining the estimate. *KernelValue* can be any of the following strings:

- 'tricubic' (default) — (1 - (dist/dmax).^3).^3
- 'gaussian' — exp(-(2*dist/dmax).^2)
- 'linear' — 1-dist/dmax

mslowess(..., 'RobustIterations', *RobustIterationsValue*, ...) specifies the number of iterations (*RobustValue*) for a robust fit. If *RobustIterationsValue* is 0 (default), no robust fit is performed. For robust smoothing, small residual values at every span are outweighed to improve the new estimate. 1 or 2 robust iterations are usually adequate, while larger values might be computationally expensive.

Note For an *X* vector that has uniformly spaced separation units, a nonrobust smoothing with *OrderValue* equal to 0 is equivalent to filtering the signal with the kernel vector.

---

mslowess(..., 'ShowPlot', *ShowPlotValue*, ...) plots the smoothed signal over the original signal. When you call mslowess without output arguments, the signals are plotted unless *ShowPlotValue* is false. When *ShowPlotValue* is true, only the first signal in *Intensities* is plotted. *ShowPlotValue* can also contain an index to one of the signals in *Intensities*.

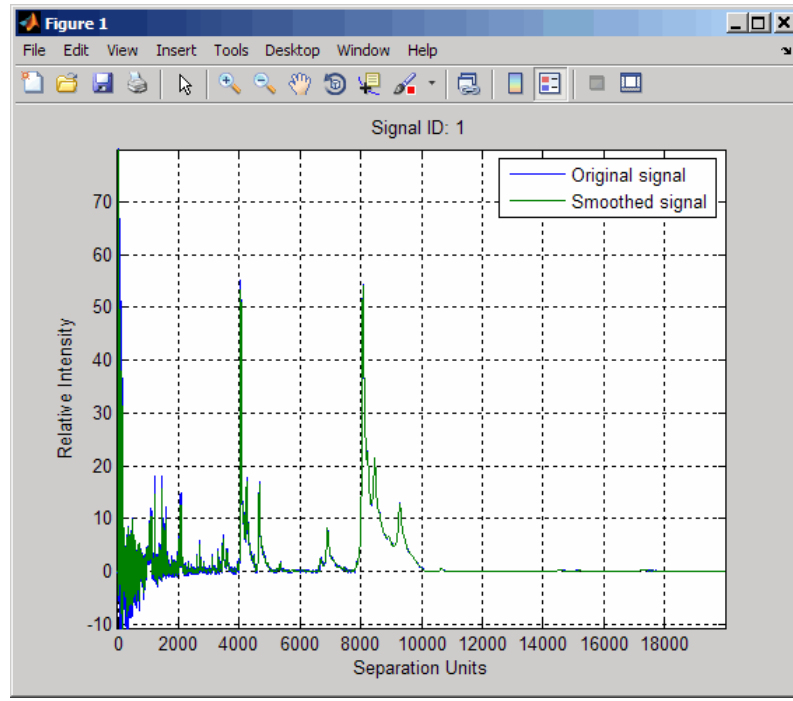
Examples

1 Load a MAT-file, included with the Bioinformatics Toolbox software, that contains some sample data.

```
load sample_lo_res
```

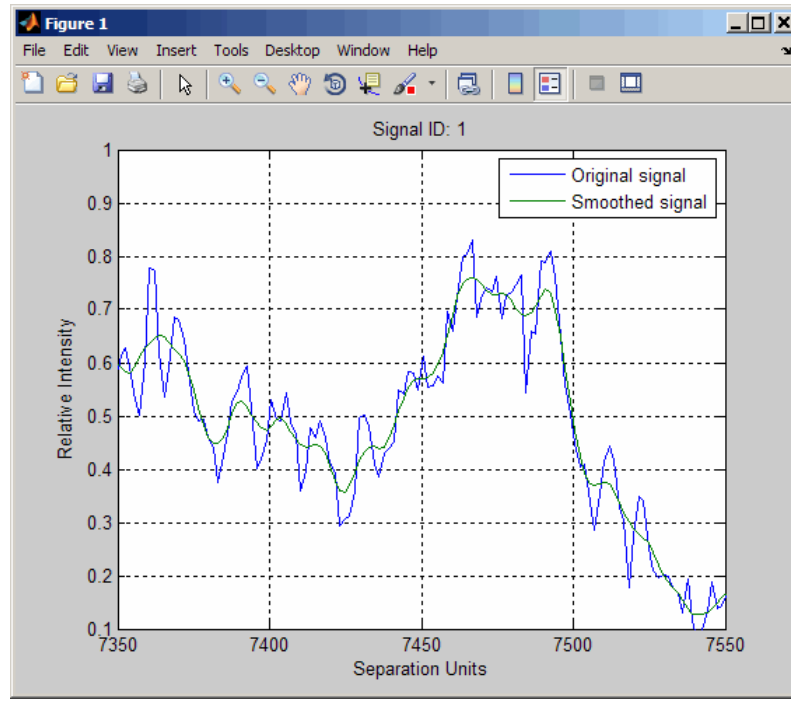
2 Smooth the spectra and draw a figure of the first spectrum with original and smoothed signals.

```
YS = mslowess(MZ_lo_res,Y_lo_res,'Showplot',true);
```



3 Zoom in on a region of the figure to see the difference in the original and smoothed signals.

```
axis([7350 7550 0.1 1.0])
```



See Also

Bioinformatics Toolbox functions: `msalign`, `msbackadj`, `msheatmap`, `msnorm`, `mspeaks`, `msresample`, `mssgolay`, `msviewer`

Bioinformatics Toolbox demo:

Preprocessing Raw Mass Spectrometry Data

msnorm

Purpose

Normalize set of signals with peaks

Syntax

```
Yout = msnorm(X, Intensities)
[Yout, NormParameters] = msnorm(...)
msnorm(X, NewY, NormParameters)
msnorm(..., 'Quantile', QuantileValue, ...)
msnorm(..., 'Limits', LimitsValue, ...)
msnorm(..., 'Consensus', ConsensusValue, ...)
msnorm(..., 'Method', MethodValue, ...)
msnorm(..., 'Max', MaxValue, ...)
```

Arguments

X	Vector of separation-unit values for a set of signals with peaks. The number of elements in the vector equals the number of rows in the matrix *Intensities*. The separation unit can quantify wavelength, frequency, distance, time, or m/z depending on the instrument that generates the signal data.
Intensities	Matrix of intensity values for a set of peaks that share the same separation-unit range. Each row corresponds to a separation-unit value, and each column corresponds to either a set of signals with peaks or a retention time. The number of rows equals the number of elements in vector *X*.

Description

Tip Use the following syntaxes with data from any separation technique that produces signal data, such as spectroscopy, NMR, electrophoresis, chromatography, or mass spectrometry.

Yout = msnorm(*X*, *Intensities*) normalizes a group of signals with peaks by standardizing the area under the curve (AUC) to the group median.

`[Yout, NormParameters] = msnorm(...)` returns a structure containing the parameters to normalize another group of signals.

`msnorm(X, NewY, NormParameters)` uses the parameter information from a previous normalization specified by *`NormParameters`* to normalize a new set of signals specified by *`NewY`* using the same parameters to select the separation-unit positions and output scale from the previous normalization. *`NormParameters`* is a structure created by `msnorm`. If a consensus proportion, *`ConsensusValue`*, was given in the previous normalization, no new separation-unit positions are selected, and normalization is performed using the same separation-unit positions.

`msnorm(..., 'PropertyName', PropertyValue, ...)` calls `msnorm` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`msnorm(..., 'Quantile', QuantileValue, ...)` specifies a 1-by-2 vector with the quantile limits for reducing the set of separation-unit values in *`X`*. For example, when *`QuantileValue`* is `[0.9 1]`, only the largest 10% of intensities in each signal are used to compute the AUC. When *`QuantileValue`* is a scalar, the scalar value represents the lower quantile limit and the upper quantile limit is set to `1`. The default value is `[0 1]` (use the whole area under the curve, AUC).

`msnorm(..., 'Limits', LimitsValue, ...)` specifies a 1-by-2 vector with a separation-unit range for picking normalization points. This parameter is useful to eliminate low-mass noise from the AUC calculation, for example the matrix noise that appears in the low-mass region of SELDI mass spectrometers. Default is `[0, max(X)]`.

`msnorm(..., 'Consensus', ConsensusValue, ...)` sets a consensus rule. To be included in the AUC, a separation-unit position must have an intensity within the quantile limits of at least part (specified by *`ConsensusValue`*) of the signals in *`Intensities`*. The same separation-unit positions are used to normalize all the signals. Enter a scalar from `0` to `1`.

Tip Use the `'Consensus'` property to eliminate low-intensity peaks and noise from the normalization.

`msnorm(..., 'Method', MethodValue, ...)` selects a method for normalizing the AUC of every signal. Enter either `'Median'` (default) or `'Mean'`.

`msnorm(..., 'Max', MaxValue, ...)`, after individually normalizing each signal, scales each signal to an overall maximum intensity specified by *`MaxValue`*. *`MaxValue`* is a scalar. If omitted, no postscaling is performed. If *`QuantileValue`* is `[1 1]`, then a single point (peak height of the tallest peak) is normalized to *`MaxValue`*.

Examples

AUC Normalization

1. Load a MAT-file, included with the Bioinformatics Toolbox software, that contains sample mass spec data, including `MZ_lo_res`, a vector of m/z values, and `Y_lo_res`, a matrix of intensity values.

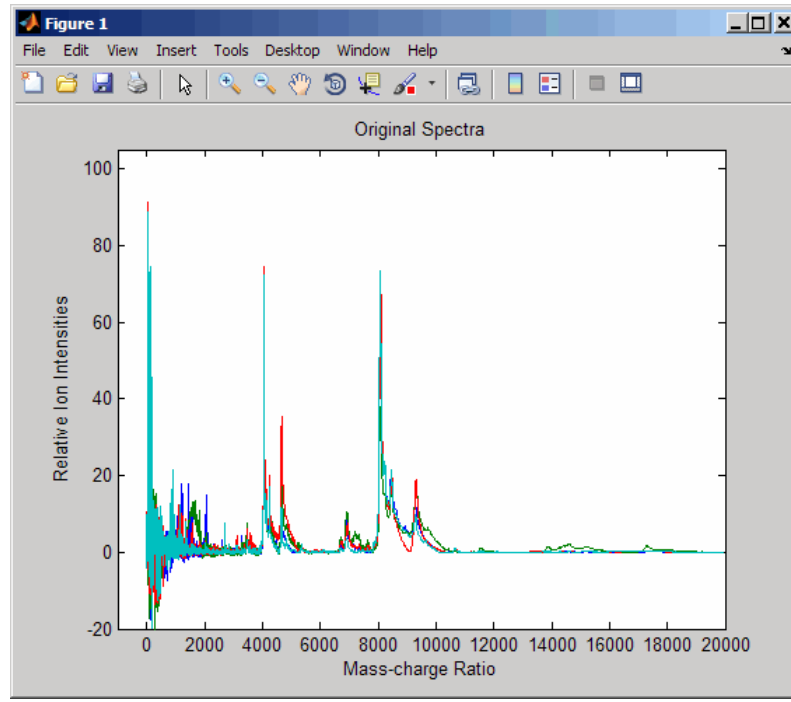
   ```
   load sample_lo_res
   ```

2. Create a subset (four signals) of the data.

   ```
   MZ = MZ_lo_res;
   Y = Y_lo_res(:,[1 2 5 6]);
   ```

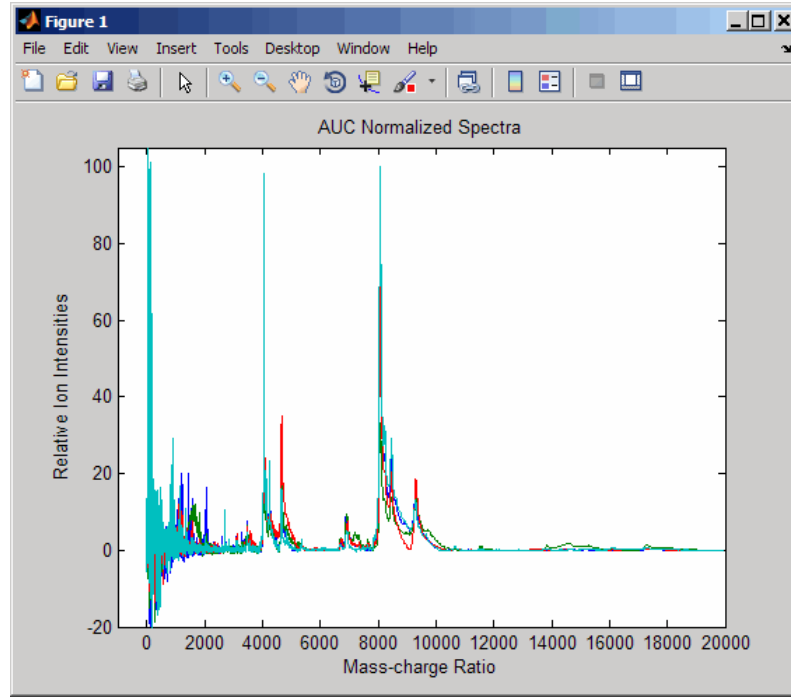
3. Plot the four spectra.

   ```
   plot(MZ, Y)
   axis([-1000 20000 -20 105])
   xlabel('Mass-charge Ratio')
   ylabel('Relative Ion Intensities')
   title('Original Spectra')
   ```



4 Normalize the area under the curve (AUC) of every spectrum to the median, eliminating low-mass (m/z < 1,000) noise, and post-rescaling such that the maximum intensity is 100. Plot the four spectra.

```
Y1 = msnorm(MZ,Y,'Limits',[1000 inf],'Max',100);
plot(MZ, Y1)
axis([-1000 20000 -20 105])
xlabel('Mass-charge Ratio')
ylabel('Relative Ion Intensities')
title('AUC Normalized Spectra')
```



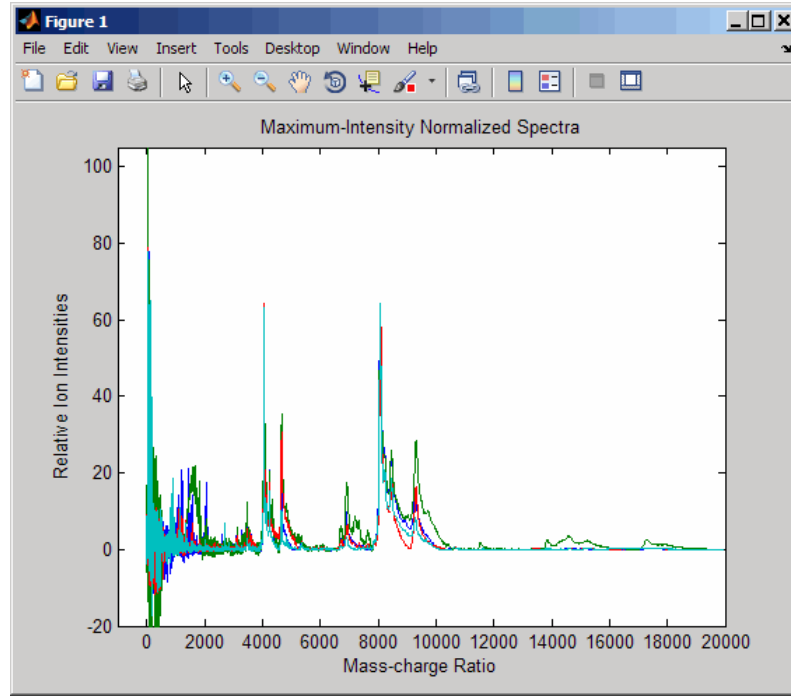
Maximum Intensity Normalization

1. If you have not already done so, complete steps 1 through 2 in AUC Normalization on page 3-1010.

2. Normalize the ion intensity of every spectrum to the maximum intensity of the single highest peak from any of the spectra in the range above 1000 m/z. Plot the four spectra.

```
Y2 = msnorm(MZ,Y,'QUANTILE', [1 1],'LIMITS',[1000 inf]);
plot(MZ, Y2)
axis([-1000 20000 -20 105])
xlabel('Mass-charge Ratio')
ylabel('Relative Ion Intensities')
```

```
title('Maximum-Intensity Normalized Spectra')
```



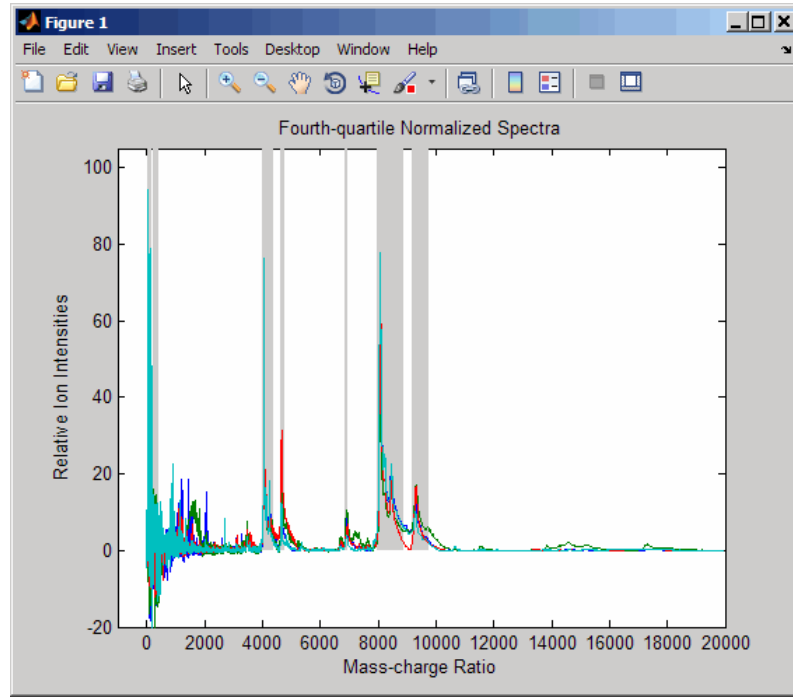
Quantile Normalization

1. If you have not already done so, complete steps 1 through 2 in AUC Normalization on page 3-1010.

2. Normalize using the data in the m/z regions where the intensities are within the fourth quartile in at least 90% of the spectrograms. Note that you can use the normalization parameters in the second output to normalize another set of data in the same m/z regions. Plot the four spectra.

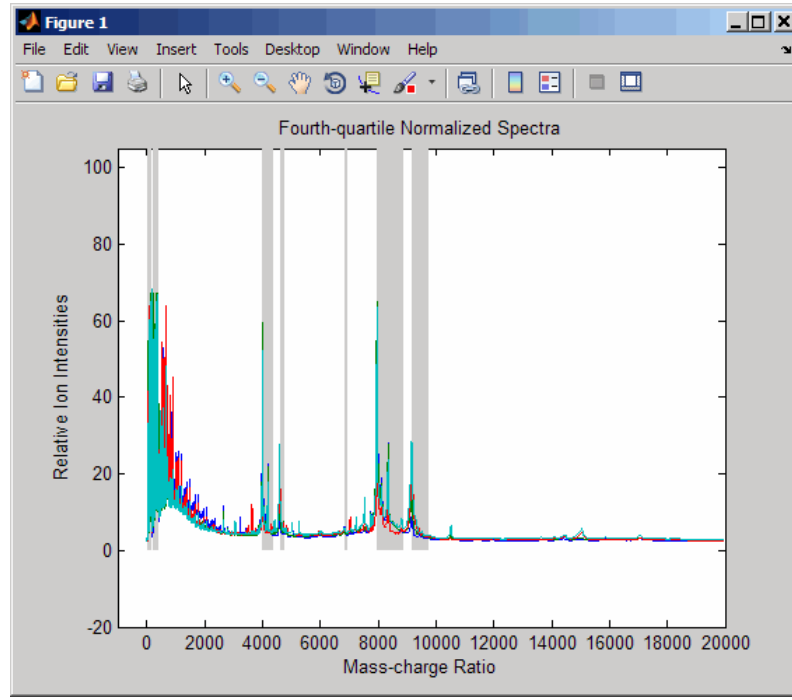
```
[Y3,S] = msnorm(MZ,Y,'Quantile',[0.75 1],'Consensus',0.9);
```

```
area(MZ,S.Xh.*1000,'LineStyle','None','FaceColor',[.8 .8 .8])
hold on
plot(MZ, Y3)
hold off
axis([-1000 20000 -20 105])
xlabel('Mass-charge Ratio')
ylabel('Relative Ion Intensities')
title('Fourth-quartile Normalized Spectra')
```



3 Use the normalization parameters in the second output of the previous step to normalize a different subset of data (four signals) using the data in the same m/z regions as the previous data set. Plot the four spectra.

```
Y4 = msnorm(MZ,Y_lo_res(:,[3 4 7 8]),S);

area(MZ,S.Xh.*1000,'LineStyle','None','FaceColor',[.8 .8 .8])
hold on
plot(MZ, Y4)
hold off
axis([-1000 20000 -20 105])
xlabel('Mass-charge Ratio')
ylabel('Relative Ion Intensities')
title('Fourth-quartile Normalized Spectra')
```



See Also

Bioinformatics Toolbox functions: `msalign`, `msbackadj`, `msheatmap`, `mslowess`, `msresample`, `mssgolay`, `msviewer`

Bioinformatics Toolbox demo:

Preprocessing Raw Mass Spectrometry Data

Purpose

Align mass spectra from multiple peak lists from LC/MS or GC/MS data set

Syntax

```
[CMZ, AlignedPeaks] = mspalign(Peaks)
[CMZ, AlignedPeaks] = mspalign(Peaks, ...'Quantile',
QuantileValue, ...)
[CMZ, AlignedPeaks] = mspalign(Peaks,
...'EstimationMethod',
   EstimationMethodValue, ...)
[CMZ, AlignedPeaks] = mspalign(Peaks,
...'CorrectionMethod',
   CorrectionMethodValue, ...)
[CMZ, AlignedPeaks] = mspalign(Peaks, ...'ShowEstimation',
   ShowEstimationValue, ...)
```

Arguments

Peaks

Cell array of peak lists from a liquid chromatography/mass spectrometry (LC/MS) or gas chromatography/mass spectrometry (GC/MS) data set. Each element in the cell array is a two-column matrix with m/z values in the first column and ion intensity values in the second column. Each element corresponds to a spectrum or retention time.

Note You can use the `mzxml2peaks` function or the `mspeaks` function to create the *Peaks* cell array.

QuantileValue

Value that determines which peaks are selected by the estimation method to create *CMZ*, the vector of common m/z values. Choices are any value ≥ `0` and ≤ `1`. Default is `0.95`.

EstimationMethodValue String specifying the method to estimate *CMZ*, the vector of common mass/charge (m/z) values. Choices are:

- `histogram` — Default method. Peak locations are clustered using a kernel density estimation approach. The peak ion intensity is used as a weighting factor. The center of all the clusters conform to the *CMZ* vector.
- `regression` — Takes a sample of the distances between observed significant peaks and regresses the inter-peak distance to create the *CMZ* vector with similar inter-element distances.

CorrectionMethodValue String specifying the method to align each peak list to the *CMZ* vector. Choices are:

- `nearest-neighbor` — Default method. For each common peak in the *CMZ* vector, its counterpart in each peak list is the peak that is closest to the common peak's m/z value.
- `shortest-path` — For each common peak in the *CMZ* vector, its counterpart in each peak list is selected using the shortest path algorithm.

ShowEstimationValue Controls the display of an assessment plot relative to the estimation method and the vector of common mass/charge (m/z) values. Choices are `true` or `false`. Default is either:

- `false` — When return values are specified.

- `true` — When return values are not specified.

Return Values

`CMZ`	Vector of common mass/charge (m/z) values estimated by the `mspalign` function.
`AlignedPeaks`	Cell array of peak lists, with the same form as *`Peaks`*, but with corrected m/z values in the first column of each matrix.

Description

`[`*`CMZ`*`, `*`AlignedPeaks`*`] = mspalign(`*`Peaks`*`)` aligns mass spectra from multiple peak lists (centroided data), by first estimating *`CMZ`*, a vector of common mass/charge (m/z) values estimated by considering the peaks in all spectra in *`Peaks`*, a cell array of peak lists, where each element corresponds to a spectrum or retention time. It then aligns the peaks in each spectrum to the values in *`CMZ`*, creating *`AlignedPeaks`*, a cell array of aligned peak lists.

`[`*`CMZ`*`, `*`AlignedPeaks`*`] = mspalign(`*`Peaks`*`, ...'`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `mspalign` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`[`*`CMZ`*`, `*`AlignedPeaks`*`] = mspalign(`*`Peaks`*`, ...'Quantile', `*`QuantileValue`*`, ...)` determines which peaks are selected by the estimation method to create *`CMZ`*, the vector of common m/z values. Choices are a scalar between `0` and `1`. Default is `0.95`.

`[`*`CMZ`*`, `*`AlignedPeaks`*`] = mspalign(`*`Peaks`*`, ...'EstimationMethod', `*`EstimationMethodValue`*`, ...)` specifies the method used to estimate *`CMZ`*, the vector of common mass/charge (m/z) values. Choices are:

- `histogram` — Default method. Peak locations are clustered using a kernel density estimation approach. The peak ion intensity is used as a weighting factor. The center of all the clusters conform to the *`CMZ`* vector.
- `regression` — Takes a sample of the distances between observed significant peaks and regresses the inter-peak distance to create the *`CMZ`* vector with similar inter-element distances.

`[`*`CMZ`*`, `*`AlignedPeaks`*`] = mspalign(`*`Peaks`*`, ...'CorrectionMethod', `*`CorrectionMethodValue`*`, ...)` specifies the method used to align each peak list to the *`CMZ`* vector. Choices are:

- `nearest-neighbor` — Default method. For each common peak in the *`CMZ`* vector, its counterpart in each peak list is the peak that is closest to the common peak's m/z value.
- `shortest-path` — For each common peak in the *`CMZ`* vector, its counterpart in each peak list is selected using the shortest path algorithm.

`[`*`CMZ`*`, `*`AlignedPeaks`*`] = mspalign(`*`Peaks`*`, ...'ShowEstimation', `*`ShowEstimationValue`*`, ...)` controls the display of an assessment plot relative to the estimation method and the estimated vector of common mass/charge (m/z) values. Choices are `true` or `false`. Default is either:

- `false` — When return values are specified.
- `true` — When return values are not specified.

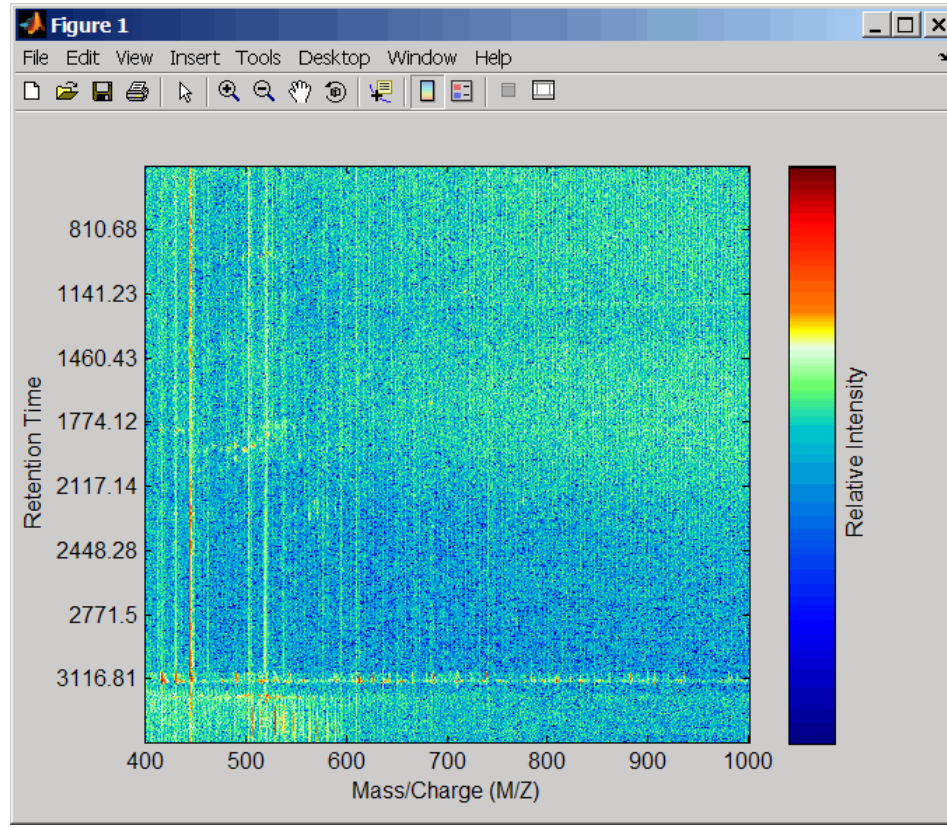
Examples

1. Load a MAT-file, included with the Bioinformatics Toolbox software, which contains liquid chromatography/mass spectrometry (LC/MS) data variables, including `peaks` and `ret_time`. `peaks` is a cell array of peak lists, where each element is a two-column matrix of m/z values and ion intensity values, and each element corresponds to a spectrum or retention time. `ret_time` is a column vector of retention times associated with the LC/MS data set.

```
load lcmsdata
```

2 Resample the unaligned data, display it in a heat map, and then overlay a dot plot.

```
[MZ,Y] = msppresample(peaks,5000);
msheatmap(MZ,ret_time,log(Y))
```



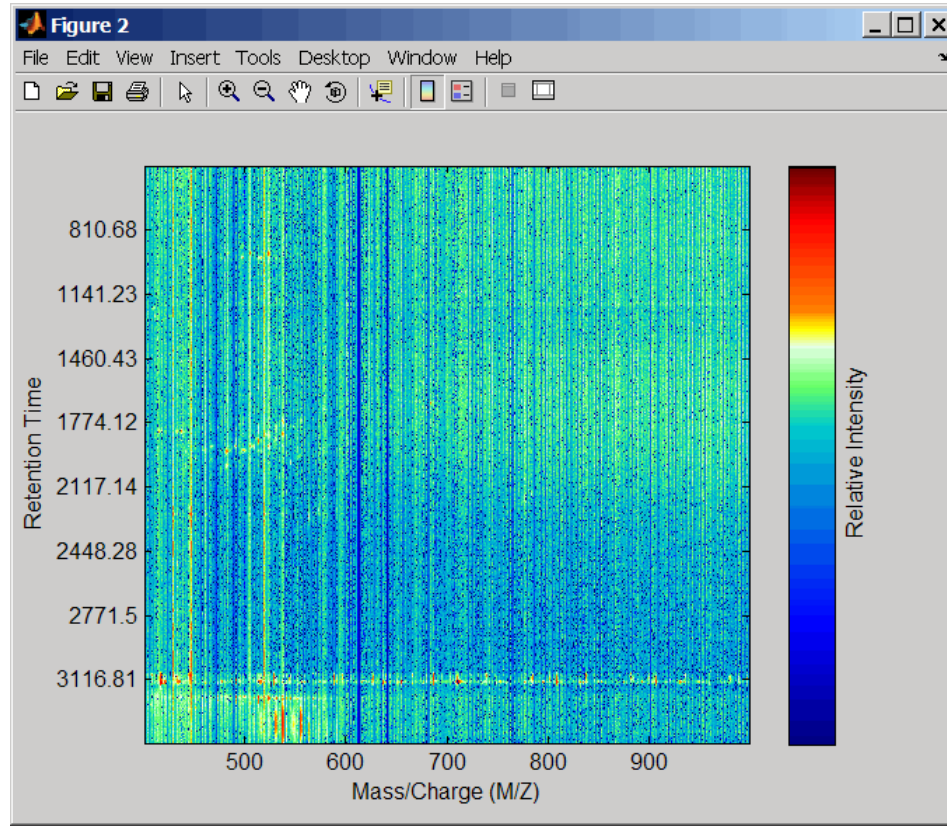

```
msdotplot(peaks,ret_time)
```

3 Align the peak lists from the mass spectra using the default estimation and correction methods.

```
[CMZ, aligned_peaks] = mspalign(peaks);
```

4 Resample the unaligned data, display it in a heat map, and then overlay a dot plot.

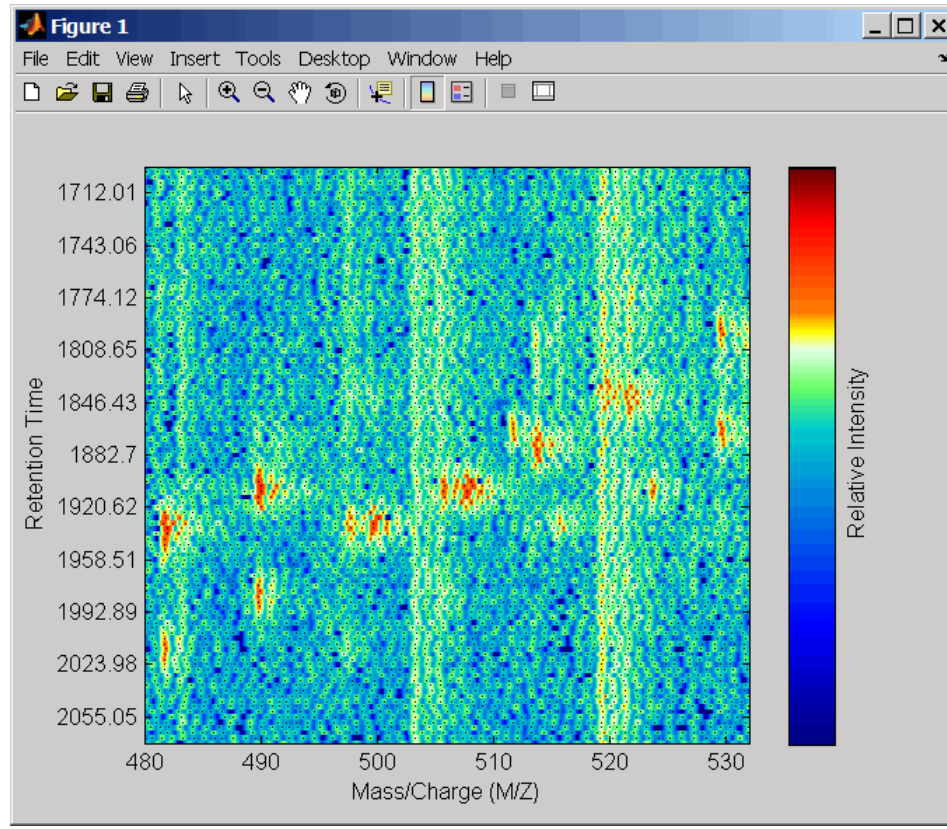
```
[MZ2,Y2] = msppresample(aligned_peaks,5000);
msheatmap(MZ2,ret_time,log(Y2))
```

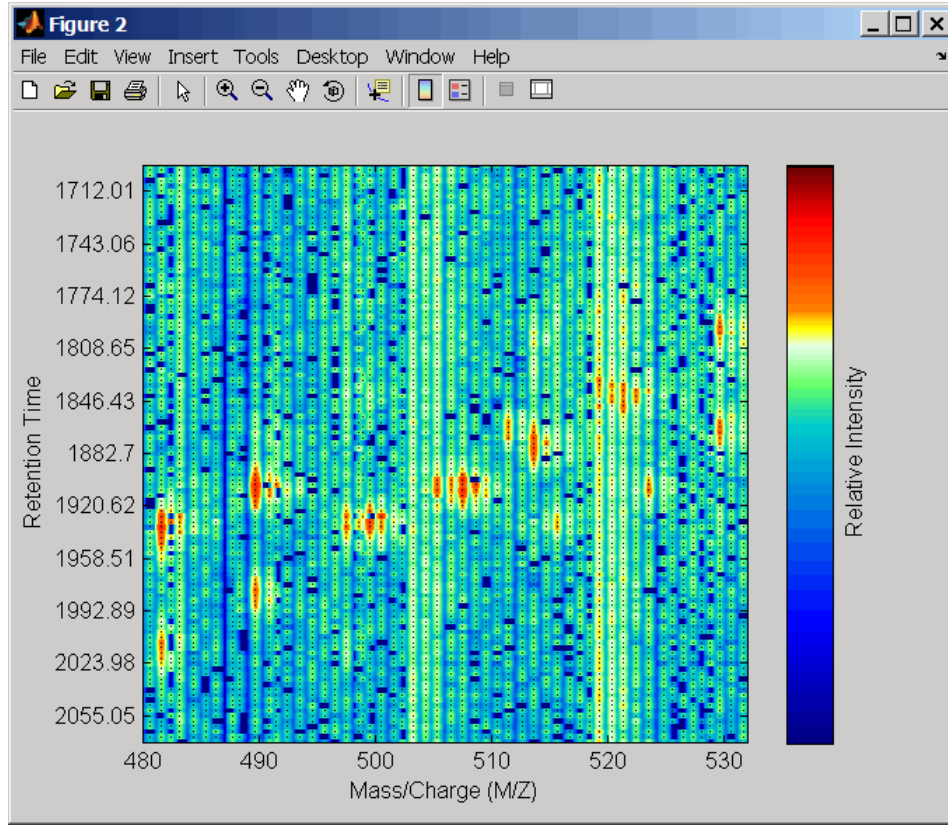


```
msdotplot(aligned_peaks,ret_time)
```

5 Link the axes of the two heat plots and zoom in to observe the detail to compare the unaligned and aligned LC/MS data sets.

```
linkaxes(findobj(0,'Tag','MSHeatMap'))
axis([480 532 375 485])
```





References

[1] Jeffries, N. (2005) Algorithms for alignment of mass spectrometry proteomic data. Bioinfomatics *21:14*, 3066–3073.

[2] Purvine, S., Kolker, N., and Kolker, E. (2004) Spectral Quality Assessment for High-Throughput Tandem Mass Spectrometry Proteomics. OMICS: A Journal of Integrative Biology *8:3*, 255–265.

See Also

Bioinformatics Toolbox functions: `msalign`, `msdotplot`, `msheatmap`, `mspeaks`, `msppresample`, `mzcdf2peaks`, `mzxml2peaks`

Purpose

Convert raw peak data to peak list (centroided data)

Syntax

```
Peaks = mspeaks(X, Intensities)
[Peaks, PFWHH] = mspeaks(X, Intensities)
[Peaks, PFWHH, PExt] = mspeaks(X, Intensities)
mspeaks(X, Intensities, ...'Base', BaseValue, ...)
mspeaks(X, Intensities, ...'Levels', LevelsValue, ...)
mspeaks(X, Intensities, ...'NoiseEstimator',
   NoiseEstimatorValue, ...)
mspeaks(X, Intensities, ...'Multiplier', MultiplierValue,
   ...)
mspeaks(X, Intensities, ...'Denoising',
DenoisingValue, ...)
mspeaks(X, Intensities, ...'PeakLocation',
PeakLocationValue,
   ...)
mspeaks(X, Intensities, ...'FWHHFilter', FWHHFilterValue,
   ...)
mspeaks(X, Intensities, ...'OverSegmentationFilter',
   OverSegmentationFilterValue, ...)
mspeaks(X, Intensities, ...'HeightFilter',
HeightFilterValue,
   ...)
mspeaks(X, Intensities, ...'ShowPlot', ShowPlotValue, ...)
mspeaks(X, Intensities, ...'Style', StyleValue, ...)
```

Description

`Peaks = mspeaks(X, Intensities)` finds relevant peaks in raw, noisy peak signal data, and creates *Peaks*, a two-column matrix, containing the separation-axis value and intensity for each peak.

`[Peaks, PFWHH] = mspeaks(X, Intensities)` returns *PFWHH*, a two-column matrix indicating the left and right locations of the full width at half height (FWHH) markers for each peak. For any peak not resolved at FWHH, `mspeaks` returns the peak shape extents instead. When *Intensities* includes multiple signals, then *PFWHH* is a cell array of matrices.

`[Peaks, PFWHH, PExt] = mspeaks(X, Intensities)` returns `PExt`, a two-column matrix indicating the left and right locations of the peak shape extents determined after wavelet denoising. When `Intensities` includes multiple signals, then `PExt` is a cell array of matrices.

`mspeaks(X, Intensities, ...'PropertyName', PropertyValue, ...)` calls `mspeaks` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each `PropertyName` in single quotation marks. Each `PropertyName` is case insensitive. These property name/property value pairs are as follows:

`mspeaks(X, Intensities, ...'Base', BaseValue, ...)` specifies the wavelet base.

`mspeaks(X, Intensities, ...'Levels', LevelsValue, ...)` specifies the number of levels for the wavelet decomposition.

`mspeaks(X, Intensities, ...'NoiseEstimator', NoiseEstimatorValue, ...)` specifies the method to estimate the threshold, `T`, to filter out noisy components in the first high-band decomposition (`y_h`).

`mspeaks(X, Intensities, ...'Multiplier', MultiplierValue, ...)` specifies the threshold multiplier constant.

`mspeaks(X, Intensities, ...'Denoising', DenoisingValue, ...)` controls the use of wavelet denoising to smooth the signal. Choices are `true` (default) or `false`.

`mspeaks(X, Intensities, ...'PeakLocation', PeakLocationValue, ...)` specifies the proportion of the peak height to use to select the points used to compute the centroid separation-axis value of the respective peak. `PeakLocationValue` must be a value $\geq$ `0` and $\leq$ `1`. Default is `1.0`.

`mspeaks(X, Intensities, ...'FWHHFilter', FWHHFilterValue, ...)` specifies the minimum full width at half height (FWHH), in separation units, for reported peaks. Peaks with FWHH below this value are excluded from the output list `Peaks`.

`mspeaks(X, Intensities, ...'OverSegmentationFilter', OverSegmentationFilterValue, ...)` specifies the minimum distance, in separation units, between neighboring peaks. When the signal is not smoothed appropriately, multiple maxima can appear to represent the same peak. Increase this filter value to join oversegmented peaks into a single peak.

`mspeaks(X, Intensities, ...'HeightFilter', HeightFilterValue, ...)` specifies the minimum height for reported peaks. Peaks with heights below this value are excluded from the output list `Peaks`.

`mspeaks(X, Intensities, ...'ShowPlot', ShowPlotValue, ...)` controls the display of a plot of the original and the smoothed signal, with the peaks included in the output matrix `Peaks` marked.

`mspeaks(X, Intensities, ...'Style', StyleValue, ...)` specifies the style for marking the peaks in the plot.

`mspeaks` finds peaks in data from any separation technique that produces signal data, such as spectroscopy, nuclear magnetic resonance (NMR), electrophoresis, chromatography, or mass spectrometry.

Inputs

X

Vector of separation-unit values for a set of signals with peaks. The number of elements in the vector equals the number of rows in the matrix *Intensities*. The separation unit can quantify wavelength, frequency, distance, time, or m/z depending on the instrument that generates the signal data.

Intensities

Matrix of intensity values for a set of peaks that share the same separation-unit range. Each row corresponds to a separation-unit value, and each column corresponds to either a set of signals with peaks or a retention time. The number of rows equals the number of elements in vector *X*.

BaseValue

Integer from 2 to 20 that specifies the wavelet base.

Default: 4

LevelsValue

Integer from 1 to 12 that specifies the number of levels for the wavelet decomposition.

Default: 10

NoiseEstimatorValue

String or scalar that specifies the method to estimate the threshold, T, to filter out noisy components in the first high-band decomposition (y_h). Choices are:

- mad — Default. Median absolute deviation, which calculates T = sqrt(2*log(*n*))*mad(*y_h*) / 0.6745, where *n* = the number of rows in the *Intensities* matrix.
- std — Standard deviation, which calculates T = std(*y_h*).
- A positive real value.

MultiplierValue

Positive real value that specifies the threshold multiplier constant.

Default: 1.0

DenoisingValue

Controls the use of wavelet denoising to smooth the signal. Choices are true (default) or false.

Tip If your data was previously smoothed, for example, with the `mslowess` or `mssgolay` function, you do not need to use wavelet denoising. Set this property to `false`.

`PeakLocationValue`

Value that specifies the proportion of the peak height to use to select the points to compute the centroid separation-axis value of the respective peak. The value must be ≥ `0` and ≤ `1`.

Note When *`PeakLocationValue`* = `1.0`, the peak location is at the maximum of the peak. When *`PeakLocationValue`* = `0`, `mspeaks` computes the peak location with all the points from the closest minimum to the left of the peak to the closest minimum to the right of the peak.

Default: `1.0`

`FWHHFilterValue`

Positive real value that specifies the minimum full width at half height (FWHH), in separation units, for reported peaks. Peaks with FWHH below this value are excluded from the output list *`Peaks`*.

Default: `0`

`OverSegmentationFilterValue`

Positive real value that specifies the minimum distance, in separation units, between neighboring peaks. When the signal is not smoothed appropriately, multiple maxima can appear to represent the same peak. Increase this filter value to join oversegmented peaks into a single peak.

Default: `0`

`HeightFilterValue`

Positive real value that specifies the minimum height for reported peaks.

Default: `0`

`ShowPlotValue`

Controls the display of a plot of the original signal and the smoothed signal, with the peaks included in the output matrix *`Peaks`* marked. Choices are `true`, `false`, or *`I`*, an integer specifying the index of a spectrum in *`Intensities`*. If set to `true`, the first spectrum in *`Intensities`* is plotted. Default is:

- `false` — When you specify return values.
- `true` — When you do not specify return values.

`StyleValue`

String specifying the style for marking the peaks in the plot. Choices are:

- `'peak'` (default) — Places a marker at the peak crest.
- `'exttriangle'` — Draws a triangle using the peak crest and the extents.
- `'fwhhtriangle'` — Draws a triangle using the peak crest and the FWHH points.
- `'extline'` — Places a marker at the peak crest and vertical lines at the extents.
- `'fwhhline'` — Places a marker at the peak crest and a horizontal line at FWHH.

Outputs

Peaks

Two-column matrix where each row corresponds to a peak. The first column contains separation-unit values (indicating the location of peaks along the separation axis). The second column contains intensity values. When *Intensities* includes multiple signals, then *Peaks* is a cell array of matrices, each containing a peak list.

PFWHH

Two-column matrix indicating the left and right locations of the full width at half height (FWHH) markers for each peak. For any peak not resolved at FWHH, mspeaks returns the peak shape extents instead. When *Intensities* includes multiple signals, then *PFWHH* is a cell array of matrices.

PExt

Two-column matrix indicating the left and right locations of the peak shape extents determined after wavelet denoising. When *Intensities* includes multiple signals, then *PExt* is a cell array of matrices.

Examples

1. Load a MAT-file, included with the Bioinformatics Toolbox software, that contains two mass spectrometry data variables, MZ_lo_res and Y_lo_res. MZ_lo_res is a vector of m/z values for a set of spectra. Y_lo_res is a matrix of intensity values for a set of mass spectra that share the same m/z range.

```
load sample_lo_res
```

2. Adjust the baseline of the eight spectra stored in Y_lo_res.

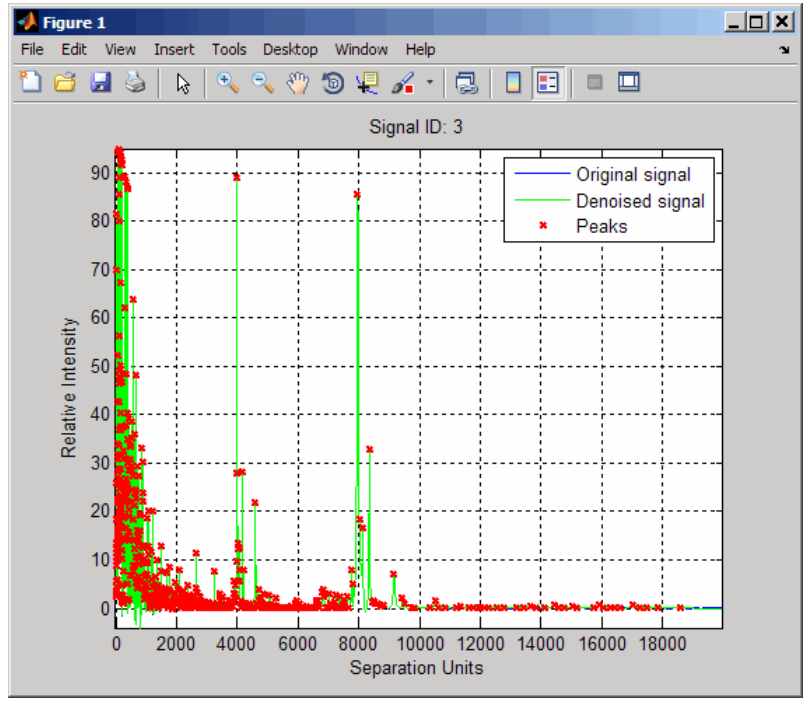
```
YB = msbackadj(MZ_lo_res,Y_lo_res);
```

3. Convert the raw mass spectrometry data to a peak list by finding the relevant peaks in each spectrum.

```
P = mspeaks(MZ_lo_res,YB);
```

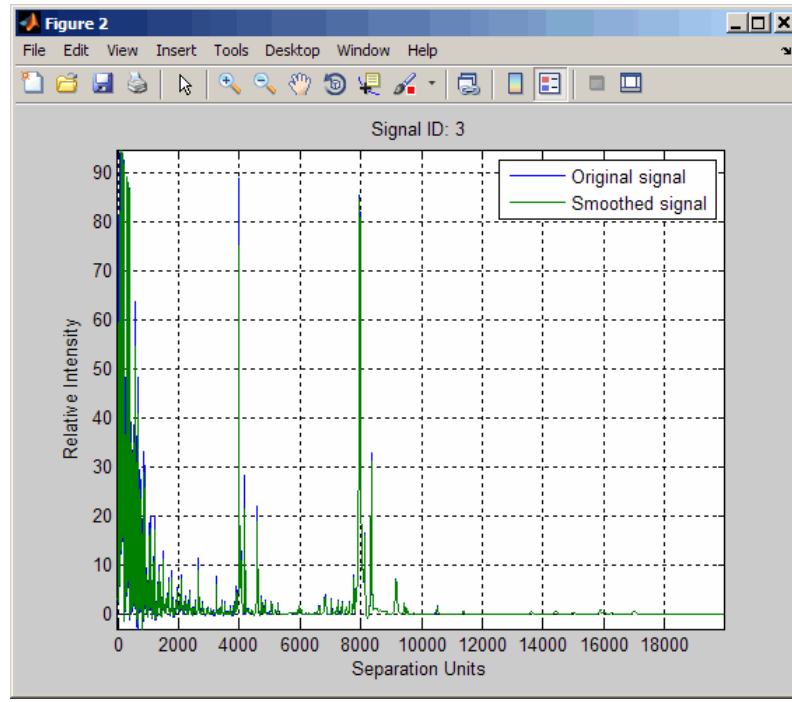
4 Plot the third spectrum in `YB`, the matrix of baseline-corrected intensity values, with the detected peaks marked.

```
P = mspeaks(MZ_lo_res,YB,'SHOWPLOT',3);
```

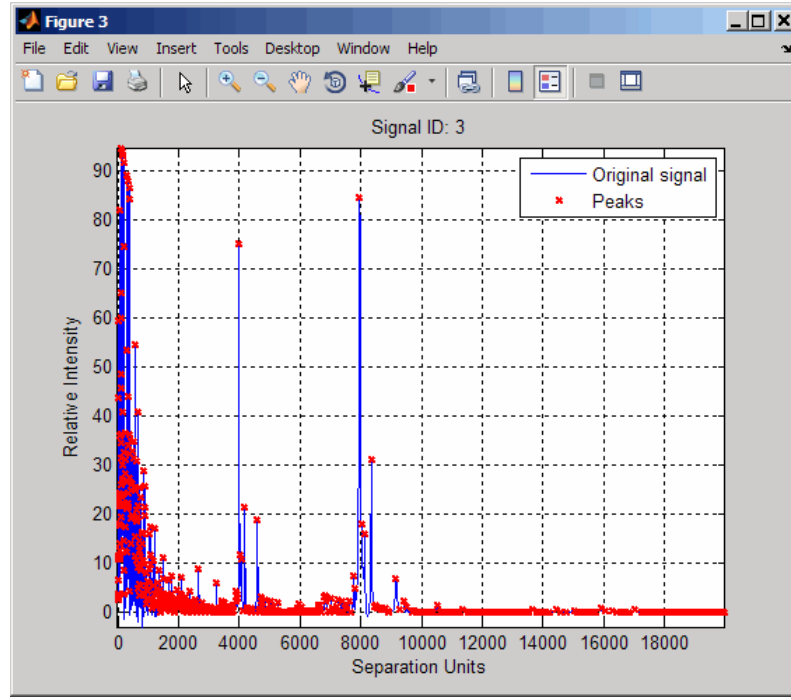


5 Smooth the signal using the `mslowess` function. Then convert the smoothed data to a peak list by finding relevant peaks and plot the third spectrum.

```
YS = mslowess(MZ_lo_res,YB,'SHOWPLOT',3);
```

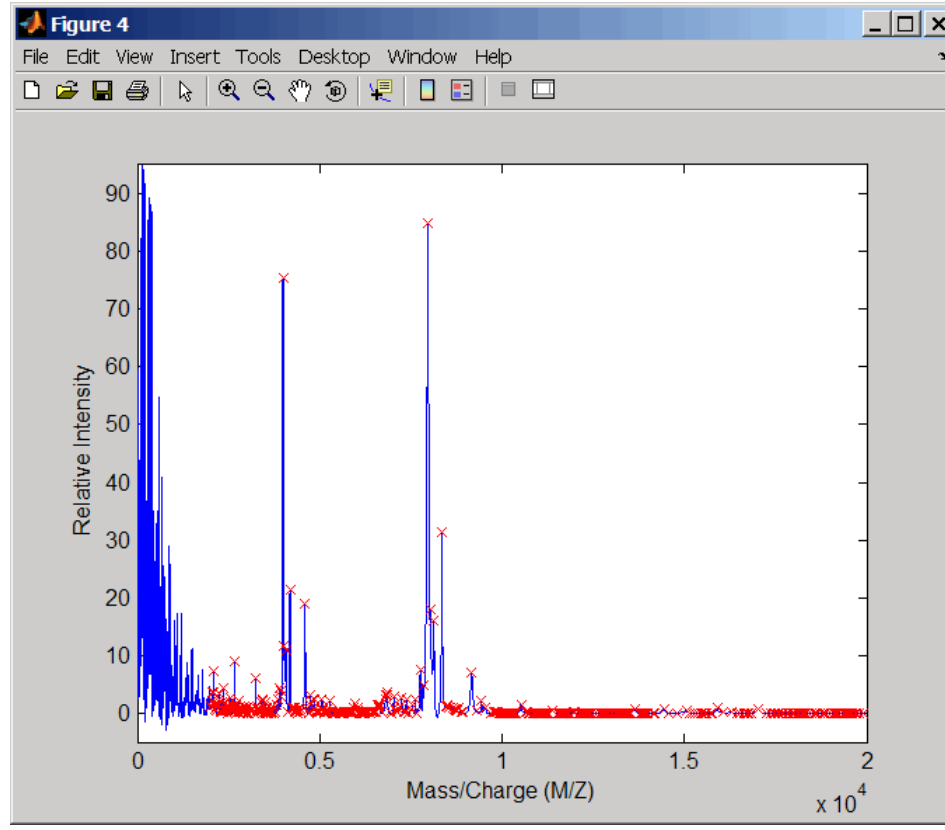



```
P = mspeaks(MZ_lo_res,YS,'DENOISING',false,'SHOWPLOT',3);
```



6 Use the `cellfun` function to remove all peaks with m/z values less than 2000 from the eight peaks listed in output `P`. Then plot the peaks of the third spectrum (in red) over its smoothed signal (in blue).

```
Q = cellfun(@(p) p(p(:,1)>2000,:),P,'UniformOutput',false);
figure
plot(MZ_lo_res,YS(:,3),'b',Q{3}(:,1),Q{3}(:,2),'rx')
xlabel('Mass/Charge (M/Z)')
ylabel('Relative Intensity')
axis([0 20000 -5 95])
```



Algorithm

`mspeaks` converts raw peak data to a peak list (centroided data) by:

1. Smoothing the signal using undecimated wavelet transform with Daubechies coefficients
2. Assigning peak locations
3. Estimating noise
4. Eliminating peaks that do not satisfy specified criteria

References

[1] Morris, J.S., Coombes, K.R., Koomen, J., Baggerly, K.A., and Kobayash, R. (2005) Feature extraction and quantification for mass spectrometry in biomedical applications using the mean spectrum. Bioinfomatics *21:9*, 1764–1775.

[2] Yasui, Y., Pepe, M., Thompson, M.L., Adam, B.L., Wright, G.L., Qu, Y., Potter, J.D., Winget, M., Thornquist, M., and Feng, Z. (2003) A data-analytic strategy for protein biomarker discovery: profiling of high-dimensional proteomic data for cancer detection. Biostatistics *4:3*, 449–463.

[3] Donoho, D.L., and Johnstone, I.M. (1995) Adapting to unknown smoothness via wavelet shrinkage. J. Am. Statist. Asso. *90*, 1200–1224.

[4] Strang, G., and Nguyen, T. (1996) Wavelets and Filter Banks (Wellesley: Cambridge Press).

[5] Coombes, K.R., Tsavachidis, S., Morris, J.S., Baggerly, K.A., Hung, M.C., and Kuerer, H.M. (2005) Improved peak detection and quantification of mass spectrometry data acquired from surface-enhanced laser desorption and ionization by denoising spectra with the undecimated discrete wavelet transform. Proteomics *5(16)*, 4107–4117.

See Also

`msbackadj` | `msdotplot` | `mslowess` | `mspalign` | `msppresample` | `mssgolay` | `cellfun`

Tutorials

- Preprocessing Raw Mass Spectrometry Data
- Visualizing and Preprocessing Hyphenated Mass Spectrometry Data Sets for Metabolite and Protein/Peptide Profiling

Purpose

Resample signal with peaks while preserving peaks

Syntax

```
[X, Intensities] = msppresample(Peaks, N)
msppresample(Peaks, N, ...'Range', RangeValue, ...)
msppresample(Peaks, N, ...'FWHH', FWHHValue, ...)
msppresample(Peaks, N, ...'ShowPlot', ShowPlotValue, ...)
```

Arguments

Peaks

Either of the following:

- Two-column matrix, where the first column contains separation-unit values and the second column contains intensity values. The separation unit can quantify wavelength, frequency, distance, time, or m/z depending on the instrument that generates the signal data.
- Cell array of peak lists, where each element is a two-column matrix of separation-unit values and intensity values, and each element corresponds to a signal or retention time.

Tip You can use the `mzxml2peaks` function or the `mspeaks` function to create the *Peaks* matrix or cell array.

N

Integer specifying the number of equally spaced points (separation-unit values) in the resampled signal.

RangeValue 1-by-2 vector specifying the minimum and maximum separation-unit values for the output matrix *Intensities*. *RangeValue* must be within [min(*inputSU*) max(*inputSU*)], where *inputSU* is the concatenated separation-unit values from the input *Peaks*. Default is the full range [min(*inputSU*) max(*inputSU*)].

FWHHValue Value that specifies the full width at half height (FWHH) in separation units. The FWHH is used to convert each peak to a Gaussian shaped curve. Default is median(diff(*inputSU*))/2, where *inputSU* is the concatenated separation-unit values from the input *Peaks*. The default is a rough approximation of resolution observed in the input data, *Peaks*.

Tip To ensure that the resolution of the peaks is preserved, set *FWHHValue* to half the distance between the two peaks of interest that are closest to each other.

ShowPlotValue Controls the display of a plot of an original and resampled signal. Choices are true, false, or *I*, an integer specifying the index of a signal in *Intensities*. If you set to true, the first signal in *Intensities* is plotted. Default is:

- false — When return values are specified.
- true — When return values are not specified.

Return Values

X	Vector of equally spaced, common separation-unit values for a set of signals with peaks. The number of elements in the vector equals *N*, or the number of rows in matrix *Intensities*.
Intensities	Matrix of reconstructed intensity values for a set of peaks that share the same separation-unit range. Each row corresponds to a separation-unit value, and each column corresponds to either a set of signals with peaks or a retention time. The number of rows equals *N*, or the number of elements in vector *X*.

Description

Tip Use the following syntaxes with data from any separation technique that produces signal data, such as spectroscopy, NMR, electrophoresis, chromatography, or mass spectrometry.

`[X, Intensities] = msppresample(Peaks, N)` resamples *Peaks*, a peak list, by converting centroided peaks to a semicontinuous, raw signal that preserves peak information. The resampled signal has *N* equally spaced points. Output *X* is a vector of *N* elements specifying the equally spaced, common separation-unit values for the set of signals with peaks. Output *Intensities* is a matrix of reconstructed intensity values for a set of peaks that share the same separation-unit range. Each row corresponds to a separation-unit value, and each column corresponds to either a set of signals with peaks or a retention time. The number of rows equals *N*.

`msppresample` uses a Gaussian kernel to reconstruct the signal. The intensity at any given separation-unit value is taken from the maximum intensity of any contributing (overlapping) peaks.

Tip msppresample is useful to prepare a set of signals for imaging functions such as msheatmap and preprocessing functions such as msbackadj and msnorm.

msppresample(*Peaks*, *N*, ... '*PropertyName*', *PropertyValue*, ...) calls msppresample with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

msppresample(*Peaks*, *N*, ...'Range', *RangeValue*, ...) specifies a separation-unit range for the output matrix *Intensities* using the minimum and maximum separation values specified in the 1-by-2 vector *RangeValue*. *RangeValue* must be within [min(*inputSU*) max(*inputSU*)], where *inputSU* is the concatenated separation-unit values from the input *Peaks*. Default is the full range [min(*inputSU*) max(*inputSU*)]

msppresample(*Peaks*, *N*, ...'FWHH', *FWHHValue*, ...) sets the full width at half height (FWHH) in separation units. The FWHH is used to convert each peak to a Gaussian shaped curve. Default is median(diff(*inputSU*))/2, where *inputSU* is the concatenated separation-unit values from the input *Peaks*. The default is a rough approximation of resolution observed in the input data, *Peaks*.

Tip To ensure that the resolution of the peaks is preserved, set *FWHHValue* to half the distance between the two peaks of interest that are closest to each other.

msppresample(*Peaks*, *N*, ...'ShowPlot', *ShowPlotValue*, ...) controls the display of a plot of an original and resampled signal. Choices are true, false, or *I*, an integer specifying the index of a signal

in *Intensities*. If you set to true, the first signal in *Intensities* is plotted. Default is:

- false — When return values are specified.
- true — When return values are not specified.

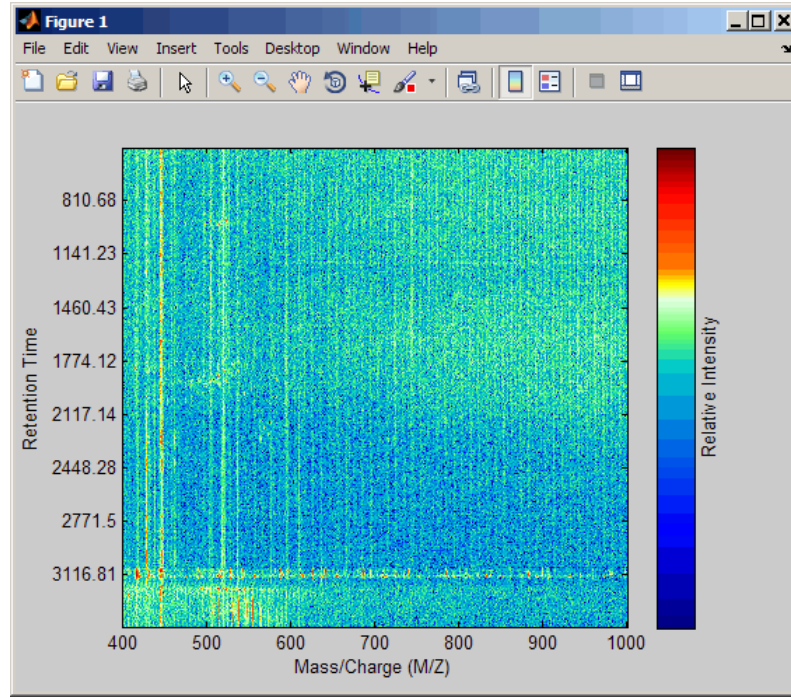
Examples

1. Load a MAT-file, included with the Bioinformatics Toolbox software, that contains liquid chromatography/mass spectrometry (LC/MS) data variables. It includes peaks, a cell array of peak lists, where each element is a two-column matrix of m/z values and ion intensity values, and each element corresponds to a spectrum or retention time.

   ```
   load lcmsdata
   ```

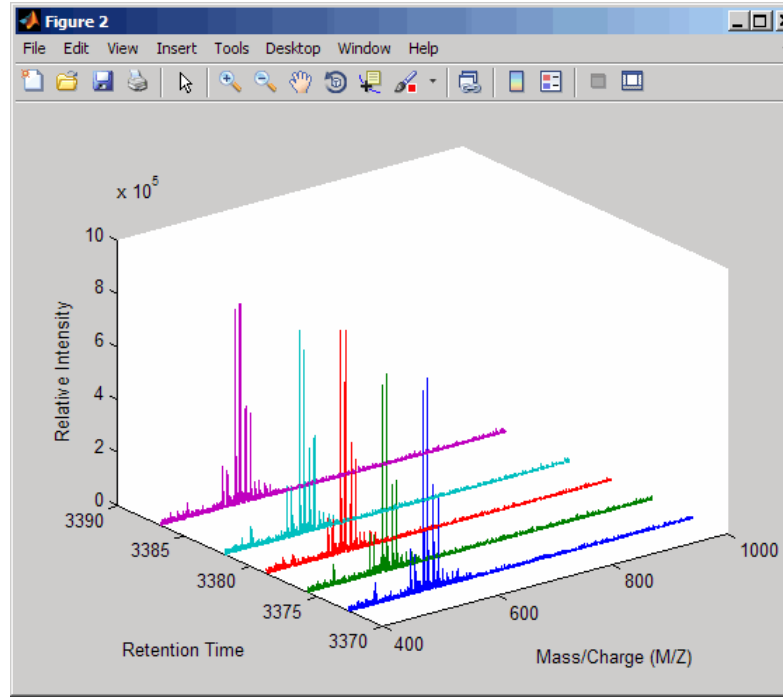
2. Resample the data, specifying 5000 m/z values in the resampled signal. Then create a heat map of the LC/MS data.

   ```
   [MZ,Y] = msppresample(peaks,5000);
   msheatmap(MZ,ret_time,log(Y))
   ```



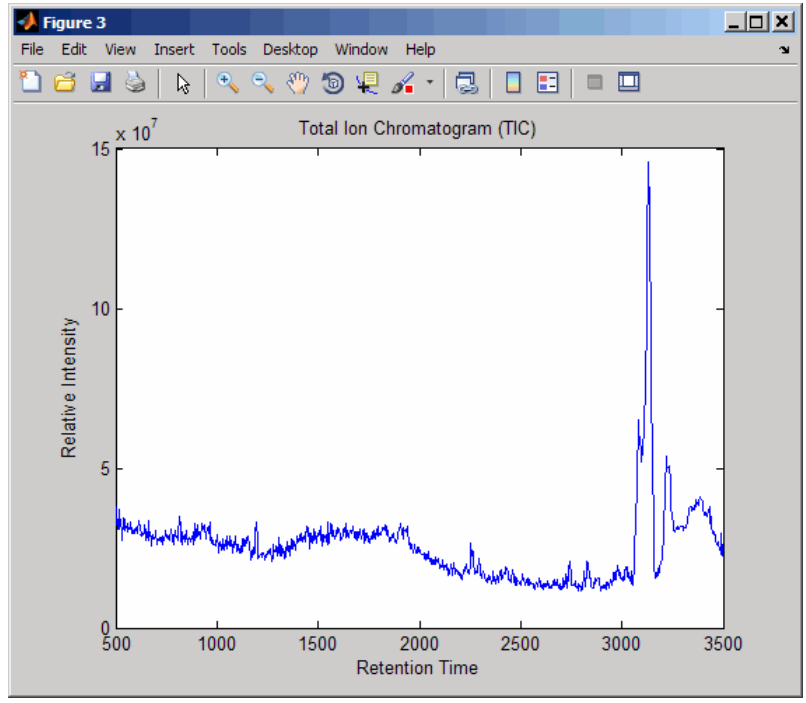
3 Plot the reconstructed profile spectra between two retention times.

```
figure
t1 = 3370;
t2 = 3390;
h = find(ret_time>t1 & ret_time<t2);
[MZ,Y] = msppresample(peaks(h),10000);
plot3(repmat(MZ,1,numel(h)),repmat(ret_time(h)',10000,1),Y)
xlabel('Mass/Charge (M/Z)')
ylabel('Retention Time')
zlabel('Relative Intensity')
```



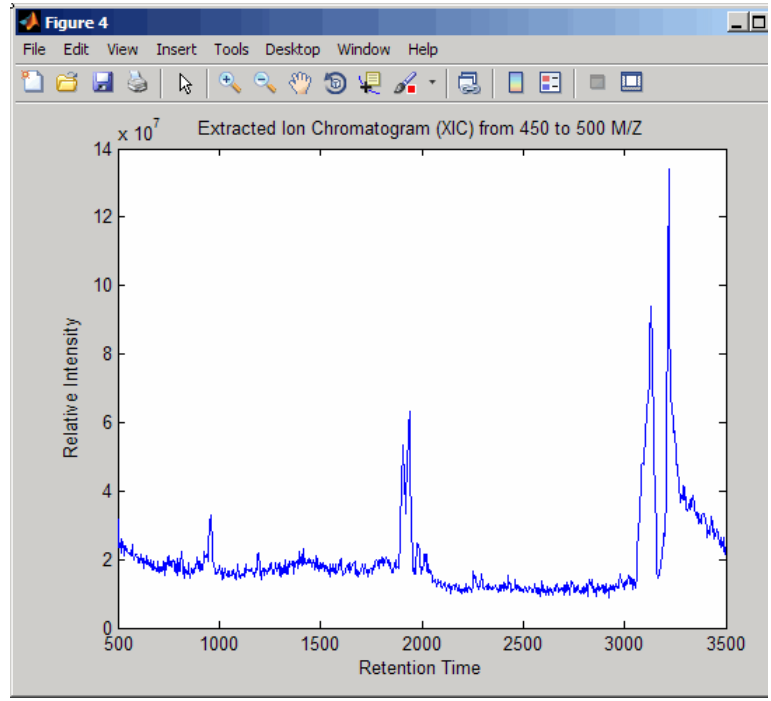
4 Resample the data to plot the Total Ion Chromatogram (TIC).

```
figure
[MZ,Y] = msppresample(peaks,5000);
plot(ret_time,sum(Y))
title('Total Ion Chromatogram (TIC)')
xlabel('Retention Time')
ylabel('Relative Intensity')
```



5 Resample the data to plot the Extracted Ion Chromatogram (XIC) in the 450 to 500 m/z range.

```
figure
[MZ,Y] = msppresample(peaks,5000,'Range',[450 500]);
plot(ret_time,sum(Y))
title('Extracted Ion Chromatogram (XIC) from 450 to 500 M/Z')
xlabel('Retention Time')
ylabel('Relative Intensity')
```



See Also

Bioinformatics Toolbox functions: `msdotplot`, `mspalign`, `mspeaks`, `msresample`, `mzcdf2peaks`, `mzcdfread`, `mzxml2peaks`, `mzxmlread`

Bioinformatics Toolbox demo:

Differential Analysis of Complex Protein and Metabolite Mixtures Using Liquid Chromatography/Mass Spectrometry (LC/MS)

msresample

Purpose

Resample signal with peaks

Syntax

```
[Xout, Intensitiesout] = msresample(X, Intensities, N)
msresample(..., 'Uniform', UniformValue, ...)
msresample(..., 'Range', RangeValue, ...)
msresample(..., 'RangeWarnOff', RangeWarnOffValue, ...)
msresample(..., 'Missing', MissingValue, ...)
msresample(..., 'Window', WindowValue, ...)
msresample(..., 'Cutoff', CutoffValue, ...)
msresample(..., 'ShowPlot', ShowPlotValue, ...)
```

Arguments

X	Vector of separation-unit values for a set of signals with peaks. The number of elements in the vector equals the number of rows in the matrix *Intensities*. The separation unit can quantify wavelength, frequency, distance, time, or m/z depending on the instrument that generates the signal data.
Intensities	Matrix of intensity values for a set of peaks that share the same separation-unit range. Each row corresponds to a separation-unit value, and each column corresponds to either a set of signals with peaks or a retention time. The number of rows equals the number of elements in vector *X*.
N	Positive integer specifying the total number of samples.

Description

Tip Use the following syntaxes with data from any separation technique that produces signal data, such as spectroscopy, NMR, electrophoresis, chromatography, or mass spectrometry.

`[Xout, Intensitiesout] = msresample(X, Intensities, N)` resamples raw noisy signal data, *Intensities*. The output signal has *N* samples with a spacing that increases linearly within the range `[min(X)`

max(*X*)]. *X* can be a linear or a quadratic function of its index. When you set input arguments such that down-sampling takes place, msresample applies a lowpass filter before resampling to minimize aliasing.

For the antialias filter, msresample uses a linear-phase FIR filter with a least-squares error minimization. The cutoff frequency is set by the largest down-sampling ratio when comparing the same regions in the *X* and *Xout* vectors.

Tip msresample is particularly useful when you have signals with different separation-unit vectors and you want to match the scales.

---

msresample(..., '*PropertyName*', *PropertyValue*, ...) calls msresample with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

msresample(..., 'Uniform', *UniformValue*, ...), when *UniformValue* is true, it forces the vector *X* to be uniformly spaced. The default value is false.

msresample(..., 'Range', *RangeValue*, ...) specifies a 1-by-2 vector with the separation-unit range for the output signal, *Intensitiesout*. *RangeValue* must be within [min(*X*) max(*X*)]. Default value is the full range [min(*X*) max(*X*)]. When *RangeValue* values exceed the values in *X*, msresample extrapolates the signal with zeros and returns a warning message.

msresample(..., 'RangeWarnOff', *RangeWarnOffValue*, ...) controls the return of a warning message when *RangeValue* values exceed the values in *X*. *RangeWarnOffValue* can be true or false (default).

msresample(..., 'Missing', *MissingValue*, ...), when *MissingValue* is true, analyzes the input vector, *X*, for dropped samples. The default value is false. If the down-sample factor is

large, checking for dropped samples might not be worth the extra computing time. Dropped samples can only be recovered if the original separation-unit values follow a linear or a quadratic function of the *X* vector index.

`msresample(..., 'Window', WindowValue, ...)` specifies the window used when calculating parameters for the lowpass filter. Enter `'Flattop'`, `'Blackman'`, `'Hamming'`, or `'Hanning'`. The default value is `'Flattop'`.

`msresample(..., 'Cutoff', CutoffValue, ...)` specifies the cutoff frequency. Enter a scalar value from `0` to `1` (Nyquist frequency or half the sampling frequency). By default, `msresample` estimates the cutoff value by inspecting the separation-unit vectors, *X* and *XOut*. However, the cutoff frequency might be underestimated if *X* has anomalies.

`msresample(..., 'ShowPlot', ShowPlotValue, ...)` plots the original and the resampled signal. When `msresample` is called without output arguments, the signals are plotted unless *ShowPlotValue* is `false`. When *ShowPlotValue* is `true`, only the first signal in *Intensities* is plotted. *ShowPlotValue* can also contain an index to one of the signals in *Intensities*.

Tip LC/MS data analysis requires extended amounts of memory from the operating system.

- If you receive errors related to memory, try the following:
  - Increase the virtual memory (swap space) for your operating system (with a recommended initial size of 3,069 and a maximum size of 16,368) as described at:

    `http://www.mathworks.com/support/tech-notes/1100/1106.html#6`

  - Set the 3 GB switch (32-bit Windows XP only) as described at:

    `http://www.mathworks.com/support/tech-notes/1100/1107.html`

- If you receive errors related to Java heap space, increase your Java heap space as described at:

  `http://www.mathworks.com/support/solutions/data/1-18I2C.html`

Examples

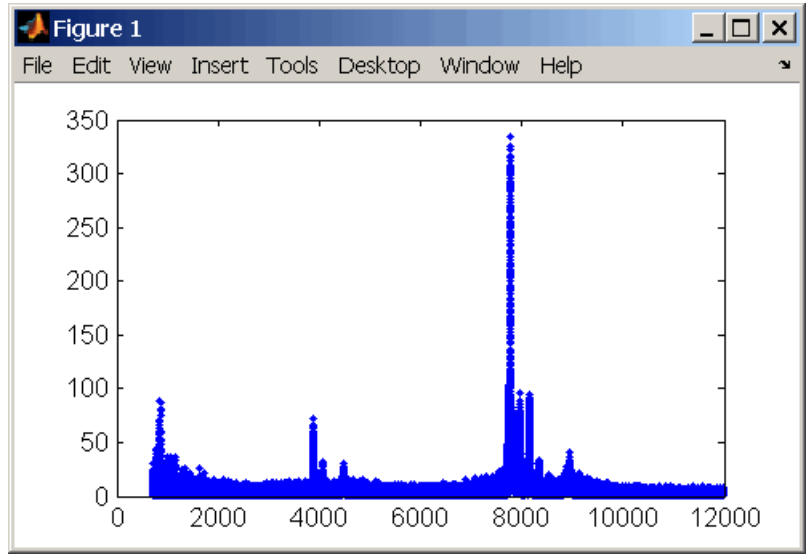
1 Load a MAT-file, included with the Bioinformatics Toolbox software, that contains mass spectrometry data, and then extract m/z and intensity value vectors.

```
load sample_hi_res;
mz = MZ_hi_res;
y = Y_hi_res;
```

2 Plot the original data to a lower resolution.

```
plot(mz, y, '.')
```

A figure appears.



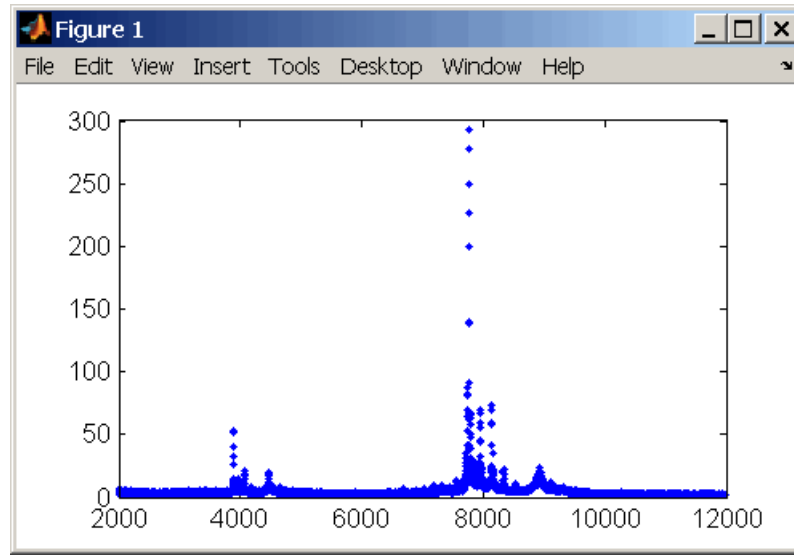
3 Resample the data.

```
[mz1,y1] = msresample(mz, y, 10000, 'range',[2000 max(mz)]);
```

4 Plot the resampled data.

```
plot(mz1,y1,'.')
```

A figure appears with the down-sampled data.



See Also

Bioinformatics Toolbox functions: `msalign`, `msbackadj`, `msheatmap`, `mslowess`, `msnorm`, `msppresample`, `mssgolay`, `msviewer`

Bioinformatics Toolbox demo:

Preprocessing Raw Mass Spectrometry Data

mssgolay

Purpose

Smooth signal with peaks using least-squares polynomial

Syntax

```
Yout = mssgolay(X, Intensities)
mssgolay(X, Intensities, ...'Span', SpanValue, ...)
mssgolay(X, Intensities, ...'Degree', DegreeValue, ...)
mssgolay(X, Intensities, ...'ShowPlot', ShowPlotValue, ...)
```

Arguments

X	Vector of separation-unit values for a set of signals with peaks. The number of elements in the vector equals the number of rows in the matrix *Intensities*. The separation unit can quantify wavelength, frequency, distance, time, or m/z depending on the instrument that generates the signal data.
Intensities	Matrix of intensity values for a set of peaks that share the same separation-unit range. Each row corresponds to a separation-unit value, and each column corresponds to either a set of signals with peaks or a retention time. The number of rows equals the number of elements in vector *X*.

Description

Tip Use the following syntaxes with data from any separation technique that produces signal data, such as spectroscopy, NMR, electrophoresis, chromatography, or mass spectrometry.

Yout = mssgolay(*X*, *Intensities*) smooths raw noisy signal data, *Intensities*, using a least-squares digital polynomial filter (Savitzky and Golay filters). The default span or frame is 15 samples.

mssgolay(*X*, *Intensities*, ...'*PropertyName*', *PropertyValue*, ...) calls mssgolay with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation

marks and is case insensitive. These property name/property value pairs are as follows:

`mssgolay(X, Intensities, ...'Span', SpanValue, ...)` modifies the frame size for the smoothing function. If *`SpanValue`* is greater than `1`, the window is the size of *`SpanValue`* in samples independent of the *`X`* vector. Higher values smooth the signal more with an increase in computation time. If *`SpanValue`* is less than `1`, the window size is a fraction of the number of points in the input data, *`X`*. For example, if *`SpanValue`* is `0.05`, the window size is equal to `5%` of the number of points in *`X`*.

Note The original algorithm by Savitzky and Golay assumes the input vector, *`X`*, has uniformly spaced separation units, while `mssgolay` also allows one that is not uniformly spaced. Therefore, the sliding frame for smoothing is centered using the closest samples in terms of the *`X`* value and not in terms of the *`X`* index.

When the input vector, *`X`*, does not have repeated values or NaN values, the algorithm is approximately twice as fast.

When the input vector, *`X`*, is evenly spaced, the least-squares fitting is performed once so that the signal is filtered with the same coefficients, and the speed of the algorithm increases considerably.

If the input vector, *`X`*, is evenly spaced and *`SpanValue`* is even, span is incremented by `1` to include both edge samples in the frame.

`mssgolay(X, Intensities, ...'Degree', DegreeValue, ...)` specifies the degree of the polynomial (*`DegreeValue`*) fitted to the points in the moving frame. The default value is `2`. *`DegreeValue`* must be smaller than *`SpanValue`*.

`mssgolay(X, Intensities, ...'ShowPlot', ShowPlotValue, ...)` plots smoothed signals over the original. When `mssgolay` is called without output arguments, the signals are plotted unless

ShowPlotValue is `false`. When *ShowPlotValue* is `true`, only the first signal in *Intensities* is plotted. *ShowPlotValue* can also contain an index to one of the signals in *Intensities*.

Examples

1. Load a MAT-file, included with the Bioinformatics Toolbox software, that contains mass spectrometry data variables, including `MZ_lo_res`, a vector of m/z values for a set of spectra, and `Y_lo_res`, a matrix of intensity values for a set of mass spectra that share the same m/z range.

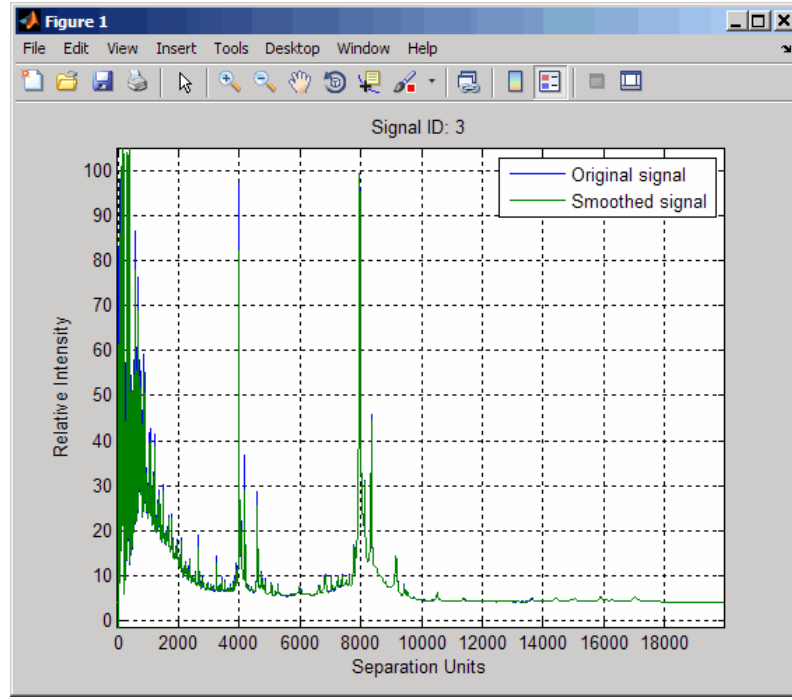
   ```
   load sample_lo_res
   ```

2. Smooth the spectrograms.

   ```
   YS = mssgolay(MZ_lo_res, Y_lo_res);
   ```

3. Plot the third spectrogram in `Y_lo_res` and its smoothed signal.

   ```
   mssgolay(MZ_lo_res,Y_lo_res,'SHOWPLOT',3);
   ```



See Also

Bioinformatics Toolbox functions: `msalign`, `msbackadj`, `msheatmap`, `mslowess`, `msnorm`, `mspeaks`, `msresample`, `msviewer`

Bioinformatics Toolbox demo:

Preprocessing Raw Mass Spectrometry Data

msviewer

Purpose

Explore mass spectrum or set of mass spectra

Syntax

```
msviewer(MZ , Y)
msviewer(..., 'Markers', MarkersValue)
msviewer(..., 'Group', GroupValue)
```

Arguments

MZ	Mass/charge vector with the range of ions in the spectra.
Y	Ion intensity vector with the same length as the mass/charge vector (*MZ*). *Y* can also be a matrix with several spectra that share the same mass/charge (*MZ*) range.

Description

`msviewer(MZ , Y)` creates a GUI to display and explore a mass spectrum, *Y*.

`msviewer(..., 'Markers', MarkersValue)` specifies a list of marker positions from the mass/charge vector, *MZ*, for exploration and easy navigation. Enter a column vector with *MZ* values.

`msviewer(..., 'Group', GroupValue)` specifies a class label for every spectrum with a different color for every class. Enter a column vector of size `[numSpectra x 1]` with integers. The default value is `[numSpectra]`.

MSViewer GUI features include the following:

- Plot mass spectra. The spectra are plotted with different colors according to their class labels.
- An overview displays a full spectrum, and a box indicates the region that is currently displayed in the main window.
- Five different zoom in options, one zoom out option, and a reset view option resize the spectrum.
- Add/focus/move/delete marker operations

- Import/Export markers from/to MATLAB workspace
- Print and preview the spectra plot
- Print the spectra plot to a MATLAB Figure window

MSViewer has five components:

- Menu bar: **File**, **Tools**, **Window**, and **Help**
- Toolbar: Zoom XY, Zoom X, Zoom Y, Reset view, Zoom out, and Help
- Main window: display the spectra
- Overview window: display the overview of a full spectrum (the average of all spectra in display)
- Marker control panel: a list of markers, Add marker, Delete marker, up and down buttons

Examples

1. Load and plot sample data

```
load sample_lo_res
msviewer(MZ_lo_res, Y_lo_res)
```

2. Add a marker by pointing to a mass peak, right-clicking, and then clicking **Add Marker**.

3. From the **File** menu, select

   - **Import Markers from Workspace** — Opens the Import Markers From MATLAB Workspace dialog. The dialog should display a list of double `Mx1` or `1xM` variables. If the selected variable is out of range, the viewer displays an error message
   - **Export Markers to Workspace** — Opens the Export Markers to MATLAB Workspace dialog. You can enter a variable name for the markers. All markers are saved. If there is no marker available, this menu item should be disabled.
   - **Print to Figure** — Prints the spectra plot in the main display to a MATLAB Figure window

4 From the **Tools** menu, click

- **Add Marker** — Opens the Add Marker dialog. Enter an m/z marker.
- **Delete Marker** — Removes the currently selected m/z marker from the **Markers** (m/z) list.
- **Next Marker** or **Previous Marker** — Moves the selection up and down the **Markers** (m/z) list.
- **Zoom XY**, **Zoom X**, **Zoom Y**, or **Zoom Out** — Changes the cursor from an arrow to crosshairs. Left-click and drag a rectangle box over an area and then release the mouse button. The display zooms the area covered by the box.

5 Move the cursor to the range window at the bottom. Click and drag the view box to a new location.

See Also

Bioinformatics Toolbox functions: `msalign`, `msbackadj`, `mslowess`, `msnorm`, `msheatmap`, `msresample`, `mssgolay`

Purpose

Align multiple sequences using progressive method

Syntax

```
SeqsMultiAligned = multialign(Seqs)
SeqsMultiAligned = multialign(Seqs, Tree)
multialign(..., 'PropertyName', PropertyValue,...)
multialign(..., 'Weights', WeightsValue)
multialign(..., 'ScoringMatrix', ScoringMatrixValue)
multialign(..., 'SMInterp', SMInterpValue)
multialign(..., 'GapOpen', GapOpenValue)
multialign(..., 'ExtendGap', ExtendGapValue)
multialign(..., 'DelayCutoff', DelayCutoffValue)
multialign(..., 'JobManager', JobManagerValue)
multialign(..., 'WaitInQueue', WaitInQueueValue)
multialign(..., 'Verbose', VerboseValue)
multialign(..., 'ExistingGapAdjust',
ExistingGapAdjustValue)
multialign(..., 'TerminalGapAdjust',
TerminalGapAdjustValue)
```

Arguments

Seqs	Vector of structures with the fields `'Sequence'` for the residues and `'Header'` or `'Name'` for the labels. *Seqs* may also be a cell array of strings or a char array.
SeqsMultiAligned	Vector of structures (same as *Seqs*) but with the field `'Sequence'` updated with the alignment. When *Seqs* is a cell or char array, *SeqsMultiAligned* is a char array with the output alignment following the same order as the input.

Tree	Phylogenetic tree calculated with either of the functions `seqlinkage` or `seqneighjoin`.
WeightsValue	Property to select the sequence weighting method. Enter either `'THG'` (default) or `'equal'`.
ScoringMatrixValue	Property to select or specify the scoring matrix. Enter an `[MxM]` matrix or `[MxMxN]` array of matrixes with`N` user-defined scoring matrices. *ScoringMatrixValue*may also be a cell array of strings with matrix names.The default is the `BLOSUM80` to `BLOSUM30` series for amino acids or a fixed matrix NUC44 for nucleotides. When passing your own series of scoring matrices make sure all of them share the same scale.
SMInterpValue	Property to specify whether linear interpolation of the scoring matrices is on or off. When `false`, scoring matrix is assigned to a fixed range depending on the distances between the two profiles (or sequences) being aligned. Default is `true`.
GapOpenValue	Scalar or a function specified using `@`. If you enter a function,`multialign` passes four values to the function: the average score for two matched residues (`sm`), the average score for two mismatched residues (`sx`), and, the length of both profiles or sequences (`len1`, `len2`). Default is `@(sm,sx,len1,len2) 5*sm`.

ExtendGapValue	Scalar or a function specified using `@`. IF you enter a function, `multiialign` passes four values to the function: the average score for two matched residues (`sm`), the average score for two mismatched residues (`sx`), and the length of both profiles or sequences (`len1`, `len2`). Default is `@(sm,sx,len1,len2) sm/4`.
DelayCutoffValue	Property to specify the threshold delay of divergent sequences. The default is unity where sequences with the closest sequence farther than the median distance are delayed.
JobManagerValue	JobManager object representing an available distributed MATLAB resource. Enter a jobmanager object returned by the Parallel Computing Toolbox™ function `findResource`.
WaitInQueueValue	Property to control waiting for a distributed MATLAB resource to be available. Enter either `true` or `false`. The default value is `false`.
VerboseValue	Property to control displaying the sequences with sequence information. Default value is `false`.
ExistingGagAdjustValue	Property to control automatic adjustment based on existing gaps. Default value is `true`.
TerminalGapAdjustValue	Property to adjusts the penalty for opening a gap at the ends of the sequence. Default value is `false`.

Description

SeqsMultiAligned = multialign(*Seqs*) performs a progressive multiple alignment for a set of sequences (*Seqs*). Pairwise distances between sequences are computed after pairwise alignment with the Gonnet scoring matrix and then by counting the proportion of sites at which each pair of sequences are different (ignoring gaps). The guide tree is calculated by the neighbor-joining method assuming equal variance and independence of evolutionary distance estimates.

SeqsMultiAligned = multialign(*Seqs*, *Tree*) uses a tree (*Tree*) as a guide for the progressive alignment. The sequences (*Seqs*) should have the same order as the leaves in the tree (*Tree*) or use a field ('Header' or 'Name') to identify the sequences.

multialign(..., '*PropertyName*', *PropertyValue*,...) enters optional arguments as property name/value pairs.

multialign(..., 'Weights', *WeightsValue*) selects the sequence weighting method. Weights emphasize highly divergent sequences by scaling the scoring matrix and gap penalties. Closer sequences receive smaller weights.

Values of the property Weights:

- 'THG'(default) — Thompson-Higgins-Gibson method using the phylogenetic tree branch distances weighted by their thickness.
- 'equal' — Assigns same weight to every sequence.

multialign(..., 'ScoringMatrix', *ScoringMatrixValue*) selects the scoring matrix (*ScoringMatrixValue*) for the progressive alignment. Match and mismatch scores are interpolated from the series of scoring matrices by considering the distances between the two profiles or sequences being aligned. The first matrix corresponds to the smallest distance and the last matrix to the largest distance. Intermediate distances are calculated using linear interpolation.

multialign(..., 'SMInterp', *SMInterpValue*), when *SMInterpValue* is false, turns off the linear interpolation of the scoring matrices. Instead, each supplied scoring matrix is assigned to

a fixed range depending on the distances between the two profiles or sequences being aligned.

`multialign(..., 'GapOpen', GapOpenValue)` specifies the initial penalty for opening a gap.

`multialign(..., 'ExtendGap', ExtendGapValue)` specifies the initial penalty for extending a gap.

`multialign(..., 'DelayCutoff', DelayCutoffValue)` specifies a threshold to delay the alignment of divergent sequences whose closest neighbor is farther than

```
(DelayCutoffValue) * (median patristic distance
between sequences)
```

`multialign(..., 'JobManager', JobManagerValue)` distributes pairwise alignments into a cluster of computers using the Parallel Computing Toolbox software.

`multialign(..., 'WaitInQueue', WaitInQueueValue)` when `WaitInQueueValue` is true, waits in the job manager queue for an available worker. When `WaitInQueueValue` is `false` (default) and there are no workers immediately available, `multialign` errors out. Use this property with the Parallel Computing Toolbox software and the `multialign` property `WaitInQueue`.

`multialign(..., 'Verbose', VerboseValue)`, when `VerboseValue` is `true`, turns on verbosity.

The remaining input optional arguments are analogous to the function `profalign` and are used through every step of the progressive alignment of profiles.

`multialign(..., 'ExistingGapAdjust', ExistingGapAdjustValue)`, if `ExistingGapAdjustValue` is `false`, turns off the automatic adjustment based on existing gaps of the position-specific penalties for opening a gap.

When `ExistingGapAdjustValue` is true, for every profile position, `profalign` proportionally lowers the penalty for opening a gap toward

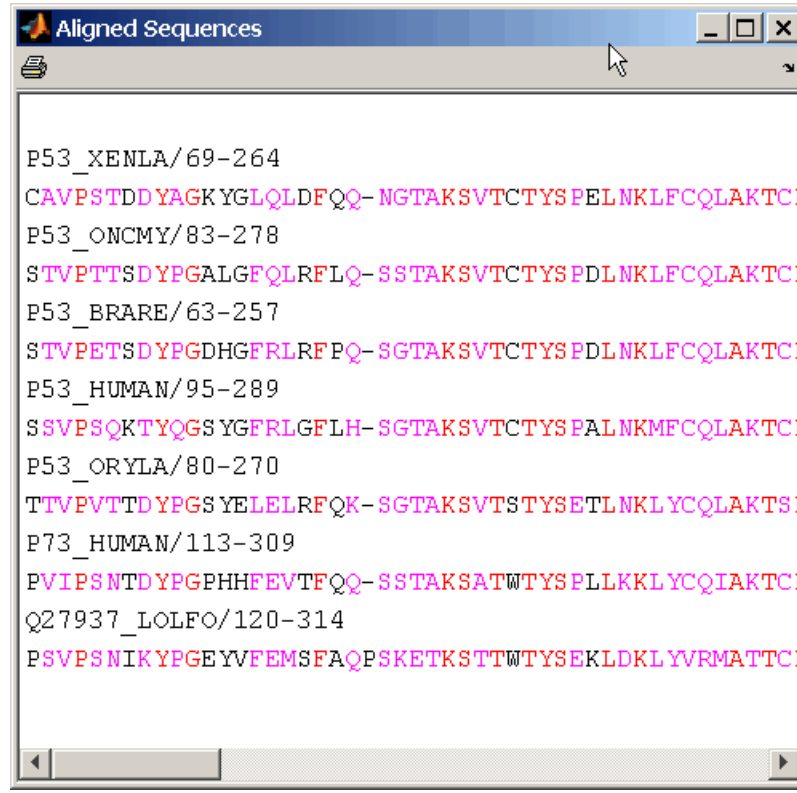
the penalty of extending a gap based on the proportion of gaps found in the contiguous symbols and on the weight of the input profile.

`multialign(..., 'TerminalGapAdjust', TerminalGapAdjustValue)`, when *`TerminalGapAdjustValue`* is `true`, adjusts the penalty for opening a gap at the ends of the sequence to be equal to the penalty for extending a gap.

Example1

1 Align seven cellular tumor antigen p53 sequences.

```
p53 = fastaread('p53samples.txt')
ma = multialign(p53,'verbose',true)
showalignment(ma)
```

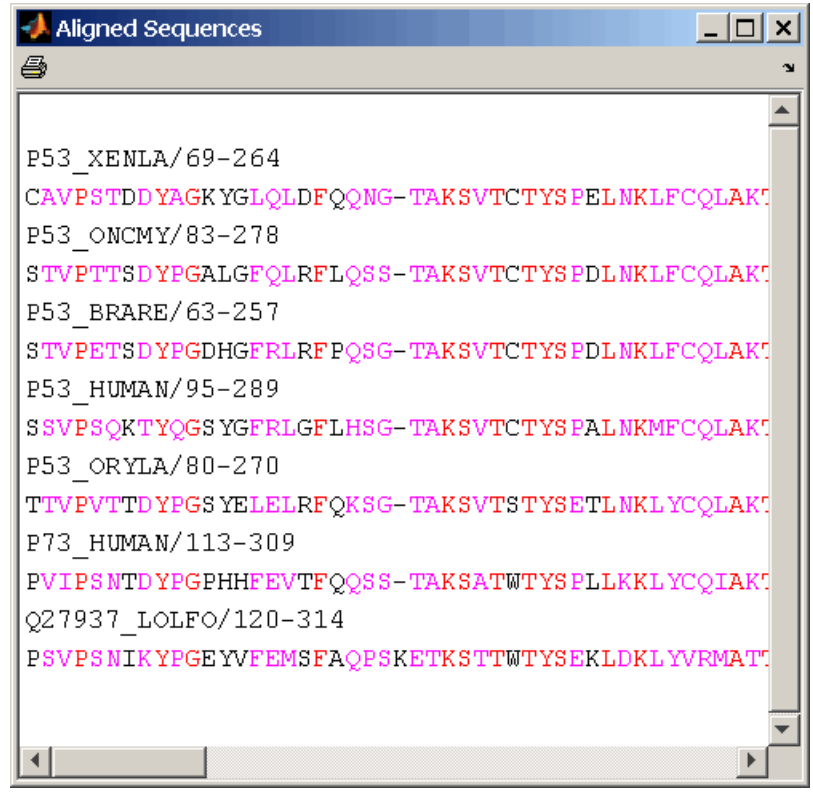


2 Use an UPGMA phylogenetic tree instead as a guiding tree.

```
dist = seqpdist(p53,'ScoringMatrix',gonnet);
tree = seqlinkage(dist,'UPGMA',p53)

Phylogenetic tree object with 7 leaves (6 branches)
```

3 Score the progressive alignment with the PAM family.

```
ma = multialign(p53,tree,'ScoringMatrix',...
                {'pam150','pam200','pam250'})
showalignment(ma)
```



Example 2

1 Enter an array of sequences.

```
seqs = {'CACGTAACATCTC','ACGACGTAACATCTTCT','AAACGTAACATCTCGC'};
```

2 Promote terminations with gaps in the alignment.

```
multialign(seqs,'terminalGapAdjust',true)

ans =
--CACGTAACATCTC--
ACGACGTAACATCTTCT
-AAACGTAACATCTCGC
```

3 Compare alignment without termination gap adjustment.

```
multialign(seqs)

ans =
CA--CGTAACATCT--C
ACGACGTAACATCTTCT
AA-ACGTAACATCTCGC
```

See Also

Bioinformatics Toolbox functions: `hmmprofalign`, `multialignread`, `multialignwrite`, `nwalign`, `profalign`, `seqprofile`, `seqconsensus`, `seqneighjoin`, `showalignment`

multialignread

Purpose

Read multiple sequence alignment file

Syntax

```
S = multialignread(File)
[Headers, Sequences] = multialignread(File)
... = multialignread(File, 'IgnoreGaps', IgnoreGapsValue)
```

Arguments

File	Multiple sequence alignment file specified by one of the following: • File name or path and file name • URL pointing to a file • MATLAB character array that contains the text of a multiple sequence alignment file You can read common multiple sequence alignment file types, such as ClustalW (`.aln`), GCG (`.msf`), and PHYLIP.
IgnoreGapsValue	Controls removing gap symbols, such as `'-'` or `'.'`, from the sequences. Choices are `true` or `false` (default).

Return Values

S	MATLAB structure array containing the following fields: • `Header` — Header information from the file. • `Sequence` — Amino acid or nucleotide sequences.
Headers	Cell array containing the header information from the file.
Sequences	Cell array containing the amino acid or nucleotide sequences.

Description

S = multialignread(*File*) reads a multiple sequence alignment file. The file contains multiple sequence lines that start with a sequence header followed by an optional number (not used by multialignread) and a section of the sequence. The multiple sequences are broken into blocks with the same number of blocks for every sequence. To view an example multiple sequence alignment file, type open aagag.aln at the MATLAB command line.

The output, *S*, is a structure array where *S*.Header contains the header information and *S*.Sequence contains the amino acid or nucleotide sequences.

[*Headers*, *Sequences*] = multialignread(*File*) reads the file into separate variables, *Headers* and *Sequences*, which are cell arrays containing header information and amino acid or nucleotide sequences, respectively.

... = multialignread(*File*, 'IgnoreGaps', *IgnoreGapsValue*) controls the removal of any gap symbol, such as '-' or '.', from the sequences. Choices are true or false (default).

Examples

Read a multiple sequence alignment of the gag polyprotein for several HIV strains.

```
gagaa = multialignread('aagag.aln')

gagaa =

1x16 struct array with fields:
    Header
    Sequence
```

See Also

Bioinformatics Toolbox functions: fastaread, gethmmalignment, multialign, multialignviewer, multialignwrite, seqconsensus, seqdisp, seqprofile

multialignviewer

Purpose

Display and interactively adjust multiple sequence alignment

Syntax

```
multialignviewer
multialignviewer(Alignment)
multialignviewer('close')
multialignviewer(..., 'Alphabet', AlphabetValue, ...)
multialignviewer(..., 'SeqHeaders', SeqHeadersValue, ...)
```

Description

`multialignviewer` opens the Multiple Sequence Alignment Viewer window, where you can display and interactively adjust a multiple sequence alignment.

`multialignviewer(Alignment)` loads a group of previously multiply aligned sequences into the Multiple Sequence Alignment Viewer window, where you can view and interactively adjust the alignment.

`multialignviewer('close')` closes the Multiple Sequence Alignment Viewer window.

`multialignviewer(..., 'PropertyName', PropertyValue, ...)` calls `multialignviewer` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each *`PropertyName`* in single quotation marks. Each *`PropertyName`* is case insensitive. These property name/property value pairs are as follows:

`multialignviewer(..., 'Alphabet', AlphabetValue, ...)` specifies the alphabet type for the sequences.

`multialignviewer(..., 'SeqHeaders', SeqHeadersValue, ...)` specifies a list of names to label the sequences in the Multiple Sequence Alignment Viewer window.

Inputs

`Alignment`

Group of multiply aligned amino acid or nucleotide sequences specified by one of the following:

- MATLAB structure containing a `Sequence` field, such as returned by `fastaread`, `gethmmalignment`, `multialign`, or `multialignread`
- MATLAB character array that contains a multiple sequence alignment, such as returned by `multialign`
- String specifying a file name, path and file name, or URL pointing to a file, where the file contains a multiple sequence alignment
- 3-by-N character array showing the pairwise alignment of two sequences, such as returned by `nwalign` or `swalign`

`AlphabetValue`

String that specifies the alphabet type for the sequences. Choices are `'AA'` for amino acids or `'NT'` for nucleotides. If you do not specify an alphabet type, `multialignviewer` attempts to determine the correct alphabet. If it cannot, it defaults to `'AA'`.

`SeqHeadersValue`

List of names to label the sequences in the Multiple Sequence Alignment Viewer window, specified by either of the following:

- MATLAB array of structures containing a `Header` or `Name` field, such as returned by `fastaread`, `gethmmalignment`, `multialign`, or `multialignread`
- Cell array of strings

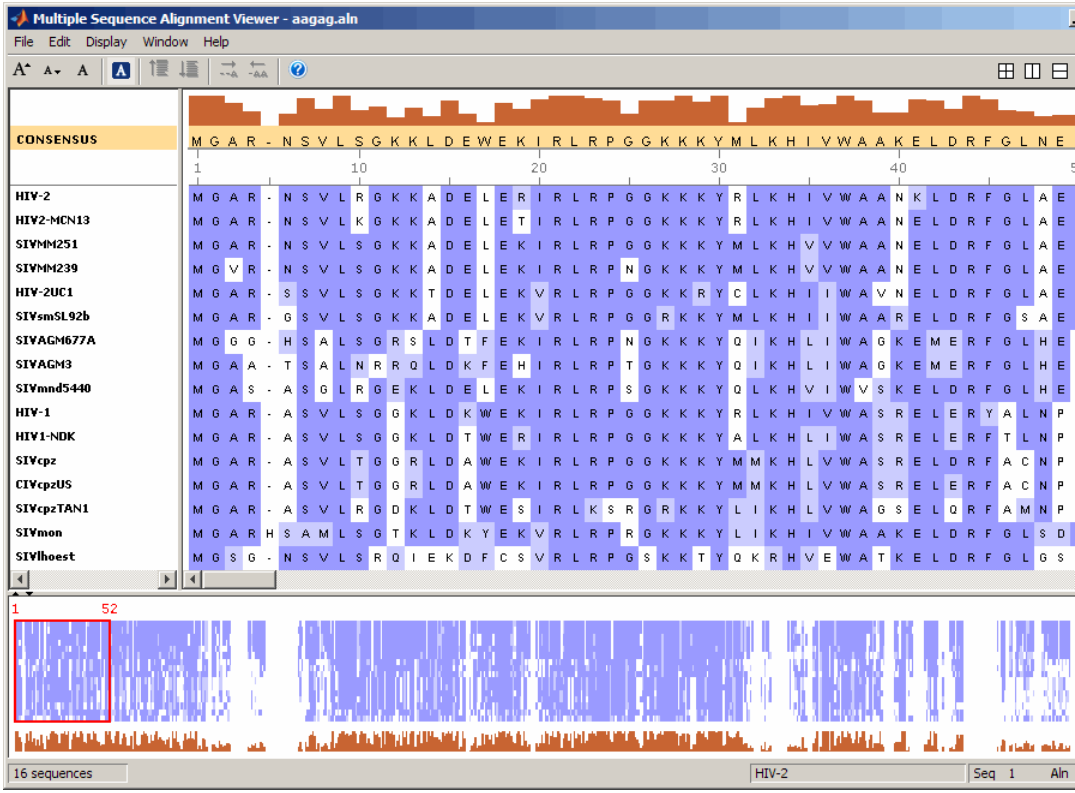
`SeqHeadersValue` must contain the same number of elements as there are sequences in *`Alignment`*.

Examples

Load a file containing a multiple sequence alignment in the Multiple Sequence Alignment Viewer window, then close the window:

```
% Load multiple sequence alignment file
% in Multiple Sequence Alignment Viewer
```

```
multialignviewer('aagag.aln')

% Close Multiple Sequence Alignment Viewer window
multialignviewer('close')
```



Alternatives

You can also display a color-coded multiple or pairwise sequence alignment using the `showalignment` function. However, the alignment displays in a MATLAB Figure window, where you cannot interact with it.

See Also

`fastaread` | `gethmmalignment` | `multialign` | `multialignread` | `multialignwrite` | `seqtool` | `showalignment` | `nwalign` | `swalign`

Tutorials

- Investigating the Bird Flu Virus

How To

- "Multiple Sequence Alignment Viewer"

multialignwrite

Purpose

Write multiple alignment to file

Syntax

```
multialignwrite(File, Alignment)
multialignwrite(..., 'Format', FormatValue, ...)
multialignwrite(..., 'Header', HeaderValue, ...)
multialignwrite(..., 'WriteCount', WriteCountValue, ...)
```

Description

`multialignwrite(File, Alignment)` writes the contents of an alignment to a ClustalW ALN-formatted (default) or MSF-formatted file.

`multialignwrite(..., 'PropertyName', PropertyValue, ...)` calls `multialignwrite` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each *`PropertyName`* in single quotation marks. Each *`PropertyName`* is case insensitive. These property name/property value pairs are as follows:

`multialignwrite(..., 'Format', FormatValue, ...)` specifies the format of the file. *`FormatValue`* can be `'ALN'` (default) or `'MSF'`.

`multialignwrite(..., 'Header', HeaderValue, ...)` specifies the first line of the file. The default for *`HeaderValue`* is `'MATLAB multiple sequence alignment'`.

`multialignwrite(..., 'WriteCount', WriteCountValue, ...)` specifies whether to add the residue counts to the end of each line. *`WriteCountValue`* can be `true` (default) or `false`.

Inputs

`Alignment`

An alignment, such as returned by the `multialign` function, represented by either a:

- Vector of structures, each containing the fields `Header` and `Sequence`
- Character array

File

String specifying either a file name or a path and file name for saving the data. If you specify only a file name, the file is saved to the MATLAB Current Folder browser.

Tip If you use an `.msf` extension when supplying a file name for *File*, the data is written to an MSF-formatted file. Otherwise, the data is written to a ClustalW ALN-formatted file.

Below the columns of the ClustalW ALN-formatted file, symbols can appear that denote:

- `*` — Residues or nucleotides in the column are identical in all sequences in the alignment.
- `:` — Conserved substitutions exist in the column for all sequences in the alignment.
- `.` — Semiconserved substitutions exist in the column for all sequences in the alignment.

For more information on these symbols, see `http://www.ebi.ac.uk/help/formats.html#aln`.

For more information on the groups of residues considered conserved and semiconserved, see section 12 in "Changes since version 1.6" at `http://web.mit.edu/clustalw_v1.83/README`.

FormatValue

String that specifies the format of *File*. Choices are `'ALN'` (default) or `'MSF'`.

Tip You can also write to an MSF-formatted file by using an `.msf` extension when supplying a file name for *File*.

HeaderValue

String that specifies the first line of the file.

Tip Use the `'Header'` property if your file header must be a specific format for a third-party software application.

Default: `'MATLAB multiple sequence alignment'`

WriteCountValue

Specifies whether to add the residue counts to the end of each line. Choices are `true` (default) or `false`.

Examples

1 Use the `fastaread` function to read `p53samples.txt`, a FASTA-formatted file included with the Bioinformatics Toolbox software, which contains seven cellular tumor antigen p53 sequences.

```
p53 = fastaread('p53samples.txt')

p53 =

7x1 struct array with fields:
    Header
    Sequence
```

2 Use the `multialign` function to align the seven cellular tumor antigen p53 sequences.

```
ma = multialign(p53,'verbose',true);
```

3 Write the alignment to a file named `p53.aln`.

```
multialignwrite('p53.aln',ma)
```

See Also

fastaread | fastawrite | gethmmalignment | multialign | multialignread | multialignviewer | phytreewrite | seqconsensus | seqdisp | seqprofile

mzcdf2peaks

Purpose

Convert mzCDF structure to peak list

Syntax

```
[Peaks, Times] = mzcdf2peaks(mzCDFStruct)
```

Arguments

mzCDFStruct	MATLAB structure containing information from a netCDF file, such as one created by the `mzcdfread` function. Its fields correspond to the variables and global attributes in a netCDF file. If a netCDF variable contains local attributes, an additional field is created, with the name of the field being the variable name appended with the `_attributes` string. The number and names of the fields will vary, depending on the mass spectrometer software, but typically there are `mass_values` and `intensity_values` fields.

Return Values

Peaks	Either of the following: • Two-column matrix, where the first column contains mass/charge (m/z) values and the second column contains ion intensity values. • Cell array of peak lists, where each element is a two-column matrix of m/z values and ion intensity values, and each element corresponds to a spectrum or retention time.
Times	Scalar of vector of retention times associated with a liquid chromatography/mass spectrometry (LC/MS) or gas chromatography/mass spectrometry (GC/MS) data set. If *Times* is a vector, the number of elements equals the number of peak lists contained in *Peaks*.

Description

`[Peaks, Times] = mzcdf2peaks(mzCDFStruct)` extracts peak information from *mzCDFStruct*, a MATLAB structure containing

information from a netCDF file, such as one created by the `mzcdfread` function, and creates *`Peaks`*, a single matrix or a cell array of matrices containing mass/charge (m/z) values and ion intensity values, and *`Times`*, a scalar or vector of retention times associated with a liquid chromatography/mass spectrometry (LC/MS) or gas chromatography/mass spectrometry (GC/MS) data set.

`mzCDFStruct` contains fields that correspond to the variables and global attributes in a netCDF file. If a netCDF variable contains local attributes, an additional field is created, with the name of the field being the variable name appended with the `_attributes` string. The number and names of the fields will vary, depending on the mass spectrometer software, but typically there are `mass_values` and `intensity_values` fields.

Examples

In the following example, the file `results.cdf` is not provided.

1. Use the `mzcdfread` function to read a netCDF file into the MATLAB software as a structure. Then extract the peak information from the structure.

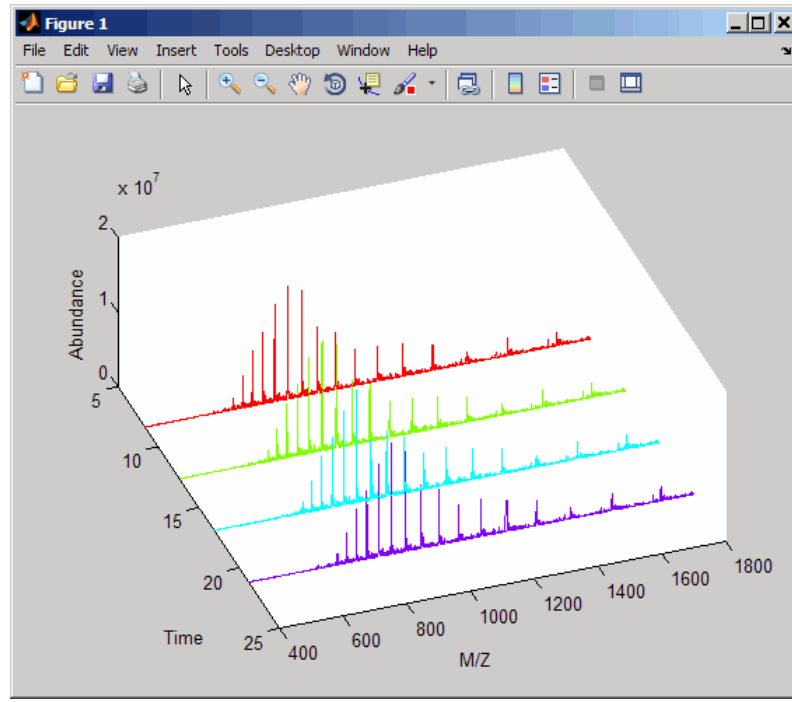
```
mzcdf_struct = mzcdfread('results.cdf');
[peaks,time] = mzcdf2peaks(mzcdf_struct)

peaks =

    [7008x2 single]
    [7008x2 single]
    [7008x2 single]
    [7008x2 single]

time =

    8.3430
   12.6130
   16.8830
   21.1530
```

2 Create a color map containing a color for each peak list (retention time).

```
colors = hsv(numel(peaks));
```

3 Create a 3-D figure of the peaks and add labels to it.

```
figure
hold on

for i = 1:numel(peaks)
    t = repmat(time(i),size(peaks{i},1),1);
    plot3(t,peaks{i}(:,1),peaks{i}(:,2),'color',colors(i,:))
end

view(70,60)
xlabel('Time')
ylabel(mzcdf_struct.mass_axis_label)
zlabel(mzcdf_struct.intensity_axis_label)
```



See Also

Bioinformatics Toolbox functions: `msdotplot`, `mspalign`, `msppresample`, `mzcdfread`

mzcdfinfo

Purpose

Return information about netCDF file containing mass spectrometry data

Syntax

```
InfoStruct = mzcdfinfo(File)
```

Arguments

File	String containing a file name, or a path and file name, of a netCDF file that contains mass spectrometry data and conforms to the ANDI/MS or the ASTM E2077-00 (2005) standard specification or earlier specifications. If you specify only a file name, that file must be on the MATLAB search path or in the current directory.

Return Values

InfoStruct	MATLAB structure containing information from a netCDF file. It includes the fields in the following table.

Description

InfoStruct = mzcdfinfo(*File*) returns a MATLAB structure, *InfoStruct*, containing summary information about a netCDF file, *File*.

File is a string containing a file name, or a path and file name, of a netCDF file that contains mass spectrometry data. The file must conform to the ANDI/MS or the ASTM E2077-00 (2005) standard specification or earlier specifications.

InfoStruct includes the following fields.

Field	Description
Filename	Name of the netCDF file.

Field	Description
FileTimeStamp	Date time stamp of the netCDF file.
FileSize	Size of the file in bytes.
NumberOfScans	Number of scans in the file.
StartTime	Run start time.
EndTime	Run end time.
TimeUnits	Units for time.
GlobalMassMin	Minimum m/z value in all scans.
GlobalMassMax	Maximum m/z value in all scans.
GlobalIntensityMin	Minimum intensity value in all scans.
GlobalIntensityMax	Maximum intensity value in all scans.
ExperimentType	Indicates if data is raw or centroided.

Note If any of the associated attributes are not in the netCDF file (because they are optional in the specifications), the value for that field will be set to `N/A` or `NaN`.

Examples

In the following example, the file `results.cdf` is not provided.

Return a MATLAB structure containing summary information about a netCDF file.

```
info = mzcdfinfo('results.cdf')

info =
```

```
                Filename: 'results.cdf'
           FileTimeStamp: '19930703134354-700'
                FileSize: 339892
           NumberOfScans: 4
               StartTime: 8.3430
                 EndTime: 21.1530
               TimeUnits: 'N/A'
           GlobalMassMin: 399.9990
           GlobalMassMax: 1.8000e+003
      GlobalIntensityMin: NaN
      GlobalIntensityMax: NaN
          ExperimentType: 'Continuum Mass Spectrum'
```

See Also

Bioinformatics Toolbox function: `mzcdfread`

Purpose

Read mass spectrometry data from netCDF file

Syntax

```
mzCDFStruct = mzcdfread(File)
mzCDFStruct = mzcdfread(File, ...'TimeRange',
TimeRangeValue, ...)
mzCDFStruct = mzcdfread(File, ...'ScanIndices',
   ScanIndicesValue, ...)
mzCDFStruct = mzcdfread(File, ...'Verbose', VerboseValue,
   ...)
```

Arguments

File

String containing a file name, or a path and file name, of a netCDF file that contains mass spectrometry data and conforms to the ANDI/MS or the ASTM E2077-00 (2005) standard specification or earlier specifications.

If you specify only a file name, that file must be on the MATLAB search path or in the current directory.

TimeRangeValue

Two-element numeric array `[Start End]` that specifies the time range in *File* for which to read spectra. Default is to read spectra from all times `[0 Inf]`.

Tip Time units are indicated in the netCDF global attributes. For summary information about the time ranges in a netCDF file, use the `mzcdfinfo` function.

Note If you specify a *TimeRangeValue*, you cannot specify a *ScanIndicesValue*.

ScanIndicesValue Positive integer, vector of integers, or a two-element numeric array `[Start_Ind End_Ind]` that specifies a scan, multiple scans, or a range of scans in *`File`* to read. `Start_Ind` and `End_Ind` are each positive integers indicating a scan index number. `Start_Ind` must be less than `End_Ind`. Default is to read all scans.

Tip For information about the scan indices in a netCDF file, check the `NumberOfScans` field in the structure returned by the `mzcdfinfo` function.

Note If you specify a *`ScanIndicesValue`*, you cannot specify *`TimeRangeValue`*.

VerboseValue Controls the display of the progress of the reading of *`File`*. Choices are `true` (default) or `false`.

Return Values

mzCDFStruct MATLAB structure containing mass spectrometry information from a netCDF file. Its fields correspond to the variables and global attributes in a netCDF file. If a netCDF variable contains local attributes, an additional field is created, with the name of the field being the variable name appended with the `_attributes` string. The number and names of the fields will vary, depending on the mass spectrometer software, but typically there are `mass_values` and `intensity_values` fields.

Description

`mzCDFStruct` `= mzcdfread(`*`File`*`)` reads a netCDF file, *`File`*, and then creates a MATLAB structure, *`mzCDFStruct`*.

File is a string containing a file name, or a path and file name, of a netCDF file that contains mass spectrometry data. The file must conform to the ANDI/MS or the ASTM E2077-00 (2005) standard specification or earlier specifications.

mzCDFStruct contains fields that correspond to the variables and global attributes in a netCDF file. If a netCDF variable contains local attributes, an additional field is created, with the name of the field being the variable name appended with the `_attributes` string. The number and names of the fields will vary, depending on the mass spectrometer software, but typically there are `mass_values` and `intensity_values` fields.

Tip LC/MS data analysis requires extended amounts of memory from the operating system.

- If you receive errors related to memory, try the following:
  - Increase the virtual memory (swap space) for your operating system (with a recommended initial size of 3,069 and a maximum size of 16,368) as described at:

    `http://www.mathworks.com/support/tech-notes/1100/1106.html#6`

  - Set the 3 GB switch (32-bit Windows XP only) as described at:

    `http://www.mathworks.com/support/tech-notes/1100/1107.html`

- If you receive errors related to Java heap space, increase your Java heap space as described at:

  `http://www.mathworks.com/support/solutions/data/1-18I2C.html`

---

mzCDFStruct = `mzcdfread(`*File*`, ...'`*PropertyName*`',` *PropertyValue*`, ...)` calls `mzcdfread` with optional properties that use property name/property value pairs. You can specify one or more

properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

mzCDFStruct = mzcdfread(*File*, ...'TimeRange', *TimeRangeValue*, ...) specifies the range of time in *File* to read. *TimeRangeValue* is a two-element numeric array [Start End]. Default is to read spectra from all times [0 Inf].

Tip Time units are indicated in the netCDF global attributes. For summary information about the time ranges in a netCDF file, use the mzcdfinfo function.

Note If you specify a *TimeRangeValue*, you cannot specify *ScanIndicesValue*.

---

mzCDFStruct = mzcdfread(*File*, ...'ScanIndices', *ScanIndicesValue*, ...) specifies a scan, multiple scans, or range of scans in *File* to read. *ScanIndicesValue* is a positive integer, vector of integers, or a two-element numeric array [Start_Ind End_Ind]. Start_Ind and End_Ind are each positive integers indicating a scan index number. Start_Ind must be less than End_Ind. Default is to read all scans.

Tip For information about the scan indices in a netCDF file, check the NumberOfScans field in the structure returned by the mzcdfinfo function.

Note If you specify a *ScanIndicesValue*, you cannot specify a *TimeRangeValue*.

mzCDFStruct = mzcdfread(*File*, ...'Verbose', *VerboseValue*, ...) controls the progress display when reading *File*. Choices are `true` (default) or `false`.

Examples

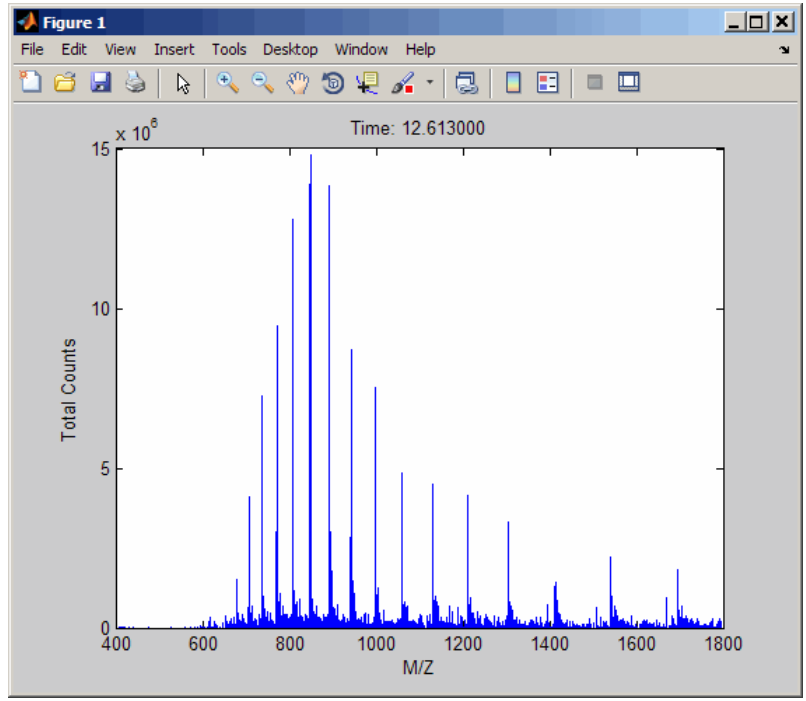
In the following example, the file `results.cdf` is not provided.

1. Read a netCDF file into the MATLAB software as a structure.

```
out = mzcdfread('results.cdf');
```

2. View the second scan in the netCDF file by creating separate variables containing the intensity and m/z values, and then plotting these values. Add a title and *x*- and *y*-axis labels using fields in the output structure.

```
idx1 = out.scan_index(2)+1;
idx2 = out.scan_index(3);
y = out.intensity_values(idx1:idx2);
z = out.mass_values(idx1:idx2);
stem(z,y,'marker','none')

title(sprintf('Time: %f',out.scan_acquisition_time(2)))
xlabel(out.mass_axis_units)
ylabel(out.intensity_axis_units)
```



See Also

Bioinformatics Toolbox functions: `jcampread`, `mzcdf2peaks`, `mzcdfinfo`, `mzxmlread`, `tgspcread`

Purpose

Convert mzXML structure to peak list

Syntax

```
[Peaks, Times] = mzxml2peaks(mzXMLStruct)
[Peaks, Times] = mzxml2peaks(mzXMLStruct,
'Levels', LevelsValue)
```

Arguments

mzXMLStruct	MATLAB structure containing information from an mzXML file, such as one created by the `mzxmlread` function. It includes the fields shown in the table below.
LevelsValue	Positive integer or vector of integers that specifies the level(s) of spectra in *mzXMLStruct* to convert, assuming the spectra are from tandem MS data sets. Default is `1`, which converts only the first-level spectra, that is, spectra containing precursor ions. Setting *LevelsValue* to `2` converts only the second-level spectra, which are the fragment spectra (created from a precursor ion).

Return Values

Peaks	Either of the following: • Two-column matrix, where the first column contains mass/charge (m/z) values and the second column contains ion intensity values. • Cell array of peak lists, where each element is a two-column matrix of m/z values and ion intensity values, and each element corresponds to a spectrum or retention time.
Times	Vector of retention times associated with a liquid chromatography/mass spectrometry (LC/MS) or gas chromatography/mass spectrometry (GC/MS) data set. The number of elements in *Times* equals the number of elements in *Peaks*.

Description

`[Peaks, Times] = mzxml2peaks(mzXMLStruct)` extracts peak information from *`mzXMLStruct`*, a MATLAB structure containing information from an mzXML file, such as one created by the `mzxmlread` function, and creates *`Peaks`*, a cell array of matrices containing mass/charge (m/z) values and ion intensity values, and *`Times`*, a vector of retention times associated with a liquid chromatography/mass spectrometry (LC/MS) or gas chromatography/mass spectrometry (GC/MS) data set. *`mzXMLStruct`* includes the following fields:

Field	Description
`scan`	Structure array containing the data pertaining to each individual scan, such as mass spectrometry level, total ion current, polarity, precursor mass (when it applies), and the spectrum data.
`index`	Structure containing indices to the positions of scan elements in the XML document.
`mzXML`	Structure containing: • Information in the root element of the mzXML schema, such as instrument details, experiment details, and preprocessing method • URLs pointing to schemas for the individual scans • Indexing approach • Digital signature calculated for the current instance of the document

`[Peaks, Times] = mzxml2peaks(mzXMLStruct, 'Levels', LevelsValue)` specifies the level(s) of the spectra in *`mzXMLStruct`* to convert, assuming the spectra are from tandem MS data sets. Default is `1`, which converts only the first-level spectra, that is, spectra containing precursor ions. Setting *`LevelsValue`* to `2` converts only the second-level spectra, which are the fragment spectra (created from a precursor ion).

Examples

Note In the following example, the file `results.mzxml` is not provided. Sample mzXML files can be found at:

- Open Proteomics Database
- Peptide Atlas Repository at the Institute for Systems Biology (ISB)
- The Sashimi Project

1. Use the `mzxmlread` function to read an mzXML file into the MATLAB software as structure. Then extract the peak information of only the first-level ions from the structure.

```
mzxml_struct = mzxmlread('results.mzxml');
[peaks,time] = mzxml2peaks(mzxml_struct);
```

2. Create a dot plot of the LC/MS data.

```
msdotplot(peaks,time)
```

See Also

Bioinformatics Toolbox functions: `msdotplot`, `mspalign`, `msppresample`, `mzxmlread`

mzxmlinfo

Purpose

Return information about mzXML file

Syntax

```
InfoStruct = mzxmlinfo(File)
InfoStruct = mzxmlinfo(File, 'NumOfLevels',
NumOfLevelsValue)
```

Arguments

File	String containing a file name, or a path and file name, of an mzXML file that conforms to the mzXML 2.1 specification or earlier specifications. If you specify only a file name, that file must be on the MATLAB search path or in the current directory.
NumOfLevelsValue	Controls the return of `NumOfLevels`, an additional field in *InfoStruct*, that contains the number of mass spectrometry (MS) levels of spectra in *File*. Choices are `true` or `false` (default).

Return Values

InfoStruct	MATLAB structure containing information from an mzXML file. It includes the fields shown in the table below.

Description

InfoStruct = `mzxmlinfo(`*File*`)` returns a MATLAB structure, *InfoStruct*, containing summary information about an mzXML file, *File*.

File is a string containing a file name, or a path and file name, of an mzXML file. The file must conform to the mzXML 2.1 specification or earlier specifications. You can view the mzXML 2.1 specification at:

```
http://sashimi.sourceforge.net/schema_revision/mzXML_2.1/Doc/mzXML_2.1_tutorial.pdf
```

InfoStruct includes the following fields.

Field	Description
`Filename`	Name of the mzXML file.
`FileModDate`	Modification date of the file.
`FileSize`	Size of the file in bytes.
`NumberOfScans`	Number of scans in the file.*
`StartTime`	Run start time.*
`EndTime`	Run end time.*
`DataProcessingIntensityCutoff`	Minimum mass/charge (m/z) intensity value.*
`DataProcessingCentroided`	Indicates if data is centroided.*
`DataProcessingDeisotoped`	Indicates if data is deisotoped.*
`DataProcessing ChargeDeconvoluted`	Indicates if data is deconvoluted.*
`DataProcessingSpotIntegration`	For LC/MALDI experiments, indicates if peaks eluting over multiple spots have been integrated into a single spot.*

***** — These fields contain `N/A` if the mzXML file does not include the associated attributes. The associated attributes are optional in the mzXML file, per the mzXML 2.1 specification.

`InfoStruct` `= mzxmlinfo(`*`File`*`, 'NumOfLevels',` *`NumOfLevelsValue`*`)` controls the return of `NumOfLevels`, an additional field in *`mzXMLInfo`*, that contains the number of mass spectrometry levels of spectra in *`File`*. Choices are `true` or `false` (default).

Examples

Note In the following example, the file `results.mzxml` is not provided. Sample mzXML files can be found at:

- Open Proteomics Database
- Peptide Atlas Repository at the Institute for Systems Biology (ISB)
- The Sashimi Project

Return a MATLAB structure containing summary information about an mzXML file.

```
info = mzxmlinfo('results.mzxml');

info =

                            Filename: 'results.mzxml'
                         FileModDate: '07-May-2008 13:39:12'
                            FileSize: 10607
                       NumberOfScans: 2
                           StartTime: 'PT0.00683333S'
                             EndTime: 'PT200.036S'
      DataProcessingIntensityCutoff: 'N/A'
           DataProcessingCentroided: 'false'
           DataProcessingDeisotoped: 'N/A'
   DataProcessingChargeDeconvoluted: 'N/A'
      DataProcessingSpotIntegration: 'N/A'
```

Return a MATLAB structure containing summary information, including the number of mass spectrometry levels, about an mzXML file.

```
info = mzxmlinfo('results.mzxml','numoflevels',true);

info =

                            Filename: 'results.mzxml'
```

```
                                FileModDate: '07-May-2008 13:39:12'
                                   FileSize: 10607
                                NumberOfScans: 2
                                    StartTime: 'PT0.00683333S'
                                      EndTime: 'PT200.036S'
                DataProcessingIntensityCutoff: 'N/A'
                     DataProcessingCentroided: 'false'
                     DataProcessingDeisotoped: 'N/A'
            DataProcessingChargeDeconvoluted: 'N/A'
               DataProcessingSpotIntegration: 'N/A'
                             NumberOfMSLevels: 2
```

See Also

Bioinformatics Toolbox function: `mzxmlread`

Purpose

Read data from mzXML file

Syntax

```
mzXMLStruct = mzxmlread(File)
mzXMLStruct = mzxmlread(File, ...'Levels',
LevelsValue, ...)
mzXMLStruct = mzxmlread(File, ...'TimeRange',
TimeRangeValue,
   ...)
mzXMLStruct = mzxmlread(File, ...'ScanIndices',
   ScanIndicesValue, ...)
mzXMLStruct = mzxmlread(File, ...'Verbose', VerboseValue,
   ...)
```

Arguments

File	String containing a file name, or a path and file name, of an mzXML file that conforms to the mzXML 2.1 specification or earlier specifications. If you specify only a file name, that file must be on the MATLAB search path or in the current directory.
LevelsValue	Positive integer or vector of integers specifying the level(s) of spectra in *File* to read. Default is to read all levels of spectra.

Tip For summary information about the levels of spectra in an mzXML file, use the `mzxmlinfo` function.

Note If you specify a *LevelsValue*, you cannot specify *TimeRangeValue* or *ScanIndicesValue*.

TimeRangeValue Two-element numeric array `[Start End]` that specifies the range of time in *`File`* to read. `Start` is a scalar between the startTime and endTime attributes of the msRun element in *`File`*. `End` is a scalar between `Start` and the endTime attribute of the msRun element in *`File`*. Default is to read spectra from all times.

Tip For summary information about the time ranges in an mzXML file, use the `mzxmlinfo` function.

Note If you specify a *`TimeRangeValue`*, you cannot specify *`LevelsValue`* or *`ScanIndicesValue`*.

ScanIndicesValue Positive integer, vector of integers, or a two-element numeric array `[Start_Ind End_Ind]` that specifies a scan, multiple scans, or a range of scans in *`File`* to read. `Start_Ind` and `End_Ind` are each positive integers indicating a scan number in the num attribute of the msRun element in *`File`*. `Start_Ind` must be less than `End_Ind`. Default is to read all scans.

Tip For summary information about the scan indices in an mzXML file, use the `mzxmlinfo` function.

Note If you specify a *ScanIndicesValue*, you cannot specify *LevelsValue* or *TimeRangeValue*.

VerboseValue Controls the display of the progress of the reading of *File*. Choices are `true` (default) or `false`.

Return Values

mzXMLStruct MATLAB structure containing information from an mzXML file. It includes the fields shown in the table below.

Description

mzXMLStruct = `mzxmlread(`*File*`)` reads an mzXML file, *File*, and then creates a MATLAB structure, *mzXMLStruct*.

File is a string containing a file name, or a path and file name, of an mzXML file. The file must conform to the mzXML 2.1 specification or earlier specifications. You can view the mzXML 2.1 specification at:

```
http://sashimi.sourceforge.net/schema_revision/mzXML_2.1/Doc/mzXML_2.1_tutorial.pdf
```

mzXMLStruct includes the following fields.

Field	Description
`scan`	Structure array containing the data pertaining to each individual scan, such as mass spectrometry level, total ion current, polarity, precursor mass (when it applies), and the spectrum data.

Field	Description
index	Structure containing indices to the positions of scan elements in the XML document.
mzXML	Structure containing: • Information in the root element of the mzXML schema, such as instrument details, experiment details, and preprocessing method • URLs pointing to schemas for the individual scans • Indexing approach • Digital signature calculated for the current instance of the document

Tip LC/MS data analysis requires extended amounts of memory from the operating system.

- If you receive errors related to memory, try the following:
  - Increase the virtual memory (swap space) for your operating system (with a recommended initial size of 3,069 and a maximum size of 16,368) as described at:

    `http://www.mathworks.com/support/tech-notes/1100/1106.html#6`

  - Set the 3 GB switch (32-bit Windows XP only) as described at:

    `http://www.mathworks.com/support/tech-notes/1100/1107.html`

- If you receive errors related to Java heap space, increase your Java heap space as described at:

  `http://www.mathworks.com/support/solutions/data/1-18I2C.html`

mzXMLStruct = mzxmlread(*File*, ...'*PropertyName*', *PropertyValue*, ...) calls mzxmlread with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

mzXMLStruct = mzxmlread(*File*, ...'Levels', *LevelsValue*, ...) specifies the level(s) of spectra in *File* to read. *LevelsValue* is a positive integer or vector of integers. Default is to read all levels of spectra.

Tip For summary information about the levels of spectra in an mzXML file, use the mzxmlinfo function.

Note If you specify a *LevelsValue*, you cannot specify *TimeRangeValue* or *ScanIndicesValue*.

---

mzXMLStruct = mzxmlread(*File*, ...'TimeRange', *TimeRangeValue*, ...) specifies the range of time in *File* to read. *TimeRangeValue* is two-element numeric array [Start End]. Start is a scalar between the startTime and endTime attributes of the msRun element in *File*. End is a scalar between Start and the endTime attribute of the msRun element in *File*. Default is to read spectra from all times.

Tip For summary information about the time ranges in an mzXML file, use the mzxmlinfo function.

Note If you specify a *TimeRangeValue*, you cannot specify *LevelsValue* or *ScanIndicesValue*.

mzXMLStruct = mzxmlread(*File*, ...'ScanIndices', *ScanIndicesValue*, ...) specifies a scan, multiple scans, or range of scans in *File* to read. *ScanIndicesValue* is a positive integer, vector of integers, or a two-element numeric array [Start_Ind End_Ind]. Start_Ind and End_Ind are each positive integers indicating a scan number in the num attribute of the msRun element in *File*. Start_Ind must be less than End_Ind. Default is to read all scan.

Tip For summary information about the scan indices in an mzXML file, use the mzxmlinfo function.

Note If you specify a *ScanIndicesValue*, you cannot specify *LevelsValue* or *TimeRangeValue*.

mzXMLStruct = mzxmlread(*File*, ...'Verbose', *VerboseValue*, ...) controls the display of the progress of the reading of *File*. Choices are true (default) or false.

Examples

Note In the following example, the file results.mzxml is not provided. Sample mzXML files can be found at:

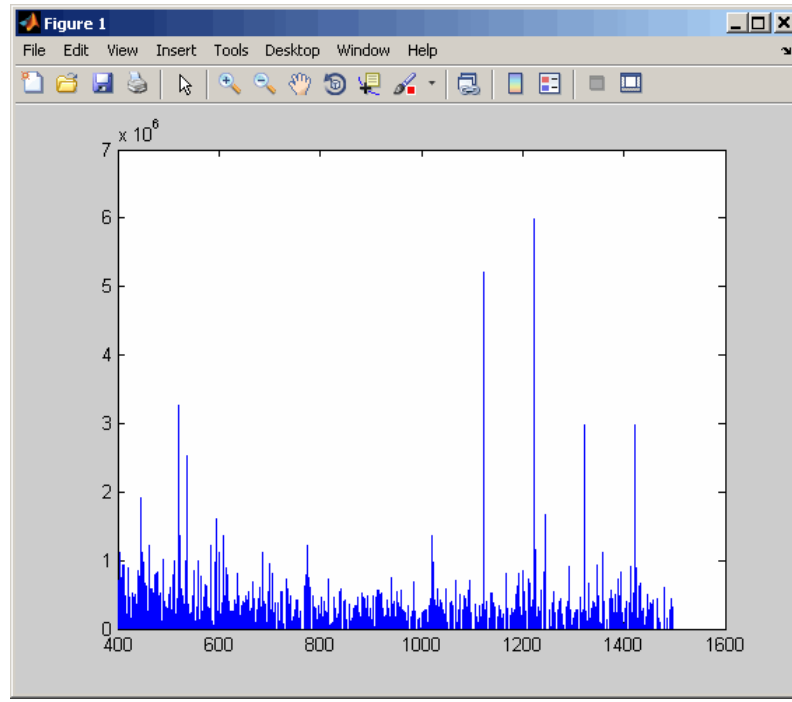
- Open Proteomics Database
- Peptide Atlas Repository at the Institute for Systems Biology (ISB)
- The Sashimi Project

1. Read an mzXML file into the MATLAB software as a structure.

```
out = mzxmlread('results.mzxml')

out =

    mzXML: [1x1 struct]
    index: [1x1 struct]
     scan: [2000x1 struct]
```

2. View the first scan in the mzXML file by creating separate variables containing the mass and charge values respectively, and then plotting these values.

```
m = out.scan(1).peaks.mz(1:2:end);
z = out.scan(1).peaks.mz(2:2:end);
stem(m,z,'marker','none')
```



See Also

Bioinformatics Toolbox functions: `jcampread`, `mzcdfread`, `mzxml2peaks`, `mzxmlinfo`, `tgspcread`

MATLAB function: `xmlread`

ndims (DataMatrix)

Purpose

Return number of dimensions in DataMatrix object

Syntax

```
N = ndims(DMObj)
```

Arguments

DMObj	DataMatrix object, such as created by `DataMatrix` (object constructor).

Return Values

N	Positive integer representing the number of dimensions in *DMObj*. The number of dimensions in a DataMatrix object is always `2`.

Description

`N = ndims(DMObj)` returns the number of dimensions in *DMObj*, a DataMatrix object. The number of dimensions in a DataMatrix object is always `2`.

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Purpose

Test DataMatrix objects for inequality

Syntax

```
T = ne(DMObj1, DMObj2)
T = DMObj1 ~= DMObj2
T = ne(DMObj1, B)
T = DMObj1 ~= B
T = ne(B, DMObj1)
T = B ~= DMObj1
```

Arguments

DMObj1, *DMObj2*	DataMatrix objects, such as created by `DataMatrix` (object constructor).
B	MATLAB numeric or logical array.

Return Values

T	Logical matrix of the same size as *DMObj1* and *DMObj2* or *DMObj1* and *B*. It contains logical `1` (true) where elements in the first input are not equal to the corresponding element in the second input, and logical `0` (false) when they are equal.

Description

T = `ne(`*DMObj1*`, `*DMObj2*`)` or the equivalent *T* = *DMObj1* `~=` *DMObj2* compares each element in DataMatrix object *DMObj1* to the corresponding element in DataMatrix object *DMObj2*, and returns *T*, a logical matrix of the same size as *DMObj1* and *DMObj2*, containing logical `1` (true) where elements in *DMObj1* are not equal to the corresponding element in *DMObj2*, and logical `0` (false) when they are equal. *DMObj1* and *DMObj2* must have the same size (number of rows and columns), unless one is a scalar (1-by-1 DataMatrix object). *DMObj1* and *DMObj2* can have different `Name` properties.

T = `ne(`*DMObj1*`, `*B*`)` or the equivalent *T* = *DMObj1* `~=` *B* compares each element in DataMatrix object *DMObj1* to the corresponding element in *B*, a numeric or logical array, and returns *T*, a logical matrix of the same size as *DMObj1* and *B*, containing logical `1` (true) where elements

in *DMObj1* are not equal to the corresponding element in *B*, and logical 0 (false) when they are equal. *DMObj1* and *B* must have the same size (number of rows and columns), unless one is a scalar.

T = ne(*B*, *DMObj1*) or the equivalent *T* = *B* ~= *DMObj1* compares each element in *B*, a numeric or logical array, to the corresponding element in DataMatrix object *DMObj1*, and returns *T*, a logical matrix of the same size as *B* and *DMObj1*, containing logical 1 (true) where elements in *B* are not equal to the corresponding element in *DMObj1*, and logical 0 (false) when they are equal. *B* and *DMObj1* must have the same size (number of rows and columns), unless one is a scalar.

MATLAB calls *T* = ne(*X*, *Y*) for the syntax *T* = *X* ~= *Y* when *X* or *Y* is a DataMatrix object.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: eq

Purpose

Count n-mers in nucleotide or amino acid sequence

Syntax

```
Nmer = nmercount(Seq, Length)
Nmer = nmercount(Seq, Length, C)
```

Arguments

Seq	One of the following: • String of codes specifying a nucleotide sequence or amino acid sequence. For valid letter codes, see the table Mapping Nucleotide Letter Codes to Integers on page 3-1121 or the table Mapping Amino Acid Letter Codes to Integers on page 3-2. • MATLAB structure containing a `Sequence` field that contains a nucleotide sequence or an amino acid sequence, such as returned by `fastaread`, `fastqread`, `emblread`, `getembl`, `genbankread`, `getgenbank`, `getgenpept`, `genpeptread`, `getpdb`, or `pdbread`.
Length	Integer specifying the length of n-mer to count.

Return Values

Nmer	Cell array containing the n-mer counts in *Seq*.

Description

Nmer = `nmercount(`*Seq*`, `*Length*`)` counts the n-mers or patterns of a specific length in *Seq*, a nucleotide sequence or amino acid sequence, and returns the n-mer counts in a cell array.

Nmer = `nmercount(`*Seq*`, `*Length*`, `*C*`)` returns only the n-mers with cardinality of at least *C*.

Examples

1 Use the `getgenpept` function to retrieve the amino acid sequence for the human insulin receptor.

```
S = getgenpept('AAA59174','SequenceOnly',true);
```

2 Count the number of four-mers in the amino acid sequence and display the first 20 rows in the cell array.

```
nmers = nmercount(S,4);
nmers(1:20,:)

ans =
    'APES'    [2]
    'DFRD'    [2]
    'ESLK'    [2]
    'FRDL'    [2]
    'GNYS'    [2]
    'LKEL'    [2]
    'SHCQ'    [2]
    'SLKD'    [2]
    'SVRI'    [2]
    'TDYL'    [2]
    'TSLA'    [2]
    'TVIN'    [2]
    'VING'    [2]
    'VPLD'    [2]
    'YALV'    [2]
    'AAAA'    [1]
    'AAAP'    [1]
    'AAEI'    [1]
    'AAEL'    [1]
    'AAFP'    [1]
```

See Also

Bioinformatics Toolbox functions: `aacount`, `basecount`, `codoncount`, `dimercount`

Purpose

Convert nucleotide sequence to amino acid sequence

Syntax

```
SeqAA = nt2aa(SeqNT)
SeqAA = nt2aa(..., 'Frame', FrameValue, ...)
SeqAA = nt2aa(..., 'GeneticCode', GeneticCodeValue, ...)
SeqAA = nt2aa(..., 'AlternativeStartCodons',
   AlternativeStartCodonsValue, ...)
SeqAA = nt2aa(..., 'ACGTOnly', ACGTOnlyValue, ...)
```

Arguments

SeqNT

One of the following:

- String of single-letter codes specifying a nucleotide sequence. For valid letter codes, see the table Mapping Nucleotide Letter Codes to Integers on page 3-1121.
- Row vector of integers specifying a nucleotide sequence. For valid integers, see the table Mapping Nucleotide Integers to Letter Codes on page 3-809.
- MATLAB structure containing a `Sequence` field that contains a nucleotide sequence, such as returned by `fastaread`, `fastqread`, `emblread`, `getembl`, `genbankread`, or `getgenbank`

Note Hyphens are valid only if the codon to which it belongs represents a gap, that is, the codon contains all hyphens. Example: `ACT---TGA`

Tip Do not use a sequence with hyphens if you specify `'all'` for *`FrameValue`*.

`FrameValue`

Integer or string specifying a reading frame in the nucleotide sequence. Choices are `1`, `2`, `3`, or `'all'`. Default is `1`.

If *`FrameValue`* is `'all'`, then *`SeqAA`* is a 3-by-1 cell array.

`GeneticCodeValue`

Integer or string specifying a genetic code number or code name from the table Genetic Code on page 3-1114. Default is `1` or `'Standard'`.

Tip If you use a code name, you can truncate the name to the first two letters of the name.

`AlternativeStartCodonsValue`

Controls the translation of alternative codons. Choices are `true` (default) or `false`.

`ACGTOnlyValue`

Controls the behavior of ambiguous nucleotide characters (`R`, `Y`, `K`, `M`, `S`, `W`, `B`, `D`, `H`, `V`, and `N`) and unknown characters. *`ACGTOnlyValue`* can be `true` (default) or `false`.

- If `true`, then the function errors if any of these characters are present.
- If `false`, then the function tries to resolve ambiguities. If it cannot, it returns `X` for the affected codon.

Return Values

SeqAA	Amino acid sequence specified by a string of single-letter codes.

Description

SeqAA = nt2aa(*SeqNT*) converts a nucleotide sequence, specified by *SeqNT*, to an amino acid sequence, returned in *SeqAA*, using the standard genetic code.

SeqAA = nt2aa(*SeqNT*, ...'*PropertyName*', *PropertyValue*, ...) calls nt2aa with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

SeqAA = nt2aa(..., 'Frame', *FrameValue*, ...) converts a nucleotide sequence for a specific reading frame to an amino acid sequence. Choices are 1, 2, 3, or 'all'. Default is 1. If *FrameValue* is 'all', then output *SeqAA* is a 3-by-1 cell array.

SeqAA = nt2aa(..., 'GeneticCode', *GeneticCodeValue*, ...) specifies a genetic code to use when converting a nucleotide sequence to an amino acid sequence. *GeneticCodeValue* can be an integer or string specifying a code number or code name from the table Genetic Code on page 3-1114. Default is 1 or 'Standard'. The amino acid to nucleotide codon mapping for the Standard genetic code is shown in the table Standard Genetic Code on page 3-1115.

Tip If you use a code name, you can truncate the name to the first two letters of the name.

SeqAA = nt2aa(..., 'AlternativeStartCodons', *AlternativeStartCodonsValue*, ...) controls the translation of alternative start codons. By default, *AlternativeStartCodonsValue* is set to true, and if the first codon of a sequence is a known alternative start codon, the codon is translated to methionine.

If this option is set to `false`, then an alternative start codon at the start of a sequence is translated to its corresponding amino acid in the genetic code that you specify, which might not necessarily be methionine. For example, in the human mitochondrial genetic code, `AUA` and `AUU` are known to be alternative start codons.

For more information about alternative start codons, see:

```
www.ncbi.nlm.nih.gov/Taxonomy/Utils/wprintgc.cgi?mode=t#SG1
```

Genetic Code

Code Number	Code Name
1	`Standard`
2	`Vertebrate Mitochondrial`
3	`Yeast Mitochondrial`
4	`Mold`, `Protozoan`, `Coelenterate Mitochondrial`, and `Mycoplasma/Spiroplasma`
5	`Invertebrate Mitochondrial`
6	`Ciliate`, `Dasycladacean`, and `Hexamita Nuclear`
9	`Echinoderm Mitochondrial`
10	`Euplotid Nuclear`
11	`Bacterial` and `Plant Plastid`
12	`Alternative Yeast Nuclear`
13	`Ascidian Mitochondrial`
14	`Flatworm Mitochondrial`
15	`Blepharisma Nuclear`
16	`Chlorophycean Mitochondrial`
21	`Trematode Mitochondrial`

Genetic Code (Continued)

Code Number	Code Name
22	Scenedesmus Obliquus Mitochondrial
23	Thraustochytrium Mitochondrial

Standard Genetic Code

Amino Acid Name	Amino Acid Code	Nucleotide Codon
Alanine	A	GCT GCC GCA GCG
Arginine	R	CGT CGC CGA CGG AGA AGG
Asparagine	N	ATT AAC
Aspartic acid (Aspartate)	D	GAT GAC
Cysteine	C	TGT TGC
Glutamine	Q	CAA CAG
Glutamic acid (Glutamate)	E	GAA GAG
Glycine	G	GGT GGC GGA GGG
Histidine	H	CAT CAC
Isoleucine	I	ATT ATC ATA
Leucine	L	TTA TTG CTT CTC CTA CTG
Lysine	K	AAA AAG
Methionine	M	ATG
Phenylalanine	F	TTT TTC
Proline	P	CCT CCC CCA CCG

Standard Genetic Code (Continued)

Amino Acid Name	Amino Acid Code	Nucleotide Codon
Serine	S	TCT TCC TCA TCG AGT AGC
Threonine	T	ACT ACC ACA ACG
Tryptophan	W	TGG
Tyrosine	Y	TAT, TAC
Valine	V	GTT GTC GTA GTG
Asparagine or Aspartic acid (Aspartate)	B	Random codon from D and N
Glutamine or Glutamic acid (Glutamate)	Z	Random codon from E and Q
Unknown amino acid (any amino acid)	X	Random codon
Translation stop	*	TAA TAG TGA
Gap of indeterminate length	-	---
Unknown character (any character or symbol not in table)	?	???

SeqAA = nt2aa(..., 'ACGTOnly', *ACGTOnlyValue*, ...) controls the behavior of ambiguous nucleotide characters (R, Y, K, M, S, W, B, D, H, V, and N) and unknown characters. *ACGTOnlyValue* can be true (default) or false. If true, then the function errors if any of these

characters are present. If `false`, then the function tries to resolve ambiguities. If it cannot, it returns `X` for the affected codon.

Examples

Converting the ND1 Gene

1. Use the `getgenbank` function to retrieve the nucleotide sequence for the human mitochondrion from the GenBank database.

```
mitochondria = getgenbank('NC_001807', 'SequenceOnly', true);
```

2. Extract the sequence for the ND1 gene from the nucleotide sequence.

```
ND1gene = mitochondria (3308:4261);
```

3. Convert the ND1 gene on the human mitochondria genome to an amino acid sequence using the Vertebrate Mitochondrial genetic code.

```
protein1 = nt2aa(ND1gene,'GeneticCode', 2);
```

4. Use the `getgenpept` function to retrieve the same amino acid sequence from the GenPept database.

```
protein2 = getgenpept('NP_536843', 'SequenceOnly', true);
```

5. Use the `isequal` function to compare the two amino acid sequences.

```
isequal (protein1, protein2)

ans =

     1
```

Converting the ND2 Gene

1. Use the `getgenbank` function to retrieve the nucleotide sequence for the human mitochondrion from the GenBank database.

```
mitochondria = getgenbank('NC_001807', 'SequenceOnly', true);
```

2 Extract the sequence for the ND2 gene from the nucleotide sequence.

```
ND2gene = mitochondria (4471:5511);
```

3 Convert the ND2 gene on the human mitochondria genome to an amino acid sequence using the Vertebrate Mitochondrial genetic code.

```
protein1 = nt2aa(ND2gene,'GeneticCode', 2);
```

Note In the `ND2gene` nucleotide sequence, the first codon is `ATT`, which is translated to `M`, while the subsequent `ATT` codons are translated to `I`. If you set `'AlternativeStartCodons'` to `false`, then the first `ATT` codon is translated to `I`, the corresponding amino acid in the Vertebrate Mitochondrial genetic code.

---

4 Use the `getgenpept` function to retrieve the same amino acid sequence from the GenPept database.

```
protein2 = getgenpept('NP_536844', 'SequenceOnly', true);
```

5 Use the `isequal` function to compare the two amino acid sequences.

```
isequal (protein1, protein2)

ans =

     1
```

Converting a Sequence with Ambiguous Characters

If you have a sequence with ambiguous or unknown nucleotide characters, you can set the `'ACGTOnly'` property to `false` to have the `nt2aa` function try to resolve them:

```
nt2aa('agttgccgacgcgcncar','ACGTOnly', false)
```

```
ans =

SCRRAQ
```

See Also

Bioinformatics Toolbox functions: `aa2nt`, `aminolookup`, `baselookup`, `codonbias`, `dnds`, `dndsml`, `geneticcode`, `isotopicdist`, `revgeneticcode`, `seqtool`

nt2int

Purpose

Convert nucleotide sequence from letter to integer representation

Syntax

```
SeqInt = nt2int(SeqChar)
SeqInt = nt2int(SeqChar, ...'Unknown', UnknownValue, ...)
SeqInt = nt2int(SeqChar, ...'ACGTOnly', ACGTOnlyValue, ...)
```

Arguments

SeqChar	One of the following: • String of codes specifying a nucleotide sequence. For valid letter codes, see the table Mapping Nucleotide Letter Codes to Integers on page 3-1121. Integers are arbitrarily assigned to IUB/IUPAC letters. • MATLAB structure containing a `Sequence` field that contains a nucleotide sequence, such as returned by `fastaread`, `fastqread`, `emblread`, `getembl`, `genbankread`, or `getgenbank`.
UnknownValue	Integer to represent unknown nucleotides. Choices are integers ≥ `0` and ≤ `255`. Default is `0`.
ACGTOnlyValue	Controls the prohibition of ambiguous nucleotides. Choices are `true` or `false` (default). If *ACGTOnlyValue* is `true`, you can enter only the characters `A`, `C`, `G`, `T`, and `U`.

Return Values

SeqInt	Nucleotide sequence specified by a row vector of integers.

Description

SeqInt = `nt2int(`*SeqChar*`)` converts *SeqChar*, a string of codes specifying a nucleotide sequence, to *SeqInt*, a row vector of integers specifying the same nucleotide sequence. For valid codes, see the

table Mapping Nucleotide Letter Codes to Integers on page 3-1121. Unknown characters (characters not in the table) are mapped to `0`. Gaps represented with hyphens are mapped to `16`.

`SeqInt` `= nt2int(`*`SeqChar`*`, ...'`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `nt2int` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`SeqInt` `= nt2int(`*`SeqChar`*`, ...'Unknown', `*`UnknownValue`*`, ...)` specifies an integer to represent unknown nucleotides. *`UnknownValue`* can be an integer ≥ `0` and ≤ `255`. Default is `0`.

`SeqInt` `= nt2int(`*`SeqChar`*`, ...'ACGTOnly', `*`ACGTOnlyValue`*`, ...)` controls the prohibition of ambiguous nucleotides (`N`, `R`, `Y`, `K`, `M`, `S`, `W`, `B`, `D`, `H`, and `V`). Choices are `true` or `false` (default). If *`ACGTOnlyValue`* is `true`, you can enter only the characters `A`, `C`, `G`, `T`, and `U`.

Mapping Nucleotide Letter Codes to Integers

Nucleotide	Code	Integer
Adenosine	A	1
Cytidine	C	2
Guanine	G	3
Thymidine	T	4
Uridine (if `'Alphabet'` set to `'RNA'`)	U	4
Purine (`A` or `G`)	R	5
Pyrimidine (`T` or `C`)	Y	6
Keto (`G` or `T`)	K	7
Amino (`A` or `C`)	M	8
Strong interaction (3 H bonds) (`G` or `C`)	S	9

Mapping Nucleotide Letter Codes to Integers (Continued)

Nucleotide	Code	Integer
Weak interaction (2 H bonds) (A or T)	W	10
Not A (C or G or T)	B	11
Not C (A or G or T)	D	12
Not G (A or C or T)	H	13
Not T or U (A or C or G)	V	14
Any nucleotide (A or C or G or T or U)	N	15
Gap of indeterminate length	-	16
Unknown (any character not in table)	*	0 (default)

Examples

Converting a Simple Sequence

Convert a nucleotide sequence from letters to integers.

```
s = nt2int('ACTGCTAGC')

s =
     1     2     4     3     2     4     1     3     2
```

Converting a Random Sequence

1. Create a random character string to represent a nucleotide sequence.

   ```
   SeqChar = randseq(20)

   SeqChar =

   TTATGACGTTATTCTACTTT
   ```

2. Convert the nucleotide sequence from letter to integer representation.

   ```
   SeqInt = nt2int(SeqChar)
   ```

```
SeqInt =

  Columns 1 through 13
     4     4     1     4     3     1     2     3     4     4     1     4

  Columns 14 through 20
     2     4     1     2     4     4     4
```

See Also

Bioinformatics Toolbox functions: `aa2int`, `baselookup`, `int2aa`, `int2nt`

ntdensity

Purpose

Plot density of nucleotides along sequence

Syntax

```
ntdensity(SeqNT)
Density = ntdensity(SeqNT)
... = ntdensity(..., 'Window', WindowValue, ...)
[Density, HighCG] = ntdensity(..., 'CGThreshold',
   CGThresholdValue, ...)
```

Arguments

SeqNT

One of the following:

- String of codes specifying a nucleotide sequence. For valid letter codes, see the table Mapping Nucleotide Letter Codes to Integers on page 3-1121.
- Row vector of integers specifying a nucleotide sequence. For valid integers, see the table Mapping Nucleotide Integers to Letter Codes on page 3-809.
- MATLAB structure containing a `Sequence` field that contains a nucleotide sequence, such as returned by `emblread`, `fastaread`, `fastqread`, `genbankread`, `getembl`, or `getgenbank`.

Note Although you can submit a sequence with nucleotides other than A, C, G, and T, ntdensity plots only A, C, G, and T.

WindowValue	Value that specifies the window length for the density calculation. Default is length(*SeqNT*)/20.
CGThresholdValue	Controls the return of indices for regions where the CG content of *SeqNT* is greater than *CGThresholdValue*. Default is 5.

Description

ntdensity(*SeqNT*) plots the density of nucleotides A, C, G, and T in sequence *SeqNT*.

Density = ntdensity(*SeqNT*) returns a MATLAB structure with the density of nucleotides A, C, G, and T.

... = ntdensity(*SeqNT*, ...'*PropertyName*', *PropertyValue*, ...) calls ntdensity with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

... = ntdensity(..., 'Window', *WindowValue*, ...) uses a window of length *WindowValue* for the density calculation. Default *WindowValue* is length(*SeqNT*)/20.

[*Density*, *HighCG*] = ntdensity(..., 'CGThreshold', *CGThresholdValue*, ...) returns indices for regions where the CG content of *SeqNT* is greater than *CGThresholdValue*. Default *CGThresholdValue* is 5.

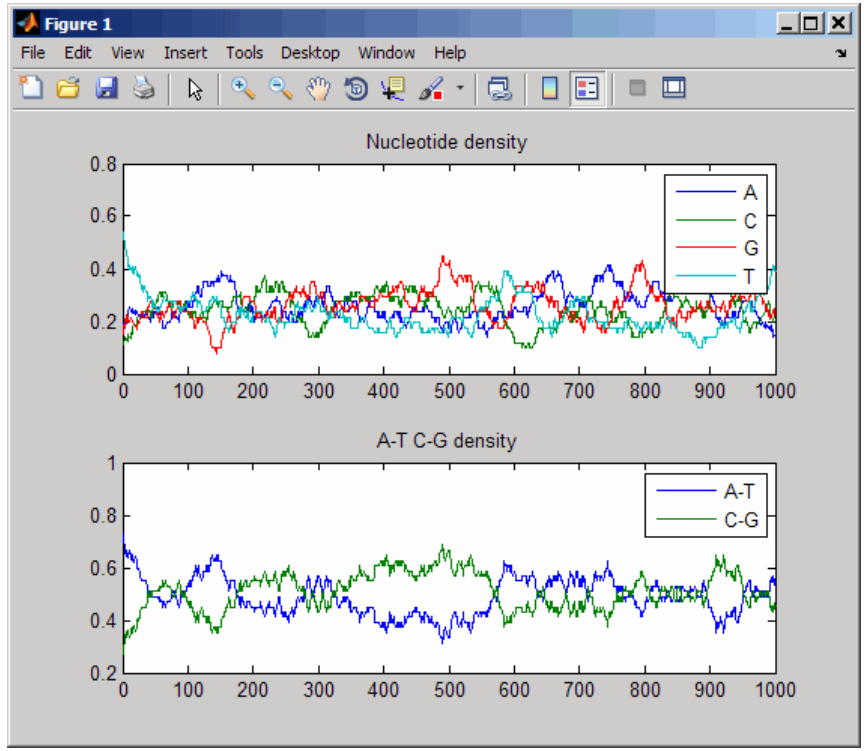
Examples

1 Create a random character string to represent a nucleotide sequence.

```
s = randseq(1000, 'alphabet', 'dna');
```

2 Plot the density of nucleotides along the sequence.

```
ntdensity(s)
```



See Also

Bioinformatics Toolbox functions: `basecount`, `codoncount`, `cpgisland`, `dimercount`

MATLAB function: `filter`

Purpose

Return NUC44 scoring matrix for nucleotide sequences

Syntax

```
ScoringMatrix = nuc44
[ScoringMatrix, MatrixInfo] = nuc44
```

Description

`ScoringMatrix = nuc44` returns the scoring matrix. The `nuc44` scoring matrix uses ambiguous nucleotide codes and probabilities rounded to the nearest integer.

Scale = `0.277316`

Expected score = `-1.7495024`, Entropy = `0.5164710` bits

Lowest score = `-4`, Highest score = `5`

Order: `A C G T R Y K M S W B D H V N`

`[ScoringMatrix, MatrixInfo] = nuc44` returns a structure with information about the matrix with fields `Name` and `Order`.

See Also

Bioinformatics Toolbox functions: `blosum`, `dayhoff`, `gonnet`, `localalign`, `nwalign`, `pam` ,`swalign`

num2goid

Purpose

Convert numbers to Gene Ontology IDs

Syntax

```
GOIDs = num2goid(X)
```

Description

`GOIDs = num2goid(X)` converts the numbers in `X` to strings with Gene Ontology IDs. IDs are a 7-digit number preceded by the prefix `GO:`, which is the standard used by the Gene Ontology database.

Examples

Get the Gene Ontology IDs of the following numbers.

```
t = [5575 5622 5623 5737 5840 30529 43226 43228 ...
     43229 43232 43234];
ids = num2goid(t)
```

See Also

Bioinformatics Toolbox functions: `geneont.geneont` (object constructor), `goannotread`

Bioinformatics Toolbox class: `geneont`

Bioinformatics Toolbox methods of geneont object: `geneont.getancestors`, `geneont.getdescendants`, `geneont.getmatrix`, `geneont.getrelatives`

Purpose

Return number of elements in DataMatrix object

Syntax

```
N = numel(DMObj)
Ns = numel(DMObj, Index1, Index2)
```

Arguments

DMObj	DataMatrix object, such as created by `DataMatrix` (object constructor).
Index1	A row or range of rows in *DMObj* specified by a positive integer or a range using the format `x:y`, where `x` is the first row and `y` is the last row.
Index2	A column or range of columns in *DMObj* specified by a positive integer or a range using the format `x:y`, where `x` is the first column and `y` is the last column.

Return Values

N	Positive integer representing the number of elements in *DMObj*, a DataMatrix object.
Ns	Positive integer representing the number of subscripted elements in *DMObj*, a DataMatrix object.

Description

`N = numel(DMObj)` returns `1`. To find the number of elements in *DMObj*, a DataMatrix object, use either of the following syntaxes:

```
prod(size(DMObj))
numel(DMObj,':',':')
```

`Ns = numel(DMObj, Index1, Index2)` returns the number of subscripted elements in *DMObj*, a DataMatrix object. *Index1* specifies a row or range of rows in *DMObj*. *Index2* specifies a column or range of columns in *DMObj*.

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

numel (DataMatrix)

Bioinformatics Toolbox object: DataMatrix object

Purpose

Globally align two sequences using Needleman-Wunsch algorithm

Syntax

```
Score = nwalign(Seq1,Seq2)
[Score, Alignment] = nwalign(Seq1,Seq2)
[Score, Alignment, Start] = nwalign(Seq1,Seq2)
... = nwalign(Seq1,Seq2, ...'Alphabet', AlphabetValue, ...)
... = nwalign(Seq1,Seq2, ...'ScoringMatrix',
    ScoringMatrixValue, ...)
... = nwalign(Seq1,Seq2, ...'Scale', ScaleValue, ...)
... = nwalign(Seq1,Seq2, ...'GapOpen', GapOpenValue, ...)
... = nwalign(Seq1,Seq2, ...'ExtendGap',
ExtendGapValue, ...)
... = nwalign(Seq1,Seq2, ...'Showscore',
ShowscoreValue, ...)
```

Arguments

Seq1, *Seq2*

Amino acid or nucleotide sequences. Enter any of the following:

- Character string of letters representing amino acids or nucleotides, such as returned by `int2aa` or `int2nt`
- Vector of integers representing amino acids or nucleotides, such as returned by `aa2int` or `nt2int`
- Structure containing a `Sequence` field

Tip For help with letter and integer representations of amino acids and nucleotides, see Amino Acid Lookup on page 3-111 or Nucleotide Lookup on page 3-122.

AlphabetValue

String specifying the type of sequence. Choices are `'AA'` (default) or `'NT'`.

ScoringMatrixValue Either of the following:

- String specifying the scoring matrix to use for the global alignment. Choices for amino acid sequences are:
  - `'BLOSUM62'`
  - `'BLOSUM30'` increasing by `5` up to `'BLOSUM90'`
  - `'BLOSUM100'`
  - `'PAM10'` increasing by `10` up to `'PAM500'`
  - `'DAYHOFF'`
  - `'GONNET'`

  Default is:
  - `'BLOSUM50'` — When *`AlphabetValue`* equals `'AA'`
  - `'NUC44'` — When *`AlphabetValue`* equals `'NT'`

  Note The above scoring matrices, provided with the software, also include a structure containing a scale factor that converts the units of the output score to bits. You can also use the `'Scale'` property to specify an additional scale factor to convert the output score from bits to another unit.

- Matrix representing the scoring matrix to use for the global alignment, such as returned by the `blosum`, `pam`, `dayhoff`, `gonnet`, or `nuc44` function.

Note If you use a scoring matrix that you created or was created by one of the above functions, the matrix does not include a scale factor. The output score will be returned in the same units as the scoring matrix. You can use the `'Scale'` property to specify a scale factor to convert the output score to another unit.

`ScaleValue`

Positive value that specifies a scale factor that is applied to the output score.

For example, if the output score is initially determined in bits, and you enter `log(2)` for *`ScaleValue`*, then `nwalign` returns *`Score`* in nats.

Default is `1`, which does not change the units of the output score.

Note If the `'ScoringMatrix'` property also specifies a scale factor, then `nwalign` uses it first to scale the output score, then applies the scale factor specified by *`ScaleValue`* to rescale the output score.

Tip Before comparing alignment scores from multiple alignments, ensure the scores are in the same units. You can use the `'Scale'` property to control the units of the output scores.

GapOpenValue	Positive value specifying the penalty for opening a gap in the alignment. Default is 8.
ExtendGapValue	Positive value specifying the penalty for extending a gap. Default is equal to *GapOpenValue*.
ShowscoreValue	Controls the display of the scoring space and the winning path of the alignment. Choices are true or false (default).

Return Values

Score	Optimal global alignment score in bits.
Alignment	3-by-N character array showing the two sequences, *Seq1* and *Seq2*, in the first and third rows, and symbols representing the optimal global alignment for them in the second row.
Start	2-by-1 vector of indices indicating the starting point in each sequence for the alignment. Because this is a global alignment, *Start* is always [1;1].

Description

Score = nwalign(*Seq1*,*Seq2*) returns the optimal global alignment score in bits. The scale factor used to calculate the score is provided by the scoring matrix.

[*Score*, *Alignment*] = nwalign(*Seq1*,*Seq2*) returns a 3-by-N character array showing the two sequences, *Seq1* and *Seq2*, in the first and third rows, and symbols representing the optimal global alignment for them in the second row. The symbol | indicates amino acids or nucleotides that match exactly. The symbol : indicates amino acids or nucleotides that are related as defined by the scoring matrix (nonmatches with a zero or positive scoring matrix value).

`[Score, Alignment, Start] = nwalign(Seq1,Seq2)` returns a 2-by-1 vector of indices indicating the starting point in each sequence for the alignment. Because this is a global alignment, `Start` is always `[1;1]`.

`... = nwalign(Seq1,Seq2, ...'PropertyName', PropertyValue, ...)` calls `nwalign` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = nwalign(Seq1,Seq2, ...'Alphabet', AlphabetValue, ...)` specifies the type of sequences. Choices are `'AA'` (default) or `'NT'`.

`... = nwalign(Seq1,Seq2, ...'ScoringMatrix', ScoringMatrixValue, ...)` specifies the scoring matrix to use for the global alignment. Default is:

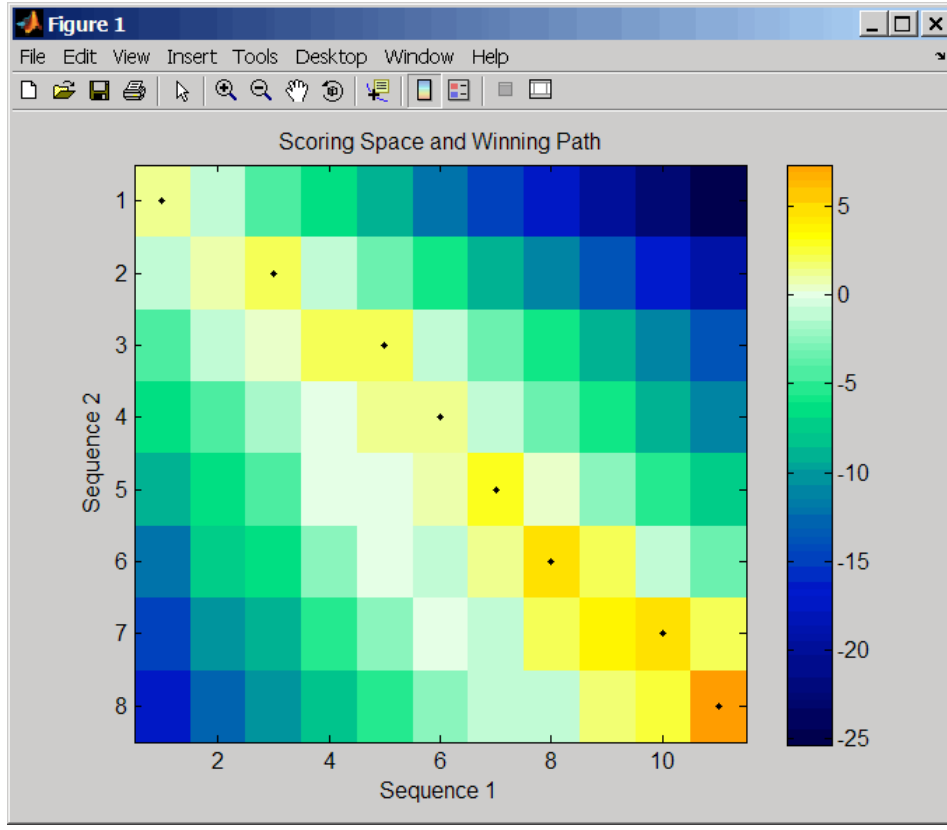
- `'BLOSUM50'` — When `AlphabetValue` equals `'AA'`
- `'NUC44'` — When `AlphabetValue` equals `'NT'`

`... = nwalign(Seq1,Seq2, ...'Scale', ScaleValue, ...)` specifies a scale factor that is applied to the output score, thereby controlling the units of the output score. Choices are any positive value.

`... = nwalign(Seq1,Seq2, ...'GapOpen', GapOpenValue, ...)` specifies the penalty for opening a gap in the alignment. Choices are any positive value. Default is `8`.

`... = nwalign(Seq1,Seq2, ...'ExtendGap', ExtendGapValue, ...)` specifies the penalty for extending a gap in the alignment. Choices are any positive value. Default is equal to `GapOpenValue`.

`... = nwalign(Seq1,Seq2, ...'Showscore', ShowscoreValue, ...)` controls the display of the scoring space and winning path of the alignment. Choices are `true` or `false` (default).



The scoring space is a heat map displaying the best scores for all the partial alignments of two sequences. The color of each (`n1,n2`) coordinate in the scoring space represents the best score for the pairing of subsequences `Seq1(1:n1)` and `Seq2(1:n2)`, where `n1` is a position in `Seq1` and `n2` is a position in `Seq2`. The best score for a pairing of specific subsequences is determined by scoring all possible alignments of the subsequences by summing matches and gap penalties.

The winning path is represented by black dots in the scoring space, and it illustrates the pairing of positions in the optimal global alignment. The color of the last point (lower right) of the winning path represents

the optimal global alignment score for the two sequences and is the *Score* output returned by nwalign.

Note The scoring space visually indicates if there are potential alternate winning paths, which is useful when aligning sequences with big gaps. Visual patterns in the scoring space can also indicate a possible sequence rearrangement.

Examples

1. Globally align two amino acid sequences using the BLOSUM50 (default) scoring matrix and the default values for the GapOpen and ExtendGap properties. Return the optimal global alignment score in bits and the alignment character array.

```
[Score, Alignment] = nwalign('VSPAGMASGYD','IPGKASYD')
Score =

    7.3333

Alignment =

VSPAGMASGYD
: | | || ||
I-P-GKAS-YD
```

2. Globally align two amino acid sequences specifying the PAM250 scoring matrix and a gap open penalty of 5.

```
[Score, Alignment] = nwalign('IGRHRYHIGG','SRYIGRG',...
                             'scoringmatrix','pam250',...
                             'gapopen',5)
Score =

    2.3333

Alignment =
```

```
IGRHRYHIG-G
 :  || || |
-S--RY-IGRG
```

3 Globally align two amino acid sequences returning the *Score* in nat units (nats) by specifying a scale factor of `log(2)`.

```
[Score, Alignment] = nwalign('HEAGAWGHEE','PAWHEAE','Scale',log(2))

Score =

    0.2310

Alignment =

HEAGAWGHE-E
    || || |
--P-AW-HEAE
```

References

[1] Durbin, R., Eddy, S., Krogh, A., and Mitchison, G. (1998). Biological Sequence Analysis (Cambridge University Press).

See Also

Bioinformatics Toolbox functions: `aa2int`, `aminolookup`, `baselookup`, `blosum`, `dayhoff`, `gonnet`, `int2aa`, `int2nt`, `localalign`, `multialign`, `nt2aa`, `nt2int`, `nuc44`, `pam`, `profalign`, `seqdotplot`, `showalignment`, `swalign`

Purpose

Calculate sequence properties of DNA oligonucleotide

Syntax

```
SeqProperties = oligoprop(SeqNT)
SeqProperties = oligoprop(SeqNT, ...'Salt', SaltValue, ...)
SeqProperties = oligoprop(SeqNT, ...'Temp', TempValue, ...)
SeqProperties = oligoprop(SeqNT, ...'Primerconc',
   PrimerconcValue, ...)
SeqProperties = oligoprop(SeqNT, ...'HPBase', HPBaseValue,
   ...)
SeqProperties = oligoprop(SeqNT, ...'HPLoop', HPLoopValue,
   ...)
SeqProperties = oligoprop(SeqNT, ...'Dimerlength',
   DimerlengthValue, ...)
```

Arguments

SeqNT	DNA oligonucleotide sequence represented by any of the following: • Character string containing the letters `A`, `C`, `G`, `T`, or `N` • Vector of integers containing the integers `1`, `2`, `3`, `4`, or `15` • Structure containing a `Sequence` field that contains a nucleotide sequence
SaltValue	Value that specifies a salt concentration in moles/liter for melting temperature calculations. Default is `0.05` moles/liter.
TempValue	Value that specifies the temperature in degrees Celsius for nearest-neighbor calculations of free energy. Default is `25` degrees Celsius.
PrimerconcValue	Value that specifies the concentration in moles/liter for melting temperature calculations. Default is `50e-6` moles/liter.

HPBaseValue	Value that specifies the minimum number of paired bases that form the neck of the hairpin. Default is 4 base pairs.
HPLoopValue	Value that specifies the minimum number of bases that form the loop of a hairpin. Default is 2 bases.
DimerlengthValue	Value that specifies the minimum number of aligned bases between the sequence and its reverse. Default is 4 bases.

Return Values

SeqProperties	Structure containing the sequence properties for a DNA oligonucleotide.

Description

SeqProperties = oligoprop(*SeqNT*) returns the sequence properties for a DNA oligonucleotide as a structure with the following fields:

Field	Description
GC	Percent GC content for the DNA oligonucleotide. Ambiguous N characters in *SeqNT* are considered to potentially be any nucleotide. If *SeqNT* contains ambiguous N characters, GC is the midpoint value, and its uncertainty is expressed by GCdelta.
GCdelta	The difference between GC (midpoint value) and either the maximum or minimum value GC could assume. The maximum and minimum values are calculated by assuming all N characters are G/C or not G/C, respectively. Therefore, GCdelta defines the possible range of GC content.

Field	Description
`Hairpins`	`H`-by-`length(`*`SeqNT`*`)` matrix of characters displaying all potential hairpin structures for the sequence *`SeqNT`*. Each row is a potential hairpin structure of the sequence, with the hairpin forming nucleotides designated by capital letters. `H` is the number of potential hairpin structures for the sequence. Ambiguous `N` characters in *`SeqNT`* are considered to potentially complement any nucleotide.
`Dimers`	`D`-by-`length(`*`SeqNT`*`)` matrix of characters displaying all potential dimers for the sequence *`SeqNT`*. Each row is a potential dimer of the sequence, with the self-dimerizing nucleotides designated by capital letters. `D` is the number of potential dimers for the sequence. Ambiguous `N` characters in *`SeqNT`* are considered to potentially complement any nucleotide.
`MolWeight`	Molecular weight of the DNA oligonucleotide. Ambiguous `N` characters in *`SeqNT`* are considered to potentially be any nucleotide. If *`SeqNT`* contains ambiguous `N` characters, `MolWeight` is the midpoint value, and its uncertainty is expressed by `MolWeightdelta`.
`MolWeightdelta`	The difference between `MolWeight` (midpoint value) and either the maximum or minimum value `MolWeight` could assume. The maximum and minimum values are calculated by assuming all `N` characters are `G` or `C`, respectively. Therefore, `MolWeightdelta` defines the possible range of molecular weight for *`SeqNT`*.

Field	Description
`Tm`	A vector with melting temperature values, in degrees Celsius, calculated by six different methods, listed in the following order: • Basic (Marmur et al., 1962) • Salt adjusted (Howley et al., 1979) • Nearest-neighbor (Breslauer et al., 1986) • Nearest-neighbor (SantaLucia Jr. et al., 1996) • Nearest-neighbor (SantaLucia Jr., 1998) • Nearest-neighbor (Sugimoto et al., 1996) Ambiguous `N` characters in *`SeqNT`* are considered to potentially be any nucleotide. If *`SeqNT`* contains ambiguous `N` characters, `Tm` is the midpoint value, and its uncertainty is expressed by `Tmdelta`.
`Tmdelta`	A vector containing the differences between `Tm` (midpoint value) and either the maximum or minimum value `Tm` could assume for each of the six methods. Therefore, `Tmdelta` defines the possible range of melting temperatures for *`SeqNT`*.
`Thermo`	`4`-by-`3` matrix of thermodynamic calculations. The rows correspond to nearest-neighbor parameters from: • Breslauer et al., 1986 • SantaLucia Jr. et al., 1996 • SantaLucia Jr., 1998 • Sugimoto et al., 1996 The columns correspond to:

Field	Description
	• delta `H` — Enthalpy in kilocalories per mole, kcal/mol • delta `S` — Entropy in calories per mole-degrees Kelvin, cal/(K)(mol) • delta `G` — Free energy in kilocalories per mole, kcal/mol Ambiguous `N` characters in *`SeqNT`* are considered to potentially be any nucleotide. If *`SeqNT`* contains ambiguous `N` characters, `Thermo` is the midpoint value, and its uncertainty is expressed by `Thermodelta`.
`Thermodelta`	`4`-by-`3` matrix containing the differences between `Thermo` (midpoint value) and either the maximum or minimum value `Thermo` could assume for each calculation and method. Therefore, `Thermodelta` defines the possible range of thermodynamic values for *`SeqNT`*.

`SeqProperties` = `oligoprop(`*`SeqNT`*`, ...'`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `oligoprop` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`SeqProperties` = `oligoprop(`*`SeqNT`*`, ...'Salt', `*`SaltValue`*`, ...)` specifies a salt concentration in moles/liter for melting temperature calculations. Default is `0.05` moles/liter.

`SeqProperties` = `oligoprop(`*`SeqNT`*`, ...'Temp', `*`TempValue`*`, ...)` specifies the temperature in degrees Celsius for nearest-neighbor calculations of free energy. Default is `25` degrees Celsius.

SeqProperties = oligoprop(*SeqNT*, ...'Primerconc', *PrimerconcValue*, ...) specifies the concentration in moles/liter for melting temperatures. Default is 50e-6 moles/liter.

SeqProperties = oligoprop(*SeqNT*, ...'HPBase', *HPBaseValue*, ...) specifies the minimum number of paired bases that form the neck of the hairpin. Default is 4 base pairs.

SeqProperties = oligoprop(*SeqNT*, ...'HPLoop', *HPLoopValue*, ...) specifies the minimum number of bases that form the loop of a hairpin. Default is 2 bases.

SeqProperties = oligoprop(*SeqNT*, ...'Dimerlength', *DimerlengthValue*, ...) specifies the minimum number of aligned bases between the sequence and its reverse. Default is 4 bases.

Examples

Calculating Properties for a DNA Sequence

1 Create a random sequence.

```
seq = randseq(25)

seq =

TAGCTTCATCGTTGACTTCTACTAA
```

2 Calculate sequence properties of the sequence.

```
S1 = oligoprop(seq)

S1 =

               GC: 36
          GCAlpha: 0
         Hairpins: [0x25 char]
           Dimers: 'tAGCTtcatcgttgacttctactaa'
        MolWeight: 7.5820e+003
    MolWeightAlpha: 0
               Tm: [52.7640 60.8629 62.2493 55.2870 54.0293 61.0614]
```

```
          TmAlpha: [0 0 0 0 0 0]
           Thermo: [4x3 double]
     ThermoAlpha: [4x3 double]
```

3 List the thermodynamic calculations for the sequence.

```
S1.Thermo

ans =

 -178.5000 -477.5700  -36.1125
 -182.1000 -497.8000  -33.6809
 -190.2000 -522.9000  -34.2974
 -191.9000 -516.9000  -37.7863
```

Calculating Properties for a DNA Sequence with Ambiguous Characters

1 Calculate sequence properties of the sequence ACGTAGAGGACGTN.

```
S2 = oligoprop('ACGTAGAGGACGTN')

S2 =

              GC: 53.5714
         GCAlpha: 3.5714
        Hairpins: 'ACGTagaggACGTn'
          Dimers: [3x14 char]
       MolWeight: 4.3329e+003
  MolWeightAlpha: 20.0150
              Tm: [38.8357 42.2958 57.7880 52.4180 49.9633 55.1330]
         TmAlpha: [1.4643 1.4643 10.3885 3.4633 0.2829 3.8074]
          Thermo: [4x3 double]
     ThermoAlpha: [4x3 double]
```

2 List the potential dimers for the sequence.

```
S2.Dimers
```

```
ans =

ACGTagaggacgtn
ACGTagaggACGTn
acgtagagGACGTN
```

References

[1] Breslauer, K.J., Frank, R., Blöcker, H., and Marky, L.A. (1986). Predicting DNA duplex stability from the base sequence. Proceedings of the National Academy of Science USA *83*, 3746–3750.

[2] Chen, S.H., Lin, C.Y., Cho, C.S., Lo, C.Z., and Hsiung, C.A. (2003). Primer Design Assistant (PDA): A web-based primer design tool. Nucleic Acids Research *31(13)*, 3751–3754.

[3] Howley, P.M., Israel, M.A., Law, M., and Martin, M.A. (1979). A rapid method for detecting and mapping homology between heterologous DNAs. Evaluation of polyomavirus genomes. The Journal of Biological Chemistry *254(11)*, 4876–4883.

[4] Marmur, J., and Doty, P. (1962). Determination of the base composition of deoxyribonucleic acid from its thermal denaturation temperature. Journal Molecular Biology *5*, 109–118.

[5] Panjkovich, A., and Melo, F. (2005). Comparison of different melting temperature calculation methods for short DNA sequences. Bioinformatics *21(6)*, 711–722.

[6] SantaLucia Jr., J., Allawi, H.T., and Seneviratne, P.A. (1996). Improved Nearest-Neighbor Parameters for Predicting DNA Duplex Stability. Biochemistry *35*, 3555–3562.

[7] SantaLucia Jr., J. (1998). A unified view of polymer, dumbbell, and oligonucleotide DNA nearest-neighbor thermodynamics. Proceedings of the National Academy of Science USA *95*, 1460–1465.

[8] Sugimoto, N., Nakano, S., Yoneyama, M., and Honda, K. (1996). Improved thermodynamic parameters and helix initiation factor to predict stability of DNA duplexes. Nucleic Acids Research *24(22)*, 4501–4505.

[9] http://www.basic.northwestern.edu/biotools/oligocalc.html for weight calculations.

See Also

Bioinformatics Toolbox functions: `isoelectric`, `molweight`, `ntdensity`, `palindromes`, `randseq`

optimalleaforder

Purpose

Determine optimal leaf ordering for hierarchical binary cluster tree

Syntax

```
Order = optimalleaforder(Tree, Dist)
Order = optimalleaforder(Tree, Dist, ...'Criteria',
CriteriaValue, ...)
Order = optimalleaforder(Tree, Dist, ...'Transformation',
   TransformationValue, ...)
```

Arguments

Tree	Hierarchical binary cluster tree represented by an (*M* - 1)-by-3 matrix, created by the `linkage` function, where *M* is the number of leaves.
Dist	Distance matrix, such as that created by the `pdist` function.
CriteriaValue	String that specifies the optimization criteria. Choices are: • `adjacent` (default) — Minimizes the sum of distances between adjacent leaves. • `group` — Minimizes the sum of distances between every leaf and all other leaves in the adjacent cluster.

TransformationValue	Either of the following:
	• String that specifies the algorithm to transform the distances in *Dist* into similarity values. Choices are:
	  - `linear` (default) — Similarity = max(all distances) - distance
	  - `quadratic` — Similarity = (max(all distances) - distance)^2
	  - `inverse` — Similarity = 1/distance

- A function handle created using @ to a function that transforms the distances in *Dist* into similarity values. The function is typically a monotonic decreasing function within the range of the distance values. The function must accept a vector input and return a vector of the same size.

Return Values

Order	Optimal leaf ordering for the hierarchical binary cluster tree represented by *Tree*.

Description

Order = optimalleaforder(*Tree*, *Dist*) returns the optimal leaf ordering for the hierarchical binary cluster tree represented by *Tree*, an (*M* - 1)-by-3 matrix, created by the linkage function, where *M* is the number of leaves. Optimal leaf ordering of a binary tree maximizes the similarity between adjacent elements (clusters or leaves) by flipping tree branches, but without dividing the clusters. The input *Dist* is a distance matrix, such as that created by the pdist function.

Order = optimalleaforder(*Tree*, *Dist*, ...'*PropertyName*', *PropertyValue*, ...) calls optimalleaforder with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

Order = optimalleaforder(*Tree*, *Dist*, ...'Criteria', *CriteriaValue*, ...) specifies the optimization criteria.

Order = optimalleaforder(*Tree*, *Dist*, ...'Transformation', *TransformationValue*, ...) specifies the algorithm to transform the distances in *Dist* into similarity values. The transformation is necessary because optimalleaforder maximizes the similarity between adjacent elements, which is comparable to minimizing the sum of distances between adjacent elements.

Examples

1. Use the `rand` function to create a 10-by-2 matrix of random values.

```
X = rand(10,2);
```

2. Use the `pdist` function to create a distance matrix containing the city block distances between the pairs of objects in matrix `X`.

```
Dist = pdist(X,'cityblock');
```

3. Use the `linkage` function to create a matrix, `Tree`, that represents a hierarchical binary cluster tree, from the distance matrix, `Dist`.

```
Tree = linkage(Dist,'average');
```

4. Use the `optimalleaforder` function to determine the optimal leaf ordering for the hierarchical binary cluster tree represented by `Tree`, using the distance matrix `Dist`.

```
order = optimalleaforder(Tree,Dist)
```

References

[1] Bar-Joseph, Z., Gifford, D.K., and Jaakkola, T.S. (2001). Fast optimal leaf ordering for hierarchical clustering. Bioinformatics *17*, Suppl 1:S22–9. PMID: 11472989.

See Also

Bioinformatics Toolbox function: `clustergram`

Statistics Toolbox functions: `linkage`, `pdist`

Purpose

Find palindromes in sequence

Syntax

```
[Position, Length] = palindromes(SeqNT)
[Position, Length, Pal] = palindromes(SeqNT)
... = palindromes(SeqNT, ..., 'Length', LengthValue, ...)
... = palindromes(SeqNT, ..., 'Complement',
ComplementValue,
   ...)
```

Arguments

SeqNT	One of the following: • String of codes specifying a nucleotide sequence. For valid letter codes, see the table Mapping Nucleotide Letter Codes to Integers on page 3-1121. • Row vector of integers specifying a nucleotide sequence. For valid integers, see the table Mapping Nucleotide Integers to Letter Codes on page 3-809. • MATLAB structure containing a `Sequence` field that contains a nucleotide sequence, such as returned by `emblread`, `fastaread`, `fastqread`, `genbankread`, `getembl`, or `getgenbank`.
LengthValue	Integer specifying a minimum length for palindromes. Default is `6`.
ComplementValue	Controls the return of complementary palindromes, that is, where the elements match their complementary pairs `A-T` (or `U`) and `C-G` instead of an exact nucleotide match. Choices are `true` or `false` (default).

Description

`[Position, Length] = palindromes(SeqNT)` finds all palindromes in sequence *`SeqNT`* with a length greater than or equal to `6`, and returns the starting indices, *`Position`*, and the lengths of the palindromes, *`Length`*.

`[Position, Length, Pal] = palindromes(SeqNT)` also returns a cell array, *`Pal`*, of the palindromes.

`... = palindromes(SeqNT, ...'PropertyName', PropertyValue, ...)` calls `palindromes` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = palindromes(SeqNT, ..., 'Length', LengthValue, ...)` finds all palindromes longer than or equal to *`LengthValue`*. Default is `6`.

`... = palindromes(SeqNT, ..., 'Complement', ComplementValue, ...)` controls the return of complementary palindromes, that is, where the elements match their complementary pairs `A-T` (or `A-U`) and `C-G` instead of an exact nucleotide match. Choices for *`ComplementValue`* are `true` or `false` (default).

Examples

Find the palindromes in a simple nucleotide sequence.

```
[p,l,s] = palindromes('GCTAGTAACGTATATATAAT')

p =
    11
    12
l =
     7
     7
s =
    'TATATAT'
    'ATATATA'
```

Find the complementary palindromes in a simple nucleotide sequence.

```
[pc,lc,sc] = palindromes('TAGCTTGTCACTGAGGCCA',...
                         'Complement',true)
pc =
     8
lc =
     7
sc =
    'TCACTGA'
```

Find the palindromes in a random nucleotide sequence.

```
a = randseq(100)

a =
TAGCTTCATCGTTGACTTCTACTAA
AAGCAAGCTCCTGAGTAGCTGGCCA
AGCGAGCTTGCTTGTGCCCGGCTGC
GGCGGTTGTATCCTGAATACGCCAT

[pos,len,pal]=palindromes(a)

pos =
    74
len =
     6
pal =
    'GCGGCG'
```

See Also

Bioinformatics Toolbox functions: `seqcomplement`, `seqrcomplement`, `seqreverse`, `seqshowwords`

MATLAB functions: `regexp`, `strfind`

Purpose

Return Point Accepted Mutation (PAM) scoring matrix

Syntax

```
ScoringMatrix = pam(N)
[ScoringMatrix, MatrixInfo] = pam(N)
... = pam(N, ...'Extended', ExtendedValue, ...)
... = pam(N, ...'Order', OrderValue, ...)
```

Arguments

N	Integer specifying the PAM scoring matrix to return. Choices are `10:10:500`.
	Tip Entering a larger value for *N* allows for sequence alignments with larger evolutionary distances.
ExtendedValue	Controls the return of the ambiguous characters (`B`, `Z`, and `X`), and the stop character (`*`), in addition to the `20` standard amino acid characters. Choices are `true` or `false` (default).
OrderValue	String that controls the order of amino acids in the scoring matrix. Choices are a string with at least the `20` standard amino acids. The default order of the output is `A R N D C Q E G H I L K M F P S T W Y V B Z X *`. If *OrderValue* does not contain the characters `B`, `Z`, `X`, and `*`, then these characters are not returned.

Description

ScoringMatrix = pam(*N*) returns the PAM*N* scoring matrix for amino acid sequences.

[*ScoringMatrix*, *MatrixInfo*] = pam(*N*) returns a structure with information about the PAM matrix. The fields in the structure are `Name`, `Scale`, `Entropy`, `Expected`, and `Order`.

`... = pam(N, ...'PropertyName', PropertyValue, ...)` calls `pam` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = pam(N, ...'Extended', ExtendedValue, ...)` controls the return of the ambiguous characters (`B`, `Z`, and `X`), and the stop character (`*`), in addition to the `20` standard amino acid characters. Choices are `true` or `false` (default).

`... = pam(N, ...'Order', OrderValue, ...)` controls the order of amino acids in the returned scoring matrix. Choices are a string with at least the `20` standard amino acids. The default ordering of the output is `A R N D C Q E G H I L K M F P S T W Y V B Z X *`. If *`OrderValue`* does not contain the extended characters `B`, `Z`, `X`, and `*`, then these characters are not returned.

PAM50 substitution matrix in `1/2` bit units, Expected score = `-3.70`, Entropy = `2.00` bits, Lowest score = `-13`, Highest score = `13`.

PAM250 substitution matrix in `1/3` bit units, Expected score = `-0.844`, Entropy = `0.354` bits, Lowest score = `-8`, Highest score = `17`.

Examples

Return the PAM50 matrix.

```
PAM50 = pam(50)
```

Return the PAM250 matrix and specify the order of amino acids in the matrix.

```
PAM250 = pam(250,'Order','CSTPAGNDEQHRKMILVFYW')
```

See Also

Bioinformatics Toolbox functions: `blosum`, `dayhoff`, `gonnet`, `localalign`, `nuc44`, `nwalign`, `swalign`

pdbdistplot

Purpose

Visualize intermolecular distances in Protein Data Bank (PDB) file

Syntax

```
pdbdistplot(PDBid)
pdbdistplot(PDBid, Distance)
```

Arguments

PDBid	String specifying a unique identifier for a protein structure record. Each structure in the PDB is represented by a 4-character alphanumeric identifier. For example, `4hhb` is the identification code for hemoglobin.
Distance	Threshold distance in angstroms shown on a spy plot. Default is 7.

Description

`pdbdistplot` displays the distances between atoms and amino acids in a PDB structure.

`pdbdistplot(`*`PDBid`*`)` retrieves the entry *`PDBid`* from the Protein Data Bank (PDB) database and creates a heat map showing interatom distances and a spy plot showing the residues where the minimum distances apart are less than 7 angstroms. *`PDBid`* is a string specifying an entry in the PDB database or the name of a variable or a file containing a PDB MATLAB structure.

`pdbdistplot(`*`PDBid`*`, `*`Distance`*`)` specifies the threshold distance shown on a spy plot.

Examples

Display a spy plot at 7 angstroms of the protein cytochrome C from albacore tuna.

```
pdbdistplot('5CYT');
```

Display a spy plot at 10 angstroms of the same structure.

```
pdbdistplot('5CYT',10);
```

See Also

Bioinformatics Toolbox functions: `getpdb`, `molviewer`, `pdbread`, `proteinplot`, `ramachandran`

pdbread

Purpose

Read data from Protein Data Bank (PDB) file

Syntax

```
PDBStruct = pdbread(File)
PDBStruct = pdbread(File, 'ModelNum', ModelNumValue)
```

Arguments

File	Either of the following: • String specifying a file name, a path and file name, or a URL pointing to a file. The referenced file is a Protein Data Bank (PDB)-formatted file (ASCII text file). If you specify only a file name, that file must be on the MATLAB search path or in the MATLAB Current Directory. • MATLAB character array that contains the text of a PDB-formatted file.
ModelNumValue	Positive integer specifying a model in a PDB-formatted file.

Return Values

PDBStruct	MATLAB structure containing a field for each PDB record.

Description

The Protein Data Bank (PDB) database is an archive of experimentally determined 3-D biological macromolecular structure data. For more information about the PDB format, see:

```
http://www.wwpdb.org/documentation/format23/v2.3.html
```

PDBStruct = pdbread(*File*) reads the data from PDB-formatted text file *File* and stores the data in the MATLAB structure, *PDBStruct*, which contains a field for each PDB record. The following table summarizes

the possible PDB records and the corresponding fields in the MATLAB structure *PDBStruct*:

PDB Database Record	Field in the MATLAB Structure
HEADER	Header
OBSLTE	Obsolete
TITLE	Title
CAVEAT	Caveat
COMPND	Compound
SOURCE	Source
KEYWDS	Keywords
EXPDTA	ExperimentData
AUTHOR	Authors
REVDAT	RevisionDate
SPRSDE	Superseded
JRNL	Journal
REMARK 1	Remark1
REMARK *N* **Note** *N* equals 2 through 999.	Remark*n* **Note** *n* equals 2 through 999.
DBREF	DBReferences
SEQADV	SequenceConflicts
SEQRES	Sequence
FTNOTE	Footnote
MODRES	ModifiedResidues

PDB Database Record	Field in the MATLAB Structure
HET	Heterogen
HETNAM	HeterogenName
HETSYN	HeterogenSynonym
FORMUL	Formula
HELIX	Helix
SHEET	Sheet
TURN	Turn
SSBOND	SSBond
LINK	Link
HYDBND	HydrogenBond
SLTBRG	SaltBridge
CISPEP	CISPeptides
SITE	Site
CRYST1	Cryst1
ORIGXn	OriginX
SCALEn	Scale
MTRIXn	Matrix
TVECT	TranslationVector
MODEL	Model
ATOM	Atom
SIGATM	AtomSD
ANISOU	AnisotropicTemp
SIGUIJ	AnisotropicTempSD
TER	Terminal

PDB Database Record	Field in the MATLAB Structure
HETATM	HeterogenAtom
CONECT	Connectivity

PDBStruct = pdbread(*File*, 'ModelNum', *ModelNumValue*) reads only the model specified by *ModelNumValue* from the PDB-formatted text file *File* and stores the data in the MATLAB structure *PDBStruct*. If *ModelNumValue* does not correspond to an existing mode number in *File*, then pdbread reads the coordinate information of all the models.

The Sequence Field

The Sequence field is also a structure containing sequence information in the following subfields:

- NumOfResidues
- ChainID
- ResidueNames — Contains the three-letter codes for the sequence residues.
- Sequence — Contains the single-letter codes for the sequence residues.

Note If the sequence has modified residues, then the ResidueNames subfield might not correspond to the standard three-letter amino acid codes. In this case, the Sequence subfield will contain the modified residue code in the position corresponding to the modified residue. The modified residue code is provided in the ModifiedResidues field.

The Model Field

The Model field is also a structure or an array of structures containing coordinate information. If the MATLAB structure contains one model, the Model field is a structure containing coordinate information for that model. If the MATLAB structure contains multiple models, the Model

field is an array of structures containing coordinate information for each model. The `Model` field contains the following subfields:

- `Atom`
- `AtomSD`
- `AnisotropicTemp`
- `AnisotropicTempSD`
- `Terminal`
- `HeterogenAtom`

The Atom Field

The `Atom` field is also an array of structures containing the following subfields:

- `AtomSerNo`
- `AtomName`
- `altLoc`
- `resName`
- `chainID`
- `resSeq`
- `iCode`
- `X`
- `Y`
- `Z`
- `occupancy`
- `tempFactor`
- `segID`
- `element`

- charge
- AtomNameStruct — Contains three subfields: chemSymbol, remoteInd, and branch.

Examples

1. Use the getpdb function to retrieve structure information from the Protein Data Bank (PDB) for the nicotinic receptor protein with identifier 1abt, and then save the data to the PDB-formatted file nicotinic_receptor.pdb in the MATLAB Current Directory.

```
getpdb('1abt', 'ToFile', 'nicotinic_receptor.pdb');
```

2. Read the data from the nicotinic_receptor.pdb file into a MATLAB structure pdbstruct.

```
pdbstruct = pdbread('nicotinic_receptor.pdb');
```

3. Read only the second model from the nicotinic_receptor.pdb file into a MATLAB structure pdbstruct_Model2.

```
pdbstruct_Model2 = pdbread('nicotinic_receptor.pdb', 'ModelNum', 2);
```

4. View the atomic coordinate information in the model fields of both MATLAB structures pdbstruct and pdbstruct_Model2.

```
pdbstruct.Model

ans =

1x4 struct array with fields:
    MDLSerNo
    Atom
    Terminal

pdbstruct_Model2.Model

ans =

    MDLSerNo: 2
```

```
            Atom: [1x1205 struct]
        Terminal: [1x2 struct]
```

5 Read the data from an URL into a MATLAB structure, `gfl_pdbstruct`.

```
gfl_pdbstruct = pdbread('http://www.rcsb.org/pdb/files/1gfl.pdb');
```

See Also

Bioinformatics Toolbox functions: `genpeptread`, `getpdb`, `molviewer`, `pdbdistplot`, `pdbsuperpose`, `pdbtransform`, `pdbwrite`

Purpose

Superpose 3-D structures of two proteins

Syntax

```
pdbsuperpose(PDB1, PDB2)
Dist = pdbsuperpose(PDB1, PDB2)
[Dist, RMSD] = pdbsuperpose(PDB1, PDB2)
[Dist, RMSD, Transf] = pdbsuperpose(PDB1, PDB2)
[Dist, RMSD, Transf, PBD2TX] = pdbsuperpose(PDB1, PDB2)
... = pdbsuperpose(..., 'ModelNum', ModelNumValue, ...)
... = pdbsuperpose(..., 'Scale', ScaleValue, ...)
... = pdbsuperpose(..., 'Translate', TranslateValue, ...)
... = pdbsuperpose(..., 'Reflection', ReflectionValue, ...)
... = pdbsuperpose(..., 'SeqAlign', SeqAlignValue, ...)
... = pdbsuperpose(..., 'Segment', SegmentValue, ...)
... = pdbsuperpose(..., 'Apply', ApplyValue, ...)
... = pdbsuperpose(..., 'Display', DisplayValue, ...)
```

Arguments

PDB1, *PDB2*

Protein structures represented by any of the following:

- String specifying a unique identifier for a protein structure record in the Protein Data Bank (PDB) database.
- Variable containing a PDB-formatted MATLAB structure, such as returned by `getpdb` or `pdbread`.
- String specifying a file name or, a path and file name. The referenced file is a PDB-formatted file. If you specify only a file name, that file must be on the MATLAB search path or in the MATLAB Current Directory.

ModelNumValue

Two-element numeric array whose elements correspond to models in *PDB1* and *PDB2* respectively when *PDB1* or *PDB2* contains multiple models. It specifies the models to consider in the

	superposition. By default, the first model in each structure is considered.
ScaleValue	Specifies whether to include a scaling component in the linear transformation. Choices are `true` or `false` (default).
TranslateValue	Specifies whether to include a translation component in the linear transformation. Choices are `true` (default) or `false`.
ReflectionValue	Specifies whether to include a reflection component in the linear transformation. Choices are: • `true` — Include reflection component. • `false` — Exclude reflection component. • `'best'` — Default. May or may not include the reflection component, depending on the best fit solution.
SeqAlignValue	Specifies whether to perform a local sequence alignment and then use only the portions of the structures corresponding to the segments that align to compute the linear transformation. Choices are `true` (default) or `false`.

Note If you set the `'SeqAlign'` property to `true`, you can also specify the following properties used by the `swalign` function:

- `'ScoringMatrix'`
- `'GapOpen'`
- `'ExtendGap'`

For more information on these properties, see `swalign`.

`SegmentValue`

Specifies the boundaries and the chain of two subsequences to consider for computing the linear transformation. *`SegmentValue`* is a cell array of strings with the following format:

```
{'start1-stop1:chain1',
'start2-stop2:chain2'}
```

You can omit the boundaries to indicate the entire chain, such as in `{'chain1', 'start2-stop2:chain2'}`. You can specify only one pair of segments at any given time, and the specified segments are assumed to contain the same number of alpha carbon atoms.

ApplyValue — Specifies the extent to which the linear transformation should be applied. Choices are:

- `'all'` — Default. Apply the linear transformation to the entire PDB2 structure.
- `'chain'` — Apply the linear transformation to the specified chain only.
- `'segment'` — Apply the linear transformation to the specified segment only.

DisplayValue — Specifies whether to display the original *PDB1* structure and the resulting transformed *PDB2TX* structure in the Molecule Viewer window using the `molviewer` function. Each structure is represented as a separate model. Choices are `true` (default) or `false`.

Return Values

Dist — Value representing a dissimilarity measure given by the sum of the squared errors between *PDB1* and *PDB2*. For more information, see `procrustes` in the Statistics Toolbox documentation.

RMSD — Scalar representing the root mean square distance between the coordinates of the *PDB1* structure and the transformed *PDB2* structure, considering only the atoms used to compute the linear transformation.

Transf

Linear transformation computed to superpose the chain of *PDB2* to the chain of *PDB1*. *Transf* is a MATLAB structure with the following fields:

- T — Orthogonal rotation and reflection component.
- b — Scale component.
- c — Translation component.

Note Only alpha carbon atom coordinates are used to compute the linear transformation.

Tip You can use the *Transf* output as input to the pdbtransform function.

PDB2TX

PDB-formatted MATLAB structure that represents the coordinates in the transformed *PDB2* protein structure.

Description

pdbsuperpose(*PDB1*, *PDB2*) computes and applies a linear transformation to superpose the coordinates of the protein structure represented in *PDB2* to the coordinates of the protein structure represented in *PDB1*. *PDB1* and *PDB2* are protein structures represented by any of the following:

- String specifying a unique identifier for a protein structure record in the PDB database.
- Variable containing a PDB-formatted MATLAB structure, such as returned by getpdb or pdbread.
- String specifying a file name or a path and file name. The referenced file is a PDB-formatted file. If you specify only a file name, that file

must be on the MATLAB search path or in the MATLAB Current Directory.

Alpha carbon atom coordinates of single chains for each structure are considered to compute the linear transformation (translation, reflection, orthogonal rotation, and scaling). By default, the first chain in each structure is considered to compute the transformation, and the transformation is applied to the entire molecule. By default, the original *PDB1* structure and the resulting transformed *PDB2* structure are displayed as separate models in the Molecule Viewer window using the `molviewer` function.

Dist = `pdbsuperpose(`*PDB1*`, `*PDB2*`)` returns a dissimilarity measure given by the sum of the squared errors between *PDB1* and *PDB2*. For more information, see `procrustes`.

`[`*Dist*`, `*RMSD*`] = pdbsuperpose(`*PDB1*`, `*PDB2*`)` also returns *RMSD*, the root mean square distance between the coordinates of the *PDB1* structure and the transformed *PDB2* structure, considering only the atoms used to compute the linear transformation.

`[`*Dist*`, `*RMSD*`, `*Transf*`] = pdbsuperpose(`*PDB1*`, `*PDB2*`)` also returns *Transf*, the linear transformation computed to superpose the chain of *PDB2* to the chain of *PDB1*. *Transf* is a MATLAB structure with the following fields:

- `T` — Orthogonal rotation and reflection component.
- `b` — Scale component.
- `c` — Translation component.

Note Only alpha carbon atom coordinates are used to compute the linear transformation.

`[Dist, RMSD, Transf, PBD2TX] = pdbsuperpose(PDB1, PDB2)` also returns *PBD2TX*, a PDB-formatted MATLAB structure that represents the coordinates in the transformed *PDB2* protein structure.

`... = pdbsuperpose(..., 'PropertyName', PropertyValue, ...)` calls `pdbsuperpose` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = pdbsuperpose(..., 'ModelNum', ModelNumValue, ...)` specifies the models to consider in the superposition when *PDB1* or *PDB2* contains multiple models. *ModelNumValue* is a two-element numeric array whose elements correspond to the models in *PDB1* and *PDB2* respectively. By default, the first model in each structure is considered.

`... = pdbsuperpose(..., 'Scale', ScaleValue, ...)` specifies whether to include a scaling component in the linear transformation. Choices are `true` or `false` (default).

`... = pdbsuperpose(..., 'Translate', TranslateValue, ...)` specifies whether to include a translation component in the linear transformation. Choices are `true` (default) or `false`.

`... = pdbsuperpose(..., 'Reflection', ReflectionValue, ...)` specifies whether to include a reflection component in the linear transformation. Choices are `true` (include reflection component), `false` (exclude reflection component), or `'best'` (may or may not include the reflection component, depending on the best fit solution). Default is `'best'`.

`... = pdbsuperpose(..., 'SeqAlign', SeqAlignValue, ...)` specifies whether to perform a local sequence alignment and then use only the portions of the structures corresponding to the segments that align to compute the linear transformation. Choices are `true` (default) or `false`.

Note If you set the `'SeqAlign'` property to `true`, you can also specify the following properties used by the `swalign` function:

- `'ScoringMatrix'`
- `'GapOpen'`
- `'ExtendGap'`

For more information on these properties, see `swalign`.

`... = pdbsuperpose(..., 'Segment', SegmentValue, ...)` specifies the boundaries and the chain of two subsequences to consider for computing the linear transformation. *`SegmentValue`* is a cell array of strings with the following format: `{'start1-stop1:chain1', 'start2-stop2:chain2'}`. You can omit the boundaries to indicate the entire chain, such as in `{'chain1', 'start2-stop2:chain2'}`. You can specify only one pair of segments at any given time, and the specified segments are assumed to contain the same number of alpha carbon atoms.

`... = pdbsuperpose(..., 'Apply', ApplyValue, ...)` specifies the extent to which the linear transformation should be applied. Choices are `'all'` (apply the linear transformation to the entire PDB2 structure), `'chain'` (apply the linear transformation to the specified chain only), or `'segment'` (apply the linear transformation to the specified segment only). Default is `'all'`.

`... = pdbsuperpose(..., 'Display', DisplayValue, ...)` specifies whether to display the original *`PDB1`* structure and the resulting transformed *`PDB2TX`* structure in the Molecule Viewer window using the `molviewer` function. Each structure is represented as a separate model. Choices are `true` (default) or `false`.

Examples

Superposing Two Hemoglobin Structures

1 Use the `getpdb` function to retrieve protein structure data from the Protein Data Bank (PDB) database for two hemoglobin structures.

```
str1 = getpdb('1dke');
str2 = getpdb('4hhb');
```

2 Superpose the first model of the two hemoglobin structures, applying the transformation to the entire molecule.

```
d = pdbsuperpose(str1, str2, 'model', [1 1], 'apply', 'all');
```

3 Superpose the two hemoglobin structures (each containing four chains), computing and applying the linear transformation chain by chain. Do not display the structures.

```
strtx = str2;
chainList1 = {str1.Sequence.ChainID};
chainList2 = {str2.Sequence.ChainID};
for i = 1:4
    [d(i), rmsd(i), tr(i), strtx] = pdbsuperpose(str1, strtx,  ...
                            'segment', {chainList1{i}; chainList2{i}}, ...
                            'apply', 'chain', 'display', false);
end
```

Superposing Two Chains of a Thioredoxin Structure

Superpose chain B on chain A of a thioredoxin structure (PDBID = 2trx), and then apply the transformation only to chain B.

```
[d, rmsd, tr] = pdbsuperpose('2trx', '2trx', 'segment', {'A', 'B'}, ...
                             'apply', 'chain')

d =

    0.0028

rmsd =
```

```
    0.6604

tr =

    T: [3x3 double]
    b: 1
    c: [109x3 double]
```

Superposing Two Calmodulin Structures

Superpose two calmodulin structures according to the linear transformation obtained using two 20 residue-long segments.

```
pdbsuperpose('1a29', '1cll', 'segment', {'10-30:A', '10-30:A'})

ans =

    0.1945
```

See Also

Bioinformatics Toolbox functions: `getpdb`, `molviewer`, `pdbread`, `pdbtransform`, `swalign`

Statistics Toolbox function: `procrustes`

Purpose

Apply linear transformation to 3-D structure of molecule

Syntax

```
pdbtransform(PDB, Transf)
PDBTX = pdbtransform(PDB, Transf)
... = pdbtransform(..., 'ModelNum', ModelNumValue, ...)
... = pdbtransform(..., 'Segment', SegmentValue, ...)
```

Arguments

PDB

Protein structure represented by any of the following:

- String specifying a unique identifier for a protein structure record in the Protein Data Bank (PDB) database.
- Variable containing a PDB-formatted MATLAB structure, such as returned by `getpdb` or `pdbread`.
- String specifying a file name or a path and file name. The referenced file is a PDB-formatted file. If you specify only a file name, that file must be on the MATLAB search path or in the MATLAB Current Directory.

Transf

MATLAB structure representing a linear transformation, which is applied to the coordinates of the molecule represented by *PDB*. *Transf* contains the following fields:

- `T` — Orthogonal rotation and reflection component.
- `b` — Scale component.
- `c` — Translation component.

Tip You can use the *Transf* structure returned by the pdbsuperpose function as input.

ModelNumValue	Positive integer that specifies the model to which to apply the transformation, when *PDB* contains multiple models. By default, the first model is considered.
SegmentValue	Specifies the extent to which the linear transformation is applied. *SegmentValue* can be either: • 'all' — The transformation is applied to the entire PDB input. • String specifying the boundaries and the chain to consider. It uses either of the following formats: 'start-stop:chain' or 'chain'. Omitting the boundaries indicates the entire chain.

Return Values

PDBTX	Transformed PDB-formatted MATLAB structure.

Description

pdbtransform(*PDB*, *Transf*) applies the linear transformation specified in *Transf*, a MATLAB structure representing a linear transformation, to the coordinates of the molecule represented by *PDB*, which can be any of the following:

- String specifying a unique identifier for a protein structure record in the PDB database.
- Variable containing a PDB-formatted MATLAB structure, such as returned by getpdb or pdbread.

- String specifying a file name or a path and file name. The referenced file is a PDB-formatted file. If you specify only a file name, that file must be on the MATLAB search path or in the MATLAB Current Directory.

PDBTX = pdbtransform(*PDB*, *Transf*) returns *PDBTX*, the transformed PDB-formatted MATLAB structure.

... = pdbtransform(...'*PropertyName*', *PropertyValue*, ...) calls pdbtransform with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

... = pdbtransform(..., 'ModelNum', *ModelNumValue*, ...) specifies the model to which to apply the transformation, when *PDB* contains multiple models. *ModelNumValue* is a positive integer. By default, the first model is considered.

... = pdbtransform(..., 'Segment', *SegmentValue*, ...) specifies the extent to which the linear transformation is applied. *SegmentValue* can be either:

- 'all' — The transformation is applied to the entire PDB input.
- String specifying the boundaries and the chain to consider. It uses either of the following formats: 'start-stop:chain' or 'chain'. Omitting the boundaries indicates the entire chain.

Examples

1 Create a MATLAB structure that defines a linear transformation.

```
transf.T = eye(3);  transf.b = 1;  transf.c = [11.8 -2.8 -32.3];
```

2 Apply the linear transformation to chain B in the thioredoxin structure, with a PDB identifier of 2trx.

```
pdbtx = pdbtransform('2trx', transf, 'segment', 'B');
```

See Also

Bioinformatics Toolbox functions: `getpdb`, `molviewer`, `pdbread`, `pdbsuperpose`

Statistics Toolbox function: `procrustes`

Purpose

Write to file using Protein Data Bank (PDB) format

Syntax

```
pdbwrite(File, PDBStruct)
PDBArray = pdbwrite(File, PDBStruct)
```

Arguments

File

String specifying either a file name or a path and file name for saving the PDB-formatted data. If you specify only a file name, the file is saved to the MATLAB Current Directory.

Tip After you save the MATLAB structure to a local PDB-formatted file, you can use the `molviewer` function to display and manipulate a 3-D image of the structure.

PDBStruct

MATLAB structure containing 3-D protein structure coordinate data, created initially by using the `getpdb` or `pdbread` functions.

Note You can edit this structure to modify its 3-D protein structure data. The coordinate information is stored in the `Model` field of *`PDBStruct`*.

Return Values

PDBArray

Character array in which each row corresponds to a line in a PDB record.

Description

`pdbwrite(`*`File`*`, `*`PDBStruct`*`)` writes the contents of the MATLAB structure *`PDBStruct`* to a PDB-formatted file (ASCII text file) whose path and file name are specified by *`File`*. In the output file, *`File`*, the

atom serial numbers are preserved. The atomic coordinate records are ordered according to their atom serial numbers.

Tip After you save the MATLAB structure to a local PDB-formatted file, you can use the `molviewer` function to display and manipulate a 3-D image of the structure.

`PDBArray` = pdbwrite(*`File`*, *`PDBStruct`*) saves the formatted PDB record, converted from the contents of the MATLAB structure *`PDBStruct`*, to *`PDBArray`*, a character array in which each row corresponds to a line in a PDB record.

Note You can edit *`PDBStruct`* to modify its 3-D protein structure data. The coordinate information is stored in the `Model` field of *`PDBStruct`*.

Examples

1. Use the `getpdb` function to retrieve structure information from the Protein Data Bank (PDB) for the green fluorescent protein with identifier `1GFL` , and store the data in the MATLAB structure `gflstruct`.

   ```
   gflstruct = getpdb('1GFL');
   ```

2. Find the *x*-coordinate of the first atom.

   ```
   gflstruct.Model.Atom(1).X

   ans =

     -14.0930
   ```

3. Edit the *x*-coordinate of the first atom.

   ```
   gflstruct.Model.Atom(1).X = -18;
   ```

Note Do not add or remove any `Atom` fields, because the `pdbwrite` function does not allow the number of elements in the structure to change.

4. Write the modified MATLAB structure `gflstruct` to a new PDB-formatted file `modified_gfl.pdb` in the `Work` directory on your `C` drive.

```
pdbwrite('c:\work\modified_gfl.pdb', gflstruct);
```

5. Use the `pdbread` function to read the modified PDB file into a MATLAB structure, then confirm that the *x*-coordinate of the first atom has changed.

```
modified_gflstruct = pdbread('c:\work\modified_gfl.pdb')
modified_gflstruct.Model.Atom(1).X

ans =

   -18
```

See Also

Bioinformatics Toolbox functions: `getpdb`, `molviewer`, `pdbread`

pdist (phytree)

Purpose

Calculate pairwise patristic distances in phytree object

Syntax

```
D = pdist(Tree)
[D, C] = pdist(Tree)
pdist(..., 'Nodes', NodesValue, ...)
pdist(..., 'Squareform', SquareformValue, ...)
pdist(..., 'Criteria', CriteriaValue, ...)
```

Arguments

Tree	phytree object created by `phytree` function (object constructor) or `phytreeread` function.
NodesValue	String that specifies the nodes included in the computation. Choices are `'leaves'` (default) or `'all'`.
SquareformValue	Controls the creation of a square matrix. Choices are `true` or `false` (default).
CriteriaValue	String that specifies the criteria used to relate pairs. Choices are `'distance'` (default) or `'levels'`.

Description

`D = pdist(Tree)` returns *D*, a vector containing the patristic distances between every possible pair of leaf nodes of *Tree*, a phylogenetic tree object. The patristic distances are computed by following paths through the branches of the tree and adding the patristic branch distances originally created with the `seqlinkage` function.

The output vector *D* is arranged in the order `((2,1), (3,1), ..., (M,1), (3,2), ..., (M,2), ..., (M,M-1))` (the lower-left triangle of the full `M`-by-`M` distance matrix). To get the distance between the `I`th and `J`th nodes `(I > J)`, use the formula `D((J-1)*(M-J/2)+I-J)`. `M` is the number of leaves.

`[D, C] = pdist(Tree)` returns in *C*, the index of the closest common parent nodes for every possible pair of query nodes.

`pdist(..., 'PropertyName', PropertyValue, ...)` calls `pdist` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`pdist(..., 'Nodes', NodesValue, ...)` specifies the nodes included in the computation. Choices are `'leaves'` (default) or `'all'`. When *`NodesValue`* is `'leaves'`, the output is ordered as before, but `M` is the total number of nodes in the tree (`NumLeaves+NumBranches`).

`pdist(..., 'Squareform', SquareformValue, ...)` controls the creation of a square matrix. Choices are `true` or `false` (default). When *`SquareformValue`* is `true`, `pdist` converts the output into a square-formatted matrix, so that `D(I,J)` denotes the distance between the `I`th and the `J`th nodes. The output matrix is symmetric and has a zero diagonal.

`pdist(..., 'Criteria', CriteriaValue, ...)` changes the criteria used to relate pairs. *`CriteriaValue`* can be `'distance'` (default) or `'levels'`.

Examples

1 Read a phylogenetic tree file into a phytree object.

```
tr = phytreeread('pf00002.tree')
```

2 Calculate the tree distances between pairs of leaves.

```
dist = pdist(tr,'nodes','leaves','squareform',true)
```

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreeread`, `phytreetool`, `seqlinkage`, `seqpdist`

Bioinformatics Toolbox object: phytree object

pfamhmmread

Purpose

Read data from PFAM HMM-formatted file

Syntax

```
HMMStruct = pfamhmmread(File)
```

Arguments

File

Either of the following:

- String specifying a file name, a path and file name, or a URL pointing to a file. The referenced file is a PFAM HMM-formatted file. If you specify only a file name, that file must be on the MATLAB search path or in the current directory.
- MATLAB character array that contains the text of a PFAM-HMM-formatted file.

Tip You can use the `gethmmprof` function with the `'ToFile'` property to retrieve HMM profile information from the PFAM database and create a PFAM HMM-formatted file.

Return Values

HMMStruct

MATLAB structure containing information from a PFAM HMM-formatted file.

Description

Note `pfamhmmread` reads version 2.0 HMMER file formats.

HMMStruct = `pfamhmmread(`*File*`)` reads *File*, a PFAM HMM-formatted file, and converts it to *HMMStruct*, a MATLAB structure containing the following fields corresponding to parameters of an HMM profile:

Field	Description
`Name`	The protein family name (unique identifier) of the HMM profile record in the PFAM database.
`PfamAccessionNumber`	The protein family accession number of the HMM profile record in the PFAM database.
`ModelDescription`	Description of the HMM profile.
`ModelLength`	The length of the profile (number of MATCH states).
`Alphabet`	The alphabet used in the model, `'AA'` or `'NT'`. **Note** `AlphaLength` is 20 for `'AA'` and 4 for `'NT'`.
`MatchEmission`	Symbol emission probabilities in the MATCH states. The format is a matrix of size `ModelLength`-by-`AlphaLength`, where each row corresponds to the emission distribution for a specific MATCH state.
`InsertEmission`	Symbol emission probabilities in the INSERT state. The format is a matrix of size `ModelLength`-by-`AlphaLength`, where each row corresponds to the emission distribution for a specific INSERT state.
`NullEmission`	Symbol emission probabilities in the MATCH and INSERT states for the NULL model. The format is a 1-by-`AlphaLength` row vector. **Note** NULL probabilities are also known as the background probabilities.

Field	Description
`BeginX`	BEGIN state transition probabilities. Format is a 1-by-`(ModelLength + 1)` row vector: `[B->D1 B->M1 B->M2 B->M3 .... B->Mend]`

`MatchX`	MATCH state transition probabilities.
	Format is a 4-by-`(ModelLength - 1)` matrix:
	`[M1->M2 M2->M3 ... M[end-1]->Mend;`
	`M1->I1 M2->I2 ... M[end-1]->I[end-1];`
	`M1->D2 M2->D3 ... M[end-1]->Dend;`
	`M1->E M2->E ... M[end-1]->E ]`

`InsertX`	INSERT state transition probabilities.
	Format is a 2-by-`(ModelLength - 1)` matrix:
	`[ I1->M2 I2->M3 ... I[end-1]->Mend;`
	`I1->I1 I2->I2 ... I[end-1]->I[end-1] ]`

`DeleteX`	DELETE state transition probabilities.
	Format is a 2-by-`(ModelLength - 1)` matrix:
	`[ D1->M2 D2->M3 ... D[end-1]->Mend ;`
	`D1->D2 D2->D3 ... D[end-1]->Dend ]`

`FlankingInsertX`	Flanking insert states (N and C) used for LOCAL profile alignment.
	Format is a 2-by-2 matrix:
	`[N->B C->T ;`
	`N->N C->C]`

Field	Description

LoopX	Loop states transition probabilities used for multiple hits alignment.
	Format is a 2-by-2 matrix:
	`[E->C  J->B ;`
	`E->J  J->J]`

NullX	Null transition probabilities used to provide scores with log-odds values also for state transitions. Format is a 2-by-1 column vector: `[G->F ; G->G]`

For more information on HMM profile models, see "HMM Profile Model" on page 3-784.

Examples

Read a URL pointing to a PFAM HMM-formatted file into a MATLAB structure.

```
site='http://pfam.sanger.ac.uk/';
hmm = pfamhmmread([site '/family/hmm?mode=ls&id=7tm_2'])

hmm =

                    Name: '7tm_2'
    PfamAccessionNumber: 'PF00002.16'
       ModelDescription: '7 transmembrane receptor (Secretin family)'
            ModelLength: 293
               Alphabet: 'AA'
          MatchEmission: [293x20 double]
         InsertEmission: [293x20 double]
           NullEmission: [1x20 double]
                 BeginX: [294x1 double]
```

```
                MatchX: [292x4 double]
               InsertX: [292x2 double]
               DeleteX: [292x2 double]
      FlankingInsertX: [2x2 double]
                LoopX: [2x2 double]
                NullX: [2x1 double]
```

Read a locally saved PFAM HMM-formatted file into a MATLAB structure.

```
pfamhmmread('pf00002.ls')
```

See Also

Bioinformatics Toolbox functions: `gethmmalignment`, `gethmmprof`, `hmmprofalign`, `hmmprofstruct`, `showhmmprof`

Purpose

Data structure containing phylogenetic tree

Description

A phytree object is a data structure containing a phylogenetic tree. Phylogenetic trees are binary rooted trees, which means that each branch is the parent of two other branches, two leaves, or one branch and one leaf. A phytree object can be ultrametric or nonultrametric.

Method Summary

Following are methods of a phytree object:

cluster (phytree)	Validate clusters in phylogenetic tree
get (phytree)	Retrieve information about phylogenetic tree object
getbyname (phytree)	Branches and leaves from phytree object
getcanonical (phytree)	Calculate canonical form of phylogenetic tree
getmatrix (phytree)	Convert phytree object into relationship matrix
getnewickstr (phytree)	Create Newick-formatted string
pdist (phytree)	Calculate pairwise patristic distances in phytree object
plot (phytree)	Draw phylogenetic tree
prune (phytree)	Remove branch nodes from phylogenetic tree
reorder (phytree)	Reorder leaves of phylogenetic tree
reroot (phytree)	Change root of phylogenetic tree
select (phytree)	Select tree branches and leaves in phytree object
subtree (phytree)	Extract phylogenetic subtree

view (phytree)	View phylogenetic tree
weights (phytree)	Calculate weights for phylogenetic tree

Property Summary

Note You cannot modify these properties directly. You can access these properties using the `get` method.

Property	Description
`NumLeaves`	Number of leaves
`NumBranches`	Number of branches
`NumNodes`	Number of nodes (`NumLeaves + NumBranches`)
`Pointers`	Branch to leaf/branch connectivity list
`Distances`	Edge length for every leaf/branch
`LeafNames`	Names of the leaves
`BranchNames`	Names of the branches
`NodeNames`	Names of all the nodes

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreeread`, `phytreetool`, `phytreewrite`, `seqlinkage`, `seqneighjoin`, `seqpdist`

Bioinformatics Toolbox methods of phytree object: `cluster`, `get`, `getbyname`, `getcanonical`, `getmatrix`, `getnewickstr`, `pdist`, `plot`, `prune`, `reroot`, `select`, `subtree`, `view`, `weights`

Purpose

Create phytree object

Syntax

```
Tree = phytree(B)
Tree = phytree(B, D)
Tree = phytree(B, C)
Tree = phytree(BC)
Tree = phytree(..., N)
Tree = phytree
```

Arguments

B	Numeric array of size `[NUMBRANCHES X 2]` in which every row represents a branch of the tree. It contains two pointers to the branch or leaf nodes, which are its children.
C	Column vector with distances for every branch.
D	Column vector with distances from every node to their parent branch.
BC	Combined matrix with pointers to branches or leaves, and distances of branches.
N	Cell array with the names of leaves and branches.

Description

Tree = phytree(*B*) creates an ultrametric phylogenetic tree object. In an ultrametric phylogenetic tree object, all leaves are the same distance from the root.

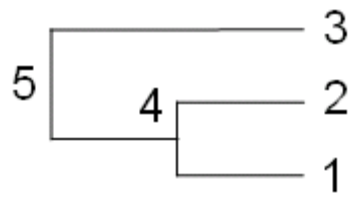
B is a numeric array of size `[NUMBRANCHES X 2]` in which every row represents a branch of the tree and it contains two pointers to the branch or leaf nodes, which are its children.

Leaf nodes are numbered from `1` to `NUMLEAVES` and branch nodes are numbered from `NUMLEAVES + 1` to `NUMLEAVES + NUMBRANCHES`. Note that because only binary trees are allowed, `NUMLEAVES = NUMBRANCHES + 1`.

Branches are defined in chronological order (for example, `B(i,:) > NUMLEAVES + i)`. As a consequence, the first row can only have pointers to leaves, and the last row must represent the root branch. Parent-child

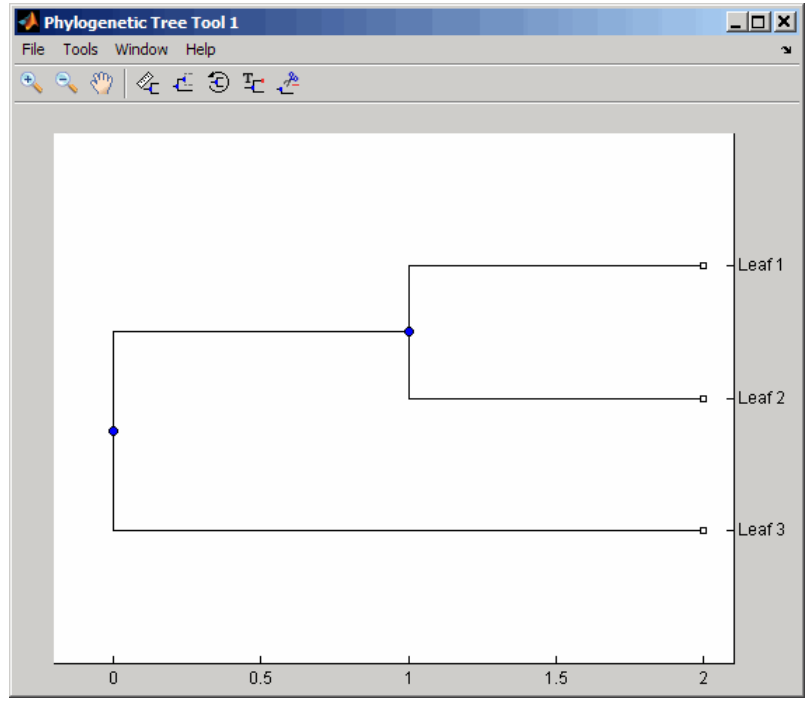
distances are set to 1, unless the child is a leaf and to satisfy the ultrametric condition of the tree its distance is increased.

Given a tree with three leaves and two branches as an example.



In the MATLAB Command Window, type

```
B = [1 2 ; 3 4]

 B =

     1     2
     3     4

tree = phytree(B)

 Phylogenetic tree object with 3 leaves (2 branches)

view(tree)
```



Tree = phytree(*B*, *D*) creates an additive (ultrametric or nonultrametric) phylogenetic tree object with branch distances defined by *D*. *D* is a numeric array of size [NUMNODES X 1] with the distances of every child node (leaf or branch) to its parent branch equal to NUMNODES = NUMLEAVES + NUMBRANCHES. The last distance in *D* is the distance of the root node and is meaningless.

```
b = [1 2 ; 3 4 ]

b =

     1     2
     3     4

d = [1; 2; 1.5; 1; 0]
```

```
d =

    1.0000
    2.0000
    1.5000
    1.0000
         0

view(phytree(b,d))
```

Tree = phytree(*B*, *C*) creates an ultrametric phylogenetic tree object with distances between branches and leaves defined by C. C is a numeric array of size [NUMBRANCHES X 1], which contains the distance from each branch to the leaves. In ultrametric trees, all of the leaves are at the same location (same distance to the root).

```
b = [1 2 ; 3 4]

b =

     1     2
     3     4

c = [1 4]'

c =

     1
     4

view(phytree(b,c))
```

Tree = phytree(*BC*) creates an ultrametric phylogenetic binary tree object with branch pointers in BC(:,[1 2]) and branch coordinates in BC(:,3). Same as phytree(B,C).

Tree = phytree(..., *N*) specifies the names for the leaves and/or the branches. *N* is a cell of strings. If NUMEL(N)==NUMLEAVES, then the names are assigned chronologically to the leaves. If NUMEL(N)==NUMBRANCHES, the names are assigned to the branch nodes. If NUMEL(N)==NUMLEAVES + NUMBRANCHES, all the nodes are named. Unassigned names default to 'Leaf #' and/or 'Branch #' as required.

Tree = phytree creates an empty phylogenetic tree object.

Examples

Create a phylogenetic tree for a set of multiply aligned sequences.

```
Sequences = multialignread('aagag.aln')
distances = seqpdist(Sequences)
tree = seqlinkage(distances)
phytreetool(tree)
```

See Also

Bioinformatics Toolbox functions: phytreeread, phytreetool, phytreewrite, seqlinkage, seqneighjoin, seqpdist

Bioinformatics Toolbox object: phytree object

Bioinformatics Toolbox methods of phytree object: cluster, get, getbyname, getcanonical, getmatrix, getnewickstr, pdist, plot, prune, reroot, select, subtree, view, weights

phytreeread

Purpose

Read phylogenetic tree file

Syntax

```
Tree = phytreeread(File)
```

Arguments

File	Newick-formatted tree files (ASCII text file). Enter a file name, a path and file name, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text for a file.
Tree	`phytree` object created with the function `phytree`.

Description

Tree = `phytreeread(`*File*`)` reads a Newick-formatted tree file and returns a phytree object in the MATLAB workspace with data from the file.

The NEWICK tree format can be found at

```
http://evolution.genetics.washington.edu/phylip/newicktree.html
```

Note This implementation allows only binary trees. Non-binary trees are translated into a binary tree with extra branches of length 0.

Examples

```
tr = phytreeread('pf00002.tree')
```

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `gethmmtree`, `phytreetool`, `phytreewrite`

Purpose

View, edit, and explore phylogenetic tree data

Syntax

```
phytreetool(Tree)
phytreetool(File)
```

Arguments

Tree	`Phytree` object created with the functions `phytree` or `phytreeread`.
File	Newick or ClustalW tree formatted file (ASCII text file) with phylogenetic tree data. Enter a file name, a path and file name, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text for a Newick file.

Description

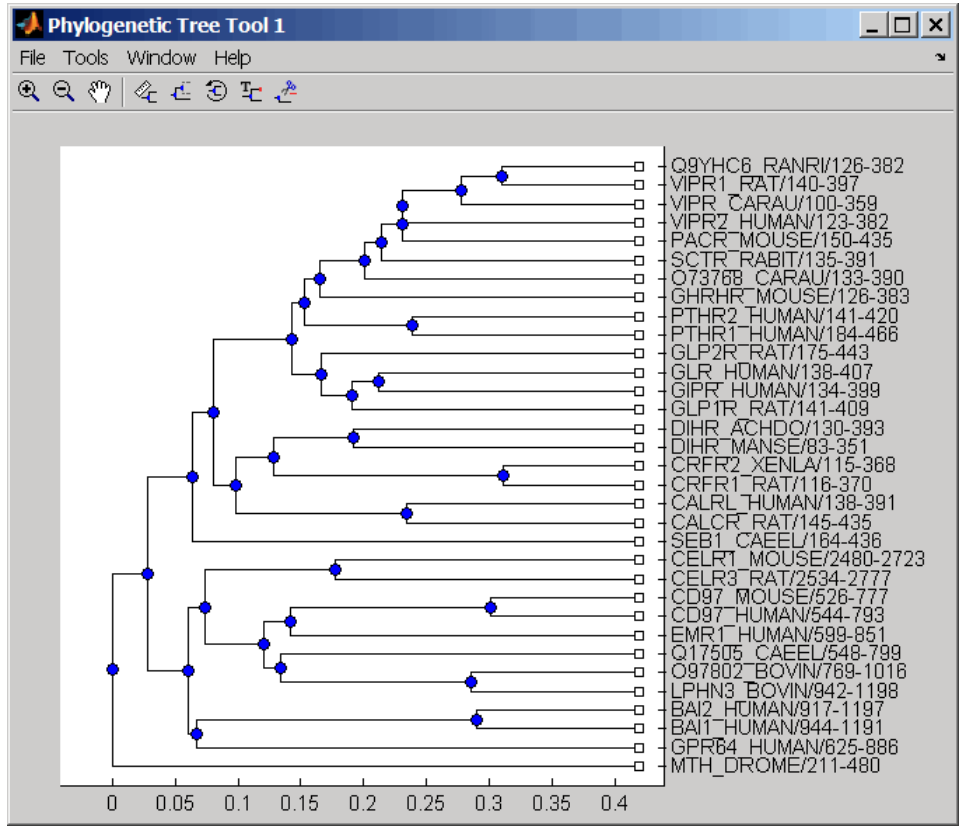
`phytreetool` is an interactive GUI that allows you to view, edit, and explore phylogenetic tree data. This GUI allows branch pruning, reordering, renaming, and distance exploring. It can also open or save Newick formatted files.

`phytreetool(Tree)` loads data from a `phytree` object in the MATLAB workspace into the GUI.

`phytreetool(File)` loads data from a Newick formatted file into the GUI.

Examples

```
tr= phytreeread('pf00002.tree')
phytreetool(tr)
```



See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreeread`, `phytreewrite`

Bioinformatics Toolbox methods of phytree object: `cluster`, `plot`, `view`

Purpose

Write phylogenetic tree object to Newick-formatted file

Syntax

```
phytreewrite(File, Tree)
phytreewrite(Tree)
phytreewrite(..., 'Distances', DistancesValue, ...)
phytreewrite(..., 'BranchNames', BranchNamesValue, ...)
```

Arguments

File	String specifying a Newick-formatted file. Enter either a file name or a path and file name supported by your operating system (ASCII text file).
Tree	Phylogenetic tree object, either created with `phytree` (object constructor function) or imported using the `phytreeread` function.

Description

`phytreewrite(File, Tree)` copies the contents of a `phytree` object from the MATLAB workspace to a file. Data in the file uses the Newick format for describing trees.

The Newick tree format can be found at

```
http://evolution.genetics.washington.edu/phylip/newicktree.html
```

`phytreewrite(Tree)` opens the Save Phylogenetic Tree As dialog box for you to enter or select a file name.

`phytreewrite(..., 'PropertyName', PropertyValue, ...)` calls `phytreewrite` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each *PropertyName* in single quotation marks. Each *PropertyName* is case insensitive. These property name/property value pairs are as follows:

`phytreewrite(..., 'Distances', DistancesValue, ...)` specifies whether to exclude the distances from the output. *DistancesValue* can be `true` (default) or `false`.

`phytreewrite(..., 'BranchNames', BranchNamesValue, ...)` specifies whether to exclude the branch names from the output. *`BranchNamesValue`* can be `true` (default) or `false`.

Examples

Read tree data from a Newick-formatted file.

```
tr = phytreeread('pf00002.tree')
```

Remove all the mouse proteins and view the pruned tree.

```
ind = getbyname(tr,'mouse');
tr = prune(tr,ind);
view(tr)
```

Write pruned tree data to a file.

```
phytreewrite('newtree.tree', tr)
```

See Also

Bioinformatics Toolbox functions: `multialignwrite`, `phytree` (object constructor), `phytreeread`, `phytreetool`, `seqlinkage`

Bioinformatics Toolbox object: `phytree object`

Bioinformatics Toolbox methods of phytree object: `getnewickstr`

Purpose

Render clustergram and dendrograms for clustergram object

Syntax

```
plot(CGObject)
plot(CGObject, HFig)
HFig = plot(...)
```

Arguments

CGObject	Clustergram object created with the function `clustergram`.
HFig	Handle to a MATLAB Figure window.

Description

`plot(`*`CGObject`*`)` renders a heat map and dendrograms for *`CGObject`*, a clustergram object, in a MATLAB Figure window.

`plot(`*`CGObject`*`, `*`HFig`*`)` renders a heat map and dendrograms for *`CGObject`*, a clustergram object, in a MATLAB Figure window with the handle *`HFig`*.

`HFig` `= plot(...)` returns the handle to the figure. The graphic properties are stored as application data in the figure handle.

Examples

Plot the clustergram object created in the Examples section of the `clustergram` function.

```
plot(cgo)
```

See Also

Bioinformatics Toolbox function: `clustergram` (object constructor)

Bioinformatics Toolbox object: clustergram object

Bioinformatics Toolbox methods of a clustergram object: `addTitle`, `addXLabel`, `addYLabel`, `get`, `set`, `view`

plot (DataMatrix)

Purpose

Draw 2-D line plot of DataMatrix object

Syntax

```
plot(DMObj1)
plot(DMObj1, DMObj2)
plot(..., LineSpec)
```

Arguments

DMObj1, *DMObj2*	DataMatrix objects, such as created by `DataMatrix` (object constructor).

Note If both *DMObj1* and *DMObj2* are input arguments, one of the inputs can be a MATLAB numeric array.

LineSpec	String specifying a line style, marker symbol, and color of the plotted lines. For more information on these specifiers, see `LineSpec`.

Description

`plot(`*DMObj1*`)` plots the columns of a DataMatrix object *DMObj1* versus their index.

`plot(`*DMObj1*`, `*DMObj2*`)` plots the data from *DMObj1* and *DMObj2*, two DataMatrix objects, or one DataMatrix object and one MATLAB numeric array.

- If *DMObj1* and *DMObj2* are both vectors, they must have the same number of elements, and `plot` plots one vector versus the other vector, creating a single line.
- If one is a vector and one a scalar, `plot` plots discrete points vertically or horizontally, at the scalar value.
- If one is a vector and one a matrix, the number of elements in the vector must equal either the number of rows or the number of columns in the matrix, and `plot` plots the vector versus each row or column in the matrix.

- If both are matrices, they must have the same size (number of rows and columns), and `plot` plots each column in *`DMObj1`* versus the corresponding column in *`DMObj2`*.

`plot(..., LineSpec)` plots all lines as defined by *`LineSpec`*, a character string specifying a line style, marker symbol, and/or color.

Note For a list of line style, marker, and color specifiers, see `LineSpec`.

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

MATLAB function: `plot`

plot (HeatMap)

Purpose

Render heat map for HeatMap object

Syntax

```
plot(HMObject)
plot(HMObject, HFig)
HFig = plot(...)
```

Arguments

HMObject	HeatMap object created with the function `HeatMap`.
HFig	Handle to a MATLAB Figure window.

Description

`plot(`*`HMObject`*`)` renders a heat map for *`HMObject`*, a HeatMap object, in a MATLAB Figure window.

`plot(`*`HMObject`*`, `*`HFig`*`)` renders a heat map for *`HMObject`*, a HeatMap object, in a MATLAB Figure window with the handle *`HFig`*.

`HFig` `= plot(...)` returns the handle to the figure. The graphic properties are stored as application data in the figure handle.

Examples

Plot the HeatMap object created in the Examples section of the `HeatMap` function.

```
plot(hmo)
```

See Also

Bioinformatics Toolbox function: `HeatMap` (object constructor)

Bioinformatics Toolbox object: HeatMap object

Bioinformatics Toolbox methods of a HeatMap object: `addTitle`, `addXLabel`, `addYLabel`, `view`

Purpose

Draw phylogenetic tree

Syntax

```
plot(Tree)
plot(Tree, ActiveBranches)
H = plot(...)
plot(..., 'Type', TypeValue, ...)
plot(..., 'Orientation', OrientationValue, ...)
plot(..., 'Rotation', RotationValue, ...)
plot(..., 'BranchLabels', BranchLabelsValue, ...)
plot(..., 'LeafLabels', LeafLabelsValue, ...)
plot(..., 'TerminalLabels', TerminalLabelsValue, ...)
plot(..., 'LLRotation', LLRotationValue, ...)
```

Arguments

Tree	Phylogenetic tree object created, such as created with the `phytree` constructor function.
ActiveBranches	Logical array of size `numBranches`-by-`1` indicating the active branches, which are displayed in the Figure window.
TypeValue	String specifying a method for drawing the phylogenetic tree. Choices are: • `'square'` (default) • `'angular'` • `'radial'` • `'equalangle'` • `'equaldaylight'`

OrientationValue String specifying the position of the root node, and hence the orientation of a phylogram or cladogram tree, when the `'Type'` property is `'square'` or `'angular'`. Choices are:

- `'left'` (default)
- `'right'`
- `'top'`
- `'bottom'`

RotationValue Scalar between `0` (default) and `360` specifying rotation angle (in degrees) of the phylogenetic tree in the Figure window, when the `'Type'` property is `'radial'`, `'equalangle'`, or `'equaldaylight'`.

BranchLabelsValue Controls the display of branch labels next to branch nodes. Choices are `true` or `false` (default).

LeafLabelsValue Controls the display of leaf labels next to leaf nodes. Choices are `true` or `false`. Default is:

- `true` — When the `'Type'` property is `'radial'`, `'equalangle'`, or `'equaldaylight'`
- `false` — When the `'Type'` property is `'square'` or `'angular'`

TerminalLabels	Controls the display of terminal labels over the axis tick labels, when the `'Type'` property is `'square'` or `'angular'`. Choices are `true` (default) or `false`.
LLRotationValue	Controls the rotation of leaf labels so that the text aligns to the root node, when the `'Type'` property is `'radial'`, `'equalangle'`, or `'equaldaylight'`. Choices are `true` or `false` (default).

Return Values

H

Structure with handles to seven graph elements. The structure includes the following fields:

- `axes`
- `BranchLines`
- `BranchDots`
- `LeafDots`
- `branchNodeLabels`
- `leafNodeLabels`
- `terminalNodeLabels`

Tip Use the `set` function with the handles in this structure and their related properties to modify the plot. For more information on the properties you can modify using the `axes` handle, see axes_props. For more information on the properties you can modify using the `BranchLines`, `BranchDots`, or `LeafDots` handle, see line_props. For more information on the properties you can modify using the `branchNodeLabels`, `leafNodeLabels`, or `terminalNodeLabels` handle, see Text Properties.

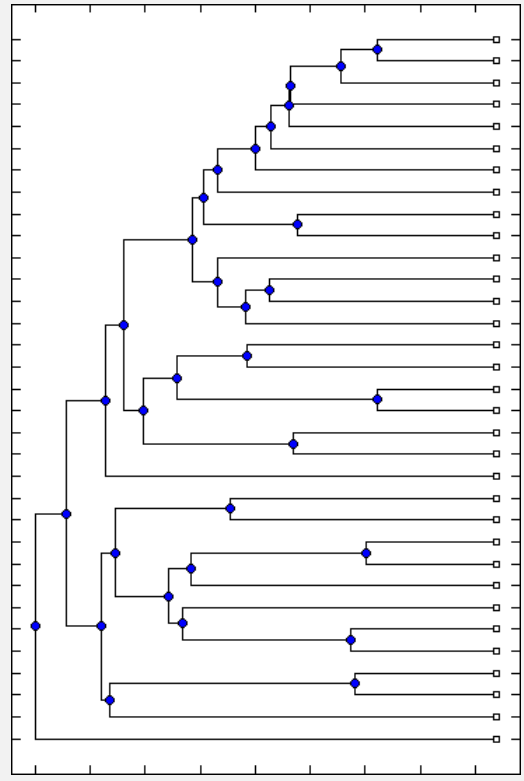
Description

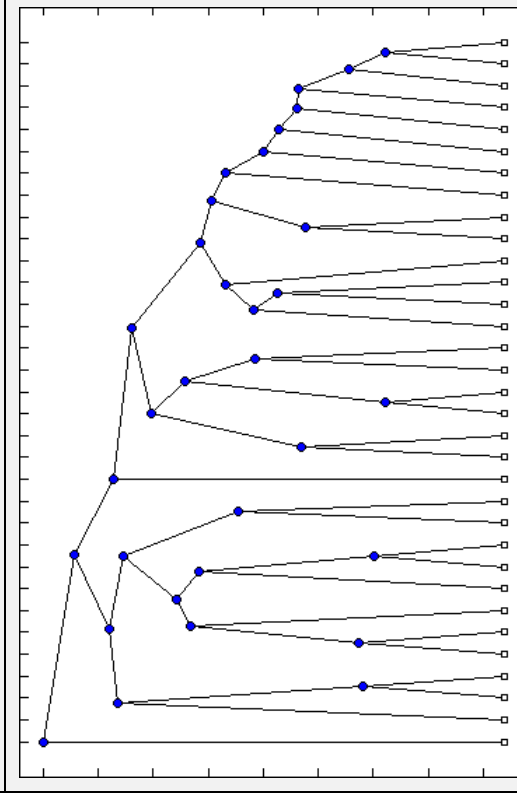
`plot(Tree)` draws a phylogenetic tree object into a figure as a phylogram. The significant distances between branches and nodes are in the horizontal direction. Vertical distances are arbitrary and have no significance.

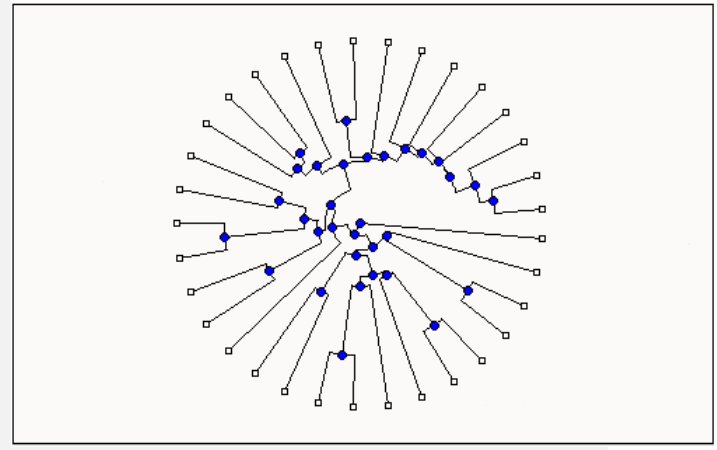
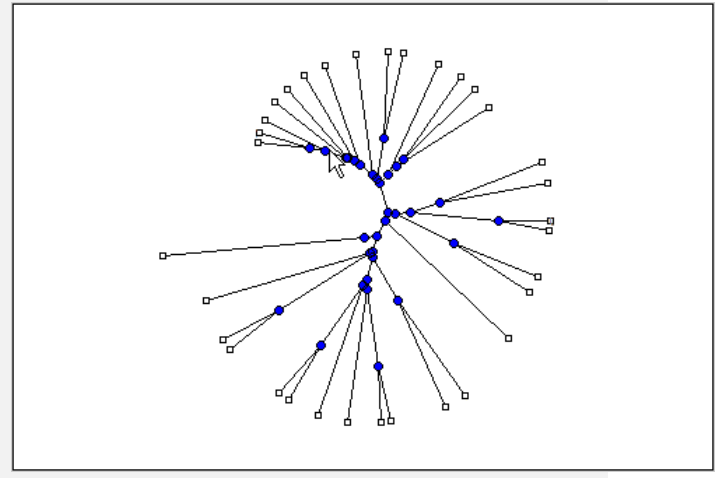
`plot(Tree, ActiveBranches)` hides the nonactive branches and all of their descendants in the Figure window. *`ActiveBranches`* is a logical array of size `numBranches`-by-`1` indicating the active branches.

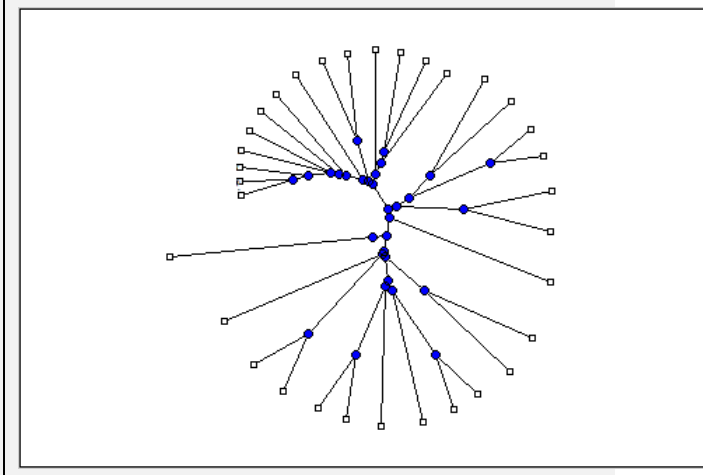
`H = plot(...)` returns a structure with handles to seven graph elements.

`plot(..., 'Type', TypeValue, ...)` specifies a method for rendering the phylogenetic tree. Choices are as follows.

Rendering Type	Description
`'square'` (default)	

Rendering Type	Description
`'angular'`	

Rendering Type	Description
`'radial'`	
`'equalangle'`	

Rendering Type	Description
	Tip This rendering type hides the significance of the root node and emphasizes clusters, thereby making it useful for visually assessing clusters and detecting outliers.
`'equaldaylight'`	 **Tip** This rendering type hides the significance of the root node and emphasizes clusters, thereby making it useful for visually assessing clusters and detecting outliers.

`plot(..., 'Orientation', OrientationValue, ...)` specifies the orientation of the root node, and hence the orientation of a phylogram or cladogram phylogenetic tree in the Figure window, when the `'Type'` property is `'square'` or `'angular'`.

`plot(..., 'Rotation', RotationValue, ...)` specifies the rotation angle (in degrees) of the phylogenetic tree in the Figure window, when the `'Type'` property is `'radial'`, `'equalangle'`, or `'equaldaylight'`. Choices are any scalar between `0` (default) and `360`.

`plot(..., 'BranchLabels', BranchLabelsValue, ...)` hides or displays branch labels next to the branch nodes. Choices are `true` or `false` (default).

`plot(..., 'LeafLabels', LeafLabelsValue, ...)` hides or displays leaf labels next to the leaf nodes. Choices are `true` or `false`. Default is:

- `true` — When the `'Type'` property is `'radial'`, `'equalangle'`, or `'equaldaylight'`
- `false` — When the `'Type'` property is `'square'` or `'angular'`

`plot(..., 'TerminalLabels', TerminalLabelsValue, ...)` hides or displays terminal labels over the axis tick labels, when the `'Type'` property is `'square'` or `'angular'`. Choices are `true` (default) or `false`.

`plot(..., 'LLRotation', LLRotationValue, ...)` controls the rotation of leaf labels so that the text aligns to the root node, when the `'Type'` property is `'radial'`, `'equalangle'`, or `'equaldaylight'`. Choices are `true` or `false` (default).

Examples

```
% Create a phytree object from a file
tr = phytreeread('pf00002.tree')
% Plot the tree and return a structure with handles to the
% graphic elements of the phytree object
h = plot(tr,'Type','radial')

% Modify the font size and color of the branch node labels
% by using one of the handles in the return structure
set(h.branchNodeLabels,'FontSize',6,'Color',[.5 .5 .5])
```

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreeread`, `phytreetool`, `seqlinkage`, `seqneighjoin`

Bioinformatics Toolbox object: phytree object

Bioinformatics Toolbox methods of phytree object: `cluster`, `view`

plus (DataMatrix)

Purpose

Add DataMatrix objects

Syntax

```
DMObjNew = plus(DMObj1, DMObj2)
DMObjNew = DMObj1 + DMObj2
DMObjNew = plus(DMObj1, B)
DMObjNew = DMObj1 + B
DMObjNew = plus(B, DMObj1)
DMObjNew = B + DMObj1
```

Arguments

DMObj1, *DMObj2*	DataMatrix objects, such as created by `DataMatrix` (object constructor).
B	MATLAB numeric or logical array.

Return Values

DMObjNew	DataMatrix object created by addition.

Description

DMObjNew = `plus(`*DMObj1*`, `*DMObj2*`)` or the equivalent *DMObjNew* = *DMObj1* + *DMObj2* performs an element-by-element addition of the DataMatrix objects *DMObj1* and *DMObj2* and places the results in *DMObjNew*, another DataMatrix object. *DMObj1* and *DMObj2* must have the same size (number of rows and columns), unless one is a scalar (1-by-1 DataMatrix object). The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*, unless *DMObj1* is a scalar; then they are the same as *DMObj2*.

DMObjNew = `plus(`*DMObj1*`, `*B*`)` or the equivalent *DMObjNew* = *DMObj1* + *B* performs an element-by-element addition of *DMObj1*, a DataMatrix object, and *B*, a numeric or logical array, and places the results in *DMObjNew*, another DataMatrix object. *DMObj1* and *B* must have the same size (number of rows and columns), unless *B* is a scalar. The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*.

DMObjNew = plus(*B*, *DMObj1*) or the equivalent *DMObjNew* = *B* + *DMObj1* performs an element-by-element addition of *B*, a numeric or logical array, and *DMObj1*, a DataMatrix object, and places the results in *DMObjNew*, another DataMatrix object. *DMObj1* and *B* must have the same size (number of rows and columns), unless *B* is a scalar. The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*.

Note Arithmetic operations between a scalar DataMatrix object and a nonscalar array are not supported.

MATLAB calls *DMObjNew* = plus(*X*, *Y*) for the syntax *DMObjNew* = *X* + *Y* when *X* or *Y* is a DataMatrix object.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: minus

power (DataMatrix)

Purpose

Array power DataMatrix objects

Syntax

```
DMObjNew = power(DMObj1, DMObj2)
DMObjNew = DMObj1 .^ DMObj2
DMObjNew = power(DMObj1, B)
DMObjNew = DMObj1 .^ B
DMObjNew = power(B, DMObj1)
DMObjNew = B .^ DMObj1
```

Arguments

DMObj1, *DMObj2*	DataMatrix objects, such as created by `DataMatrix` (object constructor).
B	MATLAB numeric or logical array.

Return Values

DMObjNew	DataMatrix object created by array power.

Description

DMObjNew = `power(`*DMObj1*`, `*DMObj2*`)` or the equivalent *DMObjNew* = *DMObj1* `.^` *DMObj2* performs an element-by-element power of the DataMatrix objects *DMObj1* and *DMObj2* and places the results in *DMObjNew*, another DataMatrix object. In other words, `power` raises each element in *DMObj1* by the corresponding element in *DMObj2*. *DMObj1* and *DMObj2* must have the same size (number of rows and columns), unless one is a scalar (1-by-1 DataMatrix object). The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*, unless *DMObj1* is a scalar; then they are the same as *DMObj2*.

DMObjNew = `power(`*DMObj1*`, `*B*`)` or the equivalent *DMObjNew* = *DMObj1* `.^` *B* performs an element-by-element power of the DataMatrix object *DMObj1* and *B*, a numeric or logical array, and places the results in *DMObjNew*, another DataMatrix object. In other words, `power` raises each element in *DMObj1* by the corresponding element in *B*. *DMObj1* and *B* must have the same size (number of rows and columns), unless *B* is a scalar. The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*.

DMObjNew = power(*B*, *DMObj1*) or the equivalent *DMObjNew* = *B* .^ *DMObj1* performs an element-by-element power of *B*, a numeric or logical array, and the DataMatrix object *DMObj1*, and places the results in *DMObjNew*, another DataMatrix object. In other words, power raises each element in *B* by the corresponding element in *DMObj1*.*DMObj1* and *B* must have the same size (number of rows and columns), unless *B* is a scalar. The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*.

Note Arithmetic operations between a scalar DataMatrix object and a nonscalar array are not supported.

MATLAB calls *DMObjNew* = power(*X*, *Y*) for the syntax *DMObjNew* = *X* .^ *Y* when *X* or *Y* is a DataMatrix object.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: times

probelibraryinfo

Purpose

Create table of probe set library information

Syntax

```
ProbeInfo = probelibraryinfo(CELStruct, CDFStruct)
```

Arguments

CELStruct	Structure created by the `affyread` function from an Affymetrix CEL file.
CDFStruct	Structure created by the `affyread` function from an Affymetrix CDF library file associated with the CEL file.

Return Values

ProbeInfo

Three-column matrix with the same number of rows as the `Probes` field of the *CELStruct*.

- Column 1 — Probe set ID/name to which the probe belongs. (Probes that do not belong to a probe set in the CDF library file have probe set ID/name equal to `0`.)
- Column 2 — Contains the probe pair number.
- Column 3 — Indicates if the probe is a perfect match (`1`) or mismatch (`-1`) probe.

Description

ProbeInfo = `probelibraryinfo(`*CELStruct*`, `*CDFStruct*`)` creates a table of information linking the probe data from *CELStruct*, a structure created from an Affymetrix CEL file, with probe set information from *CDFStruct*, a structure created from an Affymetrix CDF file.

Note Affymetrix probe pair indexing is `0`-based, while MATLAB software indexing is `1`-based. The output from `probelibraryinfo` is `1`-based.

Examples

The following example uses a sample CEL file and the CDF library file from the *E. coli* Antisense Genome array, which you can download from:

```
http://www.affymetrix.com/support/technical/sample_data/demo_data.affx
```

After you download the demo data, you will need the Affymetrix Data Transfer Tool to extract the CEL file from a DTT file. You can download the Affymetrix Data Transfer Tool from:

```
http://www.affymetrix.com/products/software/specific/dtt.affx
```

The following example assumes that the `Ecoli-antisense-121502.CEL` file is stored on the MATLAB search path or in the current directory. It also assumes that the associated CDF library file, `Ecoli_ASv2.CDF`, is stored at `D:\Affymetrix\LibFiles\Ecoli`.

1. Read the contents of a CEL file into a MATLAB structure.

```
celStruct = affyread('Ecoli-antisense-121502.CEL');
```

2. Read the contents of a CDF file into a MATLAB structure.

```
cdfStruct = affyread('D:\Affymetrix\LibFiles\Ecoli\Ecoli_ASv2.CDF');
```

3. Extract probe set library information.

```
ProbeInfo = probelibraryinfo(celStruct, cdfStruct);
```

4. Determine the probe set to which the 1104th probe belongs.

```
cdfStruct.ProbeSets(ProbeInfo(1104,1)).Name

ans =

thrA_b0002_at
```

See Also

Bioinformatics Toolbox functions: `affyread`, `celintensityread`, `probesetlink`, `probesetlookup`, `probesetplot`, `probesetvalues`

probesetlink

Purpose

Display probe set information on NetAffx Web site

Syntax

```
probesetlink(AffyStruct, PS)
URL = probesetlink(AffyStruct, PS)
probesetlink(AffyStruct, PS, ...'Source', SourceValue, ...)
probesetlink(AffyStruct, PS, ...'Browser',
BrowserValue, ...)
URL = probesetlink(AffyStruct, PS, ...'NoDisplay',
   NoDisplayValue, ...)
```

Arguments

AffyStruct	Structure created by the `affyread` function from an Affymetrix CHP file or an Affymetrix CDF library file.
PS	Probe set index or the probe set ID/name.
SourceValue	Controls the linking to the data source (for example, GenBank or Flybase) for the probe set (instead of linking to the NetAffx Web site). Choices are `true` or `false` (default).

Note This property requires the GIN library file associated with the CHP or CDF file to be located in the same directory as the CDF library file.

BrowserValue	Controls the display of the probe set information in your system's default Web browser. Choices are `true` or `false` (default).
NoDisplayValue	Controls the return of *URL* without opening a Web browser. Choices are `true` or `false` (default).

Return Values

URL	URL for the probe set information.

Description

`probesetlink(AffyStruct, PS)` opens a Web Browser window displaying information on the NetAffx Web site about a probe set specified by `PS`, a probe set index or the probe set ID/name, and `AffyStruct`, a structure created from an Affymetrix CHP file or Affymetrix CDF library file.

`URL = probesetlink(AffyStruct, PS)` also returns the URL (linking to the NetAffx Web site) for the probe set information.

`probesetlink(AffyStruct, PS, ...'PropertyName', PropertyValue, ...)` calls `probesetlink` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`probesetlink(AffyStruct, PS, ...'Source', SourceValue, ...)` controls the linking to the data source (for example, GenBank or Flybase) for the probe set (instead of linking to the NetAffx Web site). Choices are `true` or `false` (default).

Note The `'Source'` property requires the GIN library file associated with the CHP or CDF file to be located in the same directory as the CDF library file.

`probesetlink(AffyStruct, PS, ...'Browser', BrowserValue, ...)` controls the display of the probe set information in your system's default Web browser. Choices are `true` or `false` (default).

`URL = probesetlink(AffyStruct, PS, ...'NoDisplay', NoDisplayValue, ...)` controls the return of the URL without opening a Web browser. Choices are `true` or `false` (default).

Note The NetAffx Web site requires you to register and provide a user name and password.

Examples

The following example uses a sample CHP file and the CDF library file from the *E. coli* Antisense Genome array, which you can download from:

```
http://www.affymetrix.com/support/technical/sample_data/demo_data.affx
```

After you download the demo data, you will need the Affymetrix Data Transfer Tool to extract the CHP file from a DTT file. You can download the Affymetrix Data Transfer Tool from:

```
http://www.affymetrix.com/products/software/specific/dtt.affx
```

The following example assumes that the `Ecoli-antisense-121502.CHP` file is stored on the MATLAB search path or in the current directory. It also assumes that the associated CDF library file, `Ecoli_ASv2.CDF`, is stored at `D:\Affymetrix\LibFiles\Ecoli`.

1. Read the contents of a CHP file into a MATLAB structure.

```
chpStruct = affyread('Ecoli-antisense-121502.CHP',...
             'D:\Affymetrix\LibFiles\Ecoli');
```

2. Display information from the NetAffx Web site for the `argG_b3172_at` probe set.

```
probesetlink(chpStruct,'argG_b3172_at')
```

See Also

Bioinformatics Toolbox functions: `affyread`, `celintensityread`, `probelibraryinfo`, `probesetlookup`, `probesetplot`, `probesetvalues`

Purpose

Look up information for Affymetrix probe set

Syntax

```
PSStruct = probesetlookup(AffyStruct, ID)
```

Arguments

AffyStruct	Structure created by the `affyread` function from an Affymetrix CHP file or an Affymetrix CDF library file for expression assays.
ID	String or cell array of strings specifying one or more probe set IDs/names or gene IDs.

Return Values

PSStruct — Structure or array of structures containing the following fields for a probe set:

- `Identifier` — Gene ID associated with the probe set
- `ProbeSetName` — Probe set ID/name
- `CDFIndex` — Index into the CDF structure for the probe set
- `GINIndex` — Index into the GIN structure for the probe set
- `Description` — Description of the probe set
- `Source` — Source(s) of the probe set
- `SourceURL` — Source URL(s) for the probe set

Description

PSStruct = probesetlookup(*AffyStruct*, *ID*) returns a structure or an array of structures containing information for an Affymetrix probe set specified by `ID`, a string or cell array of strings specifying one or more probe set IDs/names or gene IDs, and by *AffyStruct*, a structure created from an Affymetrix CHP file or Affymetrix CDF library file for expression assays.

Note This function works with CHP files and CDF files for expression assays only. It requires that the GIN library file associated with the CHP file or CDF file to be located in the same directory as the CDF library file.

Examples

The following example uses the CDF library file from the *E. coli* Antisense Genome array, which you can download from:

```
http://www.affymetrix.com/support/technical/sample_data/demo_data.affx
```

The following example assumes that the `Ecoli_ASv2.CDF` library file is stored at `D:\Affymetrix\LibFiles\Ecoli`.

1. Read the contents of a CDF library file into a MATLAB structure.

```
cdfStruct = affyread('D:\Affymetrix\LibFiles\Ecoli\Ecoli_ASv2.CDF');
```

2. Look up the gene ID (`Identifier`) associated with the `argG_b3172_at` probe set.

```
probesetlookup(cdfStruct,'argG_b3172_at')

ans =

      Identifier: '3315278'
    ProbeSetName: 'argG_b3172_at'
        CDFIndex: 5213
        GINIndex: 3074
     Description: [1x82 char]
          Source: 'NCBI EColi Genome'
       SourceURL: [1x74 char]
```

See Also

Bioinformatics Toolbox functions: `affyread`, `celintensityread`, `probelibraryinfo`, `probesetlink`, `probesetplot`, `probesetvalues`, `rmabackadj`

Purpose

Plot Affymetrix probe set intensity values

Syntax

```
probesetplot(CELStruct, CDFStruct, PS)
probesetplot(CELStruct, CDFStruct, PS, ...'GeneName',
GeneNameValue, ...)
probesetplot(CELStruct, CDFStruct, PS, ...'Field',
   FieldValue, ...)
probesetplot(CELStruct, CDFStruct, PS, ...'ShowStats',
   ShowStatsValue, ...)
```

Arguments

CELStruct	Structure created by the `affyread` function from an Affymetrix CEL file.
CDFStruct	Structure created by the `affyread` function from an Affymetrix CDF library file associated with the CEL file.
PS	Probe set index or the probe set ID/name.
GeneNameValue	Controls whether the probe set name or the gene name is used for the title of the plot. Choices are `true` or `false` (default).

Note The `'GeneName'` property requires the GIN library file associated with the CEL and CDF files to be located in the same directory as the CDF library file from which *CDFStruct* was created.

FieldValue	String specifying the type of data to plot. Choices are: • 'Intensity' (default) • 'StdDev' • 'Background' • 'Pixels' • 'Outlier'
ShowStatsValue	Controls whether the mean and standard deviation lines are included in the plot. Choices are true or false (default).

Description

probesetplot(*CELStruct*, *CDFStruct*, *PS*) plots the PM (perfect match) and MM (mismatch) intensity values for a specified probe set. *CELStruct* is a structure created by the affyread function from an Affymetrix CEL file. *CDFStruct* is a structure created by the affyread function from an Affymetrix CDF library file associated with the CEL file. *PS* is the probe set index or the probe set ID/name.

Note MATLAB software uses 1-based indexing for probe set numbers, while the Affymetrix CDF file uses 0-based indexing for probe set numbers. For example, CDFStruct.ProbeSets(1) has a ProbeSetNumber of 0 in the ProbePairs field.

---

probesetplot(*CELStruct*, *CDFStruct*, *PS*, ...'*PropertyName*', *PropertyValue*, ...) calls probesetplot with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`probesetplot(CELStruct, CDFStruct, PS, ...'GeneName', GeneNameValue, ...)` controls whether the probe set name or the gene name is used for the title of the plot. Choices are `true` or `false` (default).

Note The `'GeneName'` property requires the GIN library file associated with the CEL and CDF files to be located in the same directory as the CDF library file from which *`CDFStruct`* was created.

`probesetplot(CELStruct, CDFStruct, PS, ...'Field', FieldValue, ...)` specifies the type of data to plot. Choices are:

- `'Intensity'` (default)
- `'StdDev'`
- `'Background'`
- `'Pixels'`
- `'Outlier'`

`probesetplot(CELStruct, CDFStruct, PS, ...'ShowStats', ShowStatsValue, ...)` controls whether the mean and standard deviation lines are included in the plot. Choices are `true` or `false` (default).

Examples

The following example use a sample CEL file and the CDF library file from the *E. coli* Antisense Genome array, which you can download from:

```
http://www.affymetrix.com/support/technical/sample_data/demo_data.affx
```

After you download the demo data, you will need the Affymetrix Data Transfer Tool to extract the CEL file from a DTT file. You can download the Affymetrix Data Transfer Tool from:

```
http://www.affymetrix.com/products/software/specific/dtt.affx
```

The following example assumes that the `Ecoli-antisense-121502.CEL` file is stored on the MATLAB search path or in the current directory. It also assumes that the associated CDF library file, `Ecoli_ASv2.CDF`, is stored at `D:\Affymetrix\LibFiles\Ecoli`.

1. Read the contents of a CEL file into a MATLAB structure.

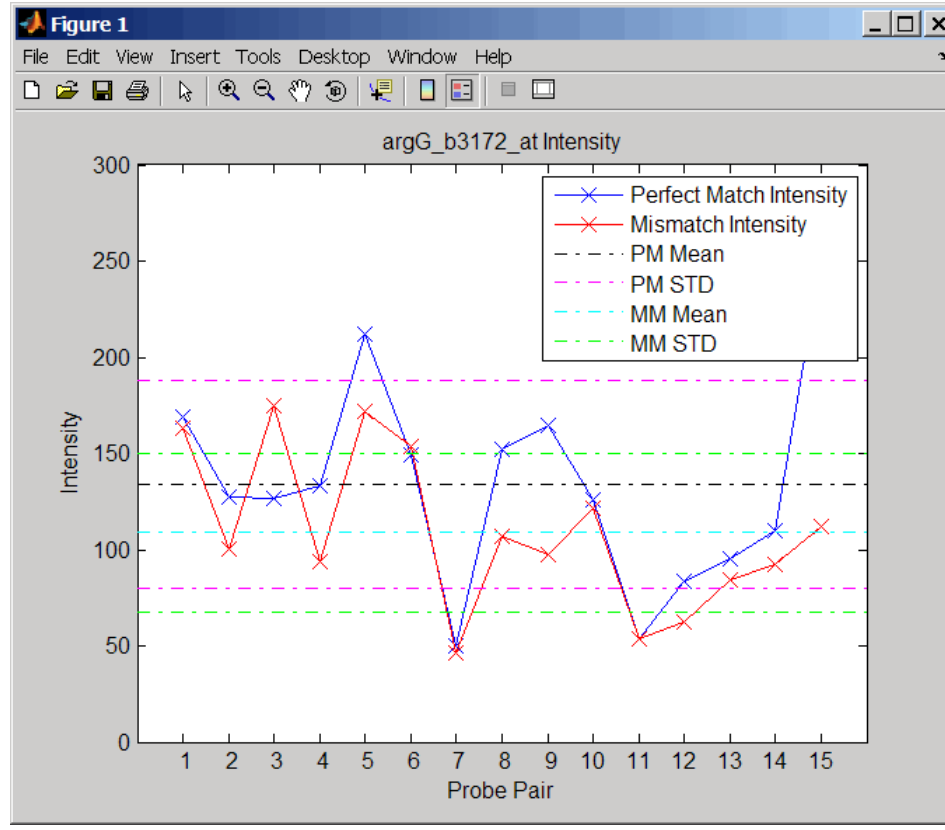
```
celStruct = affyread('Ecoli-antisense-121502.CEL');
```

2. Read the contents of a CDF file into a MATLAB structure.

```
cdfStruct = affyread('D:\Affymetrix\LibFiles\Ecoli\Ecoli_ASv2.CDF');
```

3. Plot the PM and MM intensity values of the `argG_b3172_at` probe set, including the mean and standard deviation.

```
probesetplot(celStruct, cdfStruct, 'argG_b3172_at','showstats', true)
```



See Also

Bioinformatics Toolbox functions: `affyread`, `celintensityread`, `probesetlink`, `probesetlookup`, `probesetvalues`

probesetvalues

Purpose

Create table of Affymetrix probe set intensity values

Syntax

```
PSValues = probesetvalues(CELStruct, CDFStruct, PS)
PSValues = probesetvalues(CELStruct, CDFStruct, PS,
   'Background', BackgroundValue)
ColumnNames = probesetvalues
```

Arguments

CELStruct	Structure created by the `affyread` function from an Affymetrix CEL file.
CDFStruct	Structure created by the `affyread` function from an Affymetrix CDF library file associated with the CEL file.
PS	Probe set index or the probe set ID/name.
BackgroundValue	Controls the background correction in the calculation. Choices are: • `true` (default) — Background values from the `Background` field in the *PSValues* matrix are used to calculate the probe intensity values. • `false` — Background values are not calculated. • A vector of precalculated background values (such as returned by the `zonebackadj` function) whose length is equal to the number of probes in *CELStruct*. These background values are used to calculate the probe intensity values.

Tip Including background correction in the calculation of the probe intensity values can be slow. Therefore, setting `'Background'` to `false` can speed up the calculation. However, the values returned in the `'Background'` field of the *`PSValues`* matrix will be zero.

Return Values

`PSValues`	Twenty-column matrix with one row for each probe pair in the probe set.
`ColumnNames`	Cell array of strings containing the column names of the *`PSValues`* matrix. This is returned only when you call `probesetvalues` with no input arguments.

Description

`PSValues` = `probesetvalues(`*`CELStruct`*`, `*`CDFStruct`*`, `*`PS`*`)` creates a table of intensity values for *`PS`*, a probe set, from the probe-level data in *`CELStruct`*, a structure created by the `affyread` function from an Affymetrix CEL file. *`PS`* is a probe set index or probe set ID/name from *`CDFStruct`*, a structure created by the `affyread` function from an Affymetrix CDF library file associated with the CEL file. *`PSValues`* is a twenty-column matrix with one row for each probe pair in the probe set. The columns correspond to the following fields.

Column	Field	Description
1	`'ProbeSetNumber'`	Number identifying the probe set to which the probe pair belongs.
2	`'ProbePairNumber'`	Index of the probe pair within the probe set.

Column	Field	Description
3	'UseProbePair'	This field is for backward compatibility only and is not currently used.
4	'Background'	Estimated background of probe intensity values of the probe pair.
5	'PMPosX'	*x*-coordinate of the perfect match probe.
6	'PMPosY'	*y*-coordinate of the perfect match probe.
7	'PMIntensity'	Intensity value of the perfect match probe.
8	'PMStdDev'	Standard deviation of intensity value of the perfect match probe.
9	'PMPixels'	Number of pixels in the cell containing the perfect match probe.
10	'PMOutlier'	True/false flag indicating if the perfect match probe was marked as an outlier.
11	'PMMasked'	True/false flag indicating if the perfect match probe was masked.
12	'MMPosX'	*x*-coordinate of the mismatch probe.
13	'MMPosY'	*y*-coordinate of the mismatch probe.
14	'MMIntensity'	Intensity value of the mismatch probe.
15	'MMStdDev'	Standard deviation of intensity value of the mismatch probe.
16	'MMPixels'	Number of pixels in the cell containing the mismatch probe.

Column	Field	Description
17	'MMOutlier'	True/false flag indicating if the mismatch probe was marked as an outlier.
18	'MMMasked'	True/false flag indicating if the mismatch probe was masked.
19	'GroupNumber'	Number identifying the group to which the probe pair belongs. For expression arrays, this is always 1. For genotyping arrays, this is typically 1 (allele A, sense), 2 (allele B, sense), 3 (allele A, antisense), or 4 (allele B, antisense).
20	'Direction'	Number identifying the direction of the probe pair. 1 = sense and 2 = antisense.

Note MATLAB software uses 1-based indexing for probe set numbers, while the Affymetrix CDF file uses 0-based indexing for probe set numbers. For example, CDFStruct.ProbeSets(1) has a ProbeSetNumber of 0 in the ProbePairs field.

PSValues = probesetvalues(*CELStruct*, *CDFStruct*, *PS*, 'Background', *BackgroundValue*) controls the background correction in the calculation. *BackgroundValue* can be:

- true (default) — Background values from the Background field in the *PSValues* matrix are used to calculate the probe intensity values.
- false — Background values are not calculated.
- A vector of precalculated background values (such as returned by the zonebackadj function) whose length is equal to the number of

probes in *CELStruct*. These background values are used to calculate the probe intensity values.

Tip Including background correction in the calculation of the probe intensity values can be slow. Therefore, setting `'Background'` to `false` can speed up the calculation. However, the values returned in the `'Background'` field of the *PSValues* matrix will be zero.

ColumnNames = `probesetvalues` returns a cell array of strings containing the column names of the *PSValues* matrix. *ColumnNames* is returned only when you call `probesetvalues` without input arguments. The information contained in *ColumnNames* is common to all Affymetrix GeneChip arrays.

Examples

The following example uses a sample CEL file and the CDF library file from the *E. coli* Antisense Genome array, which you can download from:

```
http://www.affymetrix.com/support/technical/sample_data/demo_data.affx
```

After you download the demo data, you will need the Affymetrix Data Transfer Tool to extract the CEL file from a DTT file. You can download the Affymetrix Data Transfer Tool from:

```
http://www.affymetrix.com/products/software/specific/dtt.affx
```

The following example assumes that the `Ecoli-antisense-121502.CEL` file is stored on the MATLAB search path or in the current directory. It also assumes that the associated CDF library file, `Ecoli_ASv2.CDF`, is stored at `D:\Affymetrix\LibFiles\Ecoli`.

1. Read the contents of a CEL file into a MATLAB structure.

   ```
   celStruct = affyread('Ecoli-antisense-121502.CEL');
   ```

2. Read the contents of a CDF file into a MATLAB structure.

```
cdfStruct = affyread('D:\Affymetrix\LibFiles\Ecoli\Ecoli_ASv2.CDF');
```

3 Use the `zonebackadj` function to return a matrix or cell array of vectors containing the estimated background values for each probe.

```
[baData,zones,background] = zonebackadj(celStruct,'cdf',cdfStruct);
```

4 Create a table of intensity values for the `argG_b3172_at` probe set.

```
psvals = probesetvalues(celStruct, cdfStruct, 'argG_b3172_at',...
         'background',background);
```

See Also

Bioinformatics Toolbox functions: `affyread`, `celintensityread`, `probelibraryinfo`, `probesetlink`, `probesetlookup`, `probesetplot`, `rmabackadj`, `zonebackadj`

profalign

Purpose

Align two profiles using Needleman-Wunsch global alignment

Syntax

```
Prof = profalign(Prof1, Prof2)
[Prof, H1, H2] = profalign(Prof1, Prof2)
profalign(..., 'ScoringMatrix', ScoringMatrixValue, ...)
profalign(..., 'GapOpen', {G1Value, G2Value}, ...)
profalign(..., 'ExtendGap', {E1Value, E2Value}, ...)
profalign(..., 'ExistingGapAdjust', ExistingGapAdjustValue,
   ...)
profalign(..., 'TerminalGapAdjust', TerminalGapAdjustValue,
   ...)
profalign(..., 'ShowScore', ShowScoreValue, ...)
```

Description

`Prof = profalign(Prof1, Prof2)` returns a new profile (*Prof*) for the optimal global alignment of two profiles (*Prof1*, *Prof2*). The profiles (*Prof1*, *Prof2*) are numeric arrays of size `[(4 or 5 or 20 or 21) x Profile Length]` with counts or weighted profiles. Weighted profiles are used to down-weight similar sequences and up-weight divergent sequences. The output profile is a numeric matrix of size `[(5 or 21) x New Profile Length]` where the last row represents gaps. Original gaps in the input profiles are preserved. The output profile is the result of adding the aligned columns of the input profiles.

`[Prof, H1, H2] = profalign(Prof1, Prof2)` returns pointers that indicate how to rearrange the columns of the original profiles into the new profile.

`profalign(..., 'PropertyName', PropertyValue, ...)` calls `profalign` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`profalign(..., 'ScoringMatrix', ScoringMatrixValue, ...)` defines the scoring matrix (*ScoringMatrixValue*) to be used for the alignment. The default is `'BLOSUM50'` for amino acids or `'NUC44'` for nucleotide sequences.

`profalign(..., 'GapOpen', {G1Value, G2Value}, ...)` sets the penalties for opening a gap in the first and second profiles respectively. *`G1Value`* and *`G2Value`* can be either scalars or vectors. When using a vector, the number of elements is one more than the length of the input profile. Every element indicates the position specific penalty for opening a gap between two consecutive symbols in the sequence. The first and the last elements are the gap penalties used at the ends of the sequence. The default gap open penalties are `{10,10}`.

`profalign(..., 'ExtendGap', {E1Value, E2Value}, ...)` sets the penalties for extending a gap in the first and second profile respectively. *`E1Value`* and *`E2Value`* can be either scalars or vectors. When using a vector, the number of elements is one more than the length of the input profile. Every element indicates the position specific penalty for extending a gap between two consecutive symbols in the sequence. The first and the last elements are the gap penalties used at the ends of the sequence. If `ExtendGap` is not specified, then extensions to gaps are scored with the same value as `GapOpen`.

`profalign(..., 'ExistingGapAdjust', ExistingGapAdjustValue, ...)`, if *`ExistingGapAdjustValue`* is `false`, turns off the automatic adjustment based on existing gaps of the position-specific penalties for opening a gap. When *`ExistingGapAdjustValue`* is `true` (default), for every profile position, `profalign` proportionally lowers the penalty for opening a gap toward the penalty of extending a gap based on the proportion of gaps found in the contiguous symbols and on the weight of the input profile.

`profalign(..., 'TerminalGapAdjust', TerminalGapAdjustValue, ...)`, when *`TerminalGapAdjustValue`* is `true`, adjusts the penalty for opening a gap at the ends of the sequence to be equal to the penalty for extending a gap. Default is `false`.

`profalign(..., 'ShowScore', ShowScoreValue, ...)`, when *`ShowScoreValue`* is `true`, displays the scoring space and the winning path.

Examples

1 Read in sequences and create profiles.

```
ma1 = ['RGTANCDMQDA';'RGTAHCDMQDA';'RRRAPCDL-DA'];
ma2 = ['RGTHCDLADAT';'RGTACDMADAA'];
p1  = seqprofile(ma1,'gaps','all','counts',true);
p2  = seqprofile(ma2,'counts',true);
```

2 Merge two profiles into a single one by aligning them.

```
p = profalign(p1,p2);
seqlogo(p)
```

3 Use the output pointers to generate the multiple alignment.

```
[p, h1, h2] = profalign(p1,p2);
ma = repmat('-',5,12);
ma(1:3,h1) = ma1;
ma(4:5,h2) = ma2;
disp(ma)
```

4 Increase the gap penalty before cysteine in the second profile.

```
gapVec = 10 + [p2(aa2int('C'),:) 0] * 10
p3 = profalign(p1,p2,'gapopen',{10,gapVec});
seqlogo(p3)
```

5 Add a new sequence to a profile without inserting new gaps into the profile.

```
gapVec = [0 inf(1,11) 0];
p4 = profalign(p3,seqprofile('PLHFMSVLWDVQQWP'),...
               'gapopen',{gapVec,10});
seqlogo(p4)
```

See Also

Bioinformatics Toolbox functions: `hmmprofalign`, `multialign`, `nwalign`, `seqprofile`, `seqconsensus`

Purpose

Open Protein Plot window to investigate properties of amino acid sequence

Syntax

```
proteinplot
proteinplot (SeqAA)
```

Arguments

SeqAA Either of the following:

- String of single-letter codes specifying an amino acid sequence. For valid letter codes, see the table Mapping Amino Acid Letter Codes to Integers on page 3-2. Unknown characters are mapped to `0`.
- MATLAB structure containing a `Sequence` field that contains an amino acid sequence, such as returned by `fastaread`, `getgenpept`, `genpeptread`, `getpdb`, or `pdbread`.

Description

The Protein Plot window lets you analyze and compare properties of a single amino acid sequence. It displays smoothed line plots of various properties such as the hydrophobicity of the amino acids in the sequence.

`proteinplot` opens the Protein Plot window.

`proteinplot (SeqAA)` opens the Protein Plot window and loads *SeqAA*, an amino acid sequence, into the window.

Tip You can analyze and compare properties of an amino acid sequence from the MATLAB command line also by using the `proteinpropplot` function.

Examples

Importing Sequences into the Protein Plot Window

You can import a sequence into the Protein Plot window from the MATLAB command line.

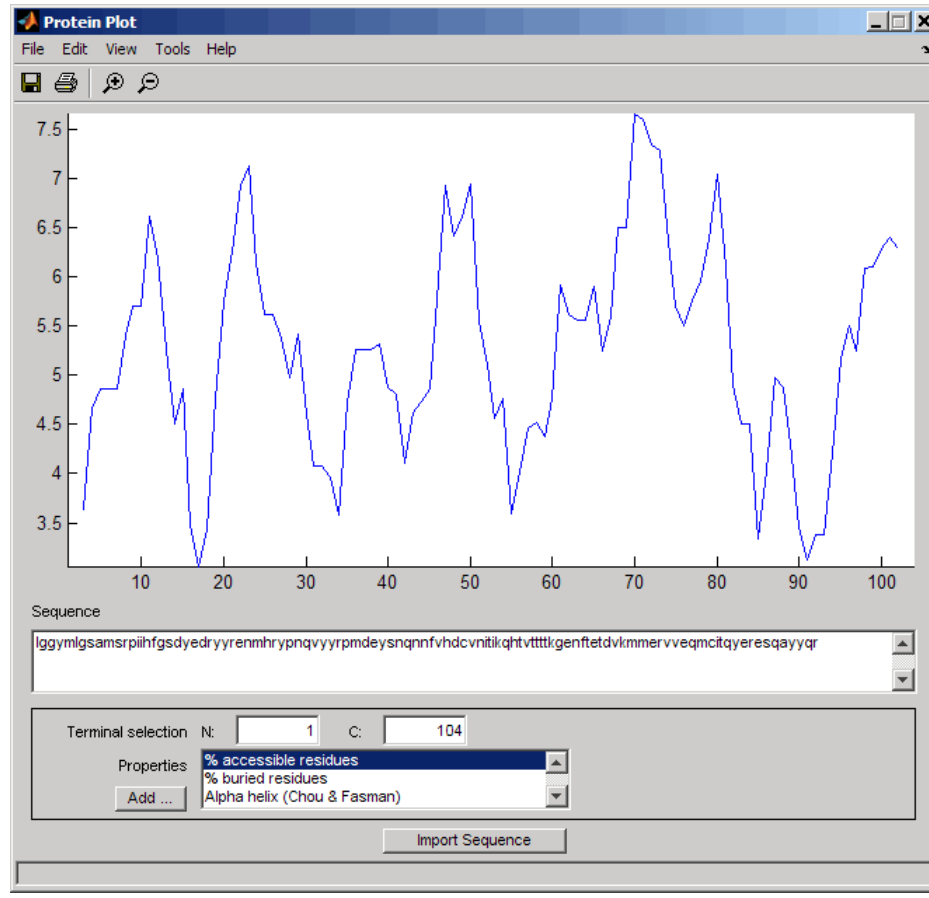
1. Retrieve an amino acid sequence from the Protein Data Bank (PDB) database.

   ```
   prion = getpdb('1HJM', 'SEQUENCEONLY', true);
   ```

2. Load the amino acid sequence into the Protein Plot window.

   ```
   proteinplot(prion)
   ```

   The Protein Plot window opens, and the sequence appears in the **Sequence** text box.



You can import a sequence after the Protein Plot window is open by doing either of the following:

- Type or paste an amino acid sequence into the **Sequence** text box.
- Click the **Import Sequence** button to open the Import dialog box From the **Import From** list, select one of the following:
  - **Workspace** — To select a variable from the MATLAB Workspace

- **Text File** — To select a text file
- **FASTA File** — To select a FASTA-formatted file
- **GenPept File** — To select a GenPept-formatted file
- **GenPept Database** — To specify an accession number in the GenPept database

Viewing Properties of Amino Acids

Select a property from the **Properties** drop-down list box to display a smoothed plot of the property values along the sequence. You can select multiple properties from the list by holding down **Shift** or **Ctrl** while selecting properties. When you select two properties, the plots are displayed using a PLOTYY-style layout, with one *y*-axis on the left and one on the right. For all other selections, a single *y*-axis is displayed. When displaying one or two properties, the *y* values displayed are the actual property values. When displaying three or more properties, the values are normalized to the range 0–1.

Accessing Information About the Properties

You can access information about the properties from the **Help** menu.

1. Select **Help > References**. The Help browser opens with a list of properties and references.
2. Scroll down to locate the property of interest.

Using Other Features in the Protein Plot Window

The **Terminal Selection** boxes (N and C) let you choose to plot only part of the sequence. By default, all of the sequence is plotted.

You can add your own properties by clicking on the **Add** button next to the **Properties** list. This opens a Property dialog box that lets you specify the value for each of the amino acids. The **Display Text** box lets you specify the text that will be displayed in the **Properties** list on the main Protein Plot window. You can also save the property values to an M-file for future use by typing a file name into the **Filename** text box.

The default smoothing method is an unweighted linear moving average with a window length of five residues. You can change this by selecting **Edit > Filter Window Options**. The dialog box lets you select the **Window Size** from `5` to `29` residues. Increasing the window size produces a smoother plot. You can modify the shape of the smoothing window by changing the **Edge Weight** factor. And you can choose the smoothing function to be a linear moving average, an exponential moving average or a linear Lowess smoothing.

The **File** menu lets you import a sequence, save the plot that you have created to a Figure file, export the data values in the figure to a workspace variable or to a MAT-file, export the figure to a normal Figure window for customizing, or print the figure.

The **Edit** menu lets you create a new property, to reset the property values to the default values, and to modify the smoothing parameters with the **Configuration Values** menu item.

The **View** menu lets you turn the toolbar on and off, and to add a legend to the plot.

The **Tools** menu lets you zoom in and zoom out of the plot, to view **Data Statistics** such as mean, minimum and maximum values of the plot, and to normalize the values of the plot from `0` to `1`.

The **Help** menu lets you view this document and to see the references for the sequence properties included with the Protein Plot window.

See Also

Bioinformatics Toolbox functions: `aacount`, `atomiccomp`, `molviewer`, `molweight`, `pdbdistplot`, `proteinpropplot`, `seqtool`

MATLAB function: `plotyy`

proteinpropplot

Purpose

Plot properties of amino acid sequence

Syntax

```
proteinpropplot (SeqAA)
proteinpropplot(SeqAA, ...'PropertyTitle',
PropertyTitleValue, ...)
proteinpropplot(SeqAA, ...'Startat', StartatValue, ...)
proteinpropplot(SeqAA, ...'Endat', EndatValue, ...)
proteinpropplot(SeqAA, ...'Smoothing', SmoothingValue, ...)
proteinpropplot(SeqAA, ...'EdgeWeight',
EdgeWeightValue, ...)
proteinpropplot(SeqAA, ...'WindowLength',
WindowLengthValue,
    ...)
```

Arguments

SeqAA

Amino acid sequence. Enter any of the following:

- Character string of letters representing an amino acid
- Vector of integers representing an amino acid, such as returned by `aa2int`
- Structure containing a `Sequence` field that contains an amino acid sequence, such as returned by `getembl`, `getgenpept`, or `getpdb`

PropertyTitleValue

String that specifies the property to plot. Default is `Hydrophobicity (Kyte & Doolittle)`. To display a list of properties to plot, enter a empty string for *PropertyTitleValue*. For example, type:

```
proteinpropplot(sequence, 'propertytitle', '')
```

Tip To access references for the properties, view the `proteinpropplot` m-file.

StartatValue	Integer that specifies the starting point for the plot from the N-terminal end of the amino acid sequence *SeqAA*. Default is 1.
EndatValue	Integer that specifies the ending point for the plot from the N-terminal end of the amino acid sequence *SeqAA*. Default is `length(`*SeqAA*`)`.
SmoothingValue	String the specifies the smoothing method. Choices are: • `linear` (default) • `exponential` • `lowess`
EdgeWeightValue	Value that specifies the edge weight used for linear and exponential smoothing methods. Decreasing this value emphasizes peaks in the plot. Choices are any value ≥0 and ≤1. Default is 1.
WindowLengthValue	Integer that specifies the window length for the smoothing method. Increasing this value gives a smoother plot that shows less detail. Default is 11.

Description

`proteinpropplot (`*SeqAA*`)` displays a plot of the hydrophobicity (Kyte and Doolittle, 1982) of the residues in sequence SeqAA.

`proteinpropplot(`*SeqAA*`, ...'`*PropertyName*`', `*PropertyValue*`, ...)` calls `proteinpropplot` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed

in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`proteinpropplot(SeqAA, ...'PropertyTitle', PropertyTitleValue, ...)` specifies a property to plot for the amino acid sequence *SeqAA*. Default is `Hydrophobicity (Kyte & Doolittle)`. To display a list of possible properties to plot, enter an empty string for *PropertyTitleValue*. For example, type:

```
proteinpropplot(sequence, 'propertytitle', '')
```

Tip To access references for the properties, view the `proteinpropplot` M-file.

`proteinpropplot(SeqAA, ...'Startat', StartatValue, ...)` specifies the starting point for the plot from the N-terminal end of the amino acid sequence *SeqAA*. Default is `1`.

`proteinpropplot(SeqAA, ...'Endat', EndatValue, ...)` specifies the ending point for the plot from the N-terminal end of the amino acid sequence *SeqAA*. Default is `length(SeqAA)`.

`proteinpropplot(SeqAA, ...'Smoothing', SmoothingValue, ...)` specifies the smoothing method. Choices are:

- `linear` (default)
- `exponential`
- `lowess`

`proteinpropplot(SeqAA, ...'EdgeWeight', EdgeWeightValue, ...)` specifies the edge weight used for linear and exponential smoothing methods. Decreasing this value emphasizes peaks in the plot. Choices are any value ≥`0` and ≤`1`. Default is `1`.

`proteinpropplot(SeqAA, ...'WindowLength', WindowLengthValue, ...)` specifies the window length for the

smoothing method. Increasing this value gives a smoother plot that shows less detail. Default is 11.

Examples

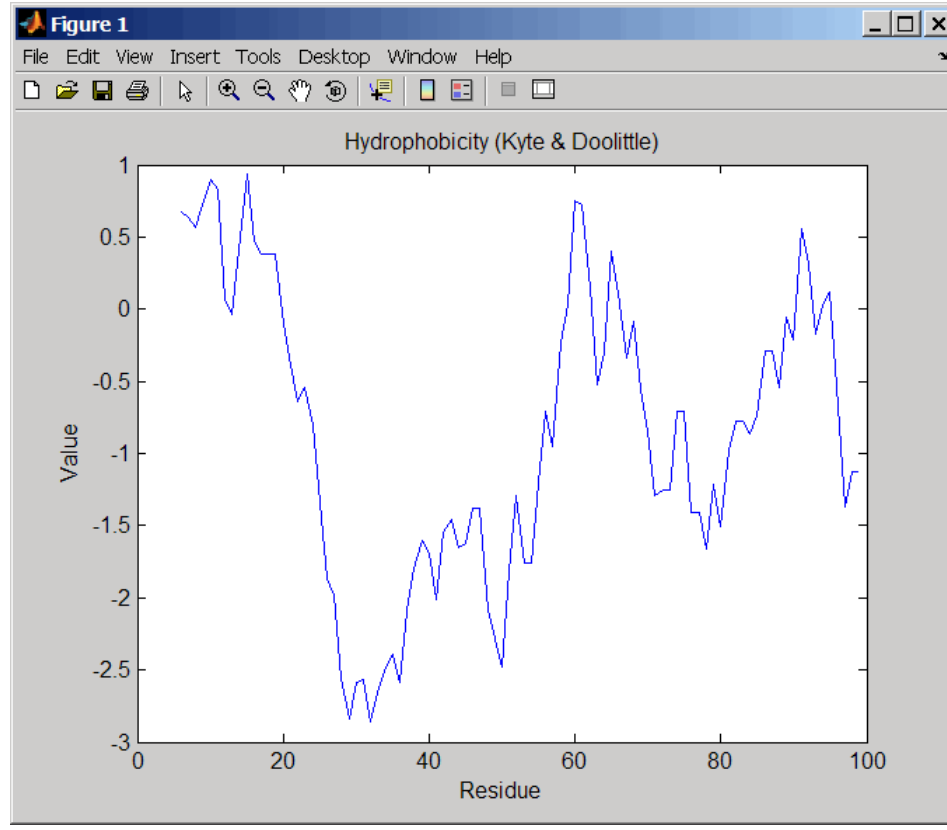
Plotting Hydrophobicity

1 Use the `getpdb` function to retrieve a protein sequence.

```
prion = getpdb('1HJM', 'SEQUENCEONLY', true);
```

2 Plot the hydrophobicity (Kyte and Doolittle, 1982) of the residues in the sequence.

```
proteinpropplot(prion)
```



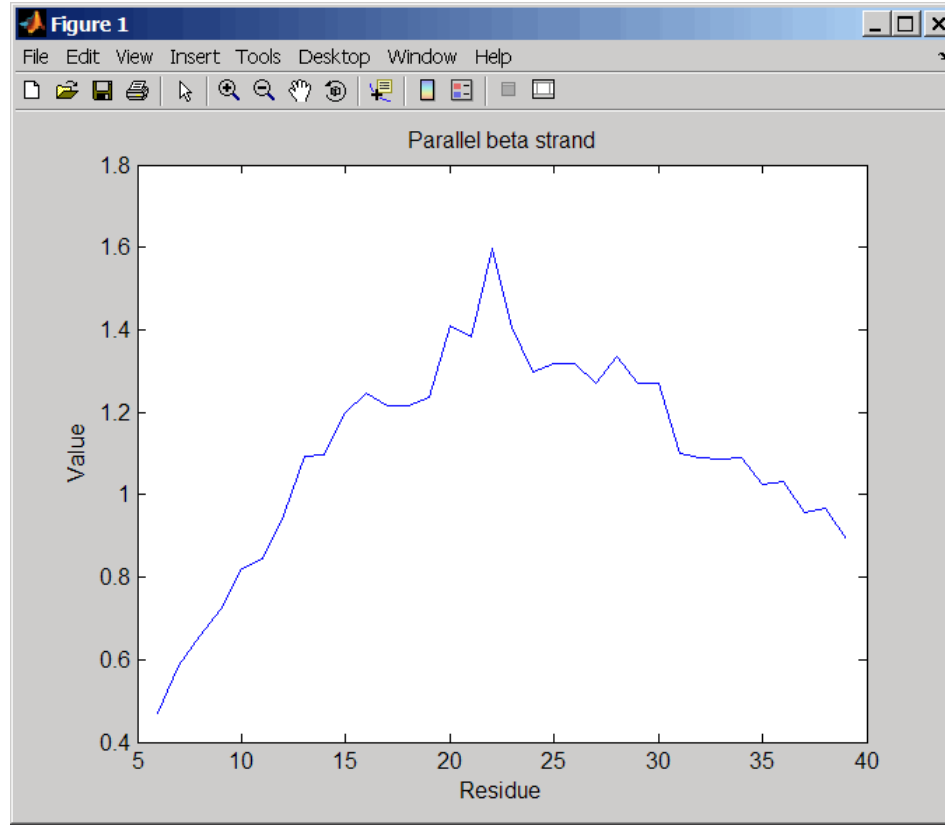
Plotting Parallel Beta Strand

1 Use the `getgenpept` function to retrieve a protein sequence.

```
s = getgenpept('aad50640');
```

2 Plot the conformational preference for parallel beta strand for the residues in the sequence.

```
proteinpropplot(s,'propertytitle','Parallel beta strand')
```



References

[1] Kyte, J., and Doolittle, R.F. (1982). A simple method for displaying the hydropathic character of a protein. J Mol Biol *157(1)*, 105–132.

See Also

Bioinformatics Toolbox functions: `aacount`, `atomiccomp`, `molviewer`, `molweight`, `pdbdistplot`, `proteinplot`, `ramachandran`, `seqtool`

MATLAB function: `plotyy`

prune (phytree)

Purpose

Remove branch nodes from phylogenetic tree

Syntax

```
T2 = prune(T1, Nodes)
T2 = prune(T1, Nodes, 'Mode','Exclusive')
```

Arguments

T1	Phylogenetic object created with the `phytree` constructor function.
Nodes	Nodes to remove from tree.
Mode	Property to control the method of pruning. Enter either `'Inclusive'` or `'Exclusive'`. The default value is `'Inclusive'`.

Description

`T2 = prune(T1, Nodes)` removes the nodes listed in the vector *Nodes* from the tree *T1*. `prune` removes any branch or leaf nodes listed in *Nodes* and all their descendants from the tree *T1*, and returns the modified tree *T2*. The parent nodes are connected to the 'brothers' as required. `Nodes` in the tree are labeled as `[1:numLeaves]` for the leaves and as `[numLeaves+1:numLeaves+numBranches]` for the branches. *Nodes* can also be a logical array of size `[numLeaves+numBranches x 1]` indicating the nodes to be removed.

`T2 = prune(T1, Nodes, 'Mode','Exclusive')` changes the `Mode` property for pruning to `'Exclusive'` and removes only the descendants of the nodes listed in the vector *Nodes*. Nodes that do not have a predecessor become leaves in the list *Nodes*. In this case, pruning is the process of reducing a tree by turning some branch nodes into leaf nodes, and removing the leaf nodes under the original branch.

Examples

Load a phylogenetic tree created from a protein family

```
tr = phytreeread('pf00002.tree');
view(tr)
```

Remove all the 'mouse' proteins

```
ind = getbyname(tr,'mouse');
tr = prune(tr,ind);
view(tr)
```

Remove potential outliers in the tree

```
[sel,sel_leaves] = select(tr,'criteria','distance',...
                              'threshold',.3,...
                              'reference','leaves',...
                              'exclude','leaves',...
                              'propagate','toleaves');
tr = prune(tr,~sel_leaves)
view(tr)
```

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreetool`

Bioinformatics Toolbox object: phytree object

Bioinformatics Toolbox methods of phytree object: `select`, `get`

bioma.ExpressionSet.pubMedID

Purpose

Retrieve or set PubMed IDs in ExpressionSet object

Syntax

```
PMIDs = pubMedID(ESObj)
NewESObj = pubMedID(ESObj, NewPMIDs)
```

Description

`PMIDs = pubMedID(ESObj)` returns a string or cell array of strings containing the PubMed IDs from a MIAME object in an ExpressionSet object.

`NewESObj = pubMedID(ESObj, NewPMIDs)` replaces the PubMed IDs in the MIAME object in `ESObj`, an ExpressionSet object, with `NewPMIDs`, a string or cell array of strings specifying new PubMed IDs, and returns `NewESObj`, a new ExpressionSet object.

Inputs

`ESObj`

Object of the `bioma.ExpressionSet` class.

`NewPMIDs`

String or cell array of strings containing new PubMed IDs.

Outputs

`PMIDs`

String or cell array of strings containing the PubMed IDs from a MIAME object in an ExpressionSet object.

`NewESObj`

Object of the `bioma.ExpressionSet` class, returned after replacing the PubMed IDs.

Examples

Construct an ExpressionSet object from `EDObj`, an ExptData object, `MDObj2`, a MetaData object containing sample variable information, and `MIAMEObj`, a MIAME object. Retrieve the PubMed identifiers stored in the MIAME object stored in the ExpressionSet object:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
```

```
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Construct MIAME object
MIAMEObj = MIAME(geoStruct);
% Import bioma package to make constructor function
% available
import bioma.*
% Construct ExpressionSet object
ESObj = ExpressionSet(EDObj, 'SData', MDObj2, 'EInfo', MIAMEObj);
% Retrieve PubMed IDs from the MIAME object
PMIDs = pubMedID(ESObj)
```

See Also

`bioma.ExpressionSet` | `bioma.data.MIAME`

How To

- “Working with ExpressionSet Objects”

Related Links

- http://www.ncbi.nlm.nih.gov/pubmed/

quantilenorm

Purpose

Quantile normalization over multiple arrays

Syntax

```
NormData = quantilenorm(Data)
NormData = quantilenorm(...,'MEDIAN', true)
NormData = quantilenorm(...,'DISPLAY', true)
```

Description

`NormData = quantilenorm(Data)`, where the columns of *`Data`* correspond to separate chips, normalizes the distributions of the values in each column.

Note If *`Data`* contains NaN values, then *`NormData`* will also contain NaN values at the corresponding positions.

`NormData = quantilenorm(...,'MEDIAN', true)` takes the median of the ranked values instead of the mean.

`NormData = quantilenorm(...,'DISPLAY', true)` plots the distributions of the columns and of the normalized data.

Examples

```
load yeastdata
normYeastValues = quantilenorm(yeastvalues,'display',1);
```

See Also

`affygcrma`, `affyrma`, `malowess`, `manorm`, `rmabackadj`, `rmasummary`

Purpose

Draw Ramachandran plot for Protein Data Bank (PDB) data

Syntax

```
ramachandran(PDBid)
ramachandran(File)
ramachandran(PDBStruct)
RamaStruct = ramachandran(...)
ramachandran(..., 'Chain', ChainValue, ...)
ramachandran(..., 'Plot', PlotValue, ...)
ramachandran(..., 'Model', ModelValue, ...)
ramachandran(..., 'Glycine', GlycineValue, ...)
ramachandran(..., 'Regions', RegionsValue, ...)
ramachandran(..., 'RegionDef', RegionDefValue, ...)
```

Arguments

PDBid

String specifying a unique identifier for a protein structure record in the PDB database.

Note Each structure in the PDB database is represented by a four-character alphanumeric identifier. For example, `4hhb` is the identifier for hemoglobin.

File

String specifying a file name or a path and file name. The referenced file is a Protein Data Bank (PDB)-formatted file. If you specify only a file name, that file must be on the MATLAB search path or in the MATLAB Current Directory.

PDBStruct

MATLAB structure containing PDB-formatted data, such as returned by `getpdb` or `pdbread`.

ChainValue

String or cell array of strings that specifies the chain(s) to compute the torsion angles for and plot.

Choices are:

- `'All'` (default) — Torsion angles for all chains are computed and plotted.
- A string specifying the chain ID, which is case sensitive.
- A cell array of strings specifying chain IDs, which are case sensitive.

PlotValue

String specifying how to plot chains. Choices are:

- `'None'` — Plots nothing.
- `'Separate'` — Plots torsion angles for all specified chains in separate plots.
- `'Combined'` (default) — Plots torsion angles for all specified chains in one combined plot.

ModelValue

Integer that specifies the structure model to consider. Default is `1`.

GlycineValue

Controls the highlighting of glycine residues with a circle in the plot. Choices are `true` or `false` (default).

RegionsValue

Controls the drawing of Ramachandran reference regions in the plot. Choices are `true` or `false` (default).

The default regions are core right-handed alpha, core beta, core left-handed alpha, and allowed, with the core regions corresponding to data points of preferred values of psi/phi angle pairs, and the allowed regions corresponding to possible, but disfavored values of psi/phi angle pairs, based on simple energy considerations. The boundaries of these default regions are based on the calculations by Morris et al., 1992.

Note If using the default colormap, red = right-handed core alpha, core beta, and core left-handed alpha, while yellow = allowed.

RegionDefValue

MATLAB structure or array of structures (if specifying multiple regions) containing information (name, color, and boundaries) for custom reference regions in a Ramachandran plot. Each structure must contain the following fields:

- `Name` — String specifying a name for the region.
- `Color` — String or three-element numeric vector of RGB values specifying a color for the region in the plot.
- `Patch` — A 2-by-N matrix of values, the first row containing torsion angle phi (Φ) values, and the second row containing torsion angle psi (Ψ) values. When psi/phi angle pairs are plotted, the data points specify boundaries for

the region. N is the number of data points needed to define the region.

Tip If you specify custom reference regions in which a smaller region is contained or covered by a larger region, list the structure for the smaller region first in the array so that it is plotted last and visible in the plot.

Return Values

RamaStruct

MATLAB structure or array of structures (if protein contains multiple chains). Each structure contains the following fields:

- `Angles`
- `ResidueNum`
- `ResidueName`
- `Chain`
- `HPoints`

For descriptions of the fields, see the following table.

Description

A Ramachandran plot is a plot of the torsion angle phi, Φ, (torsion angle between the `C-N-CA-C` atoms) versus the torsion angle psi, Ψ, (torsion angle between the `N-CA-C-N` atoms) for each residue of a protein sequence.

`ramachandran(`*`PDBid`*`)` generates the Ramachandran plot for the protein specified by the PDB database identifier *`PDBid`*.

`ramachandran(`*`File`*`)` generates the Ramachandran plot for the protein specified by *`File`*, a PDB-formatted file.

`ramachandran(PDBStruct)` generates the Ramachandran plot for the protein stored in *`PDBStruct`*, a MATLAB structure containing PDB-formatted data, such as returned by `getpdb` or `pdbread`.

`RamaStruct` `= ramachandran(...)` returns a MATLAB structure or array of structures (if protein contains multiple chains). Each structure contains the following fields.

Field	Description
`Angles`	Three-column matrix containing the torsion angles phi (Φ), psi (Ψ), and omega (ω) for each residue in the sequence, ordered by residue sequence number. The number of rows in the matrix is equal to the number of rows in the `ResidueNum` column vector, which can be used to determine which residue corresponds to each row in the `Angles` matrix. **Note** The `Angles` matrix contains a row for each number in the range of residue sequence numbers, including residue sequence numbers missing from the PDB file. Rows corresponding to residue sequence numbers missing from the PDB file contain the value `NaN`.

Field	Description
`ResidueNum`	Column vector containing the residue sequence numbers from the PDB file. **Note** The `ResidueNum` vector starts with one of the following: • The lowest residue sequence number (if the lowest residue sequence number is negative or zero) • The number `1` (if the lowest residue sequence number is positive) The `ResidueNum` vector ends with the highest residue sequence number and includes all numbers in the range, including residue sequence numbers missing from the PDB file. The angles listed in the `Angles` matrix are in the same order as the residue sequence numbers in the `ResidueNum` vector. Therefore, you can use the `ResidueNum` vector to determine which residue corresponds to each row in the `Angles` matrix.
`ResidueName`	Column vector containing the residue names for the protein.
`Chain`	A string specifying the chains in the protein.
`HPoints`	Handle to the data points in the plot.

`ramachandran(..., '`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `ramachandran` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`ramachandran(..., 'Chain', ChainValue, ...)` specifies the chain(s) to compute the torsion angles for and plot. Choices are:

- `'All'` (default) — Torsion angles for all chains are computed and plotted.
- A string specifying the chain ID, which is case sensitive.
- A cell array of strings specifying chain IDs, which are case sensitive.

`ramachandran(..., 'Plot', PlotValue, ...)` specifies how to plot chains. Choices are:

- `'None'` — Plots nothing.
- `'Separate'` — Plots torsion angles for all specified chains in separate plots.
- `'Combined'` (default) — Plots torsion angles for all specified chains in one combined plot.

`ramachandran(..., 'Model', ModelValue, ...)` specifies the structure model to consider. Default is `1`.

`ramachandran(..., 'Glycine', GlycineValue, ...)` controls the highlighting of glycine residues with a circle in the plot. Choices are `true` or `false` (default).

`ramachandran(..., 'Regions', RegionsValue, ...)` controls the drawing of Ramachandran reference regions in the plot. Choices are `true` or `false` (default).

The default regions are core right-handed alpha, core beta, core left-handed alpha, and allowed, with the core regions corresponding to data points of preferred values of psi/phi angle pairs, and the allowed regions corresponding to possible, but disfavored values of psi/phi angle pairs, based on simple energy considerations. The boundaries of these default regions are based on the calculations by Morris et al., 1992.

Note If using the default colormap, then red = core right-handed alpha, core beta, and core left-handed alpha, while yellow = allowed.

`ramachandran(..., 'RegionDef', RegionDefValue, ...)` specifies information (name, color, and boundary) for custom reference regions in a Ramachandran plot. *`RegionDefValue`* is a MATLAB structure or array of structures containing the following fields:

- `Name` — String specifying a name for the region.
- `Color` — String or three-element numeric vector of RGB values specifying a color for the region in the plot.
- `Patch` — A 2-by-N matrix of values, the first row containing torsion angle phi (Φ) values, and the second row containing torsion angle psi (Ψ) values. When psi/phi angle pairs are plotted, the data points specify a boundary for the region. N is the number of data points needed to define the region.

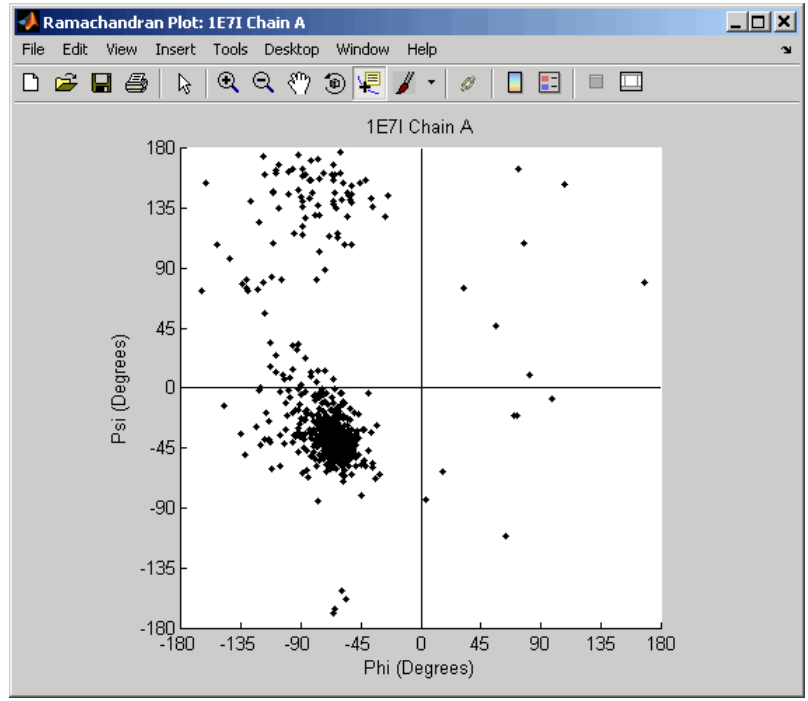
Tip If you specify custom reference regions in which a smaller region is contained or covered by a larger region, list the structure for the smaller region first in the array so that it is plotted last and visible in the plot.

Examples

Drawing a Ramachandran Plot

Draw the Ramachandran plot for the human serum albumin complexed with octadecanoic acid, which has a PDB database identifier of `1E7I`.

```
ramachandran('1E7I')
```



Drawing a Ramachandran Plot for a Specific Chain

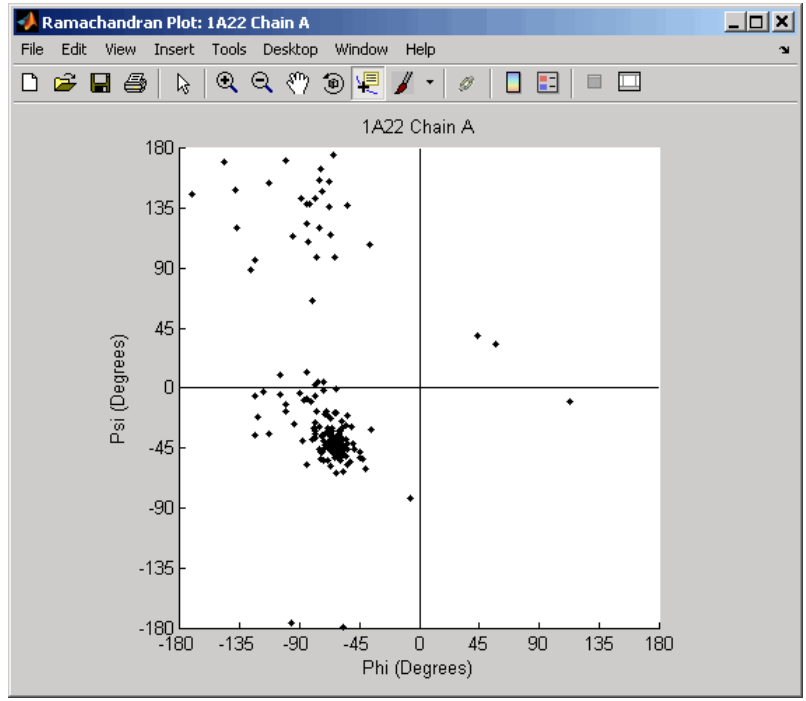
1 Use the `getpdb` function to retrieve protein structure data for the human growth hormone from the PDB database, and save the information to a file.

```
getpdb('1a22','ToFile','1a22.pdb');
```

2 Compute the torsion angles and draw the Ramachandran plot for chain A of the human growth hormone, represented in the pdb file, `1a22.pdb`.

```
ChainA1a22Struct = ramachandran('1a22.pdb','chain','A')

ChainA1a22Struct =
```

```
          Angles: [191x3 double]
      ResidueNum: [191x1 double]
     ResidueName: {191x1 cell}
           Chain: 'A'
         HPoints: 370.0012
```



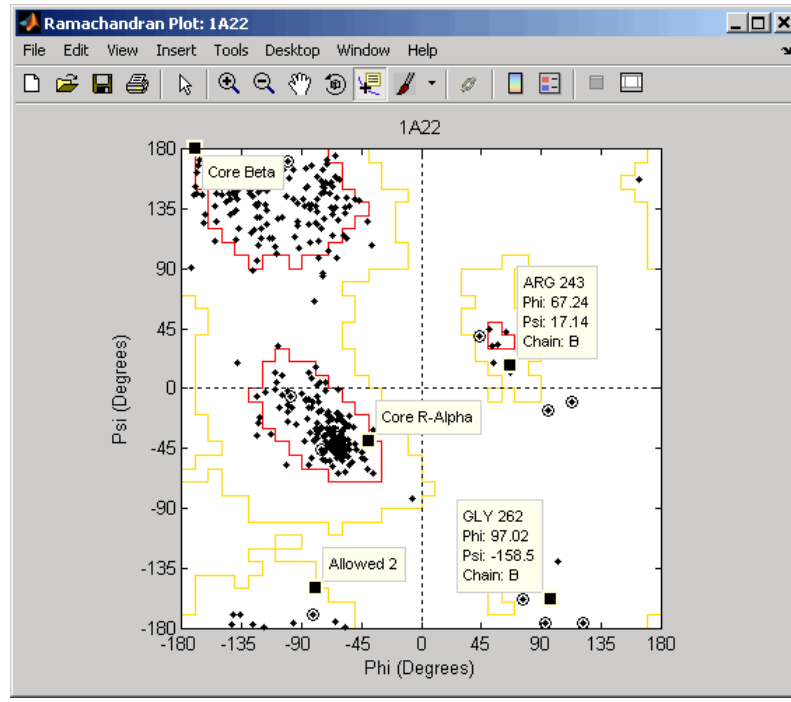
Drawing Ramachandran Plots with Highlighted Glycine Residues and Ramachandran Regions

1. Use the `getpdb` function to retrieve protein structure data for the human growth hormone from the PDB database, and store the information in a structure.

```
Struct1a22 = getpdb('1a22');
```

2 Draw a combined Ramachandran plot for all chains of the human growth hormone, represented in the pdb structure, `1a22Struct`. Highlight the glycine residues (with a circle), and draw the reference Ramachandran regions in the plot.

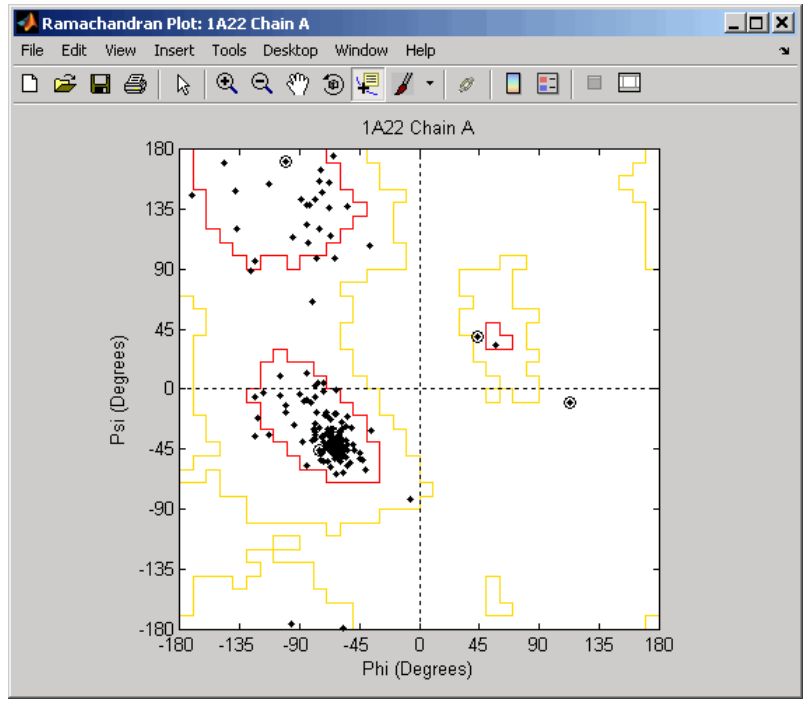
```
ramachandran(Struct1a22,'glycine',true,'regions',true);
```

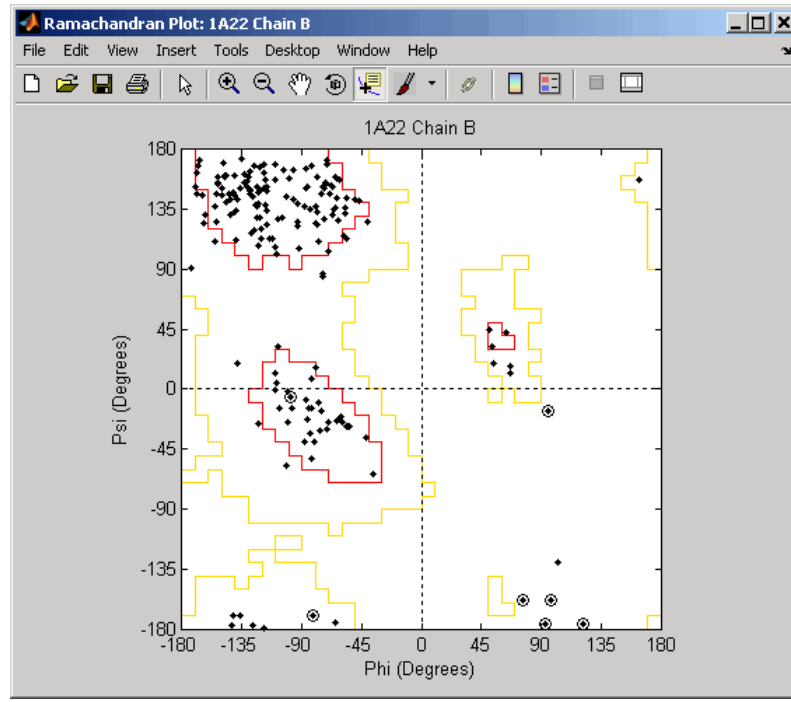


Tip Click a data point to display a data tip with information about the residue. Click a region to display a data tip defining the region. Press and hold the **Alt** key to display multiple data tips.

3 Draw a separate Ramachandran plot for each chain of the human growth hormone, represented in the pdb structure, `1a22Struct`. Highlight the glycine residues (with a circle) and draw the reference Ramachandran regions in the plot.

```
ramachandran(Struct1a22,'plot','separate','chain','all',...
             'glycine',true,'regions',true)
```





Writing a Tab-Delimited Report File from a Ramachandran Structure

1 Create an array of two structures containing torsion angles for chains A and D in the Calcium/Calmodulin-dependent protein kinase, which has a PDB database identifier of `1hkx`.

```
a = ramachandran('1hkx', 'chain', {'A', 'D'})

a =

1x2 struct array with fields:
    Angles
    ResidueNum
```

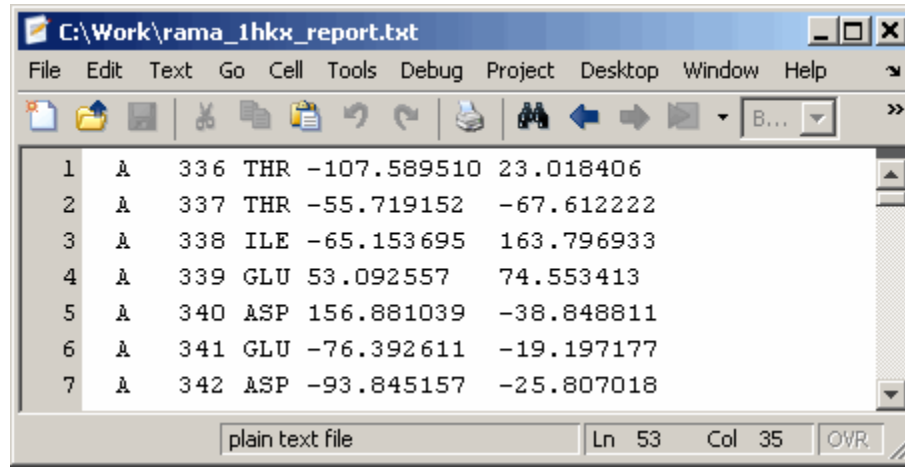
```
ResidueName
Chain
HPoints
```

2 Write a tab-delimited report file containing torsion angles phi (Φ) and psi (Ψ) for chains A and D in the Calcium/Calmodulin-dependent protein kinase.

```
fid = fopen('rama_1hkx_report.txt', 'wt');

for c = 1:numel(a)
    for i = 1:length(a(c).Angles)
        if ~all(isnan(a(c).Angles(i,:)))
            fprintf(fid,'%s\t%d\t%s\t%f\t%f\n', a(c).Chain, ...
                a(c).ResidueNum(i), a(c).ResidueName{i}, ...
                a(c).Angles(i,1:2));
        end
    end
end

fclose(fid);
```

3 View the file you created in the MATLAB Editor.

```
edit rama_1hkx_report.txt
```



References

[1] Morris, A.L., MacArthur, M.W., Hutchinson, E.G., and Thornton, J.M. (1992). Stereochemical Quality of Protein Structure Coordinates. PROTEINS: Structure, Function, and Genetics *12*, 345–364.

See Also

Bioinformatics Toolbox functions: `getpdb`, `molviewer`, `pdbdistplot`, `pdbread`, `proteinpropplot`

randfeatures

Purpose

Generate randomized subset of features

Syntax

```
[IDX, Z] = randfeatures(X, Group, 'PropertyName',
   PropertyValue...)
randfeatures(..., 'Classifier', C)
randfeatures(..., 'ClassOptions', CO)
randfeatures(..., 'PerformanceThreshold', PT)
randfeatures(..., 'ConfidenceThreshold', CT)
randfeatures(..., 'SubsetSize', SS)
randfeatures(..., 'PoolSize', PS)
randfeatures(..., 'NumberOfIndices', N)
randfeatures(..., 'CrossNorm', CN)
randfeatures(..., 'Verbose', VerboseValue)
```

Description

`[IDX, Z] = randfeatures(X, Group, 'PropertyName', PropertyValue...)` performs a randomized subset feature search reinforced by classification. `randfeatures` randomly generates subsets of features used to classify the samples. Every subset is evaluated with the apparent error. Only the best subsets are kept, and they are joined into a single final pool. The cardinality for every feature in the pool gives the measurement of the significance.

`X` contains the training samples. Every column of `X` is an observed vector. `Group` contains the class labels. `Group` can be a numeric vector or a cell array of strings; `numel(Group)` must be the same as the number of columns in `X`, and `numel(unique(Group))` must be greater than or equal to `2`. `Z` is the classification significance for every feature. `IDX` contains the indices after sorting `Z`; i.e., the first one points to the most significant feature.

`randfeatures(..., 'Classifier', C)` sets the classifier. Options are

```
'da'   (default)  Discriminant analysis
'knn'             K nearest neighbors
```

`randfeatures(..., 'ClassOptions', CO)`is a cell with extra options for the selected classifier. Defaults are

`{5,'correlation','consensus'}` for `KNN` and `{'linear'}` for `DA`. See `knnclassify` and `classify` for more information.

`randfeatures(..., 'PerformanceThreshold', PT)` sets the correct classification threshold used to pick the subsets included in the final pool. Default is `0.8` (`80%`).

`randfeatures(..., 'ConfidenceThreshold', CT)` uses the posterior probability of the discriminant analysis to invalidate classified subvectors with low confidence. This option is only valid when `Classifier` is `'da'`. Using it has the same effect as using `'consensus'` in `KNN`; i.e., it makes the selection of approved subsets very stringent. Default is `0.95.^(number of classes)`.

`randfeatures(..., 'SubsetSize', SS)` sets the number of features considered in every subset. Default is `20`.

`randfeatures(..., 'PoolSize', PS)` sets the targeted number of accepted subsets for the final pool. Default is `1000`.

`randfeatures(..., 'NumberOfIndices', N)` sets the number of output indices in `IDX`. Default is the same as the number of features.

`randfeatures(..., 'CrossNorm', CN)` applies independent normalization across the observations for every feature. Cross-normalization ensures comparability among different features, although it is not always necessary because the selected classifier properties might already account for this. Options are

```
'none' (default)  Intensities are not cross-normalized.
'meanvar'         x_new = (x - mean(x))/std(x)
'softmax'         x_new = (1+exp((mean(x)-x)/std(x)))^-1
'minmax'          x_new = (x - min(x))/(max(x)-min(x))
```

`randfeatures(..., 'Verbose', VerboseValue)`, when `Verbose` is `true`, turns off verbosity. Default is `true`.

Examples

Find a reduced set of genes that is sufficient for classification of all the cancer types in the t-matrix NCI60 data set. Load sample data.

```
load NCI60tmatrix
```

Select features.

```
I = randfeatures(X,GROUP,'SubsetSize',15,'Classifier','da');
```

Test features with a linear discriminant classifier.

```
C = classify(X(I(1:25),:)',X(I(1:25),:)',GROUP);
cp = classperf(GROUP,C);
cp.CorrectRate
```

See Also

Bioinformatics Toolbox functions: `classperf`, `crossvalind`, `knnclassify`, `rankfeatures`, `svmclassify`

Statistics Toolbox functions: `classify`, `sequentialfs`

Purpose

Generate random sequence from finite alphabet

Syntax

```
Seq = randseq(SeqLength)
Seq = randseq(SeqLength, ...'Alphabet', AlphabetValue, ...)
Seq = randseq(SeqLength, ...'Weights', WeightsValue, ...)
Seq = randseq(SeqLength, ...'FromStructure',
    FromStructureValue, ...)
Seq = randseq(SeqLength, ...'Case', CaseValue, ...)
Seq = randseq(SeqLength, ...'DataType', DataTypeValue, ...)
```

Arguments

SeqLength	Integer that specifies the number of nucleotides or amino acids in the random sequence .
AlphabetValue	String that specifies the alphabet for the sequence. Choices are `'dna'`(default), `'rna'`, or `'amino'`.
WeightsValue	Property to specify a weighted random sequence.
FromStructureValue	Property to specify a weighted random sequence using output structures from the functions from `basecount`, `dimercount`, `codoncount`, or `aacount`.
CaseValue	String that specifies the case of letters in a sequence when `Alphabet` is `'char'`. Choices are`'upper'` (default) or `'lower'`.
DataTypeValue	String that specifies the data type for a sequence. Choices are `'char'`(default) for letter sequences, and `'uint8'` or `'double'` for numeric sequences. Creates a sequence as an array of *DataType*.

Description

Seq = randseq(*SeqLength*) creates a random sequence with a length specified by *SeqLength*.

Seq = randseq(*SeqLength*, ...'*PropertyName*', *PropertyValue*, ...) calls randseq with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

Seq = randseq(*SeqLength*, ...'Alphabet', *AlphabetValue*, ...) generates a sequence from a specific alphabet.

Seq = randseq(*SeqLength*, ...'Weights', *WeightsValue*, ...) creates a weighted random sequence where the ith letter of the sequence alphabet is selected with weight W(i). The weight vector is usually a probability vector or a frequency count vector. Note that the ith element of the nucleotide alphabet is given by int2nt(i), and the ith element of the amino acid alphabet is given by int2aa(i).

Seq = randseq(*SeqLength*, ...'FromStructure', *FromStructureValue*, ...) creates a weighted random sequence with weights given by the output structure from basecount, dimercount, codoncount, or aacount.

Seq = randseq(*SeqLength*, ...'Case', *CaseValue*, ...) specifies the case for a letter sequence.

Seq = randseq(*SeqLength*, ...'DataType', *DataTypeValue*, ...) specifies the data type for the sequence array.

Examples

Generate a random DNA sequence.

```
randseq(20)

ans =
TAGCTGGCCAAGCGAGCTTG
```

Generate a random RNA sequence.

```
randseq(20,'alphabet','rna')

ans =
GCUGCGGCGGUUGUAUCCUG
```

Generate a random protein sequence.

```
randseq(20,'alphabet','amino')

ans =
DYKMCLYEFGMFGHFTGHKK
```

See Also

Statistics Toolbox functions: `hmmgenerate`, `randsample`

MATLAB functions: `rand`, `randperm`

rankfeatures

Purpose

Rank key features by class separability criteria

Syntax

```
[IDX, Z] = rankfeatures(X, Group)
[IDX, Z] = rankfeatures(X, Group, ...'Criterion',
CriterionValue, ...)
[IDX, Z] = rankfeatures(X, Group, ...'CCWeighting', ALPHA,
   ...)
[IDX, Z] = rankfeatures(X, Group, ...'NWeighting',
BETA, ...)
[IDX, Z] = rankfeatures(X, Group, ...'NumberOfIndices', N,
   ...)
[IDX, Z] = rankfeatures(X, Group, ...'CrossNorm', CN, ...)
```

Description

`[IDX, Z] = rankfeatures(X, Group)` ranks the features in `X` using an independent evaluation criterion for binary classification. `X` is a matrix where every column is an observed vector and the number of rows corresponds to the original number of features. `Group` contains the class labels.

`IDX` is the list of indices to the rows in `X` with the most significant features. `Z` is the absolute value of the criterion used (see below).

`Group` can be a numeric vector or a cell array of strings; `numel(Group)` is the same as the number of columns in `X`, and `numel(unique(Group))` is equal to `2`.

`[IDX, Z] = rankfeatures(X, Group, ...'PropertyName', PropertyValue, ...)` calls `rankfeatures` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`[IDX, Z] = rankfeatures(X, Group, ...'Criterion', CriterionValue, ...)` sets the criterion used to assess the significance of every feature for separating two labeled groups. Choices are:

- 'ttest' (default) — Absolute value two-sample t-test with pooled variance estimate.
- 'entropy' — Relative entropy, also known as Kullback-Leibler distance or divergence.
- 'bhattacharyya' — Minimum attainable classification error or Chernoff bound.
- 'roc' — Area between the empirical receiver operating characteristic (ROC) curve and the random classifier slope.
- 'wilcoxon' — Absolute value of the u-statistic of a two-sample unpaired Wilcoxon test, also known as Mann-Whitney.

Note 'ttest', 'entropy', and 'bhattacharyya' assume normal distributed classes while 'roc' and 'wilcoxon' are nonparametric tests. All tests are feature independent.

[*IDX*, *Z*] = rankfeatures(*X*, *Group*, ...'CCWeighting', *ALPHA*, ...) uses correlation information to outweigh the *Z* value of potential features using *Z* * (1-*ALPHA**(RHO)), where RHO is the average of the absolute values of the cross-correlation coefficient between the candidate feature and all previously selected features. *ALPHA* sets the weighting factor. It is a scalar value between 0 and 1. When *ALPHA* is 0 (default) potential features are not weighted. A large value of RHO (close to 1) outweighs the significance statistic; this means that features that are highly correlated with the features already picked are less likely to be included in the output list.

[*IDX*, *Z*] = rankfeatures(*X*, *Group*, ...'NWeighting', *BETA*, ...) uses regional information to outweigh the *Z* value of potential features using *Z* * (1-exp(-(DIST/*BETA*).^2)), where DIST is the distance (in rows) between the candidate feature and previously selected features. *BETA* sets the weighting factor. It is greater than or equal to 0. When BETA is 0 (default) potential features are not weighted. A small DIST (close to 0) outweighs the significance statistics of only

close features. This means that features that are close to already picked features are less likely to be included in the output list. This option is useful for extracting features from time series with temporal correlation.

BETA can also be a function of the feature location, specified using `@` or an anonymous function. In both cases `rankfeatures` passes the row position of the feature to `BETA()` and expects back a value greater than or equal to `0`.

Note You can use `'CCWeighting'` and `'NWeighting'` together.

`[`*IDX*`, `*Z*`] = rankfeatures(`*X*`, `*Group*`, ...'NumberOfIndices', `*N*`, ...)` sets the number of output indices in *IDX*. Default is the same as the number of features when *ALPHA* and *BETA* are `0`, or `20` otherwise.

`[`*IDX*`, `*Z*`] = rankfeatures(`*X*`, `*Group*`, ...'CrossNorm', `*CN*`, ...)` applies independent normalization across the observations for every feature. Cross-normalization ensures comparability among different features, although it is not always necessary because the selected criterion might already account for this. Choices are:

- `'none'` (default) — Intensities are not cross-normalized.
- `'meanvar'` — `x_new = (x - mean(x))/std(x)`
- `'softmax'` — `x_new = (1+exp((mean(x)-x)/std(x)))^-1`
- `'minmax'` — `x_new = (x - min(x))/(max(x)-min(x))`

Examples

1. Find a reduced set of genes that is sufficient for differentiating breast cancer cells from all other types of cancer in the t-matrix NCI60 data set. Load sample data.

   ```
   load NCI60tmatrix
   ```

2. Get a logical index vector to the breast cancer cells.

   ```
   BC = GROUP == 8;
   ```

3 Select features.

```
I = rankfeatures(X,BC,'NumberOfIndices',12);
```

4 Test features with a linear discriminant classifier.

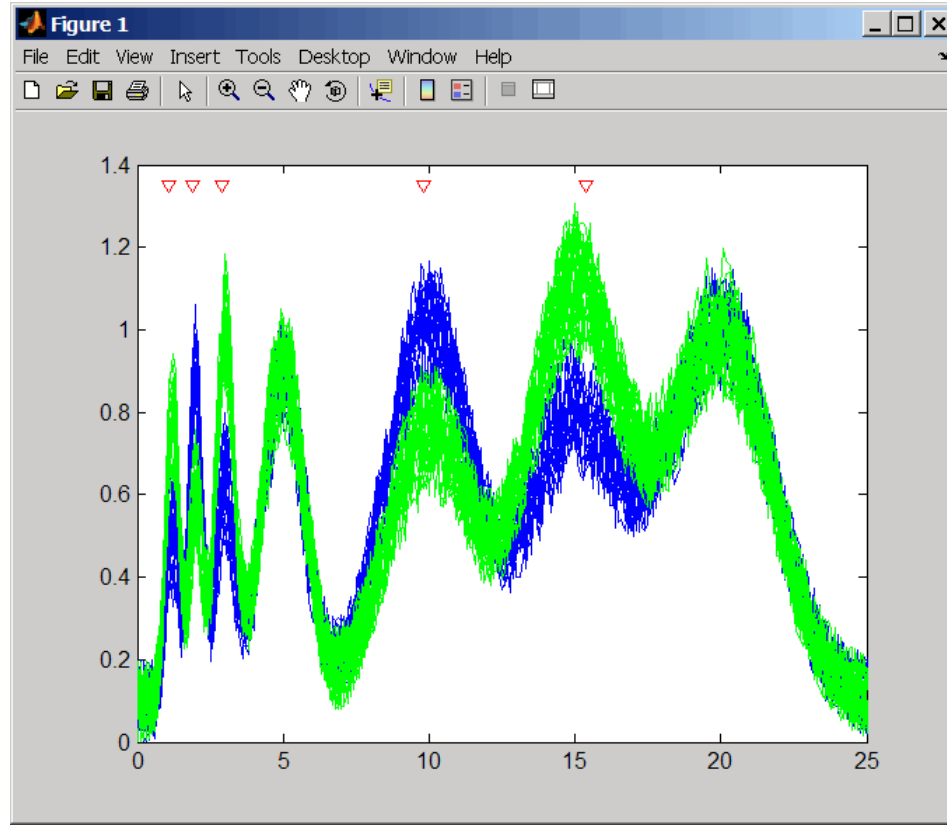
```
C = classify(X(I,:)',X(I,:)',double(BC));
cp = classperf(BC,C);
cp.CorrectRate

ans =

     1
```

5 Use cross-correlation weighting to further reduce the required number of genes.

```
I = rankfeatures(X,BC,'CCWeighting',0.7,'NumberOfIndices',8);
C = classify(X(I,:)',X(I,:)',double(BC));
cp = classperf(BC,C);
cp.CorrectRate

ans =

     1
```

6 Find the discriminant peaks of two groups of signals with Gaussian pulses modulated by two different sources.

```
load GaussianPulses
f = rankfeatures(y',grp,'NWeighting',@(x) x/10+5,'NumberOfIndices',5);
plot(t,y(grp==1,:),'b',t,y(grp==2,:),'g',t(f),1.35,'vr')
```



See Also

Bioinformatics Toolbox functions: `classperf`, `crossvalind`, `randfeatures`, `svmclassify`

Statistics Toolbox functions: `classify`, `sequentialfs`

Purpose

Right array divide DataMatrix objects

Syntax

```
DMObjNew = rdivide(DMObj1, DMObj2)
DMObjNew = DMObj1 ./ DMObj2
DMObjNew = rdivide(DMObj1, B)
DMObjNew = DMObj1 ./ B
DMObjNew = rdivide(B, DMObj1)
DMObjNew = B ./ DMObj1
```

Arguments

DMObj1, *DMObj2*	DataMatrix objects, such as created by `DataMatrix` (object constructor).
B	MATLAB numeric or logical array.

Return Values

DMObjNew	DataMatrix object created by right array division.

Description

DMObjNew = `rdivide(`*DMObj1*`, `*DMObj2*`)` or the equivalent *DMObjNew* = *DMObj1* `./` *DMObj2* performs an element-by-element right array division of the DataMatrix objects *DMObj1* and *DMObj2* and places the results in *DMObjNew*, another DataMatrix object. In other words, `rdivide` divides each element in *DMObj1* by the corresponding element in *DMObj2*. *DMObj1* and *DMObj2* must have the same size (number of rows and columns), unless one is a scalar (1-by-1 DataMatrix object). The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*, unless *DMObj1* is a scalar; then they are the same as *DMObj2*.

DMObjNew = `rdivide(`*DMObj1*`, `*B*`)` or the equivalent *DMObjNew* = *DMObj1* `./` *B* performs an element-by-element right array division of the DataMatrix object *DMObj1* and *B*, a numeric or logical array, and places the results in *DMObjNew*, another DataMatrix object. In other words, `rdivide` divides each element in *DMObj1* by the corresponding element in *B*. *DMObj1* and *B* must have the same size (number of rows and

columns), unless *B* is a scalar. The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*.

DMObjNew = rdivide(*B*, *DMObj1*) or the equivalent *DMObjNew* = *B* ./ *DMObj1* performs an element-by-element right array division of *B*, a numeric or logical array, and the DataMatrix object *DMObj1*, and places the results in *DMObjNew*, another DataMatrix object. In other words, rdivide divides each element in *B* by the corresponding element in *DMObj1*.*DMObj1* and *B* must have the same size (number of rows and columns), unless *B* is a scalar. The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*.

Note Arithmetic operations between a scalar DataMatrix object and a nonscalar array are not supported.

MATLAB calls *DMObjNew* = rdivide(*X*, *Y*) for the syntax *DMObjNew* = *X* ./ *Y* when *X* or *Y* is a DataMatrix object.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox methods of a DataMatrix object: ldivide, times

Purpose

Find restriction enzymes that cut nucleotide sequence

Syntax

```
[Enzymes, Sites] = rebasecuts(SeqNT)
rebasecuts(SeqNT, Group)
rebasecuts(SeqNT, [Q, R])
rebasecuts(SeqNT, S)
```

Arguments

SeqNT	Nucleotide sequence.
Group	Cell array of strings representing the names of valid restriction enzymes.
Q, *R*	Base positions that limit the search to all sites between base *Q* and base *R*.
S	Base position that limits the search to all sites after base *S*.

Return Values

Enzymes	Cell array with the names of restriction enzymes from REBASE®, the Restriction Enzyme Database.
Sites	Vector of cut sites identified with the base position number before every cut.

Description

`[Enzymes, Sites] = rebasecuts(SeqNT)` finds all the restriction enzymes that cut *SeqNT*, a nucleotide sequence.

`rebasecuts(SeqNT, Group)` limits the search to *Group*, a list of enzymes.

`rebasecuts(SeqNT, [Q, R])` limits the search to those enzymes that cut after the base position specified by *Q* and before the base position specified by *R*.

`rebasecuts(SeqNT, S)` limits the search to those enzymes that cut just after the base position specified by *S*.

REBASE, the Restriction Enzyme Database, is a collection of information about restriction enzymes and related proteins. For more information about REBASE, see:

```
http://rebase.neb.com/rebase/rebase.html
```

Examples

1 Create a nucleotide sequence.

```
seq = 'AGAGGGGTACGCGCTCTGAAAAGCGGGAACCTCGTGGCGCTTTATTAA';
```

2 Find all possible enzymes and cleavage sites in the sequence.

```
 [enzymes, sites] = rebasecuts(seq)
```

3 Find where restriction enzymes `CfoI` and `Tru9I` cut the sequence.

```
[enzymes, sites] = rebasecuts(seq, {'CfoI','Tru9I'})

enzymes =

    'CfoI'
    'CfoI'
    'Tru9I'

sites =

    13
    39
    45
```

4 Find all possible enzymes that cut after base 7.

```
enzymes  = rebasecuts(seq, 7)

enzymes =

    'Csp6I'
    'CviQI'
    'RsaNI'
```

5 Find all possible enzymes that cut between bases 11 and 37.

```
enzymes  = rebasecuts(seq, [11 37])

enzymes =

    'AccII'
    'AspLEI'
    'BmiI'
    'Bsh1236I'
    'BspFNI'
    'BspLI'
    'BstFNI'
    'BstHHI'
    'BstUI'
    'CfoI'
    'FnuDII'
    'GlaI'
    'HhaI'
    'Hin6I'
    'HinP1I'
    'Hpy188I'
    'HspAI'
    'MvnI'
    'NlaIV'
    'PspN4I'
    'SetI'
```

References

[1] Roberts, R.J., Vincze, T., Posfai, J., and Macelis, D. (2007). REBASE—enzymes and genes for DNA restriction and modification. Nucl. Acids Res. *35*, D269–D270.

[2] Official REBASE Web site: `http://rebase.neb.com`.

See Also

Bioinformatics Toolbox functions: `cleave`, `cleavelookup`, `restrict`, `seq2regexp`, `seqshowwords`

MATLAB function: `regexp`

Purpose

Create red and blue colormap

Syntax

```
redbluecmap(Length)
```

Arguments

Length	Positive integer that specifies the length of (or the number of colors in) the colormap. Choices are positive integers ≥ 3 or ≤ 11. Default is 11.

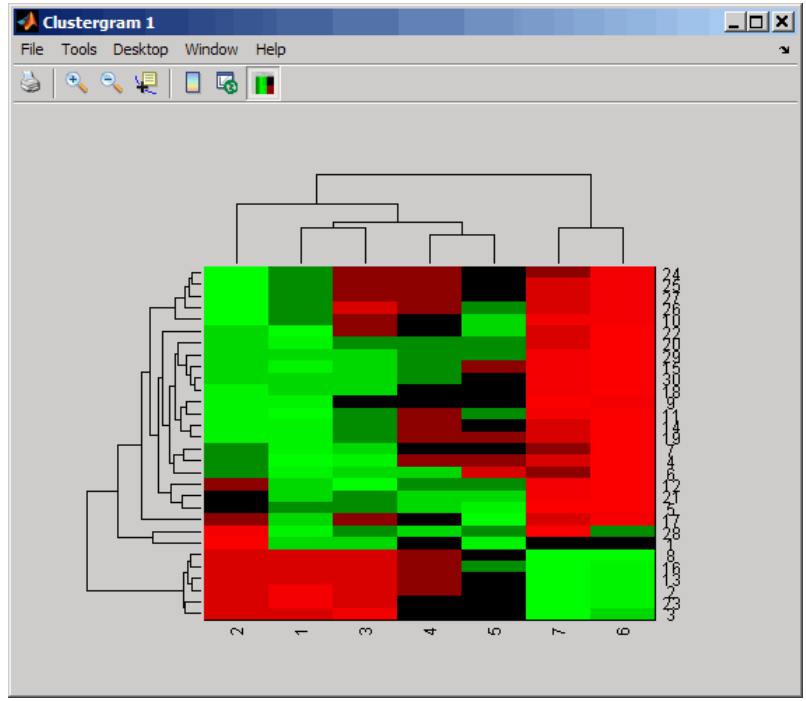
Description

`redbluecmap(Length)` returns a *Length*-by-3 matrix containing a red and blue diverging color palette. Low values are dark blue, values in the center of the map are white, and high values are dark red. *Length* is a positive integer ≥ 3 and ≤ 11, which determines the number of colors in the colormap. Default is 11.

Examples

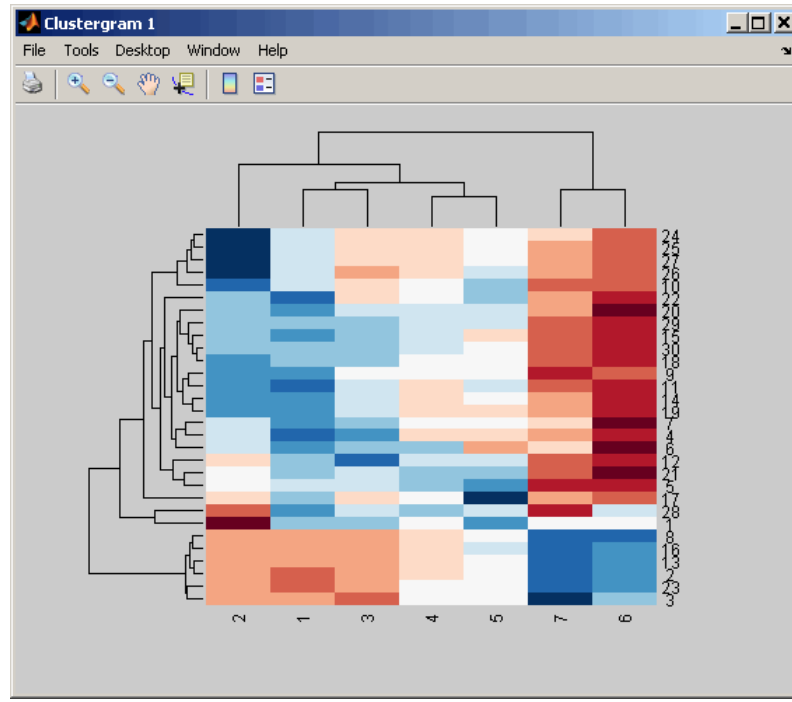
1 Load the MAT-file, provided with the Bioinformatics Toolbox software, that contains `yeastvalues`, a matrix of gene expression data. Create a clustergram object and display the dendrograms and heat map from the gene expression data in the first 30 rows of the `yeastvalues` matrix.

```
load filteredyeastdata
cgo = clustergram(yeastvalues(1:30,:))
Clustergram object with 30 rows of nodes and 7 columns of nodes.
```



2 Reset the colormap of the heat map to `redbluecmap`.

```
set(cgo,'Colormap',redbluecmap);
```



References

[1] `http://colorbrewer.org`

See Also

Bioinformatics Toolbox functions: `clustergram`, `redgreencmap`

MATLAB functions: `colormap`, `colormapeditor`

redgreencmap

Purpose

Create red and green colormap

Syntax

```
redgreencmap(Length)
redgreencmap(Length, 'Interpolation', InterpolationValue)
```

Arguments

Length	Length of the colormap. Enter either `256` or `64`. Default is the length of the colormap of the current figure.
InterpolationValue	Property that lets you set the algorithm for color interpolation. Choices are: • `'linear'` • `'quadratic'` • `'cubic'` • `'sigmoid'` (default)

Note The sigmoid interpolation is tanh.

Description

`redgreencmap(Length)` returns a *Length*-by-3 matrix containing a red and green colormap. Low values are bright green, values in the center of the map are black, and high values are red. Enter either `256` or `64` for *Length*. If *Length* is empty, the length of the map will be the same as the length of the colormap of the current figure.

`redgreencmap(Length, 'Interpolation', InterpolationValue)` lets you set the algorithm for color interpolation. Choices are:

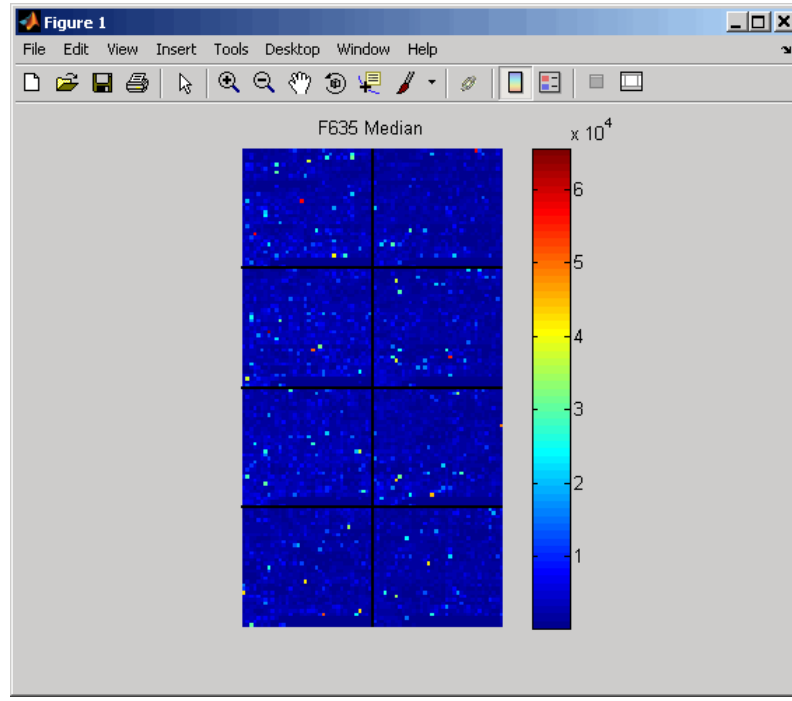
- `'linear'`
- `'quadratic'`
- `'cubic'`
- `'sigmoid'` (default)

Note The sigmoid interpolation is tanh.

Examples

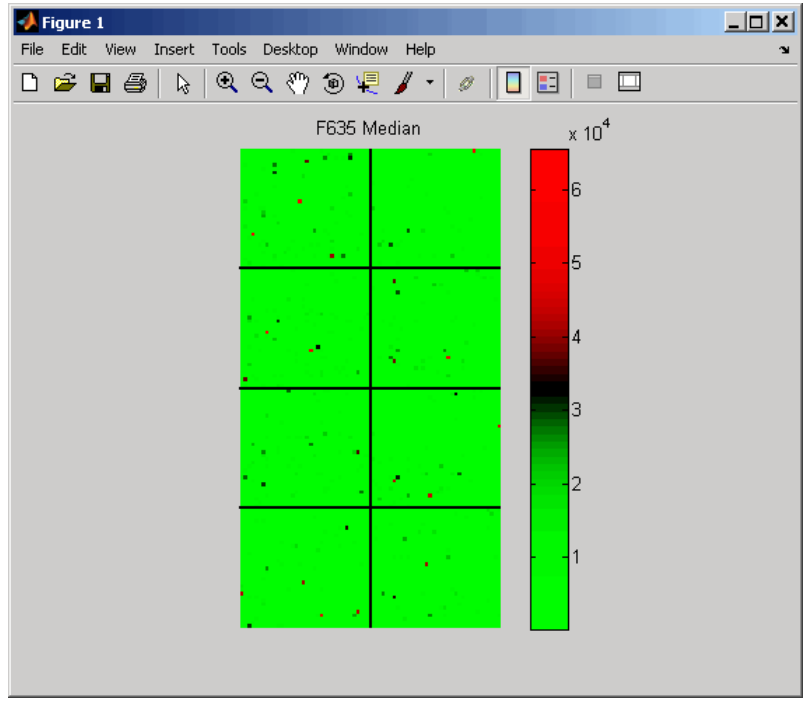
1 Create a MATLAB structure from the microarray data in a GenePix Results (GPR) file, then display an image of the `'F635 Median'` field.

```
pd = gprread('mouse_a1pd.gpr');
maimage(pd,'F635 Median')
```



2 Reset the colormap of the current figure.

```
colormap(redgreencmap)
```



See Also

Bioinformatics Toolbox function: `clustergram`, `redbluecmap`

MATLAB functions: `colormap`, `colormapeditor`

Purpose

Reorder leaves of phylogenetic tree

Syntax

```
Tree1Reordered = reorder(Tree1, Order)
[Tree1Reordered, OptimalOrder] = reorder(Tree1, Order,
   'Approximate', ApproximateValue)
[Tree1Reordered, OptimalOrder] = reorder(Tree1, Tree2)
```

Arguments

Tree1, *Tree2*	Phytree objects.
Order	Vector with position indices for each leaf.
ApproximateValue	Controls the use of the optimal leaf-ordering calculation to find the closest order possible to the suggested one without dividing the clades or producing crossing branches. Enter `true` to use the calculation. Default is `false`.

Return Values

Tree1Reordered	Phytree object with reordered leaves.
OptimalOrder	Vector of position indices for each leaf in *Tree1Reordered*, determined by the optimal leaf-ordering calculation.

Description

Tree1Reordered = `reorder(`*Tree1*`, `*Order*`)` reorders the leaves of the phylogenetic tree *Tree1*, without modifying its structure and distances, creating a new phylogenetic tree, *Tree1Reordered*. *Order* is a vector of position indices for each leaf. If *Order* is invalid, that is, if it divides the clades (or produces crossing branches), then `reorder` returns an error message.

`[`*Tree1Reordered*`, `*OptimalOrder*`] = reorder(`*Tree1*`, `*Order*`, 'Approximate', `*ApproximateValue*`)` controls the use of the optimal leaf-ordering calculation, which finds the best approximate order closest to the suggested one, without dividing the clades or producing crossing branches. Enter `true` to use the calculation and return

Tree1Reordered, the reordered tree, and *OptimalOrder*, a vector of position indices for each leaf in *Tree1Reordered*, determined by the optimal leaf-ordering calculation. Default is `false`.

`[`*Tree1Reordered*`, `*OptimalOrder*`] = reorder(`*Tree1*`, `*Tree2*`)` uses the optimal leaf-ordering calculation to reorder the leaves in *Tree1* such that it matches the order of leaves in *Tree2* as closely as possible, without dividing the clades or producing crossing branches. *Tree1Reordered* is the reordered tree, and *OptimalOrder* is a vector of position indices for each leaf in *Tree1Reordered*, determined by the optimal leaf-ordering calculation

Examples

Reordering Leaves Using a Valid Order

1 Create and view a phylogenetic tree.

```
b = [1 2; 3 4; 5 6; 7 8; 9 10];
tree = phytree(b)
   Phylogenetic tree object with 6 leaves (5 branches)
view(tree)
```

2 Reorder the leaves on the phylogenetic tree, and then view the reordered tree.

```
treeReordered = reorder(tree, [5, 6, 3, 4, 1, 2])
view(treeReordered)
```

Finding Best Approximate Order When Using an Invalid Order

1 Create a phylogenetic tree by reading a Newick-formatted tree file (ASCII text file).

```
tree = phytreeread('pf00002.tree')
    Phylogenetic tree object with 33 leaves (32 branches)
```

2 Create a row vector of the leaf names in alphabetical order.

```
[dummy,order] = sort(get(tree,'LeafNames'));
```

3 Reorder the phylogenetic tree to match as closely as possible the row vector of alphabetically ordered leaf names, without dividing the clades or having crossing branches.

```
treeReordered = reorder(tree,order,'approximate',true)
    Phylogenetic tree object with 33 leaves (32 branches)
```

4 View the original and the reordered phylogenetic trees.

```
view(tree)
view(treeReordered)
```

Reordering Leaves to Match Leaf Order in Another Phylogenetic Tree

1 Create a phylogenetic tree by reading sequence data from a FASTA file, calculating the pairwise distances between sequences, and then using the neighbor-joining method.

```
seqs = fastaread('pf00002.fa')

seqs =

33x1 struct array with fields:
    Header
    Sequence

dist = seqpdist(seqs,'method','jukes-cantor','indels','pair');
NJtree = seqneighjoin(dist,'equivar',seqs)
    Phylogenetic tree object with 33 leaves (32 branches)
```

2 Create another phylogenetic tree from the same sequence data and pairwise distances between sequences, using the single linkage method.

```
HCtree = seqlinkage(dist,'single',seqs)
    Phylogenetic tree object with 33 leaves (32 branches)
```

3 Use the optimal leaf-ordering calculation to reorder the leaves in `HCtree` such that it matches the order of leaves in `NJtree` as closely as possible, without dividing the clades or having crossing branches.

```
HCtree_reordered = reorder(HCtree,NJtree)
    Phylogenetic tree object with 33 leaves (32 branches)
```

4 View the reordered phylogenetic tree and the tree used to reorder it.

```
view(HCtree_reordered)
view(NJtree)
```

See Also

Bioinformatics Toolbox function: `phytree` (object constructor)

Bioinformatics Toolbox object: phytree object

Bioinformatics Toolbox methods of a phytree object: `get`, `getbyname`, `prune`

Purpose

Change root of phylogenetic tree

Syntax

```
Tree2 = reroot(Tree1)
Tree2 = reroot(Tree1, Node)
Tree2 = reroot(Tree1, Node, Distance)
```

Arguments

Tree1	Phylogenetic tree (`phytree` object) created with the function `phytree`.
Node	Node index returned by the phytree object method `getbyname`.
Distance	Distance from the reference branch.

Description

Tree2 = `reroot(`*Tree1*`)` changes the root of a phylogenetic tree (*Tree1*) using a midpoint method. The midpoint is the location where the mean values of the branch lengths, on either side of the tree, are equalized. The original root is deleted from the tree.

Tree2 = `reroot(`*Tree1*`, `*Node*`)` changes the root of a phylogenetic tree (*Tree1*) to a branch node using the node index (*Node*). The new root is placed at half the distance between the branch node and its parent.

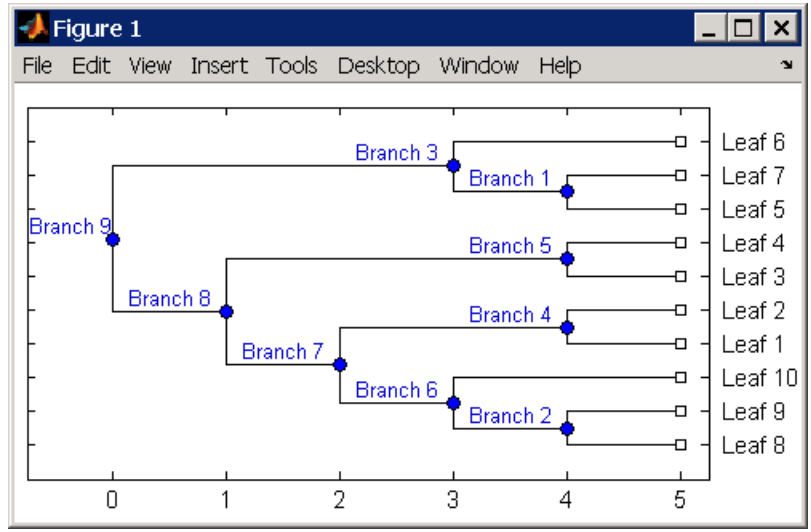
Tree2 = `reroot(`*Tree1*`, `*Node*`, `*Distance*`)` changes the root of a phylogenetic tree (*Tree1*) to a new root at a given distance (*Distance*) from the reference branch node (*Node*) toward the original root of the tree. Note: The new branch representing the root in the new tree (`Tree2`) is labeled `'Root'`.

Examples

1 Create an ultrametric tree.

```
tr_1 = phytree([5 7;8 9;6 11; 1 2;3 4;10 12;...
                14 16; 15 17;13 18])
plot(tr_1,'branchlabels',true)
```

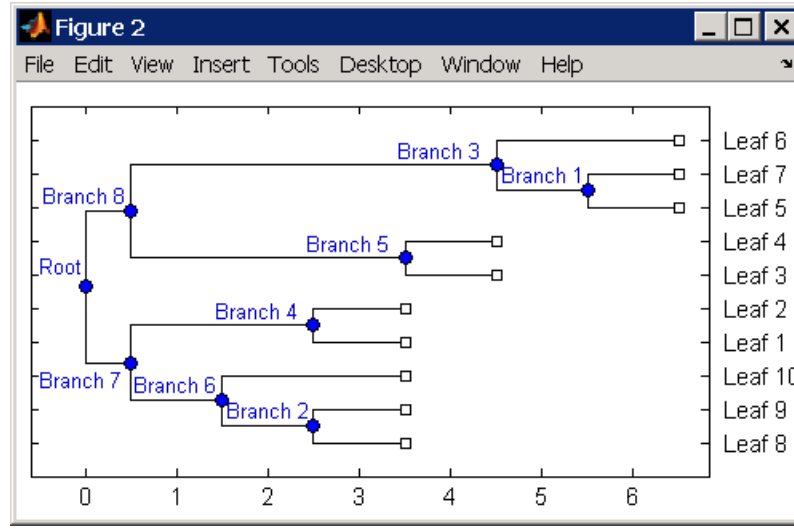
A figure with the phylogenetic tree displays.



2 Place the root at `'Branch 7'`.

```
sel = getbyname(tr_1,'Branch 7');
tr_2 =  reroot(tr_1,sel)
plot(tr_2,'branchlabels',true)
```

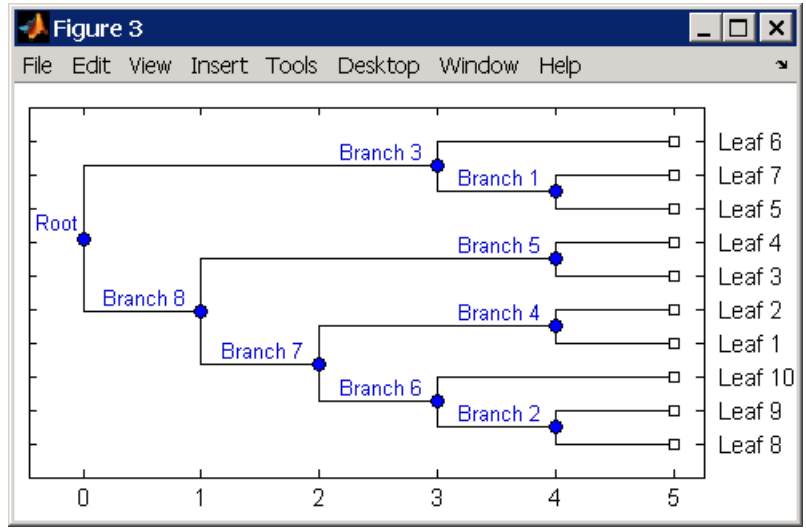
A figure of a phylogenetic tree displays with the root moved to the center of branch 7.



3 Move the root to a branch that makes the tree as ultrametric as possible.

```
tr_3 = reroot(tr_2)
plot(tr_3,'branchlabels',true)
```

A figure of the new tree displays with the root moved from the center of branch 7 to branch 8.



See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `seqneighjoin`

Bioinformatics Toolbox object: phytree object

Bioinformatics Toolbox methods of phytree object: `get`, `getbyname`, `prune`, `select`

Purpose

Split nucleotide sequence at restriction site

Syntax

```
Fragments = restrict(SeqNT, Enzyme)
Fragments = restrict(SeqNT, NTPattern, Position)
[Fragments, CuttingSites] = restrict(...)
[Fragments, CuttingSites, Lengths] = restrict(...)
... = restrict(..., 'PartialDigest', PartialDigestValue)
```

Arguments

SeqNT	One of the following: • String of codes specifying a nucleotide sequence. For valid letter codes, see the table Mapping Nucleotide Letter Codes to Integers on page 3-1121. • Row vector of integers specifying a nucleotide sequence. For valid integers, see the table Mapping Nucleotide Integers to Letter Codes on page 3-809. • MATLAB structure containing a `Sequence` field that contains a nucleotide sequence, such as returned by `fastaread`, `fastqread`, `emblread`, `getembl`, `genbankread`, or `getgenbank`.
Enzyme	String specifying a name of a restriction enzyme from REBASE, the Restriction Enzyme Database.

Tip Some enzymes specify cutting rules for both a strand and its complement strand. `restrict` applies only the cutting rule for the 5' —> 3' strand. For a workaround to applying an enzyme cutting rule for both strands, see Splitting a Double-Stranded Nucleotide Sequence on page 3-1307.

`NTPattern`	Short nucleotide sequence recognition pattern to search for in *`SeqNT`*, a larger sequence. *`NTPattern`* can be either of the following: • Character string • Regular expression
`Position`	Either of the following: • Integer specifying a position in the *`SeqNT`* to cut, relative to *`NTPattern`*. • Two-element vector specifying two positions in the *`SeqNT`* to cut, relative to *`NTPattern`*.
`PartialDigestValue`	Value from `0` to `1` (default) specifying the probability that a cleavage site will be cut.

Note Position `0` corresponds to a cut before the first base of *`NTPattern`*.

Description

`Fragments` `= restrict(`*`SeqNT`*`,` *`Enzyme`*`)` cuts *`SeqNT`*, a nucleotide sequence, into fragments at the restriction sites of *`Enzyme`*, a restriction

enzyme. The `restrict` function stores the return values in *`Fragments`*, a cell array of sequences.

`Fragments` = `restrict(`*`SeqNT`*`,` *`NTPattern`*`,` *`Position`*`)` cuts *`SeqNT`*, a nucleotide sequence, into fragments at restriction sites specified by *`NTPattern`*, a nucleotide recognition pattern, and *`Position`*.

`[`*`Fragments`*`,` *`CuttingSites`*`] = restrict(...)` returns a numeric vector with the indices representing the cutting sites. The `restrict` function adds a `0` to the beginning of the *`CuttingSites`* vector so that the number of elements in *`CuttingSites`* equals the number of elements in *`Fragments`*. You can use *`CuttingSites`* `+ 1` to point to the first base of every fragment respective to the original sequence.

`[`*`Fragments`*`,` *`CuttingSites`*`,` *`Lengths`*`] = restrict(...)` returns a numeric vector with the lengths of every fragment.

`...  = restrict(..., 'PartialDigest',` *`PartialDigestValue`*`)` simulates a partial digest where each restriction site in the sequence has a *`PartialDigestValue`* or probability of being cut.

REBASE, the Restriction Enzyme Database, is a collection of information about restriction enzymes and related proteins. For more information about REBASE or to search REBASE for the name of a restriction enzyme, see:

```
http://rebase.neb.com/rebase/rebase.html
```

Examples

Splitting a Nucleotide Sequence by Specifying an Enzyme

1 Enter a nucleotide sequence.

```
Seq = 'AGAGGGGTACGCGCTCTGAAAAGCGGGAACCTCGTGGCGCTTTATTAA';
```

2 Use the restriction enzyme `HspAI` (which specifies a recognition sequence of `GCGC` and a cleavage position of `1`) to cleave the nucleotide sequence.

```
fragmentsEnzyme = restrict(Seq,'HspAI')
```

```
fragmentsEnzyme =
    'AGAGGGGTACG'
    'CGCTCTGAAAAGCGGGAACCTCGTGG'
    'CGCTTTATTAA'
```

Splitting a Nucleotide Sequence by Specifying a Pattern and Position

1 Enter a nucleotide sequence.

```
Seq = 'AGAGGGGTACGCGCTCTGAAAAGCGGGAACCTCGTGGCGCTTTATTAA';
```

2 Use the sequence pattern `GCGC` with the point of cleavage at position `3` to cleave the nucleotide sequence.

```
fragmentsPattern = restrict(Seq,'GCGC',3)

fragmentsPattern =
    'AGAGGGGTACGCG'
    'CTCTGAAAAGCGGGAACCTCGTGGCG'
    'CTTTATTAA'
```

Splitting a Nucleotide Sequence by Specifying a Regular Expression for the Pattern

1 Enter a nucleotide sequence.

```
Seq = 'AGAGGGGTACGCGCTCTGAAAAGCGGGAACCTCGTGGCGCTTTATTAA';
```

2 Use a regular expression to specify the sequence pattern.

```
fragmentsRegExp = restrict(Seq,'GCG[^C]',3)

fragmentsRegExp =

    'AGAGGGGTACGCGCTCTGAAAAGCG'
    'GGAACCTCGTGGCGCTTTATTAA'
```

Returning the Cutting Sites and Fragment Lengths

1 Enter a nucleotide sequence.

```
Seq = 'AGAGGGGTACGCGCTCTGAAAAGCGGGAACCTCGTGGCGCTTTATTAA';
```

2 Capture the cutting sites and fragment lengths as well as the fragments.

```
[fragments, cut_sites, lengths] = restrict(Seq,'HspAI')

fragments =
    'AGAGGGGTACG'
    'CGCTCTGAAAAGCGGGAACCTCGTGG'
    'CGCTTTATTAA'

cut_sites =
     0
    11
    37

lengths =
    11
    26
    11
```

Splitting a Double-Stranded Nucleotide Sequence

Some enzymes specify cutting rules for both a strand and its complement strand. `restrict` applies only the cutting rule for the 5' —> 3' strand. You can apply this rule manually for the complement strand.

1 Enter a nucleotide sequence.

```
seq = 'CCCGCNNNNNNN';
```

2 Use the `seqcomplement` function to determine the complement strand, which is in the 3' —> 5' direction.

```
seqc = seqcomplement(seq)

seqc =

GGGCGNNNNNNN
```

3 Cut the first strand using the restriction enzyme `FauI` (which specifies a recognition sequence pattern of `CCCGC` and a cleavage position of `9`).

```
cuts_strand1 = restrict(seq, 'FauI')

cuts_strand1 =

    'CCCGCNNNN'
    'NNN'
```

4 Cut the complement strand according the rule specified by `FauI` (which specifies a recognition sequence pattern of `GGGCG` with the point of cleavage at position `11`).

```
cuts_strand2 = restrict(seqc, 'GGGCG', 11)

cuts_strand2 =

    'GGGCGNNNNNN'
    'N'
```

References

[1] Roberts, R.J., Vincze, T., Posfai, J., and Macelis, D. (2007). REBASE—enzymes and genes for DNA restriction and modification. Nucl. Acids Res. *35*, D269–D270.

[2] Official REBASE Web site: `http://rebase.neb.com`.

See Also

Bioinformatics Toolbox functions: `cleave`, `cleavelookup`, `rebasecuts`, `seq2regexp`, `seqcomplement`, `seqshowwords`

MATLAB function: `regexp`

Purpose

Return reverse mapping (amino acid to nucleotide codon) for genetic code

Syntax

```
Map = revgeneticcode
Map = revgeneticcode(GeneticCode)
Map = revgeneticcode(..., 'Alphabet', AlphabetValue, ...)
Map = revgeneticcode(..., 'ThreeLetterCodes',
   ThreeLetterCodesValue, ...)
```

Arguments

GeneticCode

Integer or string specifying a genetic code number or code name from the table Genetic Code on page 3-1311. Default is `1` or `'Standard'`.

Tip If you use a code name, you can truncate the name to the first two letters of the name.

AlphabetValue

String specifying the nucleotide alphabet to use in the map. Choices are:

- `'DNA'` (default) — Uses the symbols `A`, `C`, `G`, and `T`.
- `'RNA'` — Uses the symbols `A`, `C`, `G`, and `U`.

ThreeLetterCodesValue

Controls the use of three-letter amino acid codes as field names in the return structure *Map*. Choices are `true` for three-letter codes or `false` for one-letter codes. Default is `false`.

Return Values

Map	Structure containing the reverse mapping of amino acids to nucleotide codons for the standard genetic code. The *Map* structure contains a field for each amino acid.

Description

Map = revgeneticcode returns a structure containing the reverse mapping of amino acids to nucleotide codons for the standard genetic code. The *Map* structure contains a field for each amino acid.

Map = revgeneticcode(*GeneticCode*) returns a structure containing the reverse mapping of amino acids to nucleotide codons for the specified genetic code. *GeneticCode* is either:

- An integer or string specifying a code number or code name from the table Genetic Code on page 3-1311
- The transl_table (code) number from the NCBI Web page describing genetic codes:

  http://www.ncbi.nlm.nih.gov/Taxonomy/Utils/wprintgc.cgi?mode=c

Tip If you use a code name, you can truncate the name to the first two letters of the name.

Map = revgeneticcode(..., '*PropertyName*', *PropertyValue*, ...) calls revgeneticcode with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

Map = revgeneticcode(..., 'Alphabet', *AlphabetValue*, ...) specifies the nucleotide alphabet to use in the map. *AlphabetValue* can

be `'DNA'`, which uses the symbols `A`, `C`, `G`, and `T`, or `'RNA'`, which uses the symbols `A`, `C`, `G`, and `U`. Default is `'DNA'`.

`Map` `= revgeneticcode(..., 'ThreeLetterCodes',` *`ThreeLetterCodesValue`*`, ...)` controls the use of three-letter amino acid codes as field names in the return structure *`Map`*. *`ThreeLetterCodesValue`* can be `true` for three-letter codes or `false` for one-letter codes. Default is `false`.

Genetic Code

Code Number	Code Name
1	Standard
2	Vertebrate Mitochondrial
3	Yeast Mitochondrial
4	Mold, Protozoan, Coelenterate Mitochondrial, and Mycoplasma/Spiroplasma
5	Invertebrate Mitochondrial
6	Ciliate, Dasycladacean, and Hexamita Nuclear
9	Echinoderm Mitochondrial
10	Euplotid Nuclear
11	Bacterial and Plant Plastid
12	Alternative Yeast Nuclear
13	Ascidian Mitochondrial
14	Flatworm Mitochondrial
15	Blepharisma Nuclear
16	Chlorophycean Mitochondrial
21	Trematode Mitochondrial

Genetic Code (Continued)

Code Number	Code Name
22	Scenedesmus Obliquus Mitochondrial
23	Thraustochytrium Mitochondrial

Examples

- Return the reverse mapping of amino acids to nucleotide codons for the `Standard` genetic code.

```
map = revgeneticcode

map =

      Name: 'Standard'
         A: {'GCT'  'GCC'  'GCA'  'GCG'}
         R: {'CGT'  'CGC'  'CGA'  'CGG'  'AGA'  'AGG'}
         N: {'AAT'  'AAC'}
         D: {'GAT'  'GAC'}
         C: {'TGT'  'TGC'}
         Q: {'CAA'  'CAG'}
         E: {'GAA'  'GAG'}
         G: {'GGT'  'GGC'  'GGA'  'GGG'}
         H: {'CAT'  'CAC'}
         I: {'ATT'  'ATC'  'ATA'}
         L: {'TTA'  'TTG'  'CTT'  'CTC'  'CTA'  'CTG'}
         K: {'AAA'  'AAG'}
         M: {'ATG'}
         F: {'TTT'  'TTC'}
         P: {'CCT'  'CCC'  'CCA'  'CCG'}
         S: {'TCT'  'TCC'  'TCA'  'TCG'  'AGT'  'AGC'}
         T: {'ACT'  'ACC'  'ACA'  'ACG'}
         W: {'TGG'}
         Y: {'TAT'  'TAC'}
         V: {'GTT'  'GTC'  'GTA'  'GTG'}
```

```
      Stops: {'TAA'  'TAG'  'TGA'}
     Starts: {'TTG'  'CTG'  'ATG'}
```

- Return the reverse mapping of amino acids to nucleotide codons for the Mold, Protozoan, Coelenterate Mitochondrial, and Mycoplasma/Spiroplasma genetic code, using the rna alphabet.

```
moldmap = revgeneticcode(4,'Alphabet','rna');
```

- Return the reverse mapping of amino acids to nucleotide codons for the Flatworm Mitochondrial genetic code, using three-letter codes for the field names in the return structure.

```
wormmap = revgeneticcode('Flatworm Mitochondrial',...
                         'ThreeLetterCodes',true);
```

References

[1] NCBI Web page describing genetic codes:

```
http://www.ncbi.nlm.nih.gov/Taxonomy/Utils/wprintgc.cgi?mode=c
```

See Also

Bioinformatics Toolbox functions: `aa2nt`, `aminolookup`, `baselookup`, `geneticcode`, `nt2aa`

Purpose

Perform background adjustment on Affymetrix microarray probe-level data using Robust Multi-array Average (RMA) procedure

Syntax

```
BackAdjustedMatrix = rmabackadj(PMData)
BackAdjustedMatrix = rmabackadj(..., 'Method',
MethodValue, ...)
BackAdjustedMatrix = rmabackadj(..., 'Truncate',
   TruncateValue, ...)
BackAdjustedMatrix = rmabackadj(..., 'Showplot',
   ShowplotValue, ...)
```

Arguments

PMData	Matrix of intensity values where each row corresponds to a perfect match (PM) probe and each column corresponds to an Affymetrix CEL file. (Each CEL file is generated from a separate chip. All chips should be of the same type.)
MethodValue	Specifies the estimation method for the background adjustment model parameters. Enter either `'RMA'` (to use estimation method described by Bolstad, 2005) or `'MLE'` (to estimate the parameters using maximum likelihood). Default is `'RMA'`.
TruncateValue	Specifies the background noise model. Enter either `true` (use a truncated Gaussian distribution) or `false` (use a nontruncated Gaussian distribution). Default is `true`.
ShowplotValue	Controls the plotting of a histogram showing the distribution of PM probe intensity values (blue) and the convoluted probability distribution function (red), with estimated parameters mu, sigma and alpha. Enter either `'all'` (plot a histogram for each column or chip) or specify a subset of columns (chips) by entering the column number, list of numbers, or range of numbers. For example:

- `..., 'Showplot', 3, ...)` plots the intensity values in column 3.
- `..., 'Showplot', [3,5,7], ...)` plots the intensity values in columns 3, 5, and 7.
- `..., 'Showplot', 3:9, ...)` plots the intensity values in columns 3 to 9.

Return Values

BackAdjustedMatrix Matrix of background-adjusted probe intensity values.

Description

BackAdjustedMatrix = rmabackadj(*PMData*) returns the background adjusted values of probe intensity values in the matrix, *PMData*. Note that each row in *PMData* corresponds to a perfect match (PM) probe and each column in *PMData* corresponds to an Affymetrix CEL file. (Each CEL file is generated from a separate chip. All chips should be of the same type.) Details on the background adjustment are described by Bolstad, 2005.

BackAdjustedMatrix = rmabackadj(..., '*PropertyName*', *PropertyValue*, ...) calls rmabackadj with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

BackAdjustedMatrix = rmabackadj(..., 'Method', *MethodValue*, ...) specifies the estimation method for the background adjustment model parameters. When *MethodValue* is 'RMA', rmabackadj implements the estimation method described by Bolstad, 2005. When *MethodValue* is 'MLE', rmabackadj estimates the parameters using maximum likelihood. Default is 'RMA'.

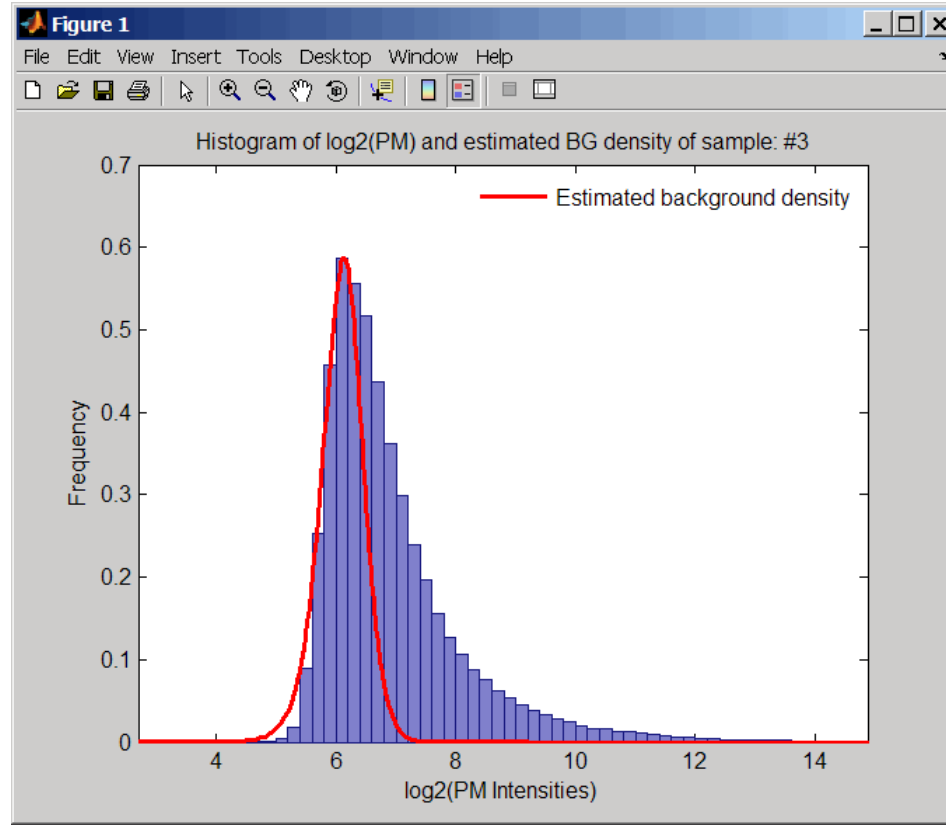
BackAdjustedMatrix = rmabackadj(..., 'Truncate', *TruncateValue*, ...) specifies the background noise model used.

When *TruncateValue* is false, rmabackadj uses nontruncated Gaussian as the background noise model. Default is true.

BackAdjustedMatrix = rmabackadj(..., 'Showplot', *ShowplotValue*, ...) lets you plot a histogram showing the distribution of PM probe intensity values (blue) and the convoluted probability distribution function (red), with estimated parameters mu, sigma and alpha. When *ShowplotValue* is 'all', rmabackadj plots a histogram for each column or chip. When *ShowplotValue* is a number, list of numbers, or range of numbers, rmabackadj plots a histogram for the indicated column number (chip).

For example:

- (..., 'Showplot', 3,...) plots the intensity values in column 3 of *PMData*.
- (..., 'Showplot', [3,5,7],...) plots the intensity values in columns 3, 5, and 7 of *PMData*.
- (..., 'Showplot', 3:9,...) plots the intensity values in columns 3 to 9 of *PMData*.



Examples

1 Load a MAT-file, included with the Bioinformatics Toolbox software, which contains Affymetrix probe-level data, including `pmMatrix`, a matrix of PM probe intensity values from multiple CEL files.

```
load prostatecancerrawdata
```

2 Perform background adjustment on the PM probe intensity values in the matrix, `pmMatrix`, creating a new matrix, `BackgroundAdjustedMatrix`.

```
BackgroundAdjustedMatrix = rmabackadj(pmMatrix);
```

3 Perform background adjustment on the PM probe intensity values in only column 3 of the matrix, `pmMatrix`, creating a new matrix, `BackgroundAdjustedChip3`.

```
BackgroundAdjustedChip3 = rmabackadj(pmMatrix(:,3));
```

The `prostatecancerrawdata.mat` file used in the previous example contains data from Best et al., 2005.

References

[1] Irizarry, R.A., Hobbs, B., Collin, F., Beazer-Barclay, Y.D., Antonellis, K.J., Scherf, U., Speed, T.P. (2003). Exploration, Normalization, and Summaries of High Density Oligonucleotide Array Probe Level Data. Biostatistics *4*, 249–264.

[2] Bolstad, B. (2005). "affy: Built-in Processing Methods" `http://www.bioconductor.org/packages/2.1/bioc/vignettes/affy/inst/doc/builtinMethods.pdf`

[3] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L., Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan, W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823–6834.

See Also

Bioinformatics Toolbox functions: `affyinvarsetnorm`, `affyread`, `affyrma`, `celintensityread`, `probelibraryinfo`, `probesetlink`, `probesetlookup`, `probesetvalues`, `quantilenorm`, `rmasummary`

Purpose

Calculate gene expression values from Affymetrix microarray probe-level data using Robust Multi-array Average (RMA) procedure

Syntax

```
ExpressionMatrix = rmasummary(ProbeIndices, Data)
ExpressionMatrix = rmasummary(ProbeIndices, Data,
'Output', OutputValue)
```

Arguments

ProbeIndices

Column vector of probe indices. The convention for probe indices is, for each probe set, to label each probe 0 to $N-1$, where N is the number of probes in the probe set.

Tip Use the `ProbeIndices` field in the structure returned by `celintensityread` as the *`ProbeIndices`* input.

Data

Matrix of natural-scale intensity values where each row corresponds to a perfect match (PM) probe and each column corresponds to an Affymetrix CEL file. (Each CEL file is generated from a separate chip. All chips should be of the same type.)

Tip Using a single-precision matrix for *`Data`* decreases memory usage.

Tip You can use the matrix from the `PMIntensities` field in the structure returned by `celintensityread` as the *`Data`* input. However, first ensure the matrix has been background adjusted, using the `rmabackadj` or `gcrmabackadj`function, and normalized, using the `quantilenorm` function.

OutputValue — Specifies the scale of the returned gene expression values. *OutputValue* can be:

- 'log'
- 'log2'
- 'log10'
- 'natural'
- @*functionname*

In the last instance, the data is transformed as defined by the function *functionname*. Default is 'log2'.

Description

ExpressionMatrix = rmasummary(*ProbeIndices*, *Data*) returns gene (probe set) expression values after calculating them from natural-scale probe intensities in the matrix *Data*, using the column vector of probe indices, *ProbeIndices*. Note that each row in *Data* corresponds to a perfect match (PM) probe, and each column corresponds to an Affymetrix CEL file. (Each CEL file is generated from a separate chip. All chips should be of the same type.) Note that the column vector *ProbeIndices* designates probes within each probe set by labeling each probe 0 to $N - 1$, where N is the number of probes in the probe set. Note that each row in *ExpressionMatrix* corresponds to a gene (probe set) and each column in *ExpressionMatrix* corresponds to an Affymetrix CEL file, which represents a single chip.

For a given probe set n, with J probe pairs, let $Yijn$ denote the background-adjusted, base 2 log transformed and quantile-normalized PM probe intensity value of chip i and probe j. $Yijn$ follows a linear additive model:

$$Yijn = Uin + Ajn + Eijn; \; i = 1, ..., I; \; j = 1, ..., J; \; n = 1, ..., N$$

where:

Uin = Gene expression of the probe set *n* on chip *i*

Ajn = Probe affinity effect for the *j*th probe in the probe set

Eijn = Residual for the *j*th probe on the *i*th chip

The RMA method assumes *A1* + *A2* + ... + *AJ* = 0 for all probe sets. A robust procedure, median polish, estimates *Ui* as the log scale measure of expression.

Note There is no column in `ExpressionMatrix` that contains probe set or gene information.

`ExpressionMatrix = rmasummary(..., 'PropertyName', PropertyValue, ...)` calls `rmasummary` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`ExpressionMatrix = rmasummary(ProbeIndices, Data, 'Output', OutputValue)` specifies the scale of the returned gene expression values. `OutputValue` can be:

- `'log'`
- `'log2'`
- `'log10'`
- `'natural'`
- `@functionname`

In the last instance, the data is transformed as defined by the function `functionname`. Default is `'log2'`.

Examples

1. Load a MAT-file, included with the Bioinformatics Toolbox software, which contains Affymetrix data variables, including `pmMatrix`, a matrix of PM probe intensity values from multiple CEL files.

```
load prostatecancerrawdata
```

2. Perform background adjustment on the PM probe intensity values in the matrix, `pmMatrix`, using the `rmabackadj` function, thereby creating a new matrix, `BackgroundAdjustedMatrix`.

```
BackgroundAdjustedMatrix = rmabackadj(pmMatrix);
```

3. Normalize the data in `BackgroundAdjustedMatrix`, using the `quantilenorm` function.

```
NormMatrix = quantilenorm(BackgroundAdjustedMatrix);
```

4. Calculate gene expression values from the probe intensities in `NormMatrix`, creating a new matrix, `ExpressionMatrix`. (Use the `probeIndices` column vector provided to supply information on the probe indices.)

```
ExpressionMatrix = rmasummary(probeIndices, NormMatrix);
```

The `prostatecancerrawdata.mat` file used in the previous example contains data from Best et al., 2005.

References

[1] Irizarry, R.A., Hobbs, B., Collin, F., Beazer-Barclay, Y.D., Antonellis, K.J., Scherf, U., Speed, T.P. (2003). Exploration, Normalization, and Summaries of High Density Oligonucleotide Array Probe Level Data. Biostatistics. *4*, 249–264.

[2] Mosteller, F., and Tukey, J. (1977). Data Analysis and Regression (Reading, Massachusetts: Addison-Wesley Publishing Company), pp. 165–202.

[3] Best, C.J.M., Gillespie, J.W., Yi, Y., Chandramouli, G.V.R., Perlmutter, M.A., Gathright, Y., Erickson, H.S., Georgevich, L.,

Tangrea, M.A., Duray, P.H., Gonzalez, S., Velasco, A., Linehan, W.M., Matusik, R.J., Price, D.K., Figg, W.D., Emmert-Buck, M.R., and Chuaqui, R.F. (2005). Molecular alterations in primary prostate cancer after androgen ablation therapy. Clinical Cancer Research *11*, 6823–6834.

See Also

`affygcrma`, `affyinvarsetnorm`, `affyrma`, `celintensityread`, `gcrmabackadj`, `mainvarsetnorm`, `malowess`, `manorm`, `quantilenorm`, `rmabackadj`

Purpose

Convert RNA sequence to DNA sequence

Syntax

```
SeqDNA = rna2dna(SeqRNA)
```

Arguments

SeqRNA RNA sequence specified by any of the following:

- Character string with the characters `A`, `C`, `G`, `U`, and ambiguous characters `R`, `Y`, `K`, `M`, `S`, `W`, `B`, `D`, `H`, `V`, `N`,
- Row vector of integers from the table Mapping Nucleotide Integers to Letter Codes on page 3-809.
- MATLAB structure containing a `Sequence` field that contains an RNA sequence, such as returned by `fastaread`, `fastqread`, `emblread`, `getembl`, `genbankread`, or `getgenbank`.

Description

SeqDNA = `rna2dna(`*SeqRNA*`)` converts an RNA sequence to a DNA sequence by converting any uracil nucleotides (`U`) in the RNA sequence to thymine nucleotides (`T`). The DNA sequence is returned in the same format as the RNA sequence. For example, if *SeqRNA* is a vector of integers, then so is *SeqDNA*.

Example

Convert an RNA sequence to a DNA sequence.

```
rna2dna('ACGAUGAGUCAUGCUU')

ans =
ACGATGAGTCATGCTT
```

See Also

Bioinformatics Toolbox function: `dna2rna`

MATLAB functions: `regexp`, `strrep`,

Purpose

Convert secondary structure of RNA sequence between bracket and matrix notations

Syntax

```
RNAStruct2 = rnaconvert(RNAStruct)
```

Arguments

RNAStruct Secondary structure of an RNA sequence represented by either:

- Bracket notation
- Connectivity matrix

Tip Use the `rnafold` function to create *RNAStruct*.

Return Values

RNAStruct2 Secondary structure of an RNA sequence represented by either:

- **Bracket notation** — String of dots and brackets, where each dot represents an unpaired base, while a pair of equally nested, opening and closing brackets represents a base pair.
- **Connectivity matrix** — Binary, upper-triangular matrix, where *RNAmatrix*`(i, j) = 1` if and only if the *i*th residue in the RNA sequence *Seq* is paired with the *j*th residue of *Seq*.

Description

RNAStruct2 = `rnaconvert(`*RNAStruct*`)` returns *RNAStruct2*, the secondary structure of an RNA sequence, in matrix notation (if *RNAStruct* is in bracket notation), or in bracket notation (if *RNAStruct* is in matrix notation).

Examples

Converting from Bracket to Matrix Notation

1 Create a string representing a secondary structure of an RNA sequence in bracket notation.

```
Bracket = '(((..((((.......)))).((.....)).))).';
```

2 Convert the secondary structure to a connectivity matrix representation.

```
Matrix = rnaconvert(Bracket);
```

Converting from Matrix to Bracket Notation

1 Create a connectivity matrix representing a secondary structure of an RNA sequence.

```
Matrix2 = zeros(12);
Matrix2(1,12) = 1;
Matrix2(2,11) = 1;
Matrix2(3,10) = 1;
Matrix2(4,9) = 1;
```

2 Convert the secondary structure to bracket notation.

```
Bracket2 = rnaconvert(Matrix2)

Bracket2 =

((((....))))
```

See Also

Bioinformatics Toolbox functions: `rnafold`, `rnaplot`

rnafold

Purpose

Predict minimum free-energy secondary structure of RNA sequence

Syntax

```
rnafold(Seq)
RNAbracket = rnafold(Seq)
[RNAbracket, Energy] = rnafold(Seq)
[RNAbracket, Energy, RNAmatrix] = rnafold(Seq)
... = rnafold(Seq, ...'MinLoopSize', MinLoopSizeValue, ...)
... = rnafold(Seq, ...'NoGU', NoGUValue, ...)
... = rnafold(Seq, ...'Progress', ProgressValue, ...)
```

Arguments

Seq	Either of the following: • String specifying an RNA sequence. • MATLAB structure containing a `Sequence` field that specifies an RNA sequence.
MinLoopSizeValue	Integer specifying the minimum size of the loops (in bases) to be considered when computing the free energy. Default is `3`.
NoGUValue	Controls whether GU or UG pairs are forbidden to form. Choices are `true` or `false` (default).
ProgressValue	Controls the display of a progress bar during the computation of the minimum free-energy secondary structure. Choices are `true` or `false` (default).

Return Values

RNAbracket	String of dots and brackets indicating the bracket notation for the minimum-free energy secondary structure of an RNA sequence. In the bracket notation, each dot represents an unpaired base, while a pair of equally nested, opening and closing brackets represents a base pair.
Energy	Value specifying the energy (in kcal/mol) of the minimum free-energy secondary structure of an RNA sequence.
RNAmatrix	Connectivity matrix representing the minimum free-energy secondary structure of an RNA sequence. A binary, upper-triangular matrix where *RNAmatrix*(i, j) = 1 if and only if the *i*th residue in the RNA sequence *Seq* is paired with the *j*th residue of *Seq*.

Description

`rnafold(`*Seq*`)` predicts and displays the secondary structure (in bracket notation) associated with the minimum free energy for the RNA sequence, *Seq*, using the thermodynamic nearest-neighbor approach.

Note For long sequences, this prediction can be time consuming. For example, a 600-nucleotide sequence can take several minutes, and sequences greater than 1000 nucleotides can take over 1 hour, depending on your system.

RNAbracket `= rnafold(`*Seq*`)` predicts and returns the secondary structure associated with the minimum free energy for the RNA sequence, *Seq*, using the thermodynamic nearest-neighbor approach. The returned structure, *RNAbracket*, is in bracket notation, that is a vector of dots and brackets, where each dot represents an unpaired

base, while a pair of equally nested, opening and closing brackets represents a base pair.

`[RNAbracket, Energy] = rnafold(Seq)` also returns *`Energy`*, the energy value (in kcal/mol) of the minimum free-energy secondary structure of the RNA sequence.

`[RNAbracket, Energy, RNAmatrix] = rnafold(Seq)` also returns *`RNAmatrix`*, a connectivity matrix representing the secondary structure associated with the minimum free energy. *`RNAmatrix`* is an upper triangular matrix where *`RNAmatrix`*`(i, j) = 1` if and only if the *`i`*th residue in the RNA sequence *`Seq`* is paired with the *`j`*th residue of *`Seq`*.

`... = rnafold(`*`Seq`*`, ...'`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `rnafold` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = rnafold(`*`Seq`*`, ...'MinLoopSize', `*`MinLoopSizeValue`*`, ...)` specifies the minimum size of the loops (in bases) to be considered when computing the free energy. Default is `3`.

`... = rnafold(`*`Seq`*`, ...'NoGU', `*`NoGUValue`*`, ...)` controls whether GU or UG pairs are forbidden to form. Choices are `true` or `false` (default).

`... = rnafold(`*`Seq`*`, ...'Progress', `*`ProgressValue`*`, ...)` controls the display of a progress bar during the computation of the minimum free-energy secondary structure. Choices are `true` or `false` (default).

Examples

Determine the minimum free-energy secondary structure (in both bracket and matrix notation) and the energy value of the following RNA sequence:

```
seq = 'ACCCCCUCCUUCCUUGGAUCAAGGGGCUCAA';
[bracket, energy, matrix] = rnafold(seq);bracket

bracket =
```

```
..(((((...((....))...)))))).....
```

References

[1] Wuchty, S., Fontana, W., Hofacker, I., and Schuster, P. (1999). Complete suboptimal folding of RNA and the stability of secondary structures. Biopolymers *49*, 145–165.

[2] Matthews, D., Sabina, J., Zuker, M., and Turner, D. (1999). Expanded sequence dependence of thermodynamic parameters improves prediction of RNA secondary structure. J. Mol. Biol. *288*, 911–940.

See Also

Bioinformatics Toolbox functions: `rnaconvert`, `rnaplot`

rnaplot

Purpose

Draw secondary structure of RNA sequence

Syntax

```
rnaplot(RNA2ndStruct)
ha = rnaplot(RNA2ndStruct)
[ha, H] = rnaplot(RNA2ndStruct)
rnaplot(RNA2ndStruct, ...'Sequence', SequenceValue, ...)
rnaplot(RNA2ndStruct, ...'Format', FormatValue, ...)
rnaplot(RNA2ndStruct, ...'Selection', SelectionValue, ...)
rnaplot(RNA2ndStruct, ...'ColorBy', ColorByValue, ...)
```

Arguments

RNA2ndStruct

Secondary structure of an RNA sequence represented by either:

- String specifying bracket notation
- Connectivity matrix

Tip Use the `rnafold` function to create *RNA2ndStruct*.

SequenceValue

Sequence of the RNA secondary structure being plotted, specified by either of the following:

- String of characters
- Structure containing a `Sequence` field that contains an RNA sequence

This information is used in the data tip displayed by clicking a base in the plot of the RNA secondary structure *RNA2ndStruct*. This information is required if you specify the `'Diagram'` format or if you specify to highlight any of the following paired selections: `'AU'`, `'UA'`, `'GC'`, `'CG'`, `'GU'` or `'UG'`.

FormatValue String specifying the format of the plot. Choices are:

- `'Circle'` (default)
- `'Diagram'`
- `'Dotdiagram'`
- `'Graph'`
- `'Mountain'`
- `'Tree'`

Note If you specify `'Diagram'`, you must also use the `'Sequence'` property to provide the RNA sequence.

SelectionValue Either of the following:

- Numeric array specifying the indices of residues to highlight in the plot.
- String specifying the subset of residues to highlight in the plot. Choices are:
  - `'Paired'`
  - `'Unpaired'`
  - `'AU'` or `'UA'`
  - `'GC'` or `'CG'`
  - `'GU'` or `'UG'`

Note If you specify `'AU'`, `'UA'`, `'GC'`, `'CG'`, `'GU'`, or `'UG'`, you must also use the `'Sequence'` property to provide the RNA sequence.

`ColorByValue` String specifying a color scheme for the plot. Choices are:

- `'State'` (default) — Color by pair state: paired bases and unpaired bases.
- `'Residue'` — Color by residue type (A, C, G, and U).
- `'Pair'` — Color by pair type (AU/UA, GC/CG, and GU/UG).

Note If you specify `'residue'` or `'pair'`, you must also use the `'Sequence'` property to provide the RNA sequence.

Note Because internal nodes of a tree correspond to paired residues, you cannot specify `'residue'` if you specify `'Tree'` for the `'Format'` property.

Return Values

ha — Handle to the figure axis.

H — A structure of handles containing a subset of the following fields, based on what you specify for the `'Selection'` and `'ColorBy'` properties:

- `Paired`
- `Unpaired`
- `A`
- `C`
- `G`
- `U`
- `AU`
- `GC`
- `GU`
- `Selected`

Description

`rnaplot(`*`RNA2ndStruct`*`)` draws the RNA secondary structure specified by *`RNA2ndStruct`*, the secondary structure of an RNA sequence represented by a string specifying bracket notation or a connectivity matrix.

`ha` `= rnaplot(`*`RNA2ndStruct`*`)` returns *`ha`*, a handle to the figure axis.

`[`*`ha`*`, `*`H`*`] = rnaplot(`*`RNA2ndStruct`*`)` also returns *`H`*, a structure of handles, which you can use to graph elements in a MATLAB Figure window.

Tip Use the handles returned in *`H`* to change properties of the graph elements, such as color, marker size, and marker type.

H contains a subset of the following fields, based on what you specify for the `'Selection'` and `'ColorBy'` properties.

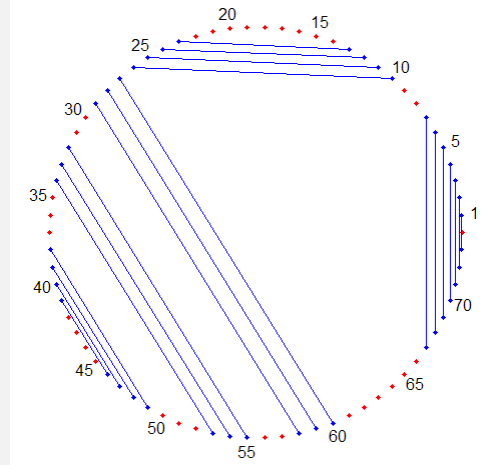
Field	Description
`Paired`	Handles to all paired residues
`Unpaired`	Handles to all unpaired residues
`A`	Handles to all A residues
`C`	Handles to all C residues
`G`	Handles to all G residues
`U`	Handles to all U residues
`AU`	Handles to all AU or UA pairs
`GC`	Handles to all GC or CG pairs
`GU`	Handles to all GU or UG pairs
`Selected`	Handles to all selected residues

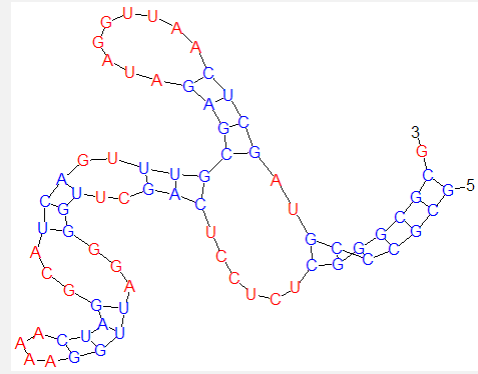
`rnaplot(`*`RNA2ndStruct`*`, ...'`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `rnaplot` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

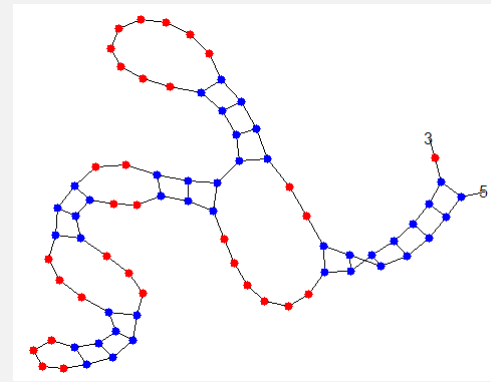
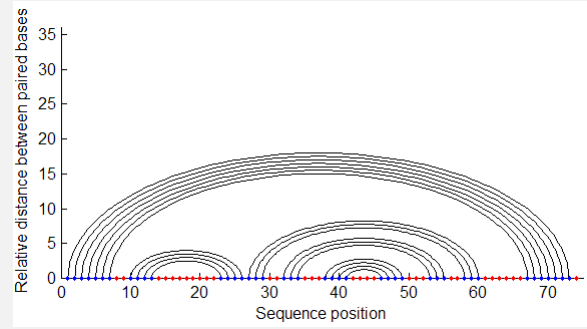
`rnaplot(`*`RNA2ndStruct`*`, ...'Sequence', `*`SequenceValue`*`, ...)` draws the RNA secondary structure specified by *`RNA2ndStruct`*, and annotates it with the sequence positions supplied by *`SequenceValue`*, the RNA sequence specified by a string of characters or a structure containing a `Sequence` field.

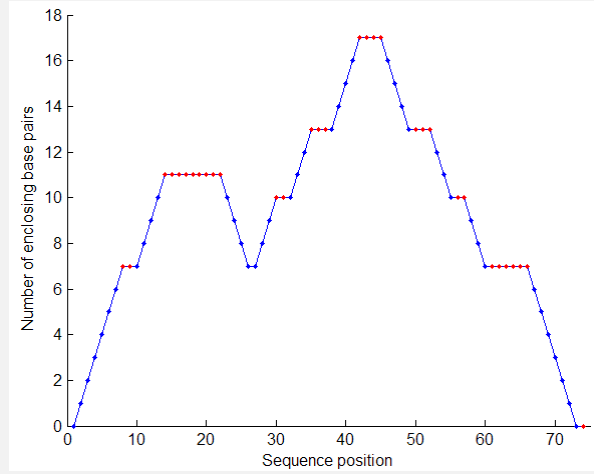
`rnaplot(`*`RNA2ndStruct`*`, ...'Format', `*`FormatValue`*`, ...)` draws the RNA secondary structure specified by *`RNA2ndStruct`*, using the format specified by *`FormatValue`*.

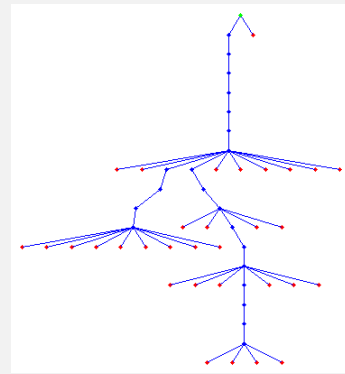
`FormatValue` is a string specifying the format of the plot. Choices are as follows.

Format	Description
`'Circle'` (default)	Each base is represented by a dot on the circumference of a circle of arbitrary size. Lines connect bases that pair with each other. 
`'Diagram'`	Two-dimensional representation of the RNA secondary structure. Each base is represented and identified by a letter. The backbone and hydrogen bonds between base pairs are represented by lines.

Format	Description
	 **Note** If you specify `'Diagram'`, you must also use the `'Sequence'` property to provide the RNA sequence.
`'Dotdiagram'`	Two-dimensional representation of the RNA secondary structure. Each base is represented and identified by a dot. The backbone and hydrogen bonds between base pairs are represented by lines.

Format	Description
	
`'Graph'`	Bases are displayed in their sequence position along the abscissa (*x*-axis) of a graph. Semi-elliptical lines connect bases that pair with each other. The height of the lines is proportional to the distance between paired bases. 

Format	Description
`'Mountain'`	Each base is represented by a dot in a two-dimensional plot, where the base position is in the abscissa (*x*-axis) and the number of base pairs enclosing a given base is in the ordinate (*y*-axis). 
`'Tree'`	Each base is represented by a node in a tree graph. Leaf nodes indicate unpaired bases, while each internal node indicates a base pair. The tree root is a fictitious node, not associated with any base in the secondary structure.

Format	Description
	 **Note** To create a tree plot, you must have accepted a Graphviz software license (free). If you have not, you will be prompted to do so.

`rnaplot(`*`RNA2ndStruct`*`, ...'Selection', `*`SelectionValue`*`, ...)` draws the RNA secondary structure specified by *`RNA2ndStruct`*, highlighting a subset of residues specified by *`SelectionValue`*. *`SelectionValue`* can be either:

- Numeric array specifying the indices of residues to highlight in the plot.
- String specifying the subset of residues to highlight in the plot. Choices are:
  - `'Paired'`
  - `'Unpaired'`
  - `'AU'` or `'UA'`
  - `'GC'` or `'CG'`

- 'GU' or 'UG'

Note If you specify 'AU', 'UA', 'GC', 'CG', 'GU', or 'UG', you must also use the 'Sequence' property to provide the RNA sequence.

rnaplot(*RNA2ndStruct*, ...'ColorBy', *ColorByValue*, ...) draws the RNA secondary structure specified by *RNA2ndStruct*, using a color scheme specified by *ColorByValue*, a string indicating a color scheme. Choices are:

- 'State' (default) — Color by pair state: paired bases and unpaired bases.
- 'Residue' — Color by residue type (A, C, G, and U).
- 'Pair' — Color by pair type (AU/UA, GC/CG, and GU/UG).

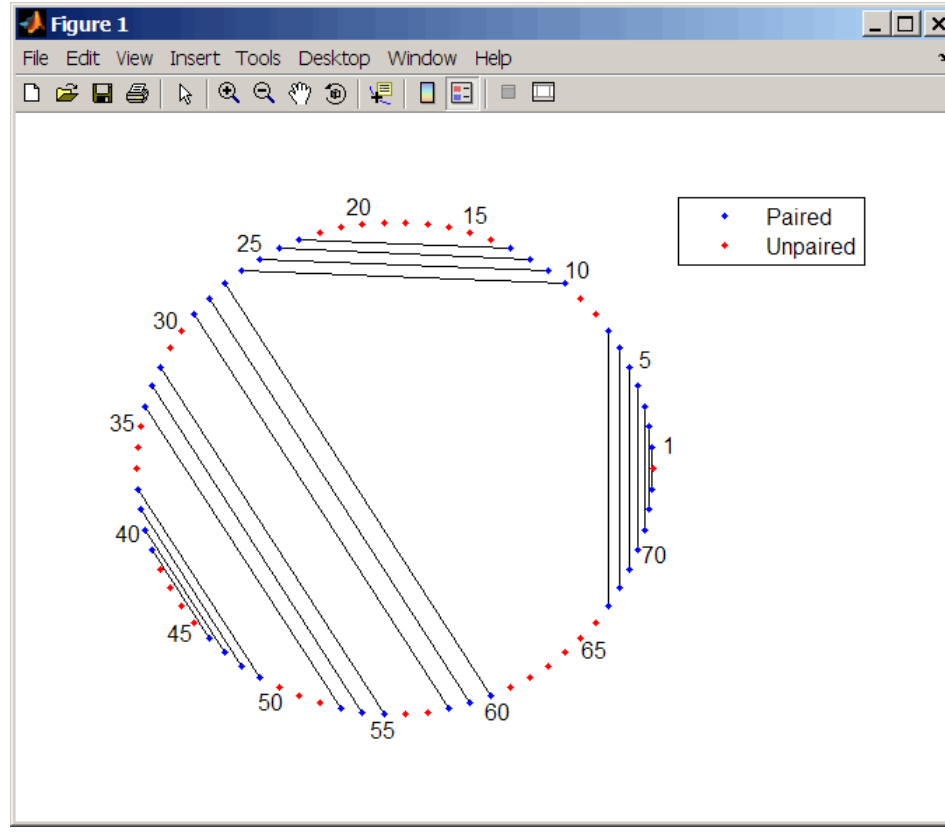
Note If you specify 'Residue' or 'Pair', you must also use the 'Sequence' property to provide the RNA sequence.

Note Because internal nodes of a tree correspond to paired residues, you cannot specify 'Residue' if you specify 'Tree' for the 'Format' property.

Examples

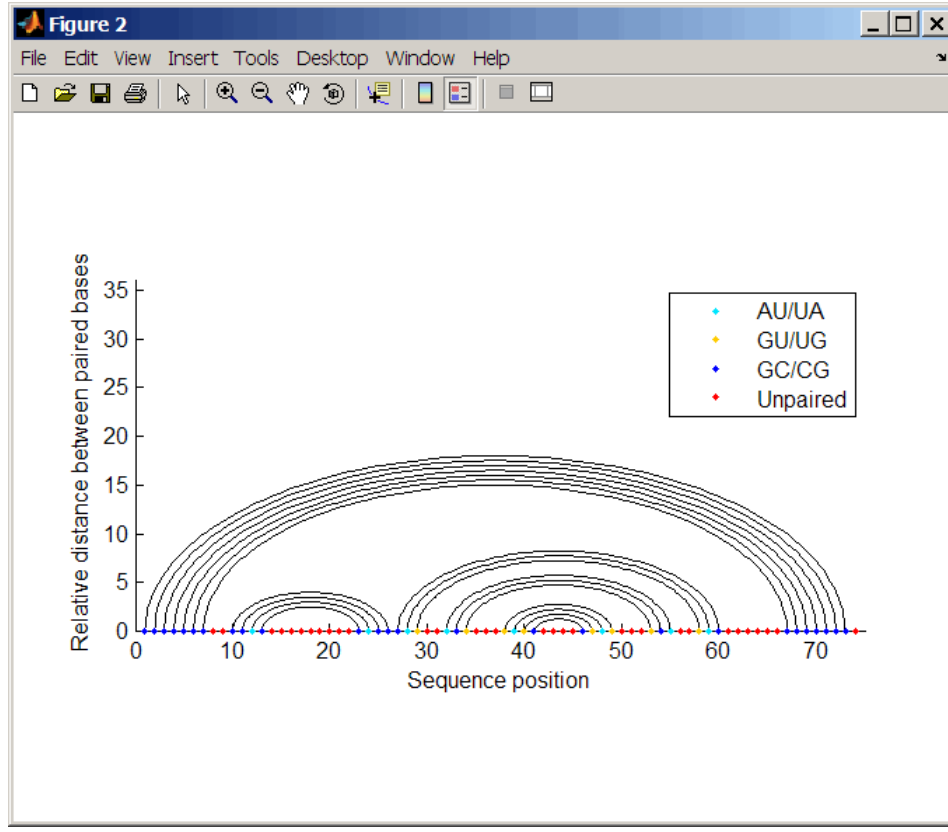
1 Determine the minimum free-energy secondary structure of an RNA sequence and plot it in circle format:

```
seq = 'GCGCCCGUAGCUCAAUUGGAUAGAGCGUUUGACUACGGAUCAAAAGGUUAGGGGUUCGACUCCUCUCGGGCGCG';
ss = rnafold(seq);
rnaplot(ss)
```



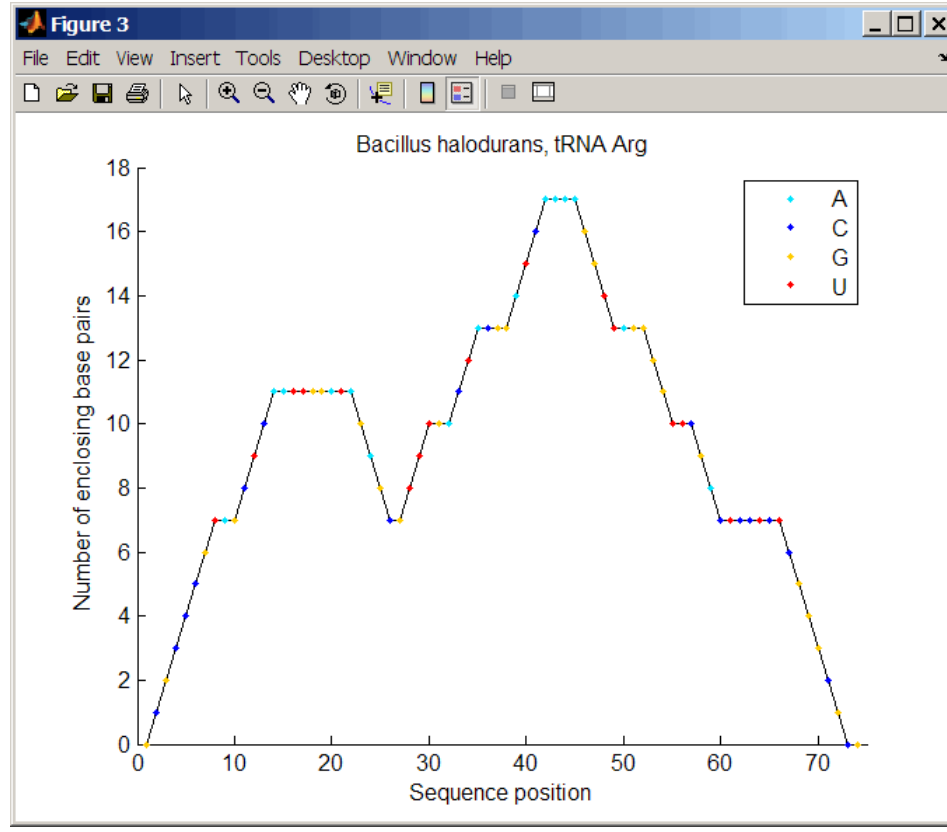
2 Plot the RNA sequence secondary structure in graph format and color it by pair type.

```
rnaplot(ss, 'sequence', seq, 'format', 'graph', 'colorby', 'pair')
```



3 Plot the RNA sequence secondary structure in mountain format and color it by residue type. Use the handle to add a title to the plot.

```
ha = rnaplot(ss, 'sequence', seq, 'format', 'mountain',...
             'colorby', 'residue')
title(ha, 'Bacillus halodurans, tRNA Arg')
```



4 Mutate the first six positions in the sequence and observe the effect the change has on the secondary structure by highlighting the first six residues.

```
seqMut = seq;
seqMut(1:6) = 'AAAAAA';
ssMut = rnafold(seqMut);
rnaplot(ss, 'sequence', seq, 'format', 'dotdiagram', 'selection', 1:6);
rnaplot(ssMut, 'sequence', seqMut, 'format', 'dotdiagram', 'selection', 1:6);
```

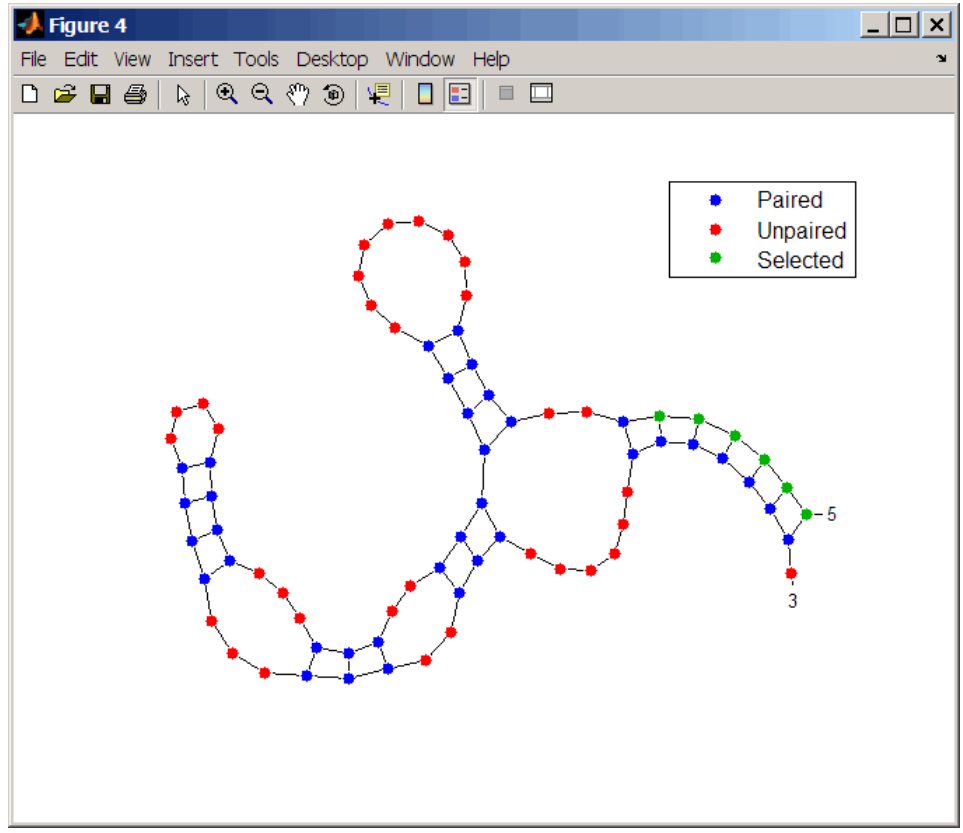
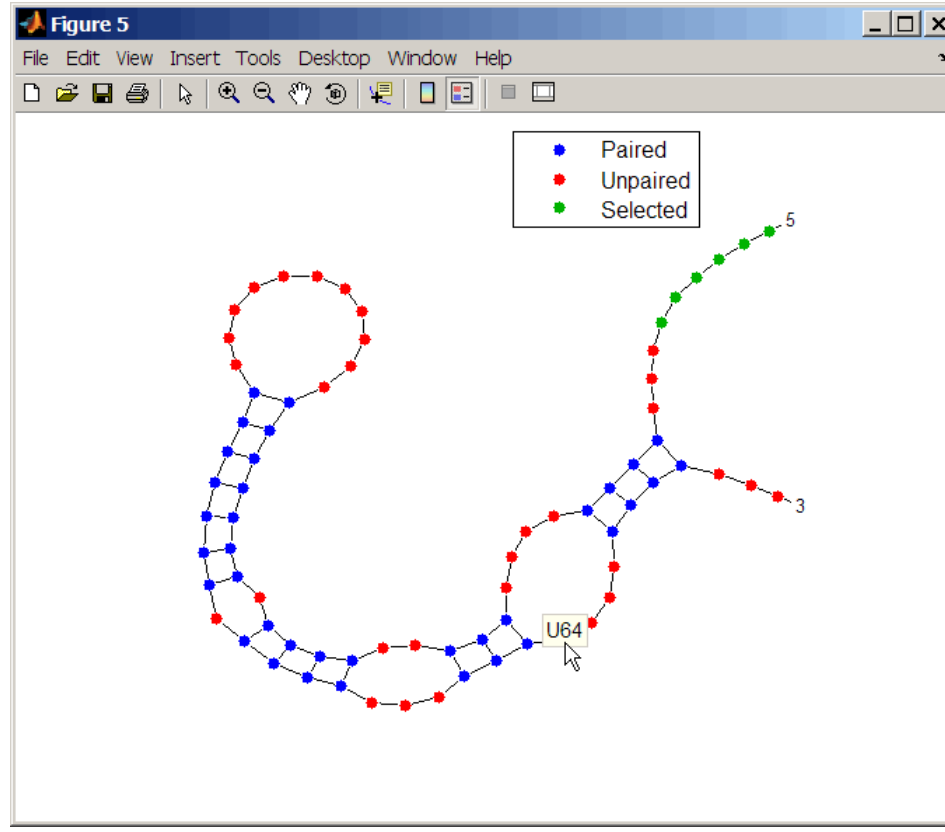


Figure 4
File Edit View Insert Tools Desktop Window Help
Paired
Unpaired
Selected
5
3



Tip If necessary, click-drag the legend to prevent it from covering the plot. Click a base in the plot to display a data tip with information on that base.

See Also

Bioinformatics Toolbox functions: `rnaconvert`, `rnafold`

rownames (DataMatrix)

Purpose

Retrieve or set row names of DataMatrix object

Syntax

```
ReturnRowNames = rownames(DMObj)
ReturnRowNames = rownames(DMObj, RowIndices)
DMObjNew = rownames(DMObj, RowIndices, RowNames)
```

Arguments

DMObj	DataMatrix object, such as created by `DataMatrix` (object constructor).
RowIndices	One or more rows in *DMObj*, specified by any of the following: • Positive integer • Vector of positive integers • String specifying a row name • Cell array of strings • Logical vector
RowNames	Row names specified by any of the following: • Numeric vector • Cell array of strings • Character array • Single string, which is used as a prefix for row names, with row numbers appended to the prefix • Logical `true` or `false` (default). If `true`, unique row names are assigned using the format `row1`, `row2`, `row3`, etc. If `false`, no row names are assigned.

Note The number of elements in *RowNames* must equal the number of elements in *RowIndices*.

Return Values

ReturnRowNames	String or cell array of strings containing row names in *DMObj*.
DMObjNew	DataMatrix object created with names specified by *RowIndices* and *RowNames*.

Description

ReturnRowNames = rownames(*DMObj*) returns *ReturnRowNames*, a cell array of strings specifying the row names in *DMObj*, a DataMatrix object.

ReturnRowNames = rownames(*DMObj*, *RowIndices*) returns the row names specified by *RowIndices*. *RowIndices* can be a positive integer, vector of positive integers, string specifying a row name, cell array of strings, or a logical vector.

DMObjNew = rownames(*DMObj*, *RowIndices*, *RowNames*) returns *DMObjNew*, a DataMatrix object with rows specified by *RowIndices* set to the names specified by *RowNames*. The number of elements in *RowIndices* must equal the number of elements in *RowNames*.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: colnames

samplealign

Purpose

Align two data sets containing sequential observations by introducing gaps

Syntax

```
[I, J] = samplealign(X, Y)
[I, J] = samplealign(X, Y, ...'Band', BandValue, ...)
[I, J] = samplealign(X, Y, ...'Width', WidthValue, ...)
[I, J] = samplealign(X, Y, ...'Gap', GapValue, ...)
[I, J] = samplealign(X, Y, ...'Quantile',
QuantileValue, ...)
[I, J] = samplealign(X, Y, ...'Distance',
DistanceValue, ...)
[I, J] = samplealign(X, Y, ...'Weights', WeightsValue, ...)
[I, J] = samplealign(X, Y, ...'ShowConstraints',
   ShowConstraintsValue, ...)
[I, J] = samplealign(X, Y, ...'ShowNetwork',
   ShowNetworkValue, ...)
[I, J] = samplealign(X, Y, ...'ShowAlignment',
   ShowAlignmentValue, ...)
```

Arguments

X, *Y*	Matrices of data where rows correspond to observations or samples, and columns correspond to features or dimensions. *X* and *Y* can have a different number of rows, but they must have the same number of columns. The first column is the reference dimension and must contain unique values in ascending order. The reference dimension could contain sample indices of the observations or a measurable value, such as time.
BandValue	Either of the following: • Scalar. • Function specified using `@(z)`, where *z* is the mid-point between a given

observation in one data set and a given observation in the other data set.

BandValue specifies a maximum allowable distance between observations (along the reference dimension only) in the two data sets, thus limiting the number of potential matches between observations in two data sets. If *S* is the value in the reference dimension for a given observation (row) in one data set, then that observation is matched only with observations in the other data set whose values in the reference dimension fall within $S \pm$ *BandValue*. Then, only these potential matches are passed to the algorithm for further scoring. Default *BandValue* is `Inf`.

WidthValue

Either of the following:

- Two-element vector, [*U*, *V*]
- Scalar that is used for both *U* and *V*

WidthValue limits the number of potential matches between observations in two data sets; that is, each observation in *X* is scored to the closest *U* observations in *Y*, and each observation in *Y* is scored to the closest *V* observations in *X*. Then, only these potential matches are passed to the algorithm for further scoring. Closeness is measured using only the first column (reference dimension) in each data set. Default is `Inf` if `'Band'` is specified; otherwise default is `10`.

GapValue

Any of the following:

- Cell array, {*G*, *H*}, where *G* is either a scalar or a function handle specified using @(*X*), and *H* is either a scalar or a function handle specified using @(*Y*). The functions @(*X*) and @(*Y*) must calculate the penalty for each observation (row) when it is matched to a gap in the other data set. The functions @(*X*) and @(*Y*) must return a column vector with the same number of rows as *X* or *Y*, containing the gap penalty for each observation (row).
- Single function handle specified using @(*Z*), which is used for both *G* and *H*. The function @(*Z*) must calculate the penalty for each observation (row) in both *X* and *Y* when it is matched to a gap in the other data set. The function @(*Z*) must take as arguments *X* and *Y*. The function @(*Z*) must return a column vector with the same number of rows as *X* or *Y*, containing the gap penalty for each observation (row).
- Scalar that is used for both *G* and *H*.

GapValue specifies the position-dependent terms for assigning gap penalties. The calculated value, *GPX*, is the gap penalty for matching observations from the first data set *X* to gaps inserted in the second data set *Y*, and is the product of two terms: *GPX* = *G* * *QMS*. The term *G* takes its value as a function of the observations in *X*. Similarly, *GPY* is the gap penalty for matching observations

from *Y* to gaps inserted in *X*, and is the product of two terms: *GPY* = *H* * *QMS*. The term *H* takes its value as a function of the observations in *Y*. By default, the term *QMS* is the 0.75 quantile of the score for the pairs of observations that are potential matches (that is, pairs that comply with the `'Band'` and `'Width'` constraints). Default *GapValue* is `1`.

QuantileValue

Scalar between `0` and `1` that specifies the quantile value used to calculate the term *QMS*, which is used by the `'Gap'` property to calculate gap penalties. Default is `0.75`.

DistanceValue

Function handle specified using `@(R,S)`. The function `@(R,S)` must:

- Calculate the distance between pairs of observations that are potential matches.
- Take as arguments, *R* and *S*, matrices that have the same number of rows and columns, and whose paired rows represent all potential matches of observations in *X* and *Y* respectively.
- Return a column vector of positive values with the same number of elements as rows in *R* and *S*.

Default is the Euclidean distance between the pairs.

Caution All columns in *X* and *Y*, including the reference dimension, are considered when calculating distances. If you do not want to include the reference dimension in the distance calculations, use the `'Weight'` property to exclude it.

WeightsValue

Either of the following:

- Logical row vector with the same number of elements as columns in *X* and *Y*, that specifies columns in *X* and *Y*.
- Numeric row vector with the same number of elements as columns in *X* and *Y*, that specifies the relative weights of the columns (features).

This property controls the inclusion/exclusion of columns (features) or the emphasis of columns (features) when calculating the distance score between observations that are potential matches, that is, when using the `'Distance'` property. Default is a logical row vector with all elements set to `true`.

Tip Using a numeric row vector for *WeightsValue* and setting some values to `0` can simplify the distance calculation when the data sets have many columns (features).

Note The weight values are not considered when using the `'Band'`, `'Width'`, or `'Gap'` property.

ShowConstraintsValue	Controls the display of the search space constrained by the specified `'Band'` and `'Width'` input parameters, thereby giving an indication of the memory required to run the algorithm with the specific `'Band'` and `'Width'` parameters on your data sets. Choices are `true` or `false` (default).
ShowNetworkValue	Controls the display of the dynamic programming network, the match scores, the gap penalties, and the winning path. Choices are `true` or `false` (default).
ShowAlignmentValue	Controls the display of the first and second columns of the *X* and *Y* data sets in the abscissa and the ordinate respectively, of a two-dimensional plot. Choices are `true`, `false` (default), or an integer specifying a column of the *X* and *Y* data sets to plot as the ordinate.

Return Values

I	Column vector containing indices of rows (observations) in *X* that match to a row (observation) in *Y*. Missing indices indicate that row (observation) is matched to a gap.
J	Column vector containing indices of rows (observations) in *Y* that match to a row (observation) in *X*. Missing indices indicate that row (observation) is matched to a gap.

Description

`[I, J] = samplealign(X, Y)` aligns the observations in two matrices of data, `X` and `Y`, by introducing gaps. `X` and `Y` are matrices of data where rows correspond to observations or samples, and columns correspond to features or dimensions. `X` and `Y` can have different number of rows, but must have the same number of columns. The first column is the reference dimension and must contain unique values in ascending order. The reference dimension could contain sample indices of the observations or a measurable value, such as time. The `samplealign` function uses a dynamic programming algorithm to minimize the sum of positive scores resulting from pairs of observations that are potential matches and the penalties resulting from the insertion of gaps. Return values `I` and `J` are column vectors containing indices that indicate the matches for each row (observation) in `X` and `Y` respectively.

Tip If you do not specify return values, `samplealign` does not run the dynamic programming algorithm. Running `samplealign` without return values, but setting the `'ShowConstraints'`, `'ShowNetwork'`, or `'ShowAlignment'` property to `true`, lets you explore the constrained search space, the dynamic programming network, or the aligned observations, without running into potential memory problems.

`[I, J] = samplealign(X, Y, ...'PropertyName', PropertyValue, ...)` calls `samplealign` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`[I, J] = samplealign(X, Y, ...'Band', BandValue, ...)` specifies a maximum allowable distance between observations (along the reference dimension only) in the two data sets, thus limiting the number of potential matches between observations in the two data sets. If `S` is the value in the reference dimension for a given observation (row) in one data set, then that observation is matched only with observations in the other data set whose values in the reference dimension fall

within *S* ± *BandValue*. Then, only these potential matches are passed to the algorithm for further scoring. *BandValue* can be a scalar or a function specified using `@(z)`, where *z* is the mid-point between a given observation in one data set and a given observation in the other data set. Default *BandValue* is `Inf`.

This constraint reduces the time and memory complexity of the algorithm from O(*MN*) to O(sqrt(*MN*)**K*), where *M* and *N* are the number of observations in *X* and *Y* respectively, and *K* is a small constant such that *K*<<*M* and *K*<<*N*. Adjust *BandValue* to the maximum expected shift between the reference dimensions in the two data sets, that is, between *X*(:,1) and *Y*(:,1).

`[I, J] = samplealign(X, Y, ...'Width', WidthValue, ...)` limits the number of potential matches between observations in two data sets; that is, each observation in *X* is scored to the closest *U* observations in *Y*, and each observation in *Y* is scored to the closest *V* observations in *X*. Then, only these potential matches are passed to the algorithm for further scoring. *WidthValue* is either a two-element vector, [*U*, *V*] or a scalar that is used for both *U* and *V*. Closeness is measured using only the first column (reference dimension) in each data set. Default is `Inf` if `'Band'` is specified; otherwise default is `10`.

This constraint reduces the time and memory complexity of the algorithm from O(*MN*) to O(sqrt(*MN*)*sqrt(*UV*)), where *M* and *N* are the number of observations in *X* and *Y* respectively, and *U* and *V* are small such that *U*<<*M* and *V*<<*N*.

Note If you specify both `'Band'` and `'Width'`, only pairs of observations that meet both constraints are considered potential matches and passed to the algorithm for scoring.

Tip Specify `'Width'` when you do not have a good estimate for the `'Band'` property. To get an indication of the memory required to run the algorithm with specific `'Band'` and `'Width'` parameters on your data sets, run `samplealign`, but do not specify return values and set `'ShowConstraints'` to `true`.

`[I, J] = samplealign(X, Y, ...'Gap', GapValue, ...)` specifies the position-dependent terms for assigning gap penalties.

GapValue is any of the following:

- Cell array, {*G*, *H*}, where *G* is either a scalar or a function handle specified using `@(X)`, and *H* is either a scalar or a function handle specified using `@(Y)`. The functions `@(X)` and `@(Y)` must calculate the penalty for each observation (row) when it is matched to a gap in the other data set. The functions `@(X)` and `@(Y)` must return a column vector with the same number of rows as *X* or *Y*, containing the gap penalty for each observation (row).
- Single function handle specified using `@(Z)`, that is used for both *G* and *H*. The function `@(Z)` must calculate the penalty for each observation (row) in both *X* and *Y* when it is matched to a gap in the other data set. The function `@(Z)` must take as arguments *X* and *Y*. The function `@(Z)` must return a column vector with the same number of rows as *X* or *Y*, containing the gap penalty for each observation (row).
- Scalar that is used for both *G* and *H*.

The calculated value, *GPX*, is the gap penalty for matching observations from the first data set *X* to gaps inserted in the second data set *Y*, and is the product of two terms: *GPX* = *G* * *QMS*. The term *G* takes its value as a function of the observations in *X*. Similarly, *GPY* is the gap penalty for matching observations from *Y* to gaps inserted in *X*, and is the product of two terms: *GPY* = *H* * *QMS*. The term *H* takes its value as a function of the observations in *Y*. By default, the term *QMS* is the 0.75 quantile of

the score for the pairs of observations that are potential matches (that is, pairs that comply with the 'Band' and 'Width' constraints).

If *G* and *H* are positive scalars, then *GPX* and *GPY* are independent of the observation where the gap is being inserted.

Default *GapValue* is 1, that is, both *G* and *H* are 1, which indicates that the default penalty for gap insertions in both sequences is equivalent to the quantile (set by the 'Quantile' property, default = 0.75) of the score for the pairs of observations that are potential matches.

Note *GapValue* defaults to a relatively safe value. However, the success of the algorithm depends on the fine tuning of the gap penalties, which is application dependent. When the gap penalties are large relative to the score of the correct matches, samplealign returns alignments with fewer gaps, but with more incorrectly aligned regions. When the gap penalties are smaller, the output alignment contains longer regions with gaps and fewer matched observations. Set 'ShowNetwork' to true to compare the gap penalties to the score of matched observations in different regions of the alignment.

[*I*, *J*] = samplealign(*X*, *Y*, ...'Quantile', *QuantileValue*, ...) specifies the quantile value used to calculate the term *QMS*, which is used by the 'Gap' property to calculate gap penalties. *QuantileValue* is a scalar between 0 and 1. Default is 0.75.

Tip Set *QuantileValue* to an empty array ([]) to make the gap penalities independent of *QMS*, that is, *GPX* and *GPY* are functions of only the *G* and *H* input parameters respectively.

[*I*, *J*] = samplealign(*X*, *Y*, ...'Distance', *DistanceValue*, ...) specifies a function to calculate the distance between pairs of observations that are potential matches. *DistanceValue* is a function handle specified using @(*R*,*S*). The function @(*R*,*S*) must take as

arguments, *R* and *S*, matrices that have the same number of rows and columns, and whose paired rows represent all potential matches of observations in *X* and *Y* respectively. The function `@(R,S)` must return a column vector of positive values with the same number of elements as rows in *R* and *S*. Default is the Euclidean distance between the pairs.

Caution

All columns in *X* and *Y*, including the reference dimension, are considered when calculating distances. If you do not want to include the reference dimension in the distance calculations, use the `'Weight'` property to exclude it.

`[I, J] = samplealign(X, Y, ...'Weights', WeightsValue, ...)` controls the inclusion/exclusion of columns (features) or the emphasis of columns (features) when calculating the distance score between observations that are potential matches, that is when using the `'Distance'` property. *WeightsValue* can be a logical row vector that specifies columns in *X* and *Y*. *WeightsValue* can also be a numeric row vector with the same number of elements as columns in *X* and *Y*, that specifies the relative weights of the columns (features). Default is a logical row vector with all elements set to `true`.

Tip Using a numeric row vector for *WeightsValue* and setting some values to `0` can simplify the distance calculation when the data sets have many columns (features).

Note The weight values are not considered when computing the constrained alignment space, that is when using the `'Band'` or `'Width'` properties, or when calculating the gap penalties, that is when using the `'Gap'` property.

`[I, J] = samplealign(X, Y, ...'ShowConstraints', ShowConstraintsValue, ...)` controls the display of the search space constrained by the input parameters `'Band'` and `'Width'`, giving an indication of the memory required to run the algorithm with specific `'Band'` and `'Width'` on your data sets. Choices are `true` or `false` (default).

`[I, J] = samplealign(X, Y, ...'ShowNetwork', ShowNetworkValue, ...)` controls the display of the dynamic programming network, the match scores, the gap penalties, and the winning path. Choices are `true` or `false` (default).

`[I, J] = samplealign(X, Y, ...'ShowAlignment', ShowAlignmentValue, ...)` controls the display of the first and second columns of the `X` and `Y` data sets in the abscissa and the ordinate respectively, of a two-dimensional plot. Links between all the potential matches that meet the constraints are displayed, and the matches belonging to the output alignment are highlighted. Choices are `true`, `false` (default), or an integer specifying a column of the `X` and `Y` data sets to plot as the ordinate.

Examples

Warping a sine wave with a smooth function to more closely follow cyclical sunspot activity

1. Load `sunspot.dat`, a data file included with the MATLAB software, that contains the variable `sunspot`, which is a two-column matrix containing variations in sunspot activity over the last 300 years. The first column is the reference dimension (years), and the second column contains sunspot activity values. Sunspot activity is cyclical, reaching a maximum about every 11 years.

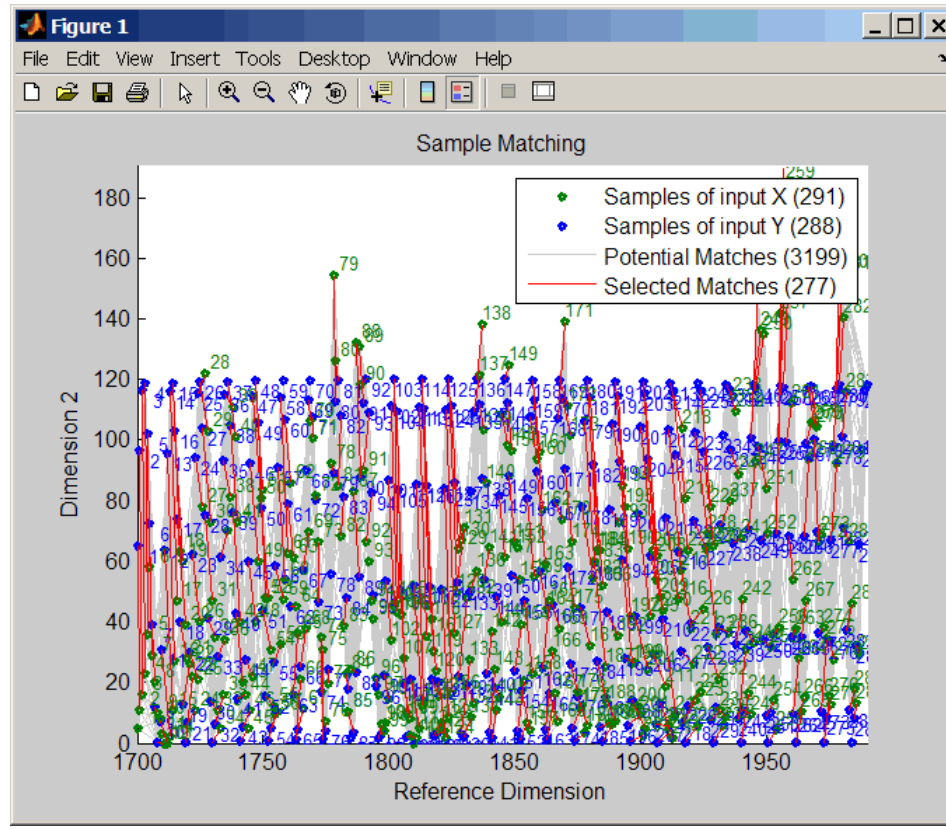
   ```
   load sunspot.dat
   ```

2. Create a sine wave with a known period of sunspot activity.

   ```
   years = (1700:1990)';
   T = 11.038;
   f = @(y) 60 + 60 * sin(y*(2*pi/T));
   ```

3 Align the observations between the sine wave and the sunspot activity by introducing gaps.

```
[i,j] = samplealign([years f(years)],sunspot,'weights',...
                    [0 1],'showalignment',true);
```

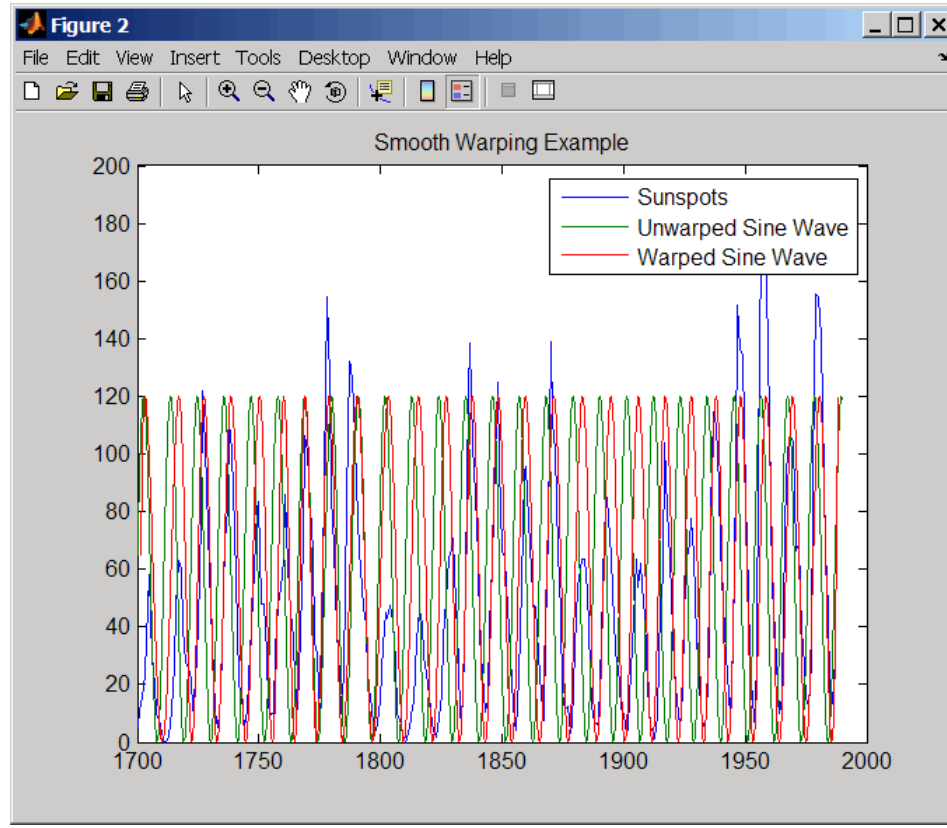


4 Estimate a smooth function to warp the sine wave.

```
[p,s,mu] = polyfit(years(i),years(j),15);
wy = @(y) polyval(p,(y-mu(1))./mu(2));
```

5 Plot the sunspot cycles, unwarped sine wave, and warped sine wave.

```
years = (1700:1/12:1990)';
figure
plot(sunspot(:,1),sunspot(:,2),years,f(years),wy(years),...
     f(years))
legend('Sunspots','Unwarped Sine Wave','Warped Sine Wave')
title('Smooth Warping Example')
```



Recovering a nonlinear warping between two signals containing noisy Gaussian peaks

1 Create two signals with noisy Gaussian peaks.

```
rand('twister',5489)
peakLoc = [30 60 90 130 150 200 230 300 380 430];
peakInt = [7 1 3 10 3 6 1 8 3 10];
time = 1:450;
comp = exp(-(bsxfun(@minus,time,peakLoc')./5).^2);
sig_1 = (peakInt + rand(1,10)) * comp + rand(1,450);
sig_2 = (peakInt + rand(1,10)) * comp + rand(1,450);
```

2 Define a nonlinear warping function.

```
wf = @(t) 1 + (t<=100).*0.01.*(t.^2) + (t>100).*...
     (310+150*tanh(t./100-3));
```

3 Warp the second signal to distort it.

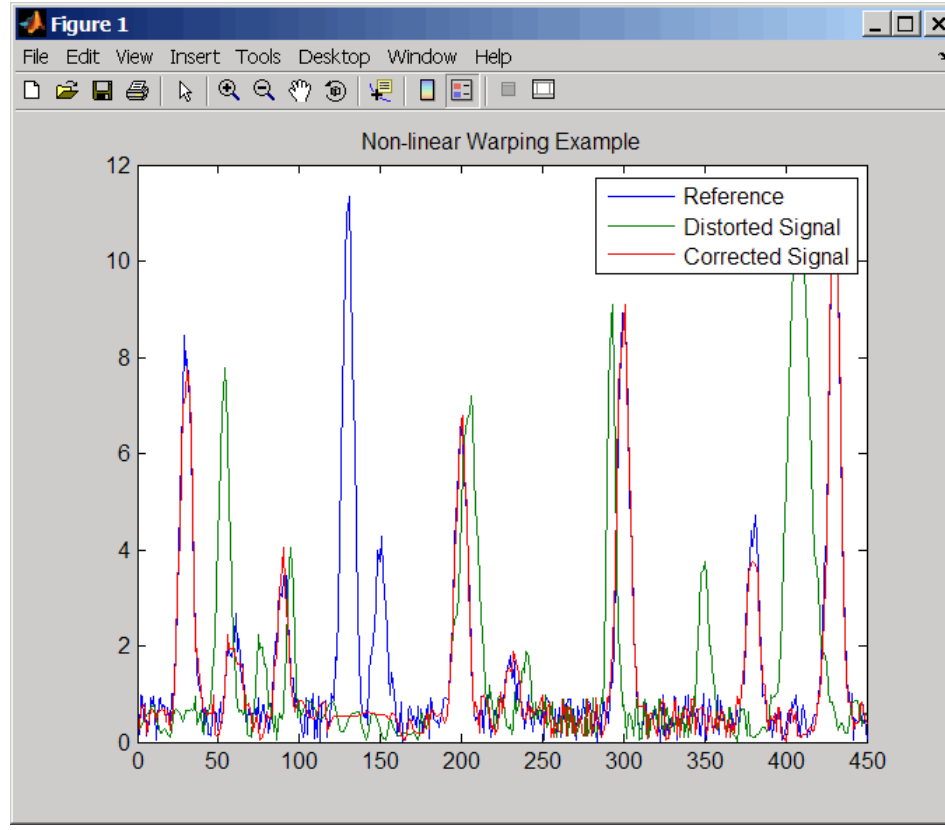
```
sig_2 = interp1(time,sig_2,wf(time),'pchip');
```

4 Align the observations between the two signals by introducing gaps.

```
[i,j] = samplealign([time;sig_1]',[time;sig_2]',...
                    'weights',[0,1],'band',35,'quantile',.5);
```

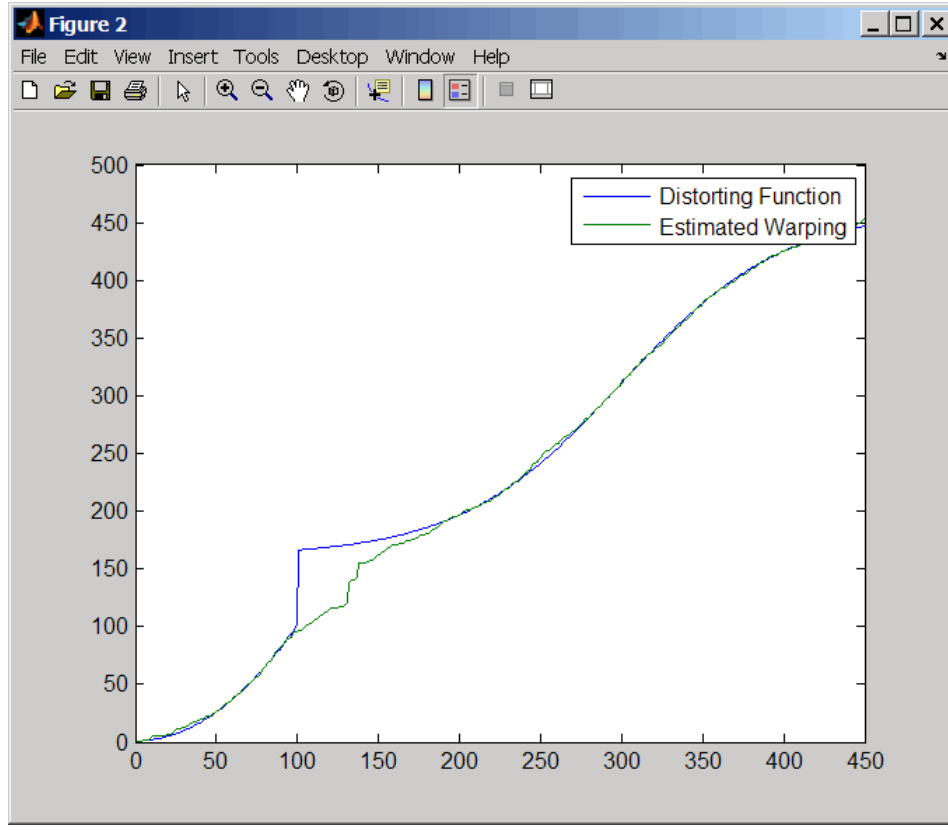
5 Plot the reference signal, distorted signal, and warped (corrected) signal.

```
figure
sig_3 = interp1(time,sig_2,interp1(i,j,time,'pchip'),'pchip');
plot(time,sig_1,time,sig_2,time,sig_3)
legend('Reference','Distorted Signal','Corrected Signal')
title('Non-linear Warping Example')
```



6 Plot the real and the estimated warping functions.

```
figure
plot(time,wf(time),time,interp1(j,i,time,'pchip'))
legend('Distorting Function','Estimated Warping')
```



Note For examples of using function handles for the `Band`, `Gap`, and `Distance` properties, see the demo Visualizing and Preprocessing Hyphenated Mass-Spectrometry Data Sets for Metabolite and Protein/Peptide Profiling.

References

[1] Myers, C.S. and Rabiner, L.R. (1981). A comparative study of several dynamic time-warping algorithms for connected word recognition. The Bell System Technical Journal *60:7*, 1389–1409.

[2] Sakoe, H. and Chiba, S. (1978). Dynamic programming algorithm optimization for spoken word recognition. IEEE Trans. Acoustics, Speech and Signal Processing *ASSP-26(1)*, 43–49.

See Also

Bioinformatics Toolbox functions: `msalign`, `msheatmap`, `mspalign`, `msppresample`, `msresample`

bioma.ExpressionSet.sampleData

Purpose

Retrieve or set sample metadata in ExpressionSet object

Syntax

```
MetaDataObj = sampleData(ESObj)
NewESObj = sampleData(ESObj, NewMetaDataObj)
```

Description

`MetaDataObj = sampleData(ESObj)` returns a MetaData object containing the sample metadata from an ExpressionSet object.

`NewESObj = sampleData(ESObj, NewMetaDataObj)` replaces the sample metadata in *`ESObj`*, an ExpressionSet object, with *`NewMetaDataObj`*, and returns *`NewESObj`*, a new ExpressionSet object.

Inputs

`ESObj`

Object of the `bioma.ExpressionSet` class.

`NewMetaDataObj`

Object of the `bioma.data.MetaData` class, containing sample metadata, stored in two dataset arrays. The sample names and variable names in *`NewMetaDataObj`* must match the sample names and variable names in the *`MetaDataObj`* being replaced in the ExpressionSet object, *`ESObj`*.

Outputs

`MetaDataObj`

Object of the `bioma.data.MetaData` class, containing the sample metadata, stored in two dataset arrays.

`NewESObj`

Object of the `bioma.ExpressionSet` class, returned after replacing the MetaData object containing the sample metadata.

Examples

Construct an ExpressionSet object from `EDObj`, an ExptData object, `MDObj2`, a MetaData object containing sample variable information, and `MIAMEObj`, a MIAME object. Retrieve the MetaData object that contains sample metadata, stored in the ExpressionSet object:

```
% Import bioma.data package to make constructor functions
```

```
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Construct MIAME object
MIAMEObj = MIAME(geoStruct);
% Import bioma package to make constructor function
% available
import bioma.*
% Construct ExpressionSet object
ESObj = ExpressionSet(EDObj, 'SData', MDObj2, 'EInfo', MIAMEObj);
% Retrieve the sample data
NewMDObj = sampleData(ESObj);
```

See Also

bioma.ExpressionSet | bioma.data.ExptData | sampleNames | featureData

How To

- "Working with ExpressionSet Objects"

bioma.ExpressionSet.sampleNames

Purpose

Retrieve or set sample names in ExpressionSet object

Syntax

```
SamNames = sampleNames(ESObj)
SamNames = sampleNames(ESObj, Subset)
NewESObj = sampleNames(ESObj, Subset, NewSamNames)
```

Description

`SamNames = sampleNames(ESObj)` returns a cell array of strings specifying all sample names in an ExpressionSet object.

`SamNames = sampleNames(ESObj, Subset)` returns a cell array of strings specifying a subset the sample names in an ExpressionSet object.

`NewESObj = sampleNames(ESObj, Subset, NewSamNames)` replaces the sample names specified by `Subset` in `ESObj`, an ExpressionSet object, with `NewSamNames`, and returns `NewESObj`, a new ExpressionSet object.

Inputs

ESObj

Object of the `bioma.ExpressionSet` class.

Subset

One of the following to specify a subset of the sample names in an ExpressionSet object:

- String specifying a sample name
- Cell array of strings specifying sample names
- Positive integer
- Vector of positive integers
- Logical vector

NewSamNames

New sample names for specific sample names within an ExpressionSet object, specified by one of the following:

- Numeric vector
- String or cell array of strings
- String, which `sampleNames` uses as a prefix for the sample names, with sample numbers appended to the prefix
- Logical `true` or `false` (default). If `true`, `sampleNames` assigns unique sample names using the format `Sample1`, `Sample2`, etc.

The number of sample names in *`NewSamNames`* must equal the number of samples specified by *`Subset`*.

Outputs

`SamNames`

Cell array of strings specifying all or some of the sample names in an ExpressionSet object. The sample names are the column names in the DataMatrix objects in the ExpressionSet object. The sample names are also the row names of the *`VarValues`* dataset array in the MetaData object in the ExpressionSet object.

`NewESObj`

Object of the `bioma.ExpressionSet` class, returned after replacing specific sample names.

Examples

Construct an ExpressionSet object from `EDObj`, an ExptData object, `MDObj2`, a MetaData object containing sample variable information, and `MIAMEObj`, a MIAME object. Retrieve the sample names from it:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
```

```
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Construct MIAME object
MIAMEObj = MIAME(geoStruct);
% Import bioma package to make constructor function
% available
import bioma.*
% Construct ExpressionSet object
ESObj = ExpressionSet(EDObj, 'SData', MDObj2, 'EInfo', MIAMEObj);
% Retrieve the sample names
SNames = sampleNames(ESObj);
```

See Also

bioma.ExpressionSet | bioma.data.ExptData | DataMatrix | bioma.data.MetaData | featureNames

How To

- “Working with ExpressionSet Objects”

Purpose

Retrieve or set sample names in ExptData object

Syntax

```
SamNames = sampleNames(EDObj)
SamNames = sampleNames(EDObj, Subset)
NewEDObj = sampleNames(EDObj, Subset, NewSamNames)
```

Description

`SamNames = sampleNames(EDObj)` returns a cell array of strings specifying all sample names in an ExptData object.

`SamNames = sampleNames(EDObj, Subset)` returns a cell array of strings specifying a subset the sample names in an ExptData object.

`NewEDObj = sampleNames(EDObj, Subset, NewSamNames)` replaces the sample names specified by `Subset` in `EDObj`, an ExptData object, with `NewSamNames`, and returns `NewEDObj`, a new ExptData object.

Inputs

EDObj

Object of the `bioma.data.ExptData` class.

Subset

One of the following to specify a subset of the sample names in an ExptData object:

- String specifying a sample name
- Cell array of strings specifying sample names
- Positive integer
- Vector of positive integers
- Logical vector

NewSamNames

New sample names for specific sample names within an ExptData object, specified by one of the following:

- Numeric vector

- String or cell array of strings
- String, which `sampleNames` uses as a prefix for the sample names, with sample numbers appended to the prefix
- Logical `true` or `false` (default). If `true`, `sampleNames` assigns unique sample names using the format `Sample1`, `Sample2`, etc.

The number of sample names in *`NewSamNames`* must equal the number of samples specified by *`Subset`*.

Outputs

`SamNames`

Cell array of strings specifying all or some of the sample names in an ExptData object. The sample names are the column names in the DataMatrix objects in the ExptData object.

`NewEDObj`

Object of the `bioma.data.ExptData` class, returned after replacing specific sample names.

Examples

Construct an ExptData object, and then retrieve the sample names from it:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Retrieve sample names
SNames = sampleNames(EDObj);
```

See Also

`bioma.data.ExptData` | `DataMatrix` | `dmNames` | `elementNames` | `featureNames`

How To

- "Working with ExptData Objects"

bioma.data.MetaData.sampleNames

Purpose

Retrieve or set sample names in MetaData object

Syntax

```
SamFeatNames = sampleNames(MDObj)
SamFeatNames = sampleNames(MDObj, Subset)
NewMDObj = sampleNames(MDObj, Subset, NewSamFeatNames)
```

Description

`SamFeatNames = sampleNames(MDObj)` returns a cell array of strings specifying all sample names in a MetaData object.

`SamFeatNames = sampleNames(MDObj, Subset)` returns a cell array of strings specifying a subset the sample names in a MetaData object.

`NewMDObj = sampleNames(MDObj, Subset, NewSamFeatNames)` replaces the sample names specified by `Subset` in `MDObj`, a MetaData object, with `NewSamFeatNames`, and returns `NewMDObj`, a new MetaData object.

Inputs

`MDObj`

Object of the `bioma.data.MetaData` class.

`Subset`

One of the following to specify a subset of the sample names in a MetaData object:

- String specifying a sample name
- Cell array of strings specifying sample names
- Positive integer
- Vector of positive integers
- Logical vector

`NewSamFeatNames`

New sample names for specific names within a MetaData object, specified by one of the following:

- Numeric vector
- String or cell array of strings
- String, which `sampleNames` uses as a prefix for the sample or feature names, with numbers appended to the prefix
- Logical `true` or `false` (default). If `true`, `sampleNames` assigns unique names using the format `Sample1`, `Sample2`, etc.

The number of names in *`NewSamFeatNames`* must equal the number of samples specified by *`Subset`*.

Outputs

`SamFeatNames`

Cell array of strings specifying all or some of the sample names in a MetaData object. The sample names are also the row names of the *`VarValues`* dataset array in the MetaData object.

`NewMDObj`

Object of the `bioma.data.MetaData` class, returned after replacing specific sample names.

Examples

Construct a MetaData object, and then retrieve the sample names from it:

```
% Import bioma.data package to make constructor function
% available
import bioma.data.*
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Retrieve the sample names
SNames = sampleNames(MDObj2)
```

See Also

`bioma.data.MetaData` | `variableDesc` | `variableValues` | `variableNames`

How To

- "Working with MetaData Objects"

bioma.ExpressionSet.sampleVarDesc

Purpose

Retrieve or set sample variable descriptions in ExpressionSet object

Syntax

```
DSVarDescriptions = sampleVarDesc(ESObj)
NewESObj = sampleVarDesc(ESObj, NewDSVarDescriptions)
```

Description

`DSVarDescriptions = sampleVarDesc(ESObj)` returns a dataset array containing the sample variable names and descriptions from the MetaData object in an ExpressionSet object.

`NewESObj = sampleVarDesc(ESObj, NewDSVarDescriptions)` replaces the sample variable descriptions in *`ESObj`*, an ExpressionSet object, with *`NewDSVarDescriptions`*, and returns *`NewESObj`*, a new ExpressionSet object.

Inputs

`ESObj`

Object of the `bioma.ExpressionSet` class.

`NewDSVarDescriptions`

Descriptions of the sample variable names, specified by either of the following:

- A new dataset array containing the sample variable names and descriptions. In this dataset array, each row corresponds to a variable. The first column contains the variable name, and the second column (`VariableDescription`) contains a description of the variable. The row names (variable names) must match the row names (variable names) in *`DSVarDescriptions`*, the dataset array being replaced in the MetaData object in the ExpressionSet object, *`ESObj`*.
- Cell array of strings containing descriptions of the sample variables. The number of elements in *`VarDesc`* must equal the number of row names (variable names) in *`DSVarDescriptions`*, the dataset array being replaced in the MetaData object in the ExpressionSet object, *`ESObj`*.

Outputs

DSVarDescriptions

A dataset array containing the sample variable names and descriptions from the MetaData object of an ExpressionSet object. In this dataset array, each row corresponds to a variable. The first column contains the variable name, and the second column (`VariableDescription`) contains a description of the variable.

NewESObj

Object of the `bioma.ExpressionSet` class, returned after replacing the dataset array containing the sample variable descriptions.

Examples

Construct an ExpressionSet object from `EDObj`, an ExptData object, `MDObj2`, a MetaData object containing sample variable information, and `MIAMEObj`, a MIAME object. Retrieve the sample variable descriptions in the ExpressionSet object:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Construct MIAME object
MIAMEObj = MIAME(geoStruct);
% Import bioma package to make constructor function
% available
import bioma.*
% Construct ExpressionSet object
ESObj = ExpressionSet(EDObj, 'SData', MDObj2, 'EInfo', MIAMEObj);
% Retrieve the sample variable descriptions
```

```
SVarDescriptions = sampleVarDesc(ESObj)
```

See Also

bioma.ExpressionSet | bioma.data.MetaData | variableDesc

How To

- “Working with ExpressionSet Objects”

Purpose

Retrieve or set sample variable names in ExpressionSet object

Syntax

```
SamVarNames = sampleVarNames(ESObj)
SamVarNames = sampleVarNames(ESObj, Subset)
NewESObj = sampleVarNames(ESObj, Subset, NewSamVarNames)
```

Description

`SamVarNames = sampleVarNames(ESObj)` returns a cell array of strings specifying all sample variable names in an ExpressionSet object.

`SamVarNames = sampleVarNames(ESObj, Subset)` returns a cell array of strings specifying a subset the sample variable names in an ExpressionSet object.

`NewESObj = sampleVarNames(ESObj, Subset, NewSamVarNames)` replaces the sample variable names specified by `Subset` in `ESObj`, an ExpressionSet object, with `NewSamVarNames`, and returns `NewESObj`, a new ExpressionSet object.

Inputs

`ESObj`

Object of the `bioma.ExpressionSet` class.

`Subset`

One of the following to specify a subset of the sample variable names in an ExpressionSet object:

- String specifying a sample variable name
- Cell array of strings specifying sample variable names
- Positive integer
- Vector of positive integers
- Logical vector

`NewSamVarNames`

New sample variable names for specific sample variable names within an ExpressionSet object, specified by one of the following:

- Numeric vector
- String or cell array of strings
- String, which `sampleVarNames` uses as a prefix for the sample variable names, with sample variable numbers appended to the prefix
- Logical `true` or `false` (default). If `true`, `sampleVarNames` assigns unique sample variable names using the format `Var1`, `Var2`, etc.

The number of sample variable names in *`NewSamVarNames`* must equal the number of sample variable names specified by *`Subset`*.

Outputs

`SamVarNames`

Cell array of strings specifying all or some of the sample variable names in an ExpressionSet object. The sample variable names are the column names of the *`VarValues`* dataset array. The sample variable names are also the row names of the *`VarDescriptions`* dataset array. Both dataset arrays are in the MetaData object in the ExpressionSet object.

`NewESObj`

Object of the `bioma.ExpressionSet` class, returned after replacing specific sample names.

Examples

Construct an ExpressionSet object from `EDObj`, an ExptData object, `MDObj2`, a MetaData object containing sample variable information, and `MIAMEObj`, a MIAME object. Retrieve the sample variable names from the ExpressionSet object:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
```

```
% Construct ExptData object
EDObj = ExptData(dmObj);
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Construct MIAME object
MIAMEObj = MIAME(geoStruct);
% Import bioma package to make constructor function
% available
import bioma.*
% Construct ExpressionSet object
ESObj = ExpressionSet(EDObj, 'SData', MDObj2, 'EInfo', MIAMEObj);
% Retrieve the sample variable names
VNames = sampleVarNames(ESObj)
```

See Also

bioma.ExpressionSet | bioma.data.MetaData | sampleNames | featureNames | featureVarNames

How To

- “Working with ExpressionSet Objects”

bioma.ExpressionSet.sampleVarValues

Purpose

Retrieve or set sample variable values in ExpressionSet object

Syntax

```
DSVarValues = sampleVarValues(ESObj)
NewESObj = sampleVarValues(ESObj, NewDSVarValues)
```

Description

`DSVarValues = sampleVarValues(ESObj)` returns a dataset array containing the measured value of each variable per sample from the MetaData object of an ExpressionSet object.

`NewESObj = sampleVarValues(ESObj, NewDSVarValues)` replaces the sample variable values in *`ESObj`*, an ExpressionSet object, with *`NewDSVarValues`*, and returns *`NewESObj`*, a new ExpressionSet object.

Inputs

`ESObj`

Object of the `bioma.ExpressionSet` class.

`NewDSVarValues`

A new dataset array containing a value for each variable per sample. In this dataset array, the columns correspond to variables and rows correspond to samples. The row names (sample names) must match the row names (sample names) in *`DSVarValues`*, the dataset array being replaced in the MetaData object in the ExpressionSet object, *`ESObj`*.

Outputs

`DSVarValues`

A dataset array containing the measured value of each variable per sample from the MetaData object of an ExpressionSet object. In this dataset array, the columns correspond to variables and rows correspond to samples.

`NewESObj`

Object of the `bioma.ExpressionSet` class, returned after replacing the dataset array containing the sample variable values.

Examples

Construct an ExpressionSet object from `EDObj`, an ExptData object, `MDObj2`, a MetaData object containing sample variable information, and `MIAMEObj`, a MIAME object. Retrieve the sample variable values in ExpressionSet object:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Construct MIAME object
MIAMEObj = MIAME(geoStruct);
% Import bioma package to make constructor function
% available
import bioma.*
% Construct ExpressionSet object
ESObj = ExpressionSet(EDObj, 'SData', MDObj2, 'EInfo', MIAMEObj);
% Retrieve the sample variable values
SVarValues = sampleVarValues(ESObj);
```

See Also

`bioma.ExpressionSet` | `bioma.data.MetaData` | `variableValues`

How To

- "Working with ExpressionSet Objects"

Purpose

Read trace data from SCF file

Syntax

```
Sample = scfread(File)
[Sample, Probability] = scfread(File)
[Sample, Probability, Comments] = scfread(File)
[A, C, G, T] = scfread (File)
[A, C, G, T, ProbA, ProbC, ProbG, ProbT] = scfread (File)
[A, C, G, T, ProbA, ProbC, ProbG, ProbT, Comments, PkIndex,
    Base] = scfread (File)
```

Arguments

File	String specifying the file name or a path and file name of an SCF formatted file.

Description

`scfread` reads data from an SCF formatted file into MATLAB structures.

Sample = `scfread(`*File*`)` reads an SCF formatted file and returns the sample data in the structure `Sample`, which contains the following fields:

Field	Description
`A`	Column vector containing intensity of A fluorescence tag
`C`	Column vector containing intensity of C fluorescence tag
`G`	Column vector containing intensity of G fluorescence tag
`T`	Column vector containing intensity of T fluorescence tag

`[`*Sample, Probability*`] = scfread(`*File*`)` also returns the probability data in the structure `Probability`, which contains the following fields:

Field	Description
peak_index	Column vector containing the position in the SCF file for the start of the data for each peak
prob_A	Column vector containing the probability of each base in the sequence being an A
prob_C	Column vector containing the probability of each base in the sequence being a C
prob_G	Column vector containing the probability of each base in the sequence being a G
prob_T	Column vector containing the probability of each base in the sequence being a T
base	Column vector containing the called bases for the sequence

`[`*`Sample, Probability, Comments`*`] = scfread(`*`File`*`)` also returns the comment information from the SCF file in a character array `Comments`.

`[`*`A, C, G, T`*`] = scfread (`*`File`*`)` returns the sample data for the four bases in separate variables.

`[`*`A, C, G, T, ProbA, ProbC, ProbG, ProbT`*`] = scfread (`*`File`*`)` also returns the probabilities data for the four bases in separate variables.

`[`*`A, C, G, T, ProbA, ProbC, ProbG, ProbT, Comments, PkIndex, Base`*`] = scfread (`*`File`*`)` also returns the peak indices and called bases in separate variables.

SCF files store data from DNA sequencing instruments. Each file includes sample data, sequence information, and the relative probabilities of each of the four bases. For more information on SCF files, see

```
http://www.mrc-lmb.cam.ac.uk/pubseq/manual/formats_unix_2.html
```

Examples

```
[sampleStruct, probStruct, Comments] = scfread('sample.scf')
sampleStruct =

    A: [10827x1 double]
    C: [10827x1 double]
    G: [10827x1 double]
    T: [10827x1 double]


probStruct =

    peak_index: [742x1 double]
        prob_A: [742x1 double]
        prob_C: [742x1 double]
        prob_G: [742x1 double]
        prob_T: [742x1 double]
          base: [742x1 char]


Comments =

SIGN=A=121,C=103,G=119,T=82
SPAC= 16.25
PRIM=0
MACH=Arkansas_SN312
DYEP=DT3700POP5{BD}v2.mob
NAME=HCIUP1D61207
LANE=6
GELN=
PROC=
RTRK=
CONV=phred version=0.990722.h
COMM=
SRCE=ABI 373A or 377
```

See Also

Bioinformatics Toolbox functions: `genbankread`, `traceplot`

Purpose

Select tree branches and leaves in phytree object

Syntax

```
S = select(Tree, N)
[S, Selleaves, Selbranches] = select(...)
select(..., 'Reference', ReferenceValue, ...)
select(..., 'Criteria', CriteriaValue, ...)
select(..., 'Threshold', ThresholdValue, ...)
select(..., 'Exclude', ExcludeValue, ...)
select(..., 'Propagate', PropagateValue, ...)
```

Arguments

Tree	Phylogenetic tree (`phytree` object) created with the function `phytree`.
N	Number of closest nodes to the root node.
ReferenceValue	Property to select a reference point for measuring distance.
CriteriaValue	Property to select a criteria for measuring distance.
ThresholdValue	Property to select a distance value. Nodes with distances below this value are selected.
ExcludeValue	Property to remove (exclude) branch or leaf nodes from the output. Enter `'none'`, `'branchs'`, or `'leaves'`. The default value is `'none'`.
PropagateValue	Property to select propagating nodes toward the leaves or the root.

Description

`S = select(Tree, N)` returns a logical vector (*S*) of size `[NumNodes x 1]` indicating the *N* closest nodes to the root node of a `phytree` object (`Tree`) where `NumNodes = NumLeaves + NumBranches`. The first criterion `select` uses is branch levels, then patristic distance (also known as tree distance). By default, `select` uses `inf` as the value of `N`, and `select(Tree)` returns a vector with values of `true`.

`[S, Selleaves, Selbranches] = select(...)` returns two additional logical vectors, one for the selected leaves and one for the selected branches.

`select(..., 'PropertyName', PropertyValue, ...)` calls `select` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`select(..., 'Reference', ReferenceValue, ...)` changes the reference point(s) to measure the closeness. `Reference` can be the root (default) or leaves. When using leaves, a node can have multiple distances to its descendant leaves (nonultrametric tree). If this the case, `select` considers the minimum distance to any descendant leaf.

`select(..., 'Criteria', CriteriaValue, ...)` changes the criteria `select` uses to measure closeness. If `C = 'levels'` (default), the first criterion is branch levels and then patristic distance. If `C = 'distance'`, the first criterion is patristic distance and then branch levels.

`select(..., 'Threshold', ThresholdValue, ...)` selects all the nodes where closeness is less than or equal to the threshold value (*`ThresholdValue`*). Notice, you can also use either of the properties `'criteria'` or `'reference'`, if `N` is not specified, then `N = infF`; otherwise you can limit the number of selected nodes by `N`.

`select(..., 'Exclude', ExcludeValue, ...)` when *`ExcludeValue`* `= 'branches'`, sets a postfilter that excludes all the branch nodes from *`S`*, or when *`ExcludeValue`* `= 'leaves'`, all the leaf nodes. The default is `'none'`.

`select(..., 'Propagate', PropagateValue, ...)` activates a postfunctionality that propagates the selected nodes to the leaves when `P=='toleaves'` or toward the root finding a common ancestor when `P == 'toroot'`. The default value is `'none'`. `P` may also be `'both'`. The `'Propagate'` property acts after the `'Exclude'` property.

Examples

```
% Load a phylogenetic tree created from a protein family:
tr = phytreeread('pf00002.tree');

% To find close products for a given protein (e.g. vipr2_human):
ind = getbyname(tr,'vipr2_human');
[sel,sel_leaves] = select(tr,'criteria','distance',...
                          'threshold',0.6,'reference',ind);
view(tr,sel_leaves)

% To find potential outliers in the tree, use
[sel,sel_leaves] = select(tr,'criteria','distance',...
                             'threshold',.3,...
                             'reference','leaves',...
                             'exclude','leaves',...
                             'propagate','toleaves');
view(tr,~sel_leaves)
```

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreetool`

Bioinformatics Toolbox object: phytree object

Bioinformatics Toolbox methods of phytree object: `get`, `pdist`, `prune`

seq2regexp

Purpose

Convert sequence with ambiguous characters to regular expression

Syntax

```
RegExp = seq2regexp(Seq)
RegExp = seq2regexp(Seq, ...'Alphabet', AlphabetValue, ...)
RegExp = seq2regexp(Seq, ...'Ambiguous',
AmbiguousValue, ...)
```

Arguments

Seq

Either of the following:

- Character string of codes specifying an amino acid or nucleotide sequence.
- Structure containing a `Sequence` field that contains an amino acid or nucleotide sequence, such as returned by `fastaread`, `fastqread`, `getembl`, `getgenbank`, `getgenpept`, or `getpdb`.

AlphabetValue

String specifying the sequence alphabet. Choices are:

- `'NT'` (default) — Nucleotide
- `'AA'` — Amino acid

AmbiguousValue

Controls whether ambiguous characters are included in *RegExp*, the regular expression return value. Choices are:

- `true` (default) — Include ambiguous characters in the return value
- `false` — Return only unambiguous characters

Return Values

RegExp

Character string of codes specifying an amino acid or nucleotide sequence in regular expression format using IUB/IUPAC codes.

Description

RegExp = seq2regexp(*Seq*) converts ambiguous amino acid or nucleotide symbols in a sequence to a regular expression format using IUB/IUPAC codes.

RegExp = seq2regexp(*Seq*, ...'*PropertyName*', *PropertyValue*, ...) calls seq2regexp with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

RegExp = seq2regexp(*Seq*, ...'Alphabet', *AlphabetValue*, ...) specifies the sequence alphabet. *AlphabetValue* can be either 'NT' for nucleotide sequences or 'AA' for amino acid sequences. Default is 'NT'.

RegExp = seq2regexp(*Seq*, ...'Ambiguous', *AmbiguousValue*, ...) controls whether ambiguous characters are included in *RegExp*, the regular expression return value. Choices are true (default) or false. For example:

- If *Seq* = 'ACGTK', and *AmbiguousValue* is true , the MATLAB software returns ACGT[GTK] with the unambiguous characters G and T and the ambiguous character K.
- If *Seq* = 'ACGTK', and *AmbiguousValue* is false, the MATLAB software returns ACGT[GT] with only the unambiguous characters.

Nucleotide Conversions

Nucleotide Code	Nucleotide	Conversion
A	Adenosine	A
C	Cytosine	C
G	Guanine	G
T	Thymidine	T
U	Uridine	U

Nucleotide Conversions (Continued)

Nucleotide Code	Nucleotide	Conversion
R	Purine	[AG]
Y	Pyrimidine	[TC]
K	Keto	[GT]
M	Amino	[AC]
S	Strong interaction (3 H bonds)	[GC]
W	Weak interaction (2 H bonds)	[AT]
B	Not A	[CGT]
D	Not C	[AGT]
H	Not G	[ACT]
V	Not T or U	[ACG]
N	Any nucleotide	[ACGT]
-	Gap of indeterminate length	-
?	Unknown	?

Amino Acid Conversion

Amino Acid Code	Amino Acid	Conversion
B	Asparagine or Aspartic acid (Aspartate)	[DN]

Amino Acid Conversion (Continued)

Amino Acid Code	Amino Acid	Conversion
Z	Glutamine or Glutamic acid (Glutamate)	[EQ]
X	Any amino acid	[A R N D C Q E G H I L K M F P S T W Y V]

Example

1 Convert a nucleotide sequence to a regular expression.

```
seq2regexp('ACWTMAN')

ans =
AC[ATW]T[ACM]A[ACGTRYKMSWBDHVN]
```

2 Convert the same nucleotide sequence, but remove ambiguous characters from the regular expression.

```
seq2regexp('ACWTMAN', 'ambiguous', false)

ans =
AC[AT]T[AC]A[ACGT]
```

See Also

Bioinformatics Toolbox functions: `restrict`, `seqwordcount`

MATLAB functions: `regexp`, `regexpi`

seqcomplement

Purpose

Calculate complementary strand of nucleotide sequence

Syntax

```
SeqC = seqcomplement(SeqNT)
```

Arguments

SeqNT — Nucleotide sequence specified by any of the following:

- Character string with the characters `A`, `C`, `G`, `T`, `U`, and ambiguous characters `R`, `Y`, `K`, `M`, `S`, `W`, `B`, `D`, `H`, `V`, `N`.
- Row vector of integers from the table Mapping Nucleotide Integers to Letter Codes on page 3-809.
- MATLAB structure containing a `Sequence` field that contains a nucleotide sequence, such as returned by `emblread`, `fastaread`, `fastqread`, `genbankread`, `getembl`, or `getgenbank`.

Description

`SeqC = seqcomplement(SeqNT)` calculates the complementary strand of a DNA or RNA nucleotide sequence. The return sequence, *SeqC*, is in the same format as *SeqNT*. For example, if *SeqNT* is a vector of integers, then so is *SeqC*.

Nucleotide in *SeqNT*	Converts to This Nucleotide in *SeqC*
A	T or U
C	G
G	C
T or U	A

Examples

Return the complement of a DNA nucleotide sequence.

```
s = 'ATCG';
seqcomplement(s)
```

```
ans =
TAGC
```

See Also

Bioinformatics Toolbox functions: `codoncount`, `palindromes`, `seqrcomplement`, `seqreverse`, `seqtool`

seqconsensus

Purpose

Calculate consensus sequence

Syntax

```
CSeq = seqconsensus(Seqs)
[CSeq, Score] = seqconsensus(Seqs)
CSeq = seqconsensus(Profile)
seqconsensus(..., 'PropertyName', PropertyValue,...)
seqconsensus(..., 'ScoringMatrix',  ScoringMatrixValue)
```

Arguments

Seqs	Set of multiply aligned amino acid or nucleotide sequences. Enter an array of strings, a cell array of strings, or an array of structures with the field `Sequence`.
Profile	Sequence profile. Enter a profile from the function `seqprofile`. `Profile` is a matrix of size `[20 (or 4) x Sequence Length]` with the frequency or count of amino acids (or nucleotides) for every position. `Profile` can also have 21 (or 5) rows if gaps are included in the consensus.
ScoringMatrixValue	Scoring matrix. The default value is `BLOSUM50` for amino acid sequences or `NUC44` for nucleotide sequences. `ScoringMatrix` can also be a `21x21`, `5x5`, `20x20`, or `4x4` numeric array. For the gap-included cases, gap scores (last row/column) are set to `mean(diag(ScoringMatrix))`for a gap matching with another gap, and set to `mean(nodiag(ScoringMatrix))` for a gap matching with another symbol

Description

CSeq = `seqconsensus(`*Seqs*`)`, for a multiply aligned set of sequences (*Seqs*), returns a string with the consensus sequence (*CSeq*). The frequency of symbols (`20` amino acids, `4` nucleotides) in the set of sequences is determined with the function `seqprofile`. For ambiguous

nucleotide or amino acid symbols, the frequency or count is added to the standard set of symbols.

`[CSeq, Score] = seqconsensus(Seqs)` returns the conservation score of the consensus sequence. Scores are computed with the scoring matrix `BLOSUM50` for amino acids or `NUC44` for nucleotides. Scores are the average euclidean distance between the scored symbol and the M-dimensional consensus value. `M` is the size of the alphabet. The consensus value is the profile weighted by the scoring matrix.

`CSeq = seqconsensus(Profile)` returns a string with the consensus sequence (`CSeq`) from a sequence profile (`Profile`).

`seqconsensus(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`seqconsensus(..., 'ScoringMatrix', ScoringMatrixValue)` specifies the scoring matrix.

The following input parameters are analogous to the function `seqprofile` when the alphabet is restricted to `'AA'` or `'NT'`.

`seqconsensus(..., 'Alphabet', AlphabetValue)`

`seqconsensus(..., 'Gaps', GapsValue)`

`seqconsensus(..., 'Ambiguous', AmbiguousValue)`

`seqconsensus(..., 'Limits', LimitsValue)`

Examples

```
seqs = fastaread('pf00002.fa');
[C,S] = seqconsensus(seqs,'limits',[50 60],'gaps','all')
```

See Also

Bioinformatics Toolbox functions: `fastaread`, `multialignread`, `multialignwrite`, `profalign`, `seqdisp`, `seqprofile`

seqdisp

Purpose

Format long sequence output for easy viewing

Syntax

```
seqdisp(Seq)
seqdisp(Seq, ...'Row', RowValue, ...)
seqdisp(Seq, ...'Column', ColumnValue, ...)
seqdisp(Seq, ...'ShowNumbers', ShowNumbersValue, ...)
```

Arguments

Seq	Nucleotide or amino acid sequence represented by any of the following: • Character array • FASTA file name • MATLAB structure with the field `Sequence` Multiply aligned sequences are allowed. FASTA files can have the file extension `fa`, `fasta`, `fas`, `fsa`, or `fst`.
RowValue	Integer that specifies the length of each row. Default is `60`.
ColumnValue	Integer that specifies the column width or number of symbols before displaying a space. Default is `10`.
ShowNumbersValue	Controls the display of numbers at the start of each row. Choices are `true` (default) to show numbers, or `false` to hide numbers.

Description

`seqdisp(Seq)` displays a sequence in rows, with a default row length of 60 and a default column width of `10`.

`seqdisp(Seq, ...'PropertyName', PropertyValue, ...)` calls `seqdisp` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each

PropertyName must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`seqdisp(`*`Seq`*`, ...'Row', `*`RowValue`*`, ...)` specifies the length of each row for the displayed sequence.

`seqdisp(`*`Seq`*`, ...'Column', `*`ColumnValue`*`, ...)` specifies the number of letters to display before adding a space. *RowValue* must be larger than and evenly divisible by *ColumnValue*.

`seqdisp(`*`Seq`*`, ...'ShowNumbers', `*`ShowNumbersValue`*`, ...)` controls the display of numbers at the start of each row. Choices are `true` (default) to show numbers, or `false` to hide numbers.

Examples

Read sequence information from the GenBank database. Display the sequence in rows with 50 letters, and within a row, separate every 10 letters with a space.

```
mouseHEXA = getgenbank('AK080777');
seqdisp(mouseHEXA, 'Row', 50, 'Column', 10)
```

Create and save a FASTA file with two sequences, and then display it.

```
hdr = ['Sequence A'; 'Sequence B'];
seq = ['TAGCTGRCCAAGGCCAAGCGAGCTTN';'ATCGACYGGTTCCGGTTCGCTCGAAN']
fastawrite('local.fa', hdr, seq);
seqdisp('local.fa', 'ShowNumbers', false')

ans =
>Sequence A
 1  TAGCTGRCCA AGGCCAAGCG AGCTTN
>Sequence B
 1  ATCGACYGGT TCCGGTTCGC TCGAAN
```

See Also

Bioinformatics Toolbox functions: `multialignread`, `multialignwrite`, `seqconsensus`, `seqlogo`, `seqprofile`, `seqshoworfs`, `seqshowwords`, `seqtool`, `getgenbank`

seqdotplot

Purpose

Create dot plot of two sequences

Syntax

```
seqdotplot(Seq1, Seq2)
seqdotplot(Seq1,Seq2, Window, Number)
Matches = seqdotplot(...)
[Matches, Matrix] = seqdotplot(...)
```

Arguments

Seq1, *Seq2*	Nucleotide or amino acid sequences. Enter two character strings. Do not enter a vector of integers. You can also enter a structure with the field `Sequence`.
Window	Enter an integer for the size of a window.
Number	Enter an integer for the number of characters within the window that match.

Description

`seqdotplot(`*Seq1*`, `*Seq2*`)` plots a figure that visualizes the match between two sequences.

`seqdotplot(`*Seq1*`,`*Seq2*`, `*Window*`, `*Number*`)` plots sequence matches when there are at least *Number* matches in a window of size *Window*.

When plotting nucleotide sequences, start with a `Window` of `11` and `Number` of `7`.

Matches `= seqdotplot(...)` returns the number of dots in the dot plot matrix.

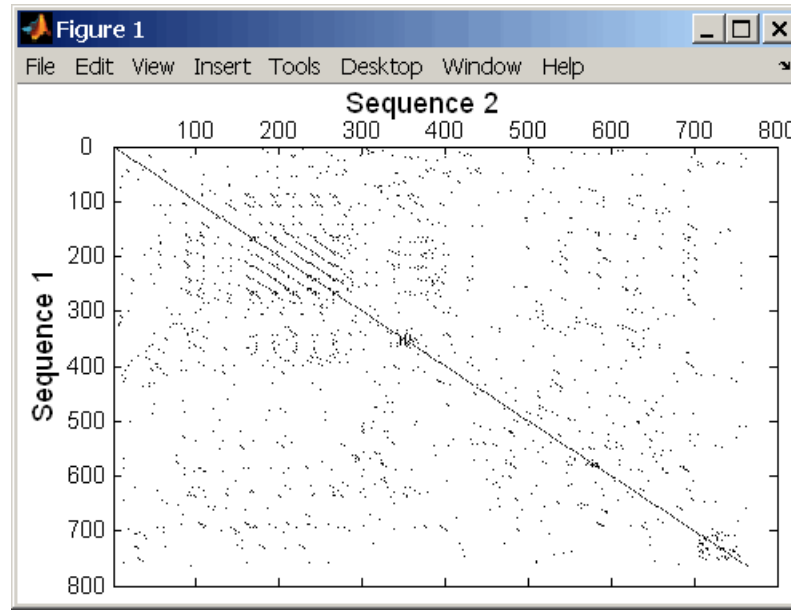
`[`*Matches*`, `*Matrix*`] = seqdotplot(...)` returns the dot plot as a sparse matrix.

Examples

This example shows the similarities between the prion protein (PrP) nucleotide sequences of two ruminants, the moufflon and the golden takin.

```
moufflon = getgenbank('AB060288','Sequence',true);
takin = getgenbank('AB060290','Sequence',true);
```

```
seqdotplot(moufflon,takin,11,7)
```



Note For the correct interpretation of a dot plot, your monitor's display resolution must be able to contain the sequence lengths. If the resolution is not adequate, `seqdotplot` resizes the image and returns a warning.

```
Matches = seqdotplot(moufflon,takin,11,7)
Matches =
        5552

[Matches, Matrix] = seqdotplot(moufflon,takin,11,7)
```

See Also

Bioinformatics Toolbox functions: `nwalign`, `swalign`

seqinsertgaps

Purpose

Insert gaps into nucleotide or amino acid sequence

Syntax

```
NewSeq = seqinsertgaps(Seq, Positions)
NewSeq = seqinsertgaps(Seq, GappedSeq)
NewSeq = seqinsertgaps(Seq, GappedSeq, Relationship)
```

Arguments

Seq	Either of the following: • String specifying a nucleotide or amino acid sequence • MATLAB structure containing a `Sequence` field
Positions	Vector of integers to specify the positions in *Seq* before which to insert a gap.
GappedSeq	Either of the following: • String specifying a nucleotide or amino acid sequence • MATLAB structure containing a `Sequence` field
Relationship	Integer specifying the relationship between *Seq* and *GappedSeq*. Choices are: • `1` — Both sequences use the same alphabet, that is both are nucleotide sequences or both are amino acid sequences. • `3` — *Seq* contains nucleotides representing codons and *GappedSeq* contains amino acids (default).

Return Values

NewSeq	Sequence with gaps inserted, represented by a string specifying a nucleotide or amino acid sequence.

Description

NewSeq = seqinsertgaps(*Seq*, *Positions*) inserts gaps in the sequence *Seq* before the positions specified by the integers in the vector *Positions*.

NewSeq = seqinsertgaps(*Seq*, *GappedSeq*) finds the gap positions in the sequence *GappedSeq*, then inserts gaps in the corresponding positions in the sequence *Seq*.

NewSeq = seqinsertgaps(*Seq*, *GappedSeq*, *Relationship*) specifies the relationship between *Seq* and *GappedSeq*. Enter 1 for *Relationship* when both sequences use the same alphabet, that is both are nucleotide sequences or both are amino acid sequences. Enter 3 for *Relationship* when *Seq* contains nucleotides representing codons and *GappedSeq* contains amino acids. Default is 3.

Examples

1. Retrieve two nucleotide sequences from the GenBank database for the neuraminidase (NA) protein of two strains of the Influenza A virus (H5N1).

```
hk01 = getgenbank('AF509094');
vt04 = getgenbank('DQ094287');
```

2. Extract the coding region from the two nucleotide sequences.

```
hk01_cds = featuresparse(hk01,'feature','CDS','Sequence',true);
vt04_cds = featuresparse(vt04,'feature','CDS','Sequence',true);
```

3. Align the amino acids sequences converted from the nucleotide sequences.

```
[sc,al]=nwalign(nt2aa(hk01_cds),nt2aa(vt04_cds),'extendgap',1);
```

4. Use the seqinsertgaps function to copy the gaps from the aligned amino acid sequences to their corresponding nucleotide sequences, thus codon-aligning them.

```
hk01_aligned = seqinsertgaps(hk01_cds,al(1,:))
vt04_aligned = seqinsertgaps(vt04_cds,al(3,:))
```

5 Once you have code aligned the two sequences, you can use them as input to other functions such as `dnds`, which calculates the synonymous and nonsynonymous substitutions rates of the codon-aligned nucleotide sequences. By setting `Verbose` to `true`, you can also display the codons considered in the computations and their amino acid translations.

```
[dn,ds] = dnds(hk01_aligned,vt04_aligned,'verbose',true)
```

See Also

Bioinformatics Toolbox functions: `dnds`, `dndsml`, `int2aa`, `int2nt`

Purpose

Construct phylogenetic tree from pairwise distances

Syntax

```
Tree = seqlinkage(Dist)
Tree = seqlinkage(Dist, Method)
Tree = seqlinkage(Dist, Method, Names)
```

Arguments

Dist	Matrix or vector of pairwise distances, such as returned by the `seqpdist` function.
Method	String that specifies a distance method. Choices are: • `'single'` • `'complete'` • `'average'` (default) • `'weighted'` • `'centroid'` • `'median'`
Names	Property to use alternative labels for leaf nodes. Enter a vector of structures, with the fields `'Header'` or `'Name'`, or a cell array of strings. In both cases the number of elements you provide must comply with the number of samples used to generate the pairwise distances in *Dist*.

Description

Tree = `seqlinkage(`*Dist*`)` returns a phylogenetic tree object from the pairwise distances, *Dist*, between the species or products. *Dist* is a matrix or vector of pairwise distances, such as returned by the `seqpdist` function.

Tree = `seqlinkage(`*Dist*`, `*Method*`)` creates a phylogenetic tree object using a specified patristic distance method. The available methods are:

`'single'`	Nearest distance (single linkage method)
`'complete'`	Furthest distance (complete linkage method)
`'average'` (default)	Unweighted Pair Group Method Average (UPGMA, group average).
`'weighted'`	Weighted Pair Group Method Average (WPGMA)
`'centroid'`	Unweighted Pair Group Method Centroid (UPGMC)
`'median'`	Weighted Pair Group Method Centroid (WPGMC)

`Tree` `= seqlinkage(`*`Dist`*`, `*`Method`*`, `*`Names`*`)` passes a list of names to label the leaf nodes (for example, species or products) in a phylogenetic tree object.

Examples

```
% Load a multiple alignment of amino acids:
seqs = fastaread('pf00002.fa');
% Measure the 'Jukes-Cantor' pairwise distances:
dist = seqpdist(seqs,'method','jukes-cantor',...
                              'indels','pair');
% Build the phylogenetic tree with the single linkage
% method and pass the names of the sequences:
tree = seqlinkage(dist,'single',seqs)
view(tree)
```

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreewrite`, `seqpdist`, `seqneighjoin`

Bioinformatics Toolbox methods of phytree object: `cluster`, `plot`, `view`

Purpose

Display sequence logo for nucleotide or amino acid sequences

Syntax

```
seqlogo(Seqs)
seqlogo(Profile)
WgtMatrix = seqlogo(...)
[WgtMatrix, Handle] = seqlogo(...)
seqlogo(..., 'Displaylogo', DisplaylogoValue, ...)
seqlogo(..., 'Alphabet', AlphabetValue, ...)
seqlogo(..., 'Startat', StartatValue, ...)
seqlogo(..., 'Endat', EndatValue, ...)
seqlogo(..., 'SSCorrection', SSCorrectionValue, ...)
```

Arguments

Seqs

Set of pairwise or multiply aligned nucleotide or amino acid sequences, represented by any of the following:

- Character array
- Cell array of strings
- Array of structures containing a `Sequence` field

Profile

Sequence profile distribution matrix with the frequency of nucleotides or amino acids for every column in the multiple alignment, such as returned by the `seqprofile` function.

The size of the frequency distribution matrix is:

- For nucleotides — `[4 x sequence length]`
- For amino acids — `[20 x sequence length]`

	If gaps were included, *Profile* may have 5 rows (for nucleotides) or 21 rows (for amino acids), but seqlogo ignores gaps.
DisplaylogoValue	Controls the display of a sequence logo. Choices are true (default) or false.
AlphabetValue	String specifying the type of sequence (nucleotide or amino acid). Choices are 'NT' (default) or 'AA'.
StartatValue	Positive integer that specifies the starting position for the sequences in *Seqs*. Default starting position is 1.
EndatValue	Positive integer that specifies the ending position for the sequences in *Seqs*. Default ending position is the maximum length of the sequences in *Seqs*.
SSCorrectionValue	Controls the use of small sample correction in the estimation of the number of bits. Choices are true (default) or false.

Return Values

WgtMatrix	Cell array containing the symbol list in *Seqs* or *Profile* and the weight matrix used to graphically display the sequence logo.
Handle	Handle to the sequence logo figure.

Description

seqlogo(*Seqs*) displays a sequence logo for *Seqs*, a set of aligned sequences. The logo graphically displays the sequence conservation at a particular position in the alignment of sequences, measured in bits. The maximum sequence conservation per site is log2(4) bits for nucleotide sequences and log2(20) bits for amino acid sequences. If

the sequence conservation value is zero or negative, no logo is displayed in that position.

`seqlogo(Profile)` displays a sequence logo for *`Profile`*, a sequence profile distribution matrix with the frequency of nucleotides or amino acids for every column in the multiple alignment, such as returned by the `seqprofile` function.

Color Code for Nucleotides

Nucleotide	Color
`A`	Green
`C`	Blue
`G`	Yellow
`T`, `U`	Red
Other	Purple

Color Code for Amino Acids

Amino Acid	Chemical Property	Color
`G S T Y C Q N`	Polar	Green
`A V L I P W F M`	Hydrophobic	Orange
`D E`	Acidic	Red
`K R H`	Basic	Blue
Other	—	Tan

`WgtMatrix` `= seqlogo(...)` returns a cell array of unique symbols in the sequence *`Seqs`* or *`Profile`*, and the information weight matrix used to graphically display the logo.

`[`*`WgtMatrix`*`,` *`Handle`*`] = seqlogo(...)` returns a handle to the sequence logo figure.

`seqlogo(`*`Seqs`*`, ...'`*`PropertyName`*`', `*`PropertyValue`*`, ...)` calls `seqpdist` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`seqlogo(..., 'Displaylogo', `*`DisplaylogoValue`*`, ...)` controls the display of a sequence logo. Choices are `true` (default) or `false`.

`seqlogo(..., 'Alphabet', `*`AlphabetValue`*`, ...)` specifies the type of sequence (nucleotide or amino acid). Choices are `'NT'` (default) or`'AA'`.

Note If you provide amino acid sequences to `seqlogo`, you must set `Alphabet` to `'AA'`.

`seqlogo(..., 'Startat', `*`StartatValue`*`, ...)` specifies the starting position for the sequences in *`Seqs`*. Default starting position is `1`.

`seqlogo(..., 'Endat', `*`EndatValue`*`, ...)` specifies the ending position for the sequences in *`Seqs`*. Default ending position is the maximum length of the sequences in *`Seqs`*.

`seqlogo(..., 'SSCorrection', `*`SSCorrectionValue`*`, ...)` controls the use of small sample correction in the estimation of the number of bits. Choices are `true` (default) or `false`.

Note A simple calculation of bits tends to overestimate the conservation at a particular location. To compensate for this overestimation, when `SSCorrection` is set to `true`, a rough estimate is applied as an approximate correction. This correction works better when the number of sequences is greater than 50.

Examples

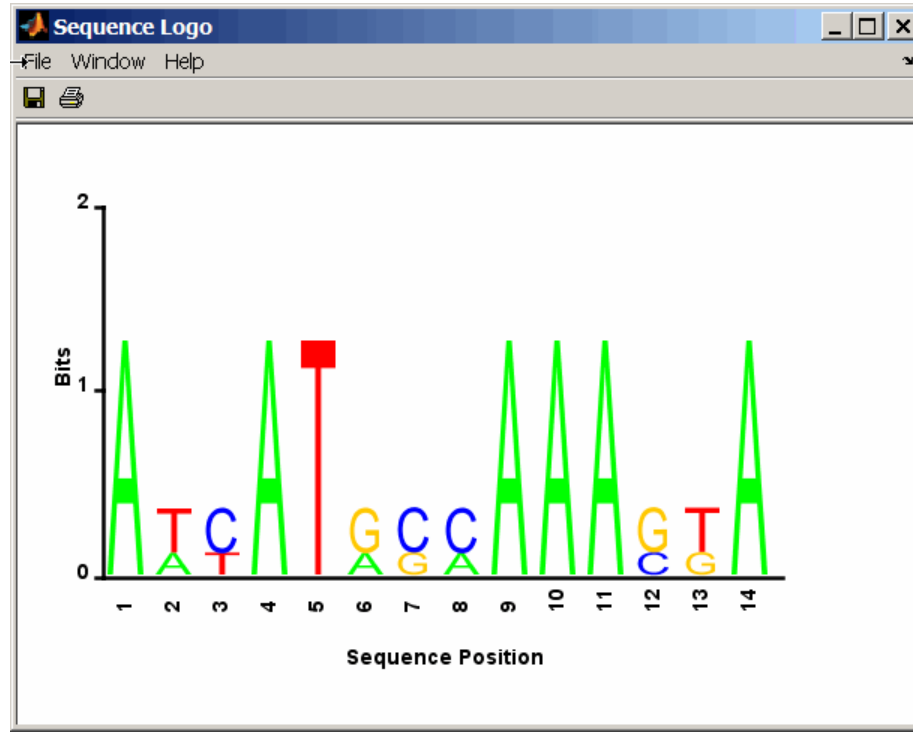
Displaying a Sequence Logo for a Nucleotide Sequence

1 Create a series of aligned nucleotide sequences.

```
S = {'ATTATAGCAAACTA',...
     'AACATGCCAAAGTA',...
     'ATCATGCAAAAGGA'}
```

2 Display the sequence logo.

```
seqlogo(S)
```



3 Notice that correction for small samples prevents you from seeing columns with information equal to `log2(4) = 2` bits, but you can turn this adjustment off.

```
seqlogo(S,'sscorrection',false)
```

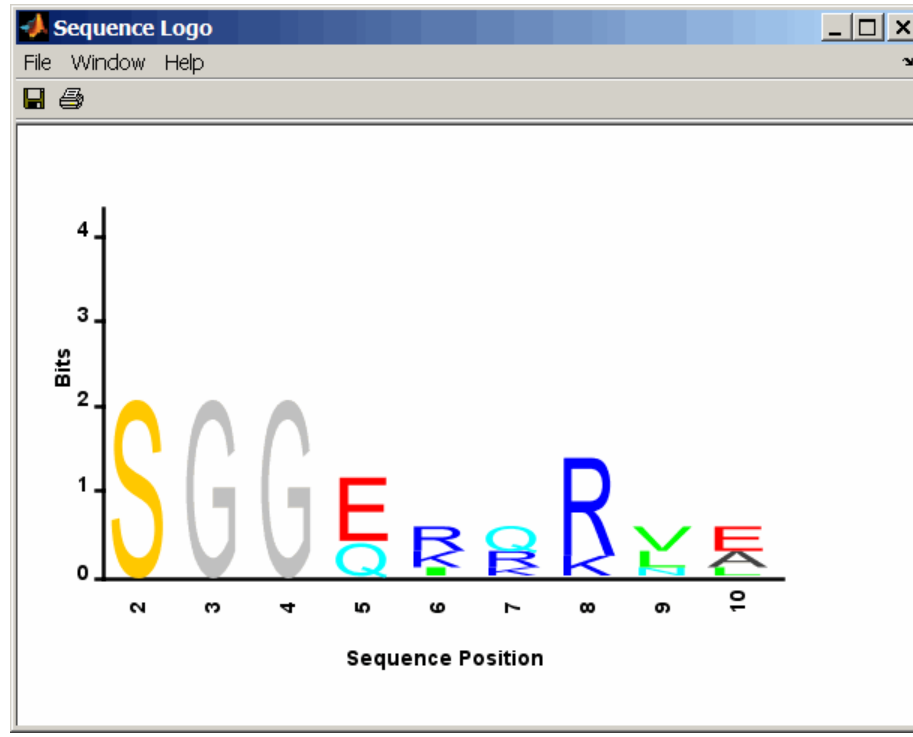
Displaying a Sequence Logo for an Amino Acid Sequence

1 Create a series of aligned amino acid sequences.

```
S2 = {'LSGGQRQRVAIARALAL',...
      'LSGGEKQRVAIARALMN',...
      'LSGGQIQRVLLARALAA',...
      'LSGGERRRLEIACVLAL',...
      'FSGGEKKKNELWQMLAL',...
      'LSGGERRRLEIACVLAL'};
```

2 Display the sequence logo, specifying an amino acid sequence and limiting the logo to sequence positions 2 through 10.

```
seqlogo(S2, 'alphabet', 'aa', 'startAt', 2, 'endAt', 10)
```



References

[1] Schneider, T.D., and Stephens, R.M. (1990). Sequence Logos: A new way to display consensus sequences. Nucleic Acids Research *18*, 6097–6100.

See Also

Bioinformatics Toolbox functions: `seqconsensus`, `seqdisp`, `seqprofile`

seqmatch

Purpose

Find matches for every string in library

Syntax

```
Index = seqmatch(Strings, Library)
```

Description

`Index = seqmatch(Strings, Library)` looks through the elements of `Library` to find strings that begin with every string in `Strings`. `Index` contains the index to the first occurrence for every string in the query. `Strings` and `Library` must be cell arrays of strings.

Examples

```
lib = {'VIPS_HUMAN', 'SCCR_RABIT', 'CALR_PIG' ,'VIPR_RAT', 'PACR_MOUSE'};
query = {'CALR','VIP'};
h = seqmatch(query,lib);
lib(h)
```

See Also

MATLAB functions: `regexp`, `strmatch`

Purpose

Neighbor-joining method for phylogenetic tree reconstruction

Syntax

```
Tree = seqneighjoin(Dist)
Tree = seqneighjoin(Dist, Method)
Tree = seqneighjoin(Dist, Method, Names)
seqneighjoin(..., 'Reroot', RerootValue)
```

Arguments

Dist	Matrix or vector returned by the `seqpdist` function.
Method	Method to compute the distances between nodes. Enter `'equivar'` (default), `'firstorder'`, or `'average'`.
Names	Vector of structures with the fields `'Header'`, `'Name'`, or a cell array of strings. In all cases the number of elements must equal the number of samples used to generate the pairwise distances in `Dist`.

Description

Tree = `seqneighjoin(`*Dist*`)` computes a phylogenetic tree object from *Dist*, pairwise distances between the species or products using the neighbor-joining method.

Tree = `seqneighjoin(`*Dist*`, `*Method*`)` specifies *Method*, a method to compute the distances of the new nodes to all other nodes at every iteration. The general expression to calculate the distances between the new node, `n`, after joining `i` and `j` and all other nodes (`k`), is given by

```
D(n,k) =  a*D(i,k) + (1-a)*D(j,k) - a*D(n,i) - (1-a)*D(n,j)
```

This expression is guaranteed to find the correct tree with additive data (minimum variance reduction).

Choices for *Method* are:

Method	Description
`'equivar'` (default)	Assumes equal variance and independence of evolutionary distance estimates (a = 1/2). Such as in Studier and Keppler, JMBE (1988).

Method	Description
`'firstorder'`	Assumes a first-order model of the variances and covariances of evolutionary distance estimates, `'a'` is adjusted at every iteration to a value between `0` and `1`. Such as in Gascuel, JMBE (1997).
`'average'`	New distances are the weighted average of previous distances while the branch distances are ignored. `D(n,k) = [ D(i,k) + D(j,k) ] /2` As in the original neighbor-joining algorithm by Saitou and Nei, JMBE (1987).

`Tree` `= seqneighjoin(`*`Dist`*`,` *`Method`*`,` *`Names`*`)` passes a list of names (*`Names`*) to label the leaf nodes (e.g., species or products) in the phylogenetic tree object.

`seqneighjoin(..., 'Reroot',` *`RerootValue`*`)`, when *`RerootValue`* is `false`, excludes rerooting the resulting tree. This is useful for observing the original linkage order followed by the algorithm. By default `seqneighjoin` reroots the resulting tree using the midpoint method.

Examples

1 Load a multiple alignment of amino acids.

```
seqs = fastaread('pf00002.fa');
```

2 Measure the Jukes-Cantor pairwise distances.

```
dist = seqpdist(seqs,'method','jukes-cantor','indels','pair');
```

3 Build the phylogenetic using the neighbor-joining algorithm.

```
tree = seqneighjoin(dist,'equivar',seqs)
view(tree)
```

References

[1] Saitou, N., and Nei, M. (1987). The neighbor-joining method: A new method for reconstructing phylogenetic trees. Molecular Biology and Evolution *4(4)*, 406–425.

[2] Gascuel, O. (1997). BIONJ: An improved version of the NJ algorithm based on a simple model of sequence data. Molecular Biology and Evolution *14* 685–695.

[3] Studier, J.A., Keppler, K.J. (1988). A note on the neighbor-joining algorithm of Saitou and Nei. Molecular Biology and Evolution *5(6)* 729–731.

See Also

Bioinformatics Toolbox functions: `multialign`, `phytree` (object constructor), `seqlinkage` (alternative method to create a phylogenetic tree), `seqpdist`

Methods of phytree object: `cluster`, `plot`, `reroot`, `view`

Purpose

Calculate pairwise distance between sequences

Syntax

```
D = seqpdist(Seqs)
D = seqpdist(Seqs, ...'Method', MethodValue, ...)
D = seqpdist(Seqs, ...'Indels', IndelsValue, ...)
D = seqpdist(Seqs, ...'Optargs', OptargsValue, ...)
D = seqpdist(Seqs, ...'PairwiseAlignment',
   PairwiseAlignmentValue, ...)
D = seqpdist(Seqs, ...'JobManager', JobManagerValue, ...)
D = seqpdist(Seqs, ...'WaitInQueue', WaitInQueueValue, ...)
D = seqpdist(Seqs, ...'SquareForm', SquareFormValue, ...)
D = seqpdist(Seqs, ...'Alphabet', AlphabetValue, ...)
D = seqpdist(Seqs, ...'ScoringMatrix', ScoringMatrixValue,
    ...)
D = seqpdist(Seqs, ...'Scale', ScaleValue, ...)
D = seqpdist(Seqs, ...'GapOpen', GapOpenValue, ...)
D = seqpdist(Seqs, ...'ExtendGap', ExtendGapValue, ...)
```

Arguments

Seqs	Any of the following: • Cell array containing nucleotide or amino acid sequences • Vector of structures containing a `Sequence` field • Matrix of characters, in which each row corresponds to a nucleotide or amino acid sequence
MethodValue	String that specifies the method for calculating pairwise distances. Default is `Jukes-Cantor`.
IndelsValue	String that specifies how to treat sites with gaps. Default is `score`.

OptargsValue — String or cell array specifying one or more input arguments required or accepted by the distance method specified by the `Method` property.

PairwiseAlignmentValue — Controls the global pairwise alignment of input sequences (using the `nwalign` function), while ignoring the multiple alignment of the input sequences (if any). Choices are `true` or `false`. Default is:

- `true` — When all input sequences do not have the same length.
- `false` — When all input sequences have the same length.

Tip If your input sequences have the same length, `seqpdist` will assume they aligned. If they are not aligned, do one of the following:

- Align the sequences before passing them to `seqpdist`, for example, using the `multialign` function.
- Set `PairwiseAlignment` to `true` when using `seqpdist`.

JobManagerValue	A `jobmanager object`, such as returned by the Parallel Computing Toolbox function `findResource`, that represents an available distributed MATLAB resource. Specifying this property distributes pairwise alignments into a cluster of computers using the Parallel Computing Toolbox software. You must have the Parallel Computing Toolbox software to use this property.
WaitInQueueValue	Controls whether `seqpdist` waits for a distributed MATLAB resource to be available when you have set the `JobManager` property. Choices are `true` or `false` (default). You must have the Parallel Computing Toolbox software to use this property.
SquareFormValue	Controls the conversion of the output into a square matrix. Choices are `true` or `false` (default).
AlphabetValue	String specifying the type of sequence (nucleotide or amino acid). Choices are `'NT'` or `'AA'` (default).
ScoringMatrixValue	String specifying the scoring matrix to use for the global pairwise alignment. Choices for amino acid sequences are: • `'PAM40'` • `'PAM250'` • `'DAYHOFF'` • `'GONNET'` • `'BLOSUM30'` increasing by `5` up to `'BLOSUM90'`

	• 'BLOSUM62' • 'BLOSUM100' Default is: • 'NUC44' (when *AlphabetValue* equals 'NT') • 'BLOSUM50' (when *AlphabetValue* equals 'AA')
ScaleValue	Positive value that specifies the scale factor used to return the score in arbitrary units. If the scoring matrix information also provides a scale factor, then both are used.
GapOpenValue	Positive integer specifying the penalty for opening a gap in the alignment. Default is 8.
ExtendedGapValue	Positive integer specifying the penalty for extending a gap. Default is equal to *GapOpenValue*.

Return Values

D	Vector containing biological distances between each pair of sequences stored in the M elements of *Seqs*.

Description

D = seqpdist(*Seqs*) returns *D*, a vector containing biological distances between each pair of sequences stored in the M sequences of *Seqs*, a cell array of sequences, a vector of structures, or a matrix or sequences.

D is a 1-by-(M*(M-1)/2) row vector corresponding to the M*(M-1)/2 pairs of sequences in Seqs. The output *D* is arranged in the order ((2,1),(3,1),..., (M,1),(3,2),...(M,2),.....(M,M-1)). This is

the lower-left triangle of the full M-by-M distance matrix. To get the distance between the *I*th and the *J*th sequences for `I > J`, use the formula `D((J-1)*(M-J/2)+I-J)`.

D = `seqpdist(`*Seqs*`, ...'`*PropertyName*`', `*PropertyValue*`, ...)` calls `seqpdist` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

D = `seqpdist(`*Seqs*`, ...'Method', `*MethodValue*`, ...)` specifies a method to compute distances between every pair of sequences. Choices are shown in the following tables.

Methods for Nucleotides and Amino Acids

Method	Description
`p-distance`	Proportion of sites at which the two sequences are different. `p` is close to `1` for poorly related sequences, and `p` is close to `0` for similar sequences. `d = p`

`Jukes-Cantor` (default)	Maximum likelihood estimate of the number of substitutions between two sequences. `p` is described with the method `p-distance`.
	
	For nucleotides:
	
	`d = -3/4 log(1-p * 4/3)`
	
	For amino acids:
	
	`d = -19/20 log(1-p * 20/19)`

`alignment-score`	Distance (`d`) between two sequences (1, 2) is computed from the pairwise alignment score between the two sequences (`score12`), and the pairwise alignment score between each sequence and itself (`score11`, `score22`) as follows:

Methods for Nucleotides and Amino Acids (Continued)

Method	Description
	`d = (1-score12/score11)* (1-score12/score22)` This option does not imply that prealigned input sequences will be realigned, it only scores them. Use with care; this distance method does not comply with the ultrametric condition. In the rare case where the score between sequences is greater than the score when aligning a sequence with itself, then `d = 0`.

Methods with No Scoring of Gaps (Nucleotides Only)

Method	Description
`Tajima-Nei`	Maximum likelihood estimate considering the background nucleotide frequencies. It can be computed from the input sequences or given by setting `Optargs` to `[gA gC gG gT]`. `gA`, `gC`, `gG`, `gT` are scalar values for the nucleotide frequencies.
`Kimura`	Considers separately the transitional nucleotide substitution and the transversional nucleotide substitution.
`Tamura`	Considers separately the transitional nucleotide substitution, the transversional nucleotide substitution, and the GC content. GC content can be computed from the input sequences or given by setting `Optargs` to the proportion of GC content (scalar value form `0` to `1`).

Methods with No Scoring of Gaps (Nucleotides Only) (Continued)

Method	Description
`Hasegawa`	Considers separately the transitional nucleotide substitution, the transversional nucleotide substitution, and the background nucleotide frequencies. Background frequencies can be computed from the input sequences or given by setting the `Optargs` property to `[gA gC gG gT]`.
`Nei-Tamura`	Considers separately the transitional nucleotide substitution between purines, the transitional nucleotide substitution between pyrimidines, the transversional nucleotide substitution, and the background nucleotide frequencies. Background frequencies can be computed from the input sequences or given by setting the `Optargs` property to `[gA gC gG gT]`.

Methods with No Scoring of Gaps (Amino Acids Only)

Method	Description
`Poisson`	Assumes that the number of amino acid substitutions at each site has a Poisson distribution.
`Gamma`	Assumes that the number of amino acid substitutions at each site has a Gamma distribution with parameter `a`. You can set `a` by using the `Optargs` property. Default is `2`.

You can also specify a user-defined distance function using `@`, for example, `@distfun`. The distance function must be of the form:

```
function D = distfun(S1, S2, OptArgsValue)
```

The `distfun` function takes the following arguments:

- *`S1`* , *`S2`* — Two sequences of the same length (nucleotide or amino acid).
- *`OptArgsValue`* — Optional problem-dependent arguments.

The `distfun` function returns a scalar that represents the distance between *`S1`* and *`S2`*.

`D` = `seqpdist(`*`Seqs`*`, ...'Indels', `*`IndelsValue`*`, ...)` specifies how to treat sites with gaps. Choices are:

- `score` (default) — Scores these sites either as a point mutation or with the alignment parameters, depending on the method selected.
- `pairwise-del` — For every pairwise comparison, it ignores the sites with gaps.
- `complete-del` — Ignores all the columns in the multiple alignment that contain a gap. This option is available only if a multiple alignment was provided as the input *`Seqs`*.

`D` = `seqpdist(`*`Seqs`*`, ...'Optargs', `*`OptargsValue`*`, ...)` passes one or more arguments required or accepted by the distance method specified by the `Method` property. Use a string or cell array to pass one or multiple input arguments. For example, you can provide the nucleotide frequencies for the `Tajima-Nei` distance method, instead of computing them from the input sequences.

`D` = `seqpdist(`*`Seqs`*`, ...'PairwiseAlignment', `*`PairwiseAlignmentValue`*`, ...)` controls the global pairwise alignment of input sequences (using the `nwalign` function), while ignoring the multiple alignment of the input sequences (if any). Default is:

- `true` — When all input sequences do not have the same length.
- `false` — When all input sequences have the same length.

Tip If your input sequences have the same length, `seqpdist` will assume they aligned. If they are not aligned, do one of the following:

- Align the sequences before passing them to `seqpdist`, for example, using the `multialign` function.
- Set `PairwiseAlignment` to `true` when using `seqpdist`.

D = `seqpdist(`*Seqs*`, ...'JobManager',` *JobManagerValue*`, ...)` distributes pairwise alignments into a cluster of computers using the Parallel Computing Toolbox software. *JobManagerValue* is a `jobmanager object` such as returned by the Parallel Computing Toolbox function `findResource`, that represents an available distributed MATLAB resource. You must have the Parallel Computing Toolbox software to use this property.

D = `seqpdist(`*Seqs*`, ...'WaitInQueue',` *WaitInQueueValue*`, ...)` controls whether `seqpdist` waits for a distributed MATLAB resource to be available when you have set the `JobManager` property. When *WaitInQueueValue* is true, `seqpdist` waits in the job manager queue for an available worker. When *WaitInQueueValue* is `false` (default) and there are no `workers` immediately available, `seqpdist` stops and displays an error message. You must have the Parallel Computing Toolbox software and have also set the `JobManager` property to use this property.

D = `seqpdist(`*Seqs*`, ...'SquareForm',` *SquareFormValue*`, ...)`, controls the conversion of the output into a square matrix such that *D*`(`*I*`,`*J*`)` denotes the distance between the *I*th and *J*th sequences. The square matrix is symmetric and has a zero diagonal. Choices are `true` or `false` (default). Setting `Squareform` to `true` is the same as using the `squareform` function in the Statistics Toolbox software.

D = `seqpdist(`*Seqs*`, ...'Alphabet',` *AlphabetValue*`, ...)` specifies the type of sequence (nucleotide or amino acid). Choices are `'NT'` or `'AA'` (default).

The remaining input properties are available when the `Method` property equals `'alignment-score'` or the `PairwiseAlignment` property equals `true`.

D = `seqpdist(`*Seqs*`, ...'ScoringMatrix',` *ScoringMatrixValue*`, ...)` specifies the scoring matrix to use for the global pairwise alignment. Default is:

- `'NUC44'` (when *AlphabetValue* equals `'NT'`)
- `'BLOSUM50'` (when *AlphabetValue* equals `'AA'`)

D = `seqpdist(`*Seqs*`, ...'Scale',` *ScaleValue*`, ...)` specifies the scale factor used to return the score in arbitrary units. Choices are any positive value. If the scoring matrix information also provides a scale factor, then both are used.

D = `seqpdist(`*Seqs*`, ...'GapOpen',` *GapOpenValue*`, ...)` specifies the penalty for opening a gap in the alignment. Choices are any positive integer. Default is `8`.

D = `seqpdist(`*Seqs*`, ...'ExtendGap',` *ExtendGapValue*`, ...)` specifies the penalty for extending a gap in the alignment. Choices are any positive integer. Default is equal to *GapOpenValue*.

Examples

1 Read amino acids alignment data into a MATLAB structure.

```
seqs = fastaread('pf00002.fa');
```

2 For every possible pair of sequences in the multiple alignment, ignore sites with gaps and score with the scoring matrix `PAM250`.

```
dist = seqpdist(seqs,'Method','alignment-score',...
                'Indels','pairwise-delete',...
                'ScoringMatrix','pam250');
```

3 Force the realignment of every pair of sequences ignoring the provided multiple alignment.

```
dist = seqpdist(seqs,'Method','alignment-score',...
```

```
                    'Indels','pairwise-delete',...
                    'ScoringMatrix','pam250',...
                    'PairwiseAlignment',true);
```

4 Measure the 'Jukes-Cantor' pairwise distances after realigning every pair of sequences, counting the gaps as point mutations.

```
dist = seqpdist(seqs,'Method','jukes-cantor',...
                'Indels','score',...
                'Scoringmatrix','pam250',...
                'PairwiseAlignment',true);
```

See Also

Bioinformatics Toolbox functions: `fastaread`, `dnds`, `dndsml`, `multialign`, `nwalign`, `phytree` (object constructor), `seqlinkage`

Bioinformatics Toolbox object: `phytree object`

Bioinformatics Toolbox method of a phytree object: `pdist`

Purpose

Calculate sequence profile from set of multiply aligned sequences

Syntax

```
Profile = seqprofile(Seqs)
[Profile, Symbols] = seqprofile(Seqs)
seqprofile(Seqs, ...'Alphabet', AlphabetValue, ...)
seqprofile(Seqs, ...'Counts', CountsValue, ...)
seqprofile(Seqs, ...'Gaps', GapsValue, ...)
seqprofile(Seqs, ...'Ambiguous', AmbiguousValue, ...)
seqprofile(Seqs, ...'Limits', LimitsValue, ...)
```

Arguments

Seqs

Set of multiply aligned sequences represented by any of the following:.

- Array of strings
- Cell array of strings
- Array of structures containing the field `Sequence`

AlphabetValue

String specifying the sequence alphabet. Choices are:

- `'NT'` — Nucleotides
- `'AA'` — Amino acids (default)
- `'none'` — No alphabet

When `Alphabet` is `'none'`, the symbol list is based on the observed symbols. Each character can be any symbol, except for a hyphen (-) and a period (.), which are reserved for gaps.

CountsValue

Controls returning frequency (ratio of counts/total counts) or counts. Choices are `true` (counts) or `false` (frequency). Default is `false`.

GapsValue	String that controls the counting of gaps in a sequence. Choices are: • `'all'` — Counts all gaps • `'noflanks'` — Counts all gaps except those at the flanks of every sequence • `'none'` — Default. Counts no gaps.
AmbiguousValue	Controls counting ambiguous symbols. Enter `'Count'` to add partial counts to the standard symbols.
LimitsValue	Specifies whether to use part of the sequence. Enter a `[1x2]` vector with the first position and the last position to include in the profile. Default is `[1,SeqLength]`.

Description

Profile = seqprofile(*Seqs*) returns *Profile*, a matrix of size [20 (or 4) x SequenceLength] with the frequency of amino acids (or nucleotides) for every column in the multiple alignment. The order of the rows is given by

- 4 nucleotides — A C G T/U
- 20 amino acids — A R N D C Q E G H I L K M F P S T W Y V

[*Profile*, *Symbols*] = seqprofile(*Seqs*) returns *Symbols*, a unique symbol list where every symbol in the list corresponds to a row in *Profile*, the profile.

seqprofile(*Seqs*, ...'*PropertyName*', *PropertyValue*, ...) calls seqprofile with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

seqprofile(*Seqs*, ...'Alphabet', *AlphabetValue*, ...) selects a nucleotide alphabet, amino acid alphabet, or no alphabet.

`seqprofile(Seqs, ...'Counts', CountsValue, ...)` when `Counts` is `true`, returns the counts instead of the frequency.

`seqprofile(Seqs, ...'Gaps', GapsValue, ...)` appends a row to the bottom of a profile (`Profile`) with the count for gaps.

`seqprofile(Seqs, ...'Ambiguous', AmbiguousValue, ...)` when `Ambiguous` is `'count'`, counts the ambiguous amino acid symbols (`B Z X`) and nucleotide symbols (`R Y K M S W B D H V N`) with the standard symbols. For example, the amino acid `X` adds a `1/20` count to every row while the amino acid `B` counts as `1/2` at the `D` and `N` rows.

`seqprofile(Seqs, ...'Limits', LimitsValue, ...)` specifies the start and end positions for the profile relative to the indices of the multiple alignment.

Examples

```
seqs = fastaread('pf00002.fa');
[P,S] = seqprofile(seqs,'limits',[50 60],'gaps','all')
```

See Also

Bioinformatics Toolbox functions: `fastaread`, `multialignread`, `multialignwrite`, `seqconsensus`, `seqdisp`, `seqlogo`

seqrcomplement

Purpose

Calculate reverse complementary strand of nucleotide sequence

Syntax

```
SeqRC = seqrcomplement(SeqNT)
```

Arguments

SeqNT Nucleotide sequence specified by any of the following:

- Character string with the characters `A`, `C`, `G`, `T`, `U`, and ambiguous characters `R`, `Y`, `K`, `M`, `S`, `W`, `B`, `D`, `H`, `V`, `N`.
- Row vector of integers from the table Mapping Nucleotide Integers to Letter Codes on page 3-809.
- MATLAB structure containing a `Sequence` field that contains a nucleotide sequence, such as returned by `emblread`, `fastaread`, `fastqread`, `genbankread`, `getembl`, or `getgenbank`.

Description

`SeqRC = seqrcomplement(SeqNT)` calculates the reverse complementary strand of a DNA or RNA nucleotide sequence. The return sequence, *SeqRC*, reads from 3' --> 5' and is in the same format as *SeqNT*. For example, if *SeqNT* is a vector of integers, then so is *SeqRC*.

Nucleotide in *SeqNT*	Converts to This Nucleotide in *SeqRC*
A	T or U
C	G
G	C
T or U	A

Examples

Return the reverse complement of a DNA nucleotide sequence.

```
s = 'ATCG'
seqrcomplement(s)
```

```
ans =
CGAT
```

See Also

Bioinformatics Toolbox functions: `codoncount`, `palindromes`, `seqcomplement`, `seqreverse`, `seqtool`

seqreverse

Purpose

Calculate reverse strand of nucleotide sequence

Syntax

```
SeqR = seqreverse(SeqNT)
```

Arguments

SeqNT — Nucleotide sequence specified by any of the following:

- Character string with the characters `A`, `C`, `G`, `T`, `U`, and ambiguous characters `R`, `Y`, `K`, `M`, `S`, `W`, `B`, `D`, `H`, `V`, `N`.
- Row vector of integers from the table Mapping Nucleotide Integers to Letter Codes on page 3-809.
- MATLAB structure containing a `Sequence` field that contains a nucleotide sequence, such as returned by `emblread`, `fastaread`, `fastqread`, `genbankread`, `getembl`, or `getgenbank`.

Description

SeqR = `seqreverse(`*SeqNT*`)` calculates the reverse strand of a DNA or RNA nucleotide sequence. The return sequence, *SeqR*, reads from 3' --> 5' and is in the same format as *SeqNT*. For example, if *SeqNT* is a vector of integers, then so is *SeqR*.

Examples

Return the reverse strand of a DNA nucleotide sequence.

```
s = 'ATCG'
seqreverse(s)
ans =
GCTA
```

See Also

Bioinformatics Toolbox functions: `codoncount`, `palindromes`, `seqcomplement`, `seqrcomplement`, `seqtool`

MATLAB function: `fliplr`

Purpose

Display open reading frames in sequence

Syntax

```
seqshoworfs(SeqNT)
seqshoworfs(SeqNT, ...'Frames', FramesValue, ...)
seqshoworfs(SeqNT, ...'GeneticCode', GeneticCodeValue, ...)
seqshoworfs(SeqNT, ...'MinimumLength', MinimumLengthValue,
    ...)
seqshoworfs(SeqNT, ...'AlternativeStartCodons',
    AlternativeStartCodonsValue, ...)
seqshoworfs(SeqNT, ...'Color', ColorValue, ...)
seqshoworfs(SeqNT, ...'Columns', ColumnsValue, ...)
```

Arguments

SeqNT	Nucleotide sequence. Enter either a character string with the characters `A`, `T` (`U`), `G`, `C`, and ambiguous characters `R`, `Y`, `K`, `M`, `S`, `W`, `B`, `D`, `H`, `V`, `N`, or a vector of integers. You can also enter a structure with the field `Sequence`.
FramesValue	Property to select the frame. Enter `1`, `2`, `3`, `-1`, `-2`, `-3`, enter a vector with integers, or `'all'`. The default value is the vector `[1 2 3]`. Frames `-1`, `-2`, and `-3` correspond to the first, second, and third reading frames for the reverse complement.
GeneticCodeValue	Genetic code name. Enter a code number or a code name from the table Genetic Code on page 3-1439.
MinimumLengthValue	Property to set the minimum number of codons in an ORF.

AlternativeStartCodonsValue Property to control using alternative start codons. Enter either `true` or `false`. The default value is `false`.

ColorValue Color to highlight the reading frame. Specify one of the following:

- Three-element numeric vector of RGB values
- String containing a predefined single-letter color code
- String containing a predefined color name

For example, to use cyan, enter `[0 1 1]`, `'c'`, or `'cyan'`. For more information on specifying colors, see `ColorSpec`.

To specify different colors for the three reading frames, use a `1`-by-`3` cell array of color values. If you are displaying reverse complement reading frames, then use a `1`-by-`6` cell array of color values.

The default color scheme is blue for the first reading frame, red for the second, and green for the third.

ColumnsValue Property to specify the number of columns in the output.

Genetic Code

Code Number	Code Name
1	Standard
2	Vertebrate Mitochondrial
3	Yeast Mitochondrial
4	Mold, Protozoan, Coelenterate Mitochondrial, and Mycoplasma/Spiroplasma
5	Invertebrate Mitochondrial
6	Ciliate, Dasycladacean, and Hexamita Nuclear
9	Echinoderm Mitochondrial
10	Euplotid Nuclear
11	Bacterial and Plant Plastid
12	Alternative Yeast Nuclear
13	Ascidian Mitochondrial
14	Flatworm Mitochondrial
15	Blepharisma Nuclear
16	Chlorophycean Mitochondrial
21	Trematode Mitochondrial
22	Scenedesmus Obliquus Mitochondrial
23	Thraustochytrium Mitochondrial

Description

`seqshoworfs` identifies and highlights all open reading frames using the standard or an alternative genetic code.

`seqshoworfs(`*`SeqNT`*`)` displays the sequence with all open reading frames highlighted, and it returns a structure of start and stop positions for each ORF in each reading frame. The standard genetic code is used with start codon `'AUG'` and stop codons `'UAA'`, `'UAG'`, and `'UGA'`.

`seqshoworfs(SeqNT, ...'PropertyName', PropertyValue, ...)` calls `seqshoworfs` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`seqshoworfs(SeqNT, ...'Frames', FramesValue, ...)` specifies the reading frames to display. The default is to display the first, second, and third reading frames with ORFs highlighted in each frame.

`seqshoworfs(SeqNT, ...'GeneticCode', GeneticCodeValue, ...)` specifies the genetic code to use for finding open reading frames.

`seqshoworfs(SeqNT, ...'MinimumLength', MinimumLengthValue, ...)` sets the minimum number of codons for an ORF to be considered valid. The default value is `10`.

`seqshoworfs(SeqNT, ...'AlternativeStartCodons', AlternativeStartCodonsValue, ...)` uses alternative start codons if `AlternativeStartCodons` is set to `true`. For example, in the human mitochondrial genetic code, `AUA` and `AUU` are known to be alternative start codons. For more details on alternative start codons, see

```
http://www.ncbi.nlm.nih.gov/Taxonomy/Utils/wprintgc.cgi?mode=t#SG1
```

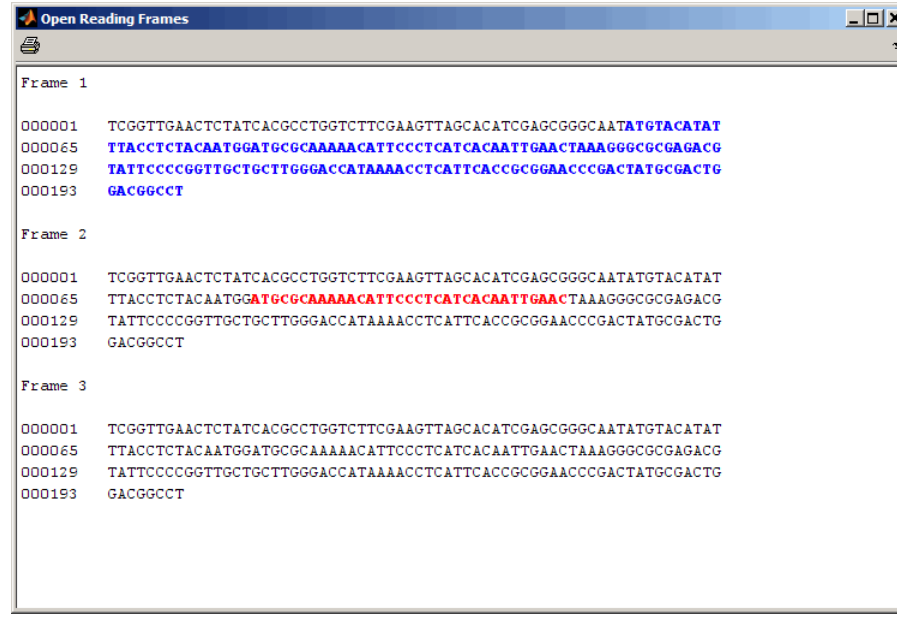
`seqshoworfs(SeqNT, ...'Color', ColorValue, ...)` specifies the color used to highlight the open reading frames in the output display. The default color scheme is blue for the first reading frame, red for the second, and green for the third.

`seqshoworfs(SeqNT, ...'Columns', ColumnsValue, ...)` specifies how many columns per line to use in the output. The default value is `64`.

Examples

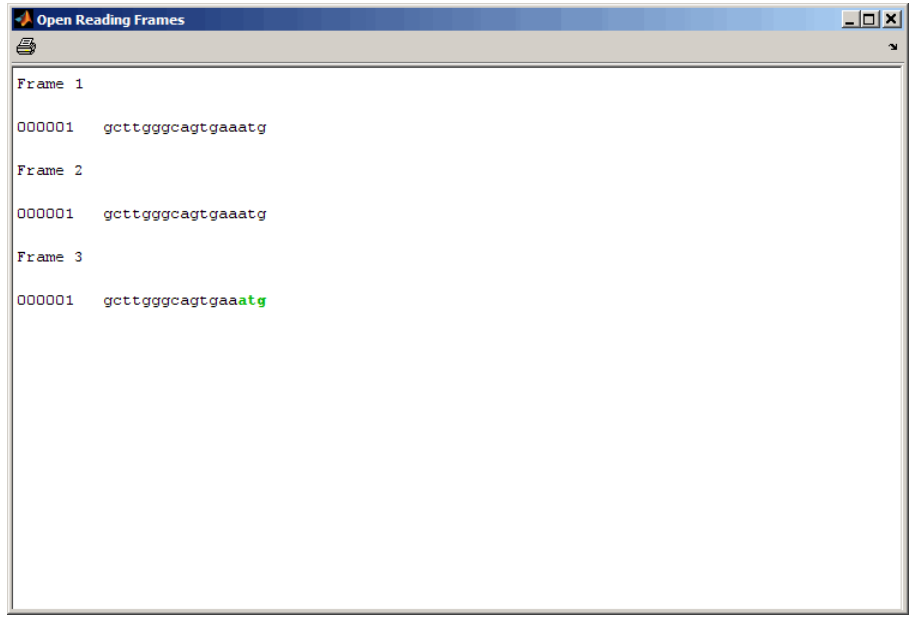
Display the open reading frames in a random nucleotide sequence.

```
s = randseq(200, 'alphabet', 'dna');
seqshoworfs(s);
```



Display the open reading frames in a GenBank sequence.

```
HLA_DQB1 = getgenbank('NM_002123');
seqshoworfs(HLA_DQB1.Sequence);
```



See Also

Bioinformatics Toolbox functions: `codoncount`, `cpgisland`, `geneticcode`, `seqdisp`, `seqshowwords`, `seqtool`, `seqwordcount`

MATLAB function: `regexp`

Purpose

Graphically display words in sequence

Syntax

```
Struct = seqshowwords(Seq, Word)
seqshowwords(Seq, Word, ...'Color', ColorValue, ...)
seqshowwords(Seq, Word, ...'Columns', ColumnsValue, ...)
seqshowwords(Seq, Word, ...'Alphabet', AlphabetValue, ...)
```

Description

`Struct = seqshowwords(Seq, Word)` opens a separate window displaying a sequence with all occurrences of one or more words highlighted. It also returns a structure containing the start and stop positions for all occurrences of the words in the sequence.

`seqshowwords(Seq, Word, ...'PropertyName', PropertyValue, ...)` calls `seqshowwords` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each *`PropertyName`* in single quotation marks. Each *`PropertyName`* is case insensitive. These property name/property value pairs are as follows:

`seqshowwords(Seq, Word, ...'Color', ColorValue, ...)` specifies the color to highlight the words in the output display of the sequence. Default is red.

`seqshowwords(Seq, Word, ...'Columns', ColumnsValue, ...)` specifies how many columns or characters per line in the output display of the sequence. Default is `64`.

`seqshowwords(Seq, Word, ...'Alphabet', AlphabetValue, ...)` specifies the alphabet for the sequence and the word or words. Choices are `'AA'` or `'NT'` (default).

Inputs

`Seq`

Amino acid or nucleotide sequence specified by any of the following:

- Character string of letters representing amino acids or nucleotides, such as returned by `int2aa` or `int2nt`.

- MATLAB structure containing a `Sequence` field, such as returned by `fastaread`, `fastqread`, `emblread`, `getembl`, `genbankread`, `getgenbank`, `getgenpept`, `genpeptread`, `getpdb`, `pdbread`, or `sffread`.

`Word`

One or more short amino acid or nucleotide sequences specified by any of the following:

- Character string of letters
- Regular expression
- Cell array of strings or regular expressions

Note If the search word or words contain amino acid or nucleotide symbols that represent multiple symbols, then `seqshowwords` shows all possible matches. For example, the symbol `R` represents either `G` or `A` (purines). If *`Word`* is `'ART'`, then `seqshowwords` shows occurrences of both `'AAT'` and `'AGT'`.

Tip If *`Word`* contains a repeating pattern, such as `'TATA'`, then `seqshowwords` does not highlight overlapping patterns of `TA` in the sequence. To highlight multiple repeats of `TA` in a sequence, use a regular expression, such as `'TA(TA)*TA'`, for *`Word`*. For more information, see "Examples" on page 3-1445.

`ColorValue`

Color to highlight all occurrences of one or more words in the sequence. Specify the color with one of the following:

- Three-element numeric vector of RGB values

- String containing a predefined single-letter color code
- String containing a predefined color name

For example, to use cyan, enter `[0 1 1]`, `'c'`, or `'cyan'`. For more information on specifying colors, see `ColorSpec`.

Default: Red, which is specified by `[1 0 0]`, `'r'`, or `'red'`

`ColumnsValue`

Positive integer specifying how many columns or characters per line in the output display of the sequence.

Default: `64`

`AlphabetValue`

String specifying the type of sequences. Choices are `'AA'` or `'NT'` (default).

Outputs

`Struct`

MATLAB structure containing the start and stop positions of all occurrences or the word or words in the sequence. It includes two fields.

Field	Description
`Start`	Row vector containing the start position of each occurrence of the search word or words.
`Stop`	Row vector containing the stop position of each occurrence of the search word or words.

Examples

Search for a word containing multiple symbols:

```
% Highlight the word 'BART' which represents 'TAGT' and 'TAAT'
seqshowwords('GCTAGTAACGTATATATAAT','BART')
```

```
ans =
    Start: [3 17]
    Stop: [6 20]

000001 GCTAGTAACGTATATATAAT
```

Search for a word that repeats, excluding overlaps:

```
% Highlight all occurrences of 'TATA', excluding those that are
% already part of another matched word.
seqshowwords('GCTATAACGTATATATATA','TATA')

ans =
    Start: [3 10 14]
    Stop: [6 13 17]

000001 GCTATAACGTATATATATA
```

Search for a word that repeats, including overlaps:

```
% Use the regular expression 'TA(TA)*TA' to highlight all multiple
% repeats of 'TA'
seqshowwords('GCTATAACGTATATATATA','TA(TA)*TA')

ans =
    Start: [3 10]
    Stop: [6 19]

000001 GCTATAACGTATATATATA
```

Search for multiple words:

```
% Use a cell array as input to highlight both the words
% 'CG' and 'GC'
seqshowwords('GCTATAACGTATATATATA',{'CG', 'GC'})


ans =

    Start: [1 8]
     Stop: [2 9]

000001    GCTATAACGTATATATATA
```

Alternatives

The `seqtool` function opens the "Sequence Tool" window, where you search for words in a sequence by selecting **Sequence > Find Word**. The Sequence Tool does not:

- Allow searching for multiple words in one step
- Return a structure containing the start and stop positions for all occurrences of the word in the sequence

See Also

`palindromes` | `cleave` | `restrict` | `seqdisp` | `seqtool` | `seqwordcount` | `strfind` | `regexp` | `ColorSpec`

Tutorials

- "Sequence Tool"

How To

- Regular Expressions

seqtool

Purpose

Open Sequence Tool window to interactively explore biological sequences

Syntax

```
seqtool
seqtool(Seq)
seqtool('close')
seqtool(Seq, 'Alphabet', AlphabetValue)
```

Arguments

Seq	Amino acid or nucleotide sequence specified by any of the following: • String of single-letter codes • Row vector of integers • MATLAB structure containing a `Sequence` field that contains an amino acid or nucleotide sequence, such as returned by `fastaread`, `fastqread`, `getgenpept`, `genpeptread`, `getpdb`, `pdbread`, `emblread`, `getembl`, `genbankread`, or `getgenbank` • String specifying a file name with an extension of .gbk, .gpt, .fasta, .fa, or .ebi.
AlphabetValue	String specifying an alphabet for the sequence, *Seq*. Default is `'AA'`, except when all of the symbols in the sequence are `A`, `C`, `G`, `T`, or `-`, then default is `'NT'`.

Description

`seqtool` opens the Sequence Tool window. For examples of using this window, see "Sequence Tool".

`seqtool(Seq)` opens the Sequence Tool window and loads *Seq*, a sequence, into the window.

`seqtool('close')` closes the Sequence Tool window.

`seqtool(`*`Seq`*`, 'Alphabet', `*`AlphabetValue`*`)` specifies an alphabet for the sequence, *`Seq`*. Default is `'AA'`, except when all of the symbols in the sequence are `A`, `C`, `G`, `T`, and `-`, then *`AlphabetValue`* defaults to `'NT'`. Use `'AA'` when you want to force an amino acid sequence alphabet.

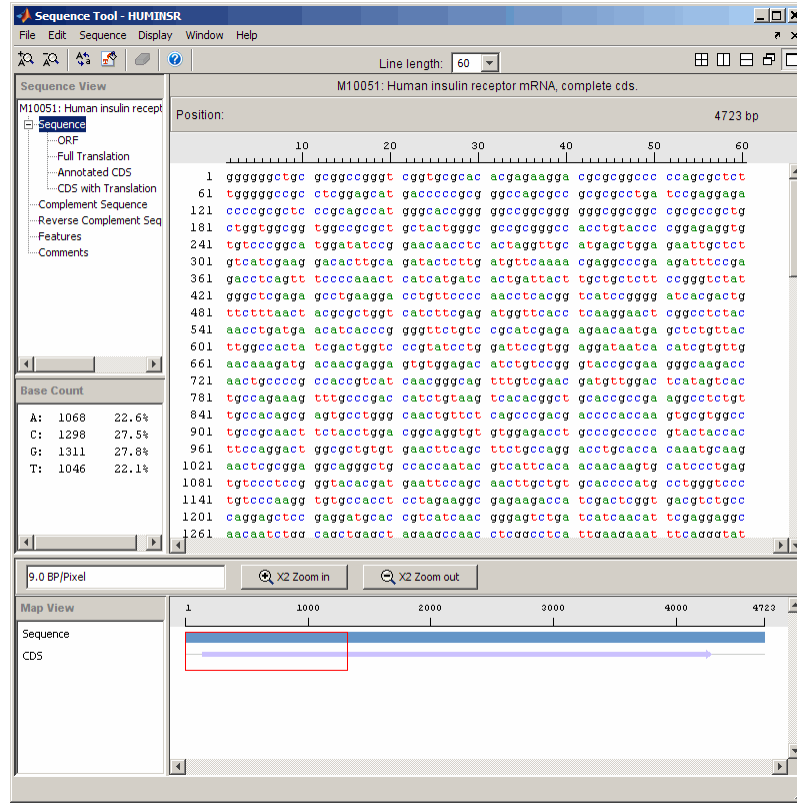
Examples

1 Retrieve a sequence from the GenBank database.

```
S = getgenbank('M10051');
```

2 Load the sequence into the Sequence Tool window.

```
seqtool(S)
```



3 Close the window.

```
seqtool('close')
```

See Also

Bioinformatics Toolbox functions: `aa2nt`, `aacount`, `aminolookup`, `basecount`, `baselookup`, `dimercount`, `emblread`, `fastaread`, `fastawrite`, `genbankread`, `geneticcode`, `genpeptread`, `getembl`, `getgenbank`, `getgenpept`, `nt2aa`, `proteinplot`, `seqcomplement`, `seqdisp`, `seqrcomplement`, `seqreverse`, `seqshoworfs`, `seqshowwords`, `seqwordcount`

Purpose

Count number of occurrences of word in sequence

Syntax

```
seqwordcount(Seq, Word)
```

Arguments

Seq	Enter a nucleotide or amino acid sequence of characters. You can also enter a structure with the field `Sequence`.
Word	Enter a short sequence of characters.

Description

`seqwordcount(Seq, Word)` counts the number of times that a word appears in a sequence, and then returns the number of occurrences of that word.

If *Word* contains nucleotide or amino acid symbols that represent multiple possible symbols (ambiguous characters), then `seqwordcount` counts all matches. For example, the symbol `R` represents either `G` or `A` (purines). For another example, if `word` equals `'ART'`, then `seqwordcount` counts occurrences of both `'AAT'` and `'AGT'`.

Examples

`seqwordcount` does not count overlapping patterns multiple times. In the following example, `seqwordcount` reports three matches. `TATATATA` is counted as two distinct matches, not three overlapping occurrences.

```
seqwordcount('GCTATAACGTATATATAT','TATA')

ans =
     3
```

The following example reports two matches (`'TAGT'` and `'TAAT'`). `B` is the ambiguous code for `G`, `T`, or `C`, while `R` is an ambiguous code for `G` and `A`.

```
seqwordcount('GCTAGTAACGTATATATAAT','BART')

ans =
     2
```

See Also

Bioinformatics Toolbox functions: `codoncount`, `seqshoworfs`, `seqshowwords`, `seqtool`, `seq2regexp`

MATLAB function: `strfind`

Purpose

Set property of biograph object

Syntax

```
set(BGobj)
set(BGobj, 'PropertyName')
set(BGobj, 'PropertyName', PropertyValue)
set(BGobj, 'Property1Name', Property1Value,
'Property2Name',
   Property2Value, ...)
```

Arguments

BGobj	Biograph object created with the function `biograph`.
PropertyName	Property name for a biograph object.
PropertyValue	Value of the property specified by *PropertyName*.

Description

`set(`*BGobj*`)` displays possible values for all properties that have a fixed set of property values in *BGobj*, a biograph object.

`set(`*BGobj*`, '`*PropertyName*`')` displays possible values for a specific property that has a fixed set of property values in *BGobj*, a biograph object.

`set(`*BGobj*`, '`*PropertyName*`', `*PropertyValue*`)` sets the specified property of *BGobj*, a biograph object.

`set(`*BGobj*`, '`*Property1Name*`', `*Property1Value*`, '`*Property2Name*`', `*Property2Value*`, ...)` sets the specified properties of *BGobj*, a biograph object.

Properties of a Biograph Object

Property	Description
`ID`	String to identify the biograph object. Default is `''`.
`Label`	String to label the biograph object. Default is `''`.

Properties of a Biograph Object (Continued)

Property	Description
`Description`	String that describes the biograph object. Default is `''`.
`LayoutType`	String that specifies the algorithm for the layout engine. Choices are: • `'hierarchical'` (default) — Uses a topological order of the graph to assign levels, and then arranges the nodes from top to bottom, while minimizing crossing edges. • `'radial'` — Uses a topological order of the graph to assign levels, and then arranges the nodes from inside to outside of the circle, while minimizing crossing edges. • `'equilibrium'` — Calculates layout by minimizing the energy in a dynamic spring system.
`EdgeType`	String that specifies how edges display. Choices are: • `'straight'` • `'curved'` (default) • `'segmented'` **Note** Curved or segmented edges occur only when necessary to avoid obstruction by nodes. Biograph objects with `LayoutType` equal to `'equilibrium'` or `'radial'` cannot produce curved or segmented edges.

Properties of a Biograph Object (Continued)

Property	Description
`Scale`	Positive number that post-scales the node coordinates. Default is `1`.
`LayoutScale`	Positive number that scales the size of the nodes before calling the layout engine. Default is `1`.
`EdgeTextColor`	Three-element numeric vector of RGB values. Default is `[0, 0, 0]`, which defines black.
`EdgeFontSize`	Positive number that sets the size of the edge font in points. Default is `8`.
`ShowArrows`	Controls the display of arrows with the edges. Choices are `'on'` (default) or `'off'`.
`ArrowSize`	Positive number that sets the size of the arrows in points. Default is `8`.
`ShowWeights`	Controls the display of text indicating the weight of the edges. Choices are `'on'` (default) or `'off'`.
`ShowTextInNodes`	String that specifies the node property used to label nodes when you display a biograph object using the `view` method. Choices are: • `'Label'` — Uses the `Label` property of the node object (default). • `'ID'` — Uses the `ID` property of the node object. • `'None'`
`NodeAutoSize`	Controls precalculating the node size before calling the layout engine. Choices are `'on'` (default) or `'off'`.

Properties of a Biograph Object (Continued)

Property	Description
`NodeCallback`	User-defined callback for all nodes. Enter the name of a function, a function handle, or a cell array with multiple function handles. After using the `view` function to display the biograph object in the Biograph Viewer, you can double-click a node to activate the first callback, or right-click and select a callback to activate. Default is the anonymous function, `@(node) inspect(node)`, which displays the Property Inspector dialog box.
`EdgeCallback`	User-defined callback for all edges. Enter the name of a function, a function handle, or a cell array with multiple function handles. After using the `view` function to display the biograph object in the Biograph Viewer, you can double-click an edge to activate the first callback, or right-click and select a callback to activate. Default is the anonymous function, `@(edge) inspect(edge)`, which displays the Property Inspector dialog box.
`CustomNodeDrawFcn`	Function handle to a customized function to draw nodes. Default is `[]`.

Properties of a Biograph Object (Continued)

Property	Description
`Nodes`	Read-only column vector with handles to node objects of a biograph object. The size of the vector is the number of nodes. For properties of node objects, see Properties of a Node Object on page 3-131.
`Edges`	Read-only column vector with handles to edge objects of a biograph object. The size of the vector is the number of edges. For properties of edge objects, see Properties of an Edge Object on page 3-133.

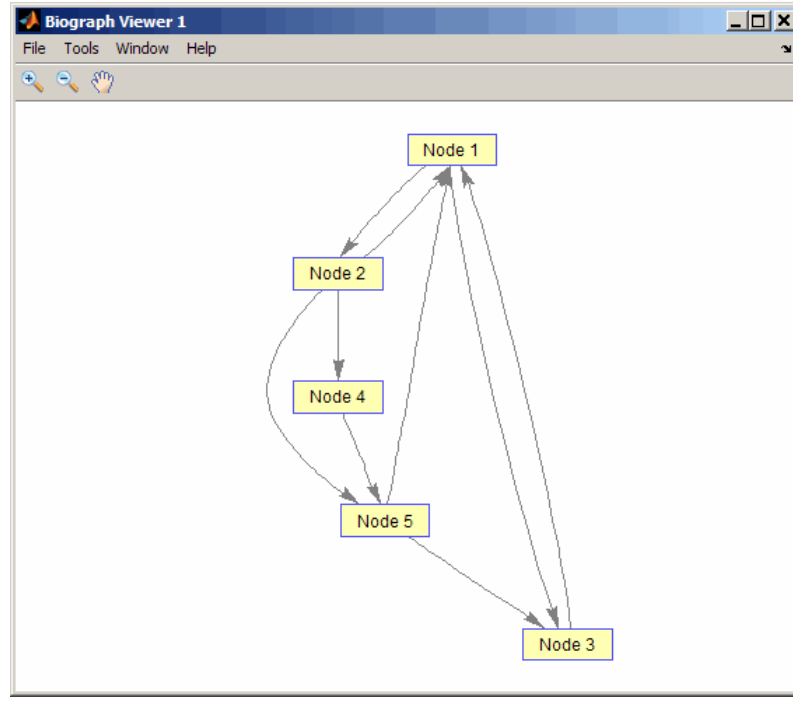
Examples

1 Create a biograph object with default node IDs.

```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];
bg = biograph(cm)
Biograph object with 5 nodes and 9 edges.
```

2 Use the `view` method to display the biograph object.

```
view(bg)
```

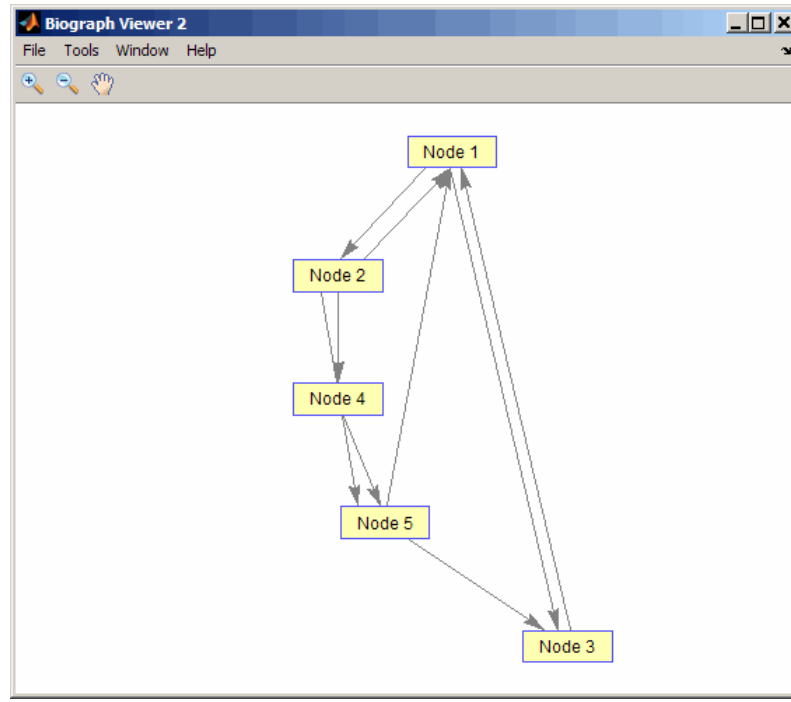


3 Use the `set` method to change the edge lines from curved to straight.

```
set(bg, 'EdgeType', 'straight')
```

4 Display the biograph object again.

```
view(bg)
```



See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox method of a biograph object: `get`

set (clustergram)

Purpose

Set property of clustergram object

Syntax

```
set(CGobj)
set(CGobj, 'PropertyName')
set(CGobj, 'PropertyName', PropertyValue)
set(CGobj, 'Property1Name', Property1Value,
'Property2Name',
   Property2Value, ...)
```

Arguments

CGobj	Clustergram object created with the function `clustergram`.
PropertyName	Property name for a clustergram object.

Description

Note You cannot set the properties of a clustergram object if you created it using the **Export Group to Workspace** command in the Clustergram window.

`set(`*`CGobj`*`)` displays possible values for all properties that have a fixed set of property values in *CGobj*, a clustergram object.

`set(`*`CGobj`*`, '`*`PropertyName`*`')` displays possible values for a specific property that has a fixed set of property values in *CGobj*, a clustergram object.

`set(`*`CGobj`*`, '`*`PropertyName`*`', `*`PropertyValue`*`)` sets the specified property of *CGobj*, a clustergram object.

`set(`*`CGobj`*`, '`*`Property1Name`*`', `*`Property1Value`*`, '`*`Property2Name`*`', `*`Property2Value`*`, ...)` sets the specified properties of *CGobj*, a clustergram object.

Properties of a Clustergram Object

Property	Description
`RowLabels`	Vector of numbers or cell array of text strings to label the rows in the dendrogram and heat map. Default is a vector of values `1` through *M*, where *M* is the number of rows in *`Data`*, the matrix of data used by the `clustergram` function to create the clustergram object.
`ColumnLabels`	Vector of numbers or cell array of text strings to label the columns in the dendrogram and heat map. Default is a vector of values `1` through *N*, where *N* is the number of columns in *`Data`*, the matrix of data used by the `clustergram` function to create the clustergram object.
`Standardize`	Numeric value that specifies the dimension for standardizing the values in *`Data`*, the matrix of data used to create the clustergram object. The standardized values are transformed so that the mean is 0 and the standard deviation is 1 in the specified dimension. Choices are: • `1` — Standardize along the columns of data. • `2` — Standardize along the rows of data. • `3` — Do not perform standardization.

Properties of a Clustergram Object (Continued)

Property	Description
`Cluster`	Numeric value that specifies the dimension for clustering the values in *`Data`*, the matrix of data used to create the clustergram object. Choices are: • `1` — Cluster rows of data only. • `2` — Cluster columns of data only. • `3` — Cluster rows of data, then cluster columns of row-clustered data.
`RowPdist`	String that specifies the distance metric to pass to the `pdist` function (Statistics Toolbox software) to use to calculate the pairwise distances between rows. For information on choices, see the `pdist` function. **Note** If the distance metric requires extra arguments, then *`RowPdistValue`* is a cell array. For example, to use the Minkowski distance with exponent `P`, you would use `{'minkowski', P}`.

Properties of a Clustergram Object (Continued)

Property	Description
`ColumnPdist`	String that specifies the distance metric to pass to the `pdist` function (Statistics Toolbox software) to use to calculate the pairwise distances between columns. For information on choices, see the `pdist` function. **Note** If the distance metric requires extra arguments, then *`ColumnPdistValue`* is a cell array. For example, to use the Minkowski distance with exponent `P`, you would use `{'minkowski', P}`.
`Linkage`	String or two-element cell array of strings that specifies the linkage method to pass to the `linkage` function (Statistics Toolbox software) to use to create the hierarchical cluster tree for rows and columns. If a two-element cell array of strings, the first element is used for linkage between rows, and the second element is used for linkage between columns. For information on choices, see the `linkage` function.
`Dendrogram`	Scalar or two-element numeric vector or cell array that specifies the `'colorthreshold'` property to pass to the `dendrogram` function (Statistics Toolbox software) to create the dendrogram plot. If a two-element numeric vector or cell array, the first element is for the rows, and the second element is for the columns. For more information, see the `dendrogram` function.

Properties of a Clustergram Object (Continued)

Property	Description
`OptimalLeafOrder`	Property to enable or disable the optimal leaf ordering calculation, which determines the leaf order that maximizes the similarity between neighboring leaves. Choices are `true` (enable) or `false` (disable). **Tip** Disabling the optimal leaf ordering calculation can be useful when working with large data sets because this calculation uses a large amount of memory and can be very time consuming.
`LogTrans`	Controls the $\log_2$ transform of *`Data`*, the matrix of data used to create the clustergram object, from natural scale. Choices are `true` or `false`.
`ColorMap`	Either of the following: • *M*-by-3 matrix of RGB values • Name or function handle of a function that returns a colormap, such as `redgreencmap` or `redbluecmap`
`DisplayRange`	Positive scalar that specifies the display range of standardized values. For example, if you specify `redgreencmap` for the `'ColorMap'` property, pure red represents values ≥ `DisplayRange`, and pure green represents values ≤ –`DisplayRange`.

Properties of a Clustergram Object (Continued)

Property	Description
`SymmetricRange`	Property to force the color scale of the heat map to be symmetric around zero. Choices are `true` or `false`.
`Ratio`	Either of the following: • Scalar • Two-element vector It specifies the ratio of space that the row and column dendrograms occupy relative to the heat map. If `Ratio` is a scalar, it is used as the ratio for both dendrograms. If `Ratio` is a two-element vector, the first element is used for the ratio of the row dendrogram width to the heat map width, and the second element is used for the ratio of the column dendrogram height to the heat map height. The second element is ignored for one-dimensional clustergrams.
`Impute`	Any of the following: • Name of a function that imputes missing data. • Handle to a function that imputes missing data. • Cell array where the first element is the name of or handle to a function that imputes missing data and the remaining elements are property name/property value pairs used as inputs to the function.

Properties of a Clustergram Object (Continued)

Property	Description
`RowMarkers`	Optional structure array for annotating the groups (clusters) of rows determined by the `clustergram` function. Each structure in the array represents a group of rows and contains the following fields: • `GroupNumber` — Number to annotate the row group. • `Annotation` — String specifying text to annotate the row group. • `Color` — String or three-element vector of RGB values specifying a color, which is used to label the row group. For more information on specifying colors, see `colorspec`. If this field is empty, default is `'blue'`.
`ColumnMarkers`	Optional structure array for annotating groups (clusters) of columns determined by the `clustergram` function. Each structure in the array represents a group of rows and contains the following fields: • `GroupNumber` — Number to annotate the column group. • `Annotation` — String specifying text to annotate the column group. • `Color` — String or three-element vector of RGB values specifying a color, which is used to label the column group. For more information on specifying colors, see `colorspec`. If this field is empty, default is `'blue'`.

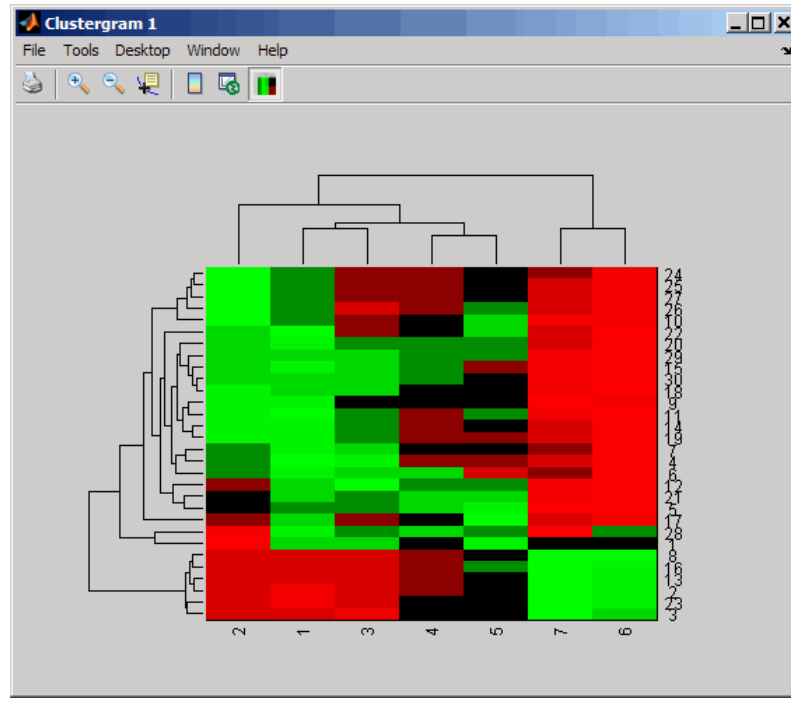
Examples

1 Load the MAT-file, provided with the Bioinformatics Toolbox software, that contains filtered yeast data. This MAT-file includes three variables: `yeastvalues`, a matrix of gene expression data, `genes`, a cell array of GenBank accession numbers for labeling the rows in `yeastvalues`, and `times`, a vector of time values for labeling the columns in `yeastvalues`.

```
load filteredyeastdata
```

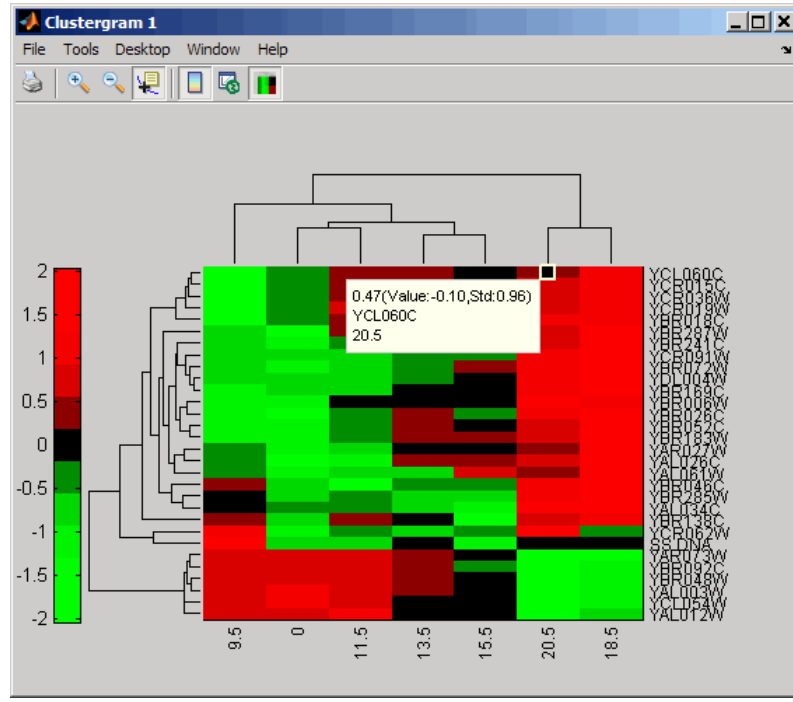
2 Create a clustergram object and display the dendrograms and heat map from the gene expression data in the first 30 rows of the `yeastvalues` matrix.

```
cgo = clustergram(yeastvalues(1:30,:))
Clustergram object with 30 rows of nodes and 7 column of nodes.
```



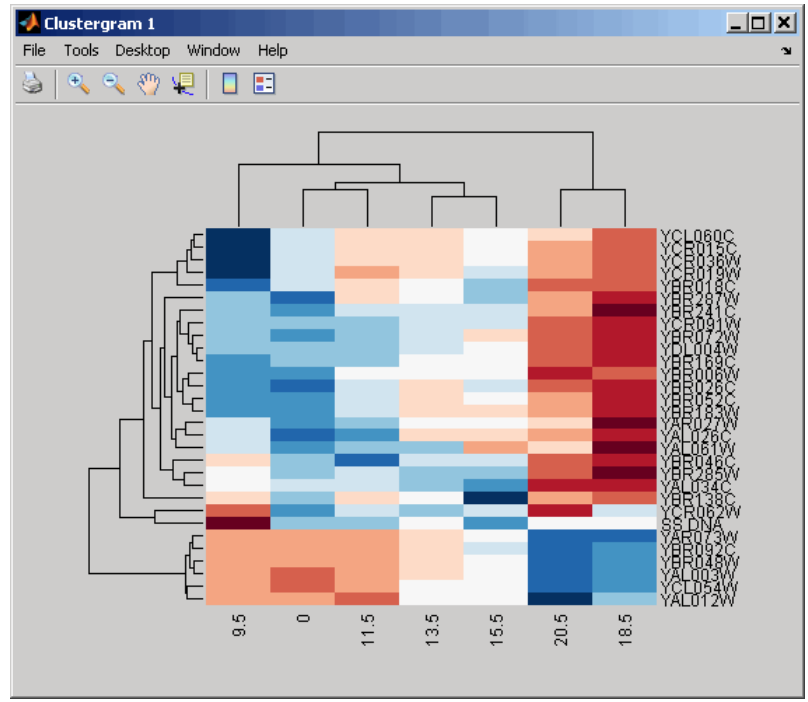
3 Use the `set` method and the `genes` and `times` vectors to add meaningful row and column labels to the clustergram.

```
set(cgo,'RowLabels',genes(1:30),'ColumnLabels',times)
```



4 Reset the colormap of the heat map to `redbluecmap`.

```
set(cgo,'Colormap',redbluecmap);
```



See Also

Bioinformatics Toolbox function: `clustergram` (object constructor)

Bioinformatics Toolbox object: clustergram object

Bioinformatics Toolbox methods of a clustergram object: `get`, `plot`, `view`

set (DataMatrix)

Purpose

Set property of DataMatrix object

Syntax

```
set(DMObj)
set(DMObj, 'PropertyName')
DMObj = set(DMObj, 'PropertyName', PropertyValue)
DMObj = set(DMObj, 'Property1Name', Property1Value,
   'Property2Name', Property2Value, ...)
```

Arguments

DMObj	DataMatrix object, such as created by `DataMatrix` (object constructor).
PropertyName	Property name of a DataMatrix object.
PropertyValue	Value of the property specified by *PropertyName*.

Description

`set(`*DMObj*`)` displays possible values for all properties that have a fixed set of property values in *DMObj*, a DataMatrix object.

`set(`*DMObj*`, '`*PropertyName*`')` displays possible values for a specific property that has a fixed set of property values in *DMObj*, a DataMatrix object.

DMObj `= set(`*DMObj*`, '`*PropertyName*`', `*PropertyValue*`)` sets the specified property of *DMObj*, a DataMatrix object.

DMObj `= set(`*DMObj*`, '`*Property1Name*`', `*Property1Value*`, '`*Property2Name*`', `*Property2Value*`, ...)` sets the specified properties of *DMObj*, a DataMatrix object.

Properties of a DataMatrix Object

Property	Description
`Name`	String that describes the DataMatrix object. Default is `''`.

Properties of a DataMatrix Object (Continued)

Property	Description
`RowNames`	Empty array or cell array of strings that specifies the names for the rows, typically gene names or probe identifiers. The number of elements in the cell array must equal the number of rows in the matrix. Default is an empty array.
`ColNames`	Empty array or cell array of strings that specifies the names for the columns, typically sample identifiers. The number of elements in the cell array must equal the number of columns in the matrix.
`NRows`	Positive number that specifies the number of rows in the matrix. **Note** You cannot modify this property directly. You can access it using the `get` method.
`NCols`	Positive number that specifies the number of columns in the matrix. **Note** You cannot modify this property directly. You can access it using the `get` method.

Properties of a DataMatrix Object (Continued)

Property	Description
`NDims`	Positive number that specifies the number of dimensions in the matrix. **Note** You cannot modify this property directly. You can access it using the `get` method.
`ElementClass`	String that specifies the class type, such as `single` or `double`. **Note** You cannot modify this property directly. You can access it using the `get` method.

Examples

1. Load the MAT-file, provided with the Bioinformatics Toolbox software, that contains yeast data. This MAT-file includes three variables: `yeastvalues`, a matrix of gene expression data, `genes`, a cell array of GenBank accession numbers for labeling the rows in `yeastvalues`, and `times`, a vector of time values for labeling the columns in `yeastvalues`.

   ```
   load filteredyeastdata
   ```

2. Import the microarray object package so that the `DataMatrix` constructor function will be available.

   ```
   import bioma.data.*
   ```

3. Create a DataMatrix object from the gene expression data in the first 30 rows of the `yeastvalues` matrix.

   ```
   dmo = DataMatrix(yeastvalues(1:30,:));
   ```

4 Use the `get` method to display the properties of the DataMatrix object, `dmo`.

```
get(dmo)
```

```
           Name: ''
        RowNames: []
        ColNames: []
           NRows: 30
           NCols: 7
           NDims: 2
     ElementClass: 'double'
```

Notice that the `RowNames` and `ColNames` fields are empty.

5 Use the `set` method and the `genes` and `times` variables to specify row names and column names for the DataMatrix object, `dmo`.

```
dmo = set(dmo,'RowNames',genes(1:30),'ColNames',times)
```

6 Use the `get` method to display the properties of the DataMatrix object, `dmo`.

```
get(dmo)
```

```
           Name: ''
        RowNames: {30x1 cell}
        ColNames: {'   0'  ' 9.5'  '11.5'  '13.5'  '15.5'  '18.5'  '20.5'}
           NRows: 30
           NCols: 7
           NDims: 2
     ElementClass: 'double'
```

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: `get`

Purpose

Return information about SFF file

Syntax

```
InfoStruct = sffinfo(File)
```

Description

`InfoStruct = sffinfo(File)` returns a MATLAB structure containing summary information about a Standard Flowgram Format (SFF) file.

Inputs

`File`

String specifying a file name or path and file name of an SFF file produced by version 1.0 of the Genome Sequencer System data analysis software from 454 Life Sciences®. If you specify only a file name, that file must be on the MATLAB search path or in the current folder.

Outputs

`InfoStruct`

MATLAB structure containing summary information about an SFF file. The structure contains the following fields.

Field	Description
`Filename`	Name of the file.
`FileModDate`	Modification date of the file.
`FileSize`	Size of the file in bytes.
`Version`	Version number of the file.
`FlowgramCode`	Code of the format used to encode flowgram values.
`NumberOfReads`	Number of sequence reads in the file.
`NumberOfFlowsPerRead`	Number of flows for each read.
`FlowChars`	Bases used in each flow.
`KeySequence`	String of bases in the key sequence.

Examples

The SFF file, `SRR013472.sff`, used in this example is not provided with the Bioinformatics Toolbox software. You can download sample SFF files from:

```
http://www.ncbi.nlm.nih.gov/Traces/sra/sra.cgi?cmd=show&f=main&m=main&s=main
```

Return a summary of the contents of an SFF file:

```
info = sffinfo('SRR013472.sff')

info =

                Filename: 'SRR013472.sff'
            FileModDate: '23-Feb-2009 15:14:36'
                FileSize: 6632392
                 Version: [0 0 0 1]
            FlowgramCode: 1
           NumberOfReads: 3546
    NumberOfFlowsPerRead: 440
               FlowChars: [1x440 char]
             KeySequence: 'TCAG'
```

See Also

`fastqread` | `fastqwrite` | `fastqinfo` | `fastainfo` | `fastaread` | `fastawrite` | `sffread`

Tutorials

- Working with SFF Files from the 454 Genome Sequencer FLX System

Related Links

-
.

sffread

Purpose

Read data from SFF file

Syntax

```
SFFStruct = sffread(File)
sffread(..., 'Blockread', BlockreadValue, ...)
sffread(..., 'Feature', FeatureValue, ...)
```

Description

`SFFStruct = sffread(File)` reads a Standard Flowgram Format (SFF) file and returns the data in a MATLAB array of structures.

`sffread(..., 'PropertyName', PropertyValue, ...)` calls `sffread` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each *`PropertyName`* in single quotation marks. Each *`PropertyName`* is case insensitive. These property name/property value pairs are as follows:

`sffread(..., 'Blockread', BlockreadValue, ...)` reads a single sequence entry or block of sequence entries from an SFF file containing multiple sequences.

`sffread(..., 'Feature', FeatureValue, ...)` specifies the information to include in the return structure.

Inputs

`File`

String specifying a file name or path and file name of an SFF file produced by version 1.0 of the Genome Sequencer System data analysis software from 454 Life Sciences. If you specify only a file name, that file must be on the MATLAB search path or in the current folder.

`BlockreadValue`

Scalar or vector that controls the reading of a single sequence entry or block of sequence entries from an SFF file containing multiple sequences. Enter a scalar *`N`*, to read the *`N`*th entry in the file. Enter a 1-by-2 vector [*`M1, M2`*], to read a block of entries starting at the *`M1`* entry and ending at the *`M2`* entry. To read all remaining entries in the file starting at the *`M1`* entry, enter a positive value for *`M1`* and enter `Inf` for *`M2`*.

FeatureValue

String specifying the information to include in the output structure. The string includes letters from the alphabet `H`, `S`, `Q`, `C`, `F`, and `I`, which represent the fields `Header`, `Sequence`, `Quality`, `Clipping`, `FlowgramValue`, and `FlowgramIndex`, respectively.

Default: `'HSQ'`

Outputs

SFFStruct

Array of structures containing information from an SFF file. There is one structure for each read or entry in the file. Each structure contains one or more of the following fields.

Field	Description
`Header`	Universal accession number.
`Sequence`	Numeric representation of nucleotide sequence.
`Quality`	Per-base quality scores.
`Clipping`	Clipping boundary positions.
`FlowgramValue`	Sequence of flowgram intensity values.
`FlowgramIndex`	Sequence of flowgram intensity indices.

Examples

The SFF file, `SRR013472.sff`, used in these examples is not provided with the Bioinformatics Toolbox software. You can download sample SFF files from:

```
http://www.ncbi.nlm.nih.gov/Traces/sra/sra.cgi?cmd=show&f=main&m=main&s=main
```

Read an entire SFF file:

```
% Read the contents of an entire SFF file into an
% array of structures
reads = sffread('SRR013472.sff')
```

```
reads =

3546x1 struct array with fields:
    Header
    Sequence
    Quality
```

Read a block of entries from an SFF file:

```
% Read only the header and sequence information of the
% first five reads from an SFF file into an array of structures
reads5 = sffread('SRR013472.sff', 'block', [1 5], 'feature', 'hs')

reads5 =

5x1 struct array with fields:
    Header
    Sequence
```

See Also

`fastqread` | `fastqwrite` | `fastqinfo` | `fastainfo` | `fastaread` | `fastawrite` | `sffinfo`

Tutorials

- Working with SFF Files from the 454 Genome Sequencer FLX System

Related Links

-
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Purpose

Solve shortest path problem in biograph object

Syntax

```
[dist, path, pred] = shortestpath(BGObj, S)
[dist, path, pred] = shortestpath(BGObj, S, T)
[...] = shortestpath(..., 'Directed', DirectedValue, ...)
[...] = shortestpath(..., 'Method', MethodValue, ...)
[...] = shortestpath(..., 'Weights', WeightsValue, ...)
```

Arguments

BGObj	Biograph object created by `biograph` (object constructor).
S	Node in graph represented by an N-by-N adjacency matrix extracted from a biograph object, *BGObj*.
T	Node in graph represented by an N-by-N adjacency matrix extracted from a biograph object, *BGObj*.
DirectedValue	Property that indicates whether the graph represented by the N-by-N adjacency matrix extracted from a biograph object, *BGObj*, is directed or undirected. Enter `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.
MethodValue	String that specifies the algorithm used to find the shortest path. Choices are: • `'Bellman-Ford'` — Assumes weights of the edges to be nonzero entries in the N-by-N adjacency matrix. Time complexity is `O(N*E)`, where `N` and `E` are the number of nodes and edges respectively. • `'BFS'` — Breadth-first search. Assumes all weights to be equal, and nonzero entries in the N-by-N adjacency matrix to represent edges. Time complexity is `O(N+E)`, where `N` and `E` are the number of nodes and edges respectively. • `'Acyclic'` — Assumes the graph represented by the N-by-N adjacency matrix extracted from a

biograph object, *BGObj*, to be a directed acyclic graph and that weights of the edges are nonzero entries in the N-by-N adjacency matrix. Time complexity is O(N+E), where N and E are the number of nodes and edges respectively.

- 'Dijkstra' — Default algorithm. Assumes weights of the edges to be positive values in the N-by-N adjacency matrix. Time complexity is O(log(N)*E), where N and E are the number of nodes and edges respectively.

WeightsValue Column vector that specifies custom weights for the edges in the N-by-N adjacency matrix extracted from a biograph object, *BGObj*. It must have one entry for every nonzero value (edge) in the N-by-N adjacency matrix. The order of the custom weights in the vector must match the order of the nonzero values in the N-by-N adjacency matrix when it is traversed column-wise. This property lets you use zero-valued weights. By default, shortestpaths gets weight information from the nonzero entries in the N-by-N adjacency matrix.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

[*dist*, *path*, *pred*] = shortestpath(*BGObj*, *S*) determines the single-source shortest paths from node *S* to all other nodes in the graph represented by an N-by-N adjacency matrix extracted from a biograph object, *BGObj*. Weights of the edges are all nonzero entries in the N-by-N adjacency matrix. *dist* are the N distances from the source to every node (using Infs for nonreachable nodes and 0 for the source node). *path* contains the winning paths to every node. *pred* contains the predecessor nodes of the winning paths.

`[dist, path, pred] = shortestpath(BGObj, S, T)` determines the single source-single destination shortest path from node `S` to node `T`.

`[...] = shortestpath(..., 'PropertyName', PropertyValue, ...)` calls `shortestpath` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each `PropertyName` must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[...] = shortestpath(..., 'Directed', DirectedValue, ...)` indicates whether the graph represented by the N-by-N adjacency matrix extracted from a biograph object, `BGObj`, is directed or undirected. Set `DirectedValue` to `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.

`[...] = shortestpath(..., 'Method', MethodValue, ...)` lets you specify the algorithm used to find the shortest path. Choices are:

- `'Bellman-Ford'` — Assumes weights of the edges to be nonzero entries in the N-by-N adjacency matrix. Time complexity is `O(N*E)`, where `N` and `E` are the number of nodes and edges respectively.
- `'BFS'` — Breadth-first search. Assumes all weights to be equal, and nonzero entries in the N-by-N adjacency matrix to represent edges. Time complexity is `O(N+E)`, where `N` and `E` are the number of nodes and edges respectively.
- `'Acyclic'` — Assumes the graph represented by the N-by-N adjacency matrix extracted from a biograph object, `BGObj`, to be a directed acyclic graph and that weights of the edges are nonzero entries in the N-by-N adjacency matrix. Time complexity is `O(N+E)`, where `N` and `E` are the number of nodes and edges respectively.
- `'Dijkstra'` — Default algorithm. Assumes weights of the edges to be positive values in the N-by-N adjacency matrix. Time complexity is `O(log(N)*E)`, where `N` and `E` are the number of nodes and edges respectively.

`[...] = shortestpath(..., 'Weights', WeightsValue, ...)` lets you specify custom weights for the edges. *`WeightsValue`* is a column vector having one entry for every nonzero value (edge) in the N-by-N adjacency matrix extracted from a biograph object, *`BGObj`*. The order of the custom weights in the vector must match the order of the nonzero values in the N-by-N adjacency matrix when it is traversed column-wise. This property lets you use zero-valued weights. By default, `shortestpath` gets weight information from the nonzero entries in the N-by-N adjacency matrix.

References

[1] Dijkstra, E.W. (1959). A note on two problems in connexion with graphs. Numerische Mathematik *1*, 269–271.

[2] Bellman, R. (1958). On a Routing Problem. Quarterly of Applied Mathematics *16(1)*, 87–90.

[3] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphshortestpath`

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `isdag`, `isomorphism`, `isspantree`, `maxflow`, `minspantree`, `topoorder`, `traverse`

Purpose

Display color-coded sequence alignment

Syntax

```
showalignment(Alignment)
showalignment(..., 'MatchColor', MatchColorValue, ...)
showalignment(..., 'SimilarColor' SimilarColorValue, ...)
showalignment(..., 'StartPointers',
StartPointersValue, ...)
showalignment(..., 'Columns', ColumnsValue, ...)
showalignment(..., 'TerminalGap', TerminalGapValue, ...)
```

Description

`showalignment(Alignment)` displays a color-coded sequence alignment in a MATLAB Figure window.

`showalignment(..., 'PropertyName', PropertyValue, ...)` calls `showalignment` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each *`PropertyName`* in single quotation marks. Each *`PropertyName`* is case insensitive. These property name/property value pairs are as follows:

`showalignment(..., 'MatchColor', MatchColorValue, ...)` specifies the color to highlight matching characters in the output display.

`showalignment(..., 'SimilarColor' SimilarColorValue, ...)` specifies the color to highlight similar characters in the output display.

`showalignment(..., 'StartPointers', StartPointersValue, ...)` specifies the starting indices in the original sequences of a local pairwise alignment.

`showalignment(..., 'Columns', ColumnsValue, ...)` specifies the number of characters to display in one row when displaying a pairwise alignment, and labels the start of each row with the sequence positions.

`showalignment(..., 'TerminalGap', TerminalGapValue, ...)` controls the inclusion or exclusion of terminal gaps from the count of matches and similar residues when displaying a pairwise alignment. *`TerminalGapValue`* can be `true` (default) or `false`.

Inputs

Alignment

Pairwise or multiple sequence alignment specified by one of the following:

- 3-by-N character array showing the pairwise alignment of two sequences, such as returned by `nwalign` or `swalign`
- MATLAB structure containing a `Sequence` field, such as returned by `fastaread`, `gethmmalignment`, `multialign`, or `multialignread`
- MATLAB character array that contains a multiple sequence alignment, such as returned by `multialign`

MatchColorValue

Color to highlight matching characters in the output display. Specify the color with one of the following:

- Three-element numeric vector of RGB values
- String containing a predefined single-letter color code
- String containing a predefined color name

For example, to use cyan, enter `[0 1 1]`, `'c'`, or `'cyan'`. For more information on specifying colors, see `ColorSpec`.

Default: Red, which is specified by `[1 0 0]`, `'r'`, or `'red'`

SimilarColorValue

Color to highlight similar characters in the output display. Specify the color with one of the following:

- Three-element numeric vector of RGB values
- String containing a predefined single-letter color code
- String containing a predefined color name

For example, to use cyan, enter `[0 1 1]`, `'c'`, or `'cyan'`. For more information on specifying colors, see `ColorSpec`.

Default: Magenta, which is specified by `[1 0 1]`, `'m'`, or `'magenta'`

`StartPointersValue`

Two-element vector that specifies the starting indices in the original sequences of a local pairwise alignment.

Tip You can use the third output returned by `swalign` as the *`StartPointersValue`*.

`ColumnsValue`

Scalar that specifies the number of characters to display in one row when displaying a pairwise alignment.

Default: `64`

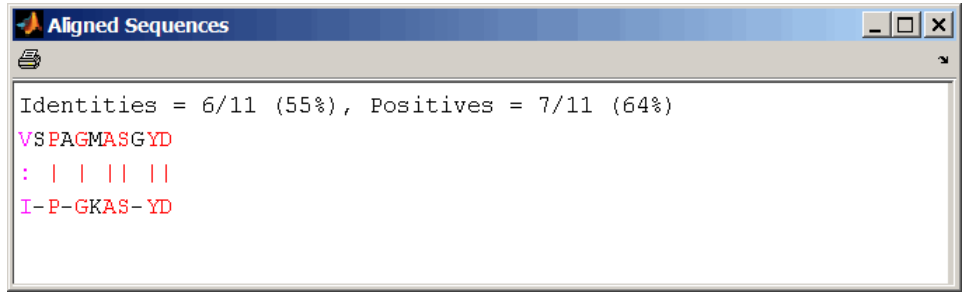
`TerminalGapValue`

Specifies whether to include or exclude terminal gaps from the count of matches and similar residues when displaying a pairwise alignment. Choices are `true` (default) or `false`.

Examples

Display a pairwise sequence alignment:

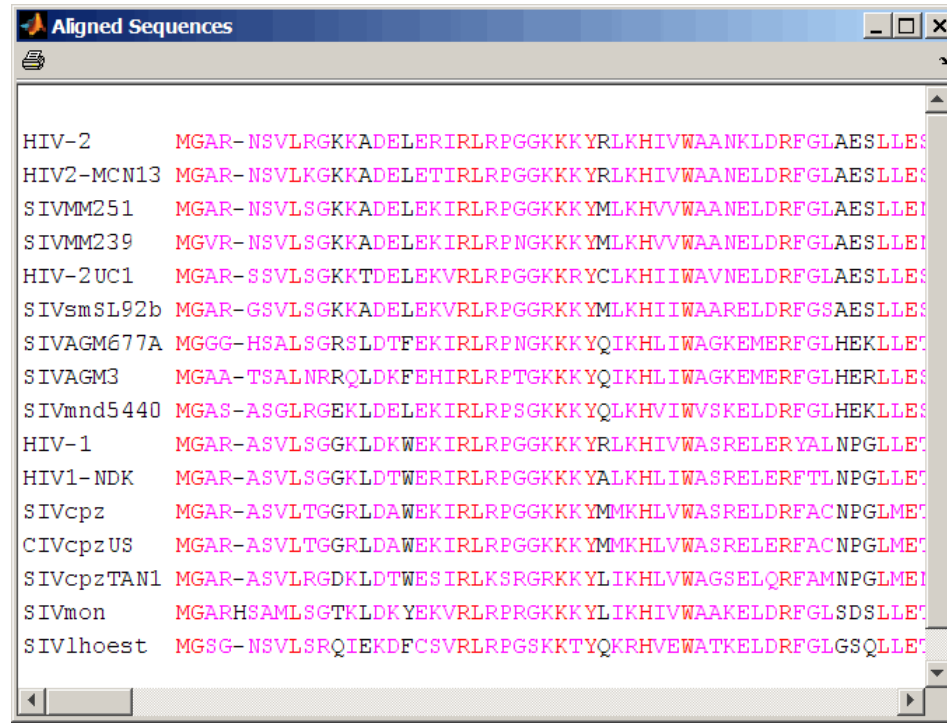
```
% Globally align two amino acid sequences
[Score, Alignment] = nwalign('VSPAGMASGYD','IPGKASYD');
% Display the color-coded alignment
showalignment(Alignment);
```



Notice that for pairwise sequence alignments, matching and similar characters appear in red and magenta respectively..

Display a multiple sequence alignment

```
% Read a multiple-sequence alignment file
gag = multialignread('aagag.aln');
% Display the color-coded alignment
showalignment(gag)
```



Notice that for multiple sequence alignments, highly conserved positions appear in red and conserved positions appear in magenta.

Tip To view a multiple-sequence alignment and interact with it, use the `multialignviewer` function.

Alternatives

You can also display a multiple or pairwise sequence alignment using the `multialignviewer` function. The alignment displays in the Multiple Sequence Alignment Viewer window, where you can view and interactively adjust a sequence alignment.

See Also

`multialign` | `multialignviewer` | `nwalign` | `swalign` | `ColorSpec` | `gethmmalignment` | `fastaread` | `multialignread` | `localalign`

Tutorials

- Aligning Pairs of Sequences

Purpose

Plot hidden Markov model (HMM) profile

Syntax

```
showhmmprof(Model)
showhmmprof(Model, ...'Scale', ScaleValue, ...)
showhmmprof(Model, ...'Order', OrderValue, ...)
```

Arguments

Model	Hidden Markov model created by the function `gethmmprof` or `pfamhmmread`.
ScaleValue	Property to select a probability scale. Enter one of the following values: • `'logprob'` — Log probabilities • `'prob'` — Probabilities • `'logodds'` — Log-odd ratios
OrderValue	Property to specify the order of the amino acid alphabet. Enter a character string with the 20 standard amino acids characters `A R N D C Q E G H I L K M F P S T W Y V`. The ambiguous characters `B Z X` are not allowed.

Description

`showhmmprof(Model)` plots a profile hidden Markov model described by the structure *Model*.

`showhmmprof(..., 'PropertyName', PropertyValue, ...)` calls `showhmmprof` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`showhmmprof(Model, ...'Scale', ScaleValue, ...)` specifies the scale to use. If log probabilities (*ScaleValue*=`'logprob'`), probabilities (*ScaleValue*=`'prob'`), or log-odd ratios (*ScaleValue*=`'logodds'`). To compute the log-odd ratios, the null model probabilities are used for symbol emission and equally distributed transitions are used for the null transition probabilities. The default *ScaleValue* is `'logprob'`.

`showhmmprof(`*`Model`*`, ...'Order', `*`OrderValue`*`, ...)` specifies the order in which the symbols are arranged along the vertical axis. This option allows you reorder the alphabet and group the symbols according to their properties.

Examples

1 Load a model example.

```
model = pfamhmmread('pf00002.ls');
```

2 Plot the profile.

```
showhmmprof(model, 'Scale', 'logodds')
```

3 Order the alphabet by hydrophobicity.

```
hydrophobic = 'IVLFCMAGTSWYPHNDQEKR';
```

4 Plot the profile.

```
showhmmprof(model, 'Order', hydrophobic)
```

See Also

Bioinformatics Toolbox functions: `gethmmprof`, `hmmprofalign`, `hmmprofestimate`, `hmmprofgenerate`, `hmmprofstruct`, `pfamhmmread`

Purpose

Convert DataMatrix object to single-precision array

Syntax

```
B = single(DMObj)
B = single(DMObj, Rows)
B = single(DMObj, Rows, Cols)
```

Arguments

DMObj	DataMatrix object, such as created by `DataMatrix` (object constructor).
Rows, *Cols*	Row(s) or column(s) in *DMObj*, specified by one of the following: • Scalar • Vector of positive integers • String specifying a row or column name • Cell array of row or column names • Logical vector

Return Values

B	MATLAB numeric array.

Description

B = `single(`*DMObj*`)` converts *DMObj*, a DataMatrix object, to a single-precision array, which it returns in *B*.

B = `single(`*DMObj*`, `*Rows*`)` converts a subset of *DMObj*, a DataMatrix object, specified by *Rows*, to a single-precision array, which it returns in *B*. *Rows* can be a positive integer, vector of positive integers, string specifying a row name, cell array of row names, or a logical vector.

B = `single(`*DMObj*`, `*Rows*`, `*Cols*`)` converts a subset of *DMObj*, a DataMatrix object, specified by *Rows* and *Cols*, to a single-precision array, which it returns in*B*. *Cols* can be a positive integer, vector of

positive integers, string specifying a column name, cell array of column names, or a logical vector.

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: `double`

Purpose

Return size of ExpressionSet object

Syntax

```
NFeatSam = size(ESObj)
[NFeatures, NSamples] = size(ESObj)
DimLength = size(ESObj, Dim)
```

Description

`NFeatSam = size(ESObj)` returns a two-element row vector containing the number of features and number of samples in an ExpressionSet object.

`[NFeatures, NSamples] = size(ESObj)` returns the number of features and number of samples in an ExpressionSet object as separate variables.

`DimLength = size(ESObj, Dim)` returns the length of the dimension specified by `Dim`.

Inputs

ESObj

Object of the `bioma.ExpressionSet` class.

Dim

Scalar specifying the dimension of the ExpressionSet object. Choices are:

- `1` — Features
- `2` — Samples

Examples

Construct an ExpressionSet object from `EDObj`, an ExptData object, `MDObj2`, a MetaData object containing sample variable information, and `MIAMEObj`, a MIAME object. Determine the number of features and samples in the ExpressionSet object:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
```

```
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
EDObj = ExptData(dmObj);
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Create a MATLAB structure containing GEO Series data
geoStruct = getgeodata('GSE4616');
% Construct MIAME object
MIAMEObj = MIAME(geoStruct);
% Import bioma package to make constructor function
% available
import bioma.*
% Construct ExpressionSet object
ESObj = ExpressionSet(EDObj, 'SData', MDObj2, 'EInfo', MIAMEObj);
% Retrieve the number of features and samples
NumFeatSam = size(ESObj)
```

See Also

bioma.ExpressionSet | bioma.data.ExptData | DataMatrix

How To

- “Working with ExpressionSet Objects”

Purpose

Return size of ExptData object

Syntax

```
NFeatSam = size(EDObj)
[NFeatures, NSamples] = size(EDObj)
DimLength = size(EDObj, Dim)
```

Description

`NFeatSam = size(EDObj)` returns a two-element row vector containing the number of features and number of samples in an ExptData object.

`[NFeatures, NSamples] = size(EDObj)` returns the number of features and number of samples in an ExptData object as separate variables.

`DimLength = size(EDObj, Dim)` returns the length of the dimension specified by `Dim`.

Inputs

EDObj

Object of the `bioma.data.ExptData` class.

Dim

Scalar specifying the dimension of the ExptData object. Choices are:

- `1` — Features
- `2` — Samples

Examples

Construct an ExptData object, and then determine the number of features and samples in it:

```
% Import bioma.data package to make constructor functions
% available
import bioma.data.*
% Create DataMatrix object from .txt file containing
% expression values from microarray experiment
dmObj = DataMatrix('File', 'mouseExprsData.txt');
% Construct ExptData object
```

```
EDObj = ExptData(dmObj);
% Retrieve the number of features and samples
NumFeatSam = size(EDObj)
```

See Also

`bioma.data.ExptData`

How To

- "Working with ExptData Objects"

Purpose

Return size of MetaData object

Syntax

```
NSamVar = size(MDObj)
[NSamples, NVariables] = size(MDObj)
DimLength = size(MDObj, Dim)
```

Description

`NSamVar = size(MDObj)` returns a two-element row vector containing the number of samples or features and number of variables in a MetaData object.

`[NSamples, NVariables] = size(MDObj)` returns the number of samples or features and the number of variables in a MetaData object as separate variables.

`DimLength = size(MDObj, Dim)` returns the length of the dimension specified by `Dim`.

Inputs

MDObj

Object of the `bioma.data.MetaData` class.

Dim

Scalar specifying the dimension of the MetaData object. Choices are:

- `1` — Samples
- `2` — Variables

Examples

Construct a MetaData object, and then determine the number of samples and variables in it:

```
% Import bioma.data package to make constructor function
% available
import bioma.data.*
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Retrieve the number of samples and variables
```

```
NumSamVar = size(MDObj2)
```

See Also

bioma.data.MetaData

How To

- “Working with MetaData Objects”

Purpose

Sort columns of DataMatrix object in ascending or descending order

Syntax

```
DMObjNew = sortcols(DMObj1)
DMObjNew = sortcols(DMObj1, Row)
DMObjNew = sortcols(DMObj1, 'ColName')
DMObjNew = sortcols(DMObj1, ..., Mode)
[DMObjNew, Indices] = sortcols(DMObj1, ...)
```

Arguments

DMObj1	DataMatrix object, such as created by `DataMatrix` (object constructor).
Row	One or more rows in *DMObj1* by which to sort the columns. Choices are: • Positive integer • Vector of positive integers • String specifying a row name • Cell array of strings specifying multiple row names • Logical vector
`'ColName'`	String that specifies to sort the columns by the column names.
Mode	String specifying the order by which to sort the columns. Choices are `'ascend'` (default) or `'descend'`.

Return Values

DMObjNew	DataMatrix object created from sorting the columns of another DataMatrix object.
Indices	Index vector that links *DMObj1* to *DMObjNew*. In other words, *DMObjNew* = *DMObj1*`(:,idx)`.

Description

DMObjNew = `sortcols(`*DMObj1*`)` sorts the columns in *DMObj1* in ascending order based on the elements in the first row. For any

columns that have equal elements in a row, sorting is based on the row immediately below.

DMObjNew = sortcols(*DMObj1*, *Row*) sorts the columns in *DMObj1* in ascending order based on the elements in the specified row. Any columns that have equal elements in the specified row are sorted based on the elements in the next specified row.

DMObjNew = sortcols(*DMObj1*, 'ColName') sorts the columns in *DMObj1* in ascending order according to the column names.

DMObjNew = sortcols(*DMObj1*, ..., *Mode*) specifies the order of the sort. *Mode* can be 'ascend' (default) or 'descend'.

[*DMObjNew*, *Indices*] = sortcols(*DMObj1*, ...) returns *Indices*, an index vector that links *DMObj1* to *DMObjNew*. In other words, *DMObjNew* = *DMObj1*(:,idx).

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: sortrows

Purpose

Sort rows of DataMatrix object in ascending or descending order

Syntax

```
DMObjNew = sortrows(DMObj1)
DMObjNew = sortrows(DMObj1, Column)
DMObjNew = sortrows(DMObj1, 'RowName')
DMObjNew = sortrows(DMObj1, ..., Mode)
[DMObjNew, Indices] = sortrows(DMObj1, ...)
```

Arguments

DMObj1	DataMatrix object, such as created by `DataMatrix` (object constructor).
Column	One or more columns in *DMObj1* by which to sort the rows. Choices are: • Positive integer • Vector of positive integers • String specifying a column name • Cell array of strings specifying multiple column names • Logical vector
`'RowName'`	String that specifies to sort the rows by the row names.
Mode	String specifying the order by which to sort the rows. Choices are `'ascend'` (default) or `'descend'`.

Return Values

DMObjNew	DataMatrix object created from sorting the rows of another DataMatrix object.
Indices	Index vector that links *DMObj1* to *DMObjNew*. In other words, *DMObjNew* = *DMObj1*`(idx,:)`.

Description

DMObjNew = `sortrows(`*DMObj1*`)` sorts the rows in *DMObj1* in ascending order based on the elements in the first column. For any rows that have

equal elements in a column, sorting is based on the column immediately to the right.

DMObjNew = sortrows(*DMObj1*, *Column*) sorts the rows in *DMObj1* in ascending order based on the elements in the specified column. Any rows that have equal elements in the specified column are sorted based on the elements in the next specified column.

DMObjNew = sortrows(*DMObj1*, 'RowName') sorts the rows in *DMObj1* in ascending order according to the row names.

DMObjNew = sortrows(*DMObj1*, ..., *Mode*) specifies the order of the sort. *Mode* can be 'ascend' (default) or 'descend'.

[*DMObjNew*, *Indices*] = sortrows(*DMObj1*, ...) returns *Indices*, an index vector that links *DMObj1* to *DMObjNew*. In other words, *DMObjNew* = *DMObj1*(idx,:).

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox method of a DataMatrix object: sortcols

Purpose

Read data from SPOT file

Syntax

```
SPOTData = sptread(File)
SPOTData = sptread(File, 'CleanColNames',
CleanColNamesValue)
```

Arguments

File	Either of the following: • String specifying a file name, a path and file name, or a URL pointing to a file. The referenced file is a SPOT-formatted file (ASCII text file). If you specify only a file name, that file must be on the MATLAB search path or in the MATLAB Current Directory. • MATLAB character array that contains the text of a SPOT-formatted file.
CleanColNamesValue	Controls the use of valid MATLAB variable names.

Description

SPOTData = sptread(*File*) reads *File*, a SPOT-formatted file, and creates *SPOTData*, a MATLAB structure containing the following fields:

```
Header
Data
Blocks
Columns
Rows
IDs
ColumnNames
Indices
Shape
```

SPOTData = sptread(*File*, 'CleanColNames', *CleanColNamesValue*) controls the use of valid MATLAB variable names. The column names in the SPOT-formatted file contain periods and some characters that cannot be used in MATLAB variable names. If you plan to use the column names as variable names in a function, use this option with `CleanColNames` set to `true` and the function will return the field `ColumnNames` with valid variable names.

The `Indices` field of the structure includes the indices that you can use for plotting heat maps of the data.

Examples

1. Read in a sample SPOT file and plot the median foreground intensity for the 635 nm channel. Note that the example file `spotdata.txt` is not provided with the Bioinformatics Toolbox software.

```
spotStruct = sptread('spotdata.txt')
maimage(spotStruct,'Rmedian');
```

2. Alternately, create a similar plot using more basic graphics commands.

```
Rmedian = magetfield(spotStruct,'Rmedian');
imagesc(Rmedian(spotStruct.Indices));
colormap bone
colorbar
```

See Also

Bioinformatics Toolbox functions: `affyread`, `agferead`, `celintensityread`, `geoseriesread`, `geosoftread`, `gprread`, `ilmnbsread`, `imageneread`, `maboxplot`, `magetfield`

Purpose

Return standard deviation values in DataMatrix object

Syntax

```
S = std(DMObj)
S = std(DMObj, Flag)
S = std(DMObj, Flag, Dim)
S = std(DMObj, Flag, Dim, IgnoreNaN)
```

Arguments

DMObj	DataMatrix object, such as created by `DataMatrix` (object constructor).
Flag	Scalar specifying how to normalize the data. Choices are: • `0` — Default. Normalizes using a sample size of $N - 1$, unless $N = 1$, in which case, normalizes using a sample size of `1`. • `1` — Normalizes using a sample size of N. N = the number of elements in each column or row, as specified by *Dim*. For more information on the normalization equations, see the MATLAB function `std`.
Dim	Scalar specifying the dimension of *DMObj* to calculate the standard deviations. Choices are: • `1` — Default. Returns standard deviation values for elements in each column. • `2` — Returns standard deviation values for elements in each row.
IgnoreNaN	Specifies if NaNs should be ignored. Choices are `true` (default) or `false`.

Return Values

S	Either of the following: • Row vector containing the standard deviation values from elements in each column in *DMObj* (when *Dim* = 1) • Column vector containing the standard deviation values from elements in each row in *DMObj* (when *Dim* = 2)

Description

S = std(*DMObj*) returns the standard deviation values of the elements in the columns of a DataMatrix object, treating NaNs as missing values. The data is normalized using a sample size of $N - 1$, where N = the number of elements in each column. *S* is a row vector containing the standard deviation values for elements in each column in *DMObj*.

S = std(*DMObj*, *Flag*) specifies how to normalize the data. If *Flag* = 0, normalizes using a sample size of $N - 1$. If *Flag* = 1, normalizes using a sample size of N. N = the number of elements in each column or row, as specified by *Dim*. For more information on the normalization equations, see the MATLAB function std. Default *Flag* = 0.

S = std(*DMObj*, *Flag*, *Dim*) returns the standard deviation values of the elements in the columns or rows of a DataMatrix object, as specified by *Dim*. If *Dim* = 1, returns *S*, a row vector containing the standard deviation values for elements in each column in *DMObj*. If *Dim* = 2, returns *S*, a column vector containing the standard deviation values for elements in each row in *DMObj*. Default *Dim* = 1.

S = std(*DMObj*, *Flag*, *Dim*, *IgnoreNaN*) specifies if NaNs should be ignored. *IgnoreNaN* can be true (default) or false.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox methods of a DataMatrix object: mean, median, var

Purpose

Extract phylogenetic subtree

Syntax

```
Tree2 = subtree(Tree1, Nodes)
```

Description

`Tree2 = subtree(Tree1, Nodes)` extracts a new subtree (*Tree2*) where the new root is the first common ancestor of the *Nodes* vector from *Tree1*. Nodes in the tree are indexed as `[1:NUMLEAVES]` for the leaves and as `[NUMLEAVES+1:NUMLEAVES+NUMBRANCHES]` for the branches. Nodes can also be a logical array of following sizes `[NUMLEAVES+NUMBRANCHES x 1]`, `[NUMLEAVES x 1]` or `[NUMBRANCHES x 1]`.

Examples

1 Load a phylogenetic tree created from a protein family.

```
tr = phytreeread('pf00002.tree')
```

2 Get the subtree that contains the VIPS and CGRR human proteins.

```
sel = getbyname(tr,{'vips_human','cgrr_human'});
sel = any(sel,2);
tr =  subtree(tr,sel)
view(tr);
```

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor)

Bioinformatics Toolbox object: phytree object

Bioinformatics Toolbox methods of phytree object: `get`, `getbyname`, `prune`, `select`

sum (DataMatrix)

Purpose

Return sum of elements in DataMatrix object

Syntax

```
S = sum(DMObj)
S = sum(DMObj, Dim)
S = sum(DMObj, Dim, IgnoreNaN)
```

Arguments

DMObj	DataMatrix object, such as created by `DataMatrix` (object constructor).
Dim	Scalar specifying the dimension of *DMObj* to calculate the sums. Choices are: • `1` — Default. Returns sum of elements in each column. • `2` — Returns sum of elements in each row.
IgnoreNaN	Specifies if NaNs should be ignored. Choices are `true` (default) or `false`.

Return Values

S	Either of the following: • Row vector containing the sums of the elements in each column in *DMObj* (when *Dim* = 1) • Column vector containing the sums of the elements in each row in *DMObj* (when *Dim* = 2)

Description

S = `sum(`*DMObj*`)` returns the sum of the elements in the columns of a DataMatrix object, treating NaNs as missing values. *S* is a row vector containing the sums of the elements in each column in *DMObj*. If the values in *DMObj* are `single`s, then *S* is a `single`; otherwise, *S* is a `double`.

S = `sum(`*DMObj*`, `*Dim*`)` returns the sum of the elements in the columns or rows of a DataMatrix object, as specified by *Dim*. If *Dim* = 1, returns

S, a row vector containing the sums of the elements in each column in *DMObj*. If *Dim* = 2, returns *S*, a column vector containing the sums of the elements in each row in *DMObj*. Default *Dim* = 1.

S = sum(*DMObj*, *Dim*, *IgnoreNaN*) specifies if NaNs should be ignored. *IgnoreNaN* can be `true` (default) or `false`.

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox methods of a DataMatrix object: `max`, `min`

svmclassify

Purpose

Classify data using support vector machine

Syntax

```
Group = svmclassify(SVMStruct, Sample)
Group = svmclassify(SVMStruct, Sample, 'Showplot',
ShowplotValue)
```

Description

`Group = svmclassify(SVMStruct, Sample)` classifies each row of the data in `Sample` using the information in a support vector machine classifier structure `SVMStruct`, created using the `svmtrain` function. `Sample` must have the same number of columns as the data used to train the classifier in `svmtrain`. `Group` indicates the group to which each row of `Sample` has been assigned.

`Group = svmclassify(SVMStruct, Sample, 'Showplot', ShowplotValue)` controls the plotting of the sample data in the figure created using the `Showplot` property with the `svmtrain` function.

Examples

1. Load the sample data, which includes Fisher's iris data of 5 measurements on a sample of 150 irises.

   ```
   load fisheriris
   ```

2. Create `data`, a two-column matrix containing sepal length and sepal width measurements for 150 irises.

   ```
   data = [meas(:,1), meas(:,2)];
   ```

3. From the `species` vector, create a new column vector, `groups`, to classify data into two groups: Setosa and non-Setosa.

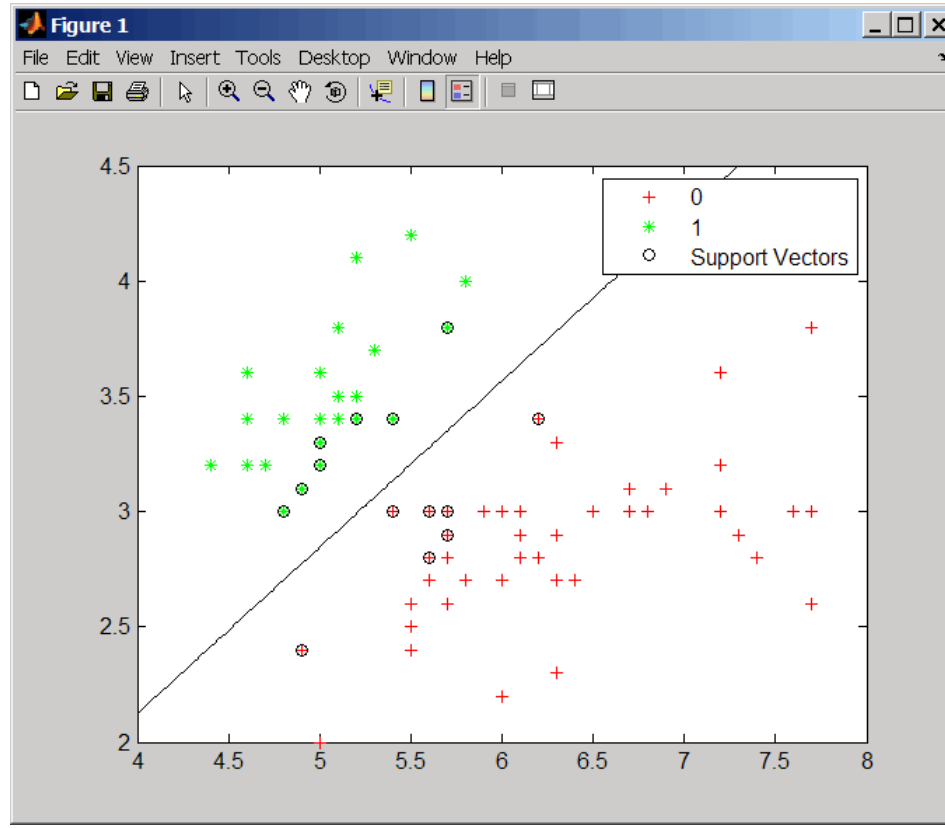
   ```
   groups = ismember(species,'setosa');
   ```

4. Randomly select training and test sets.

   ```
   [train, test] = crossvalind('holdOut',groups);
   cp = classperf(groups);
   ```

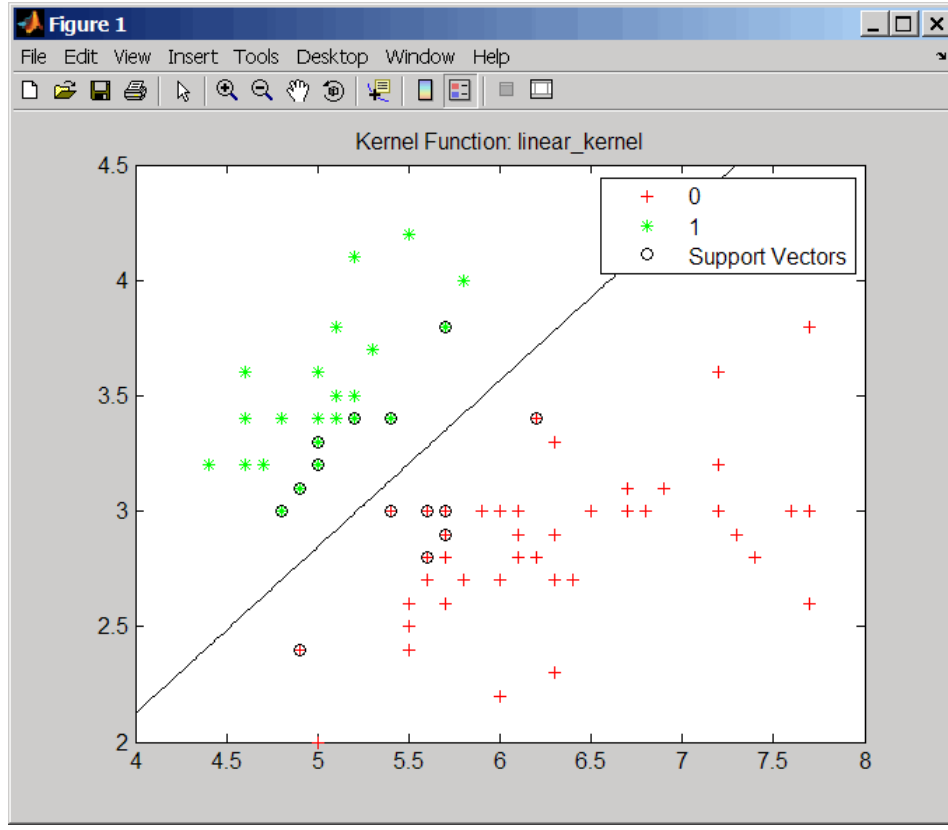
5 Use the `svmtrain` function to train an SVM classifier using a linear kernel function and plot the grouped data.

```
svmStruct = svmtrain(data(train,:),groups(train),'showplot',true);
```



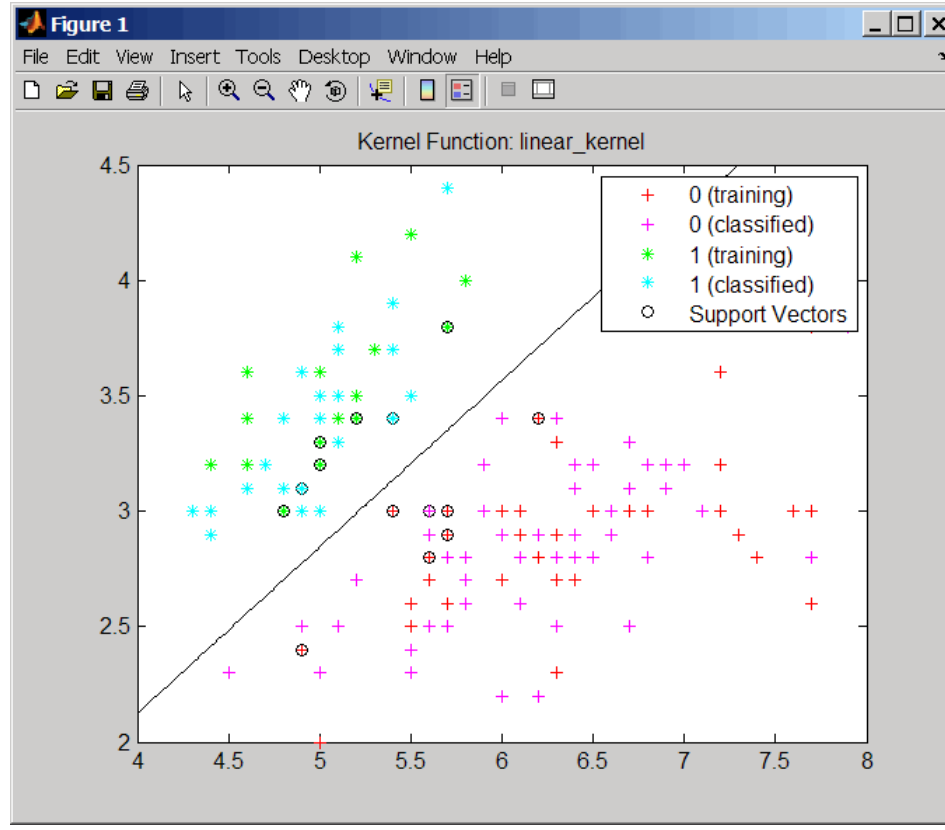
6 Add a title to the plot, using the `KernelFunction` field from the `svmStruct` structure as the title.

```
title(sprintf('Kernel Function: %s',...
              func2str(svmStruct.KernelFunction)),...
              'interpreter','none');
```



7 Classify the test set using a support vector machine.

```
classes = svmclassify(svmStruct,data(test,:),'showplot',true);
```

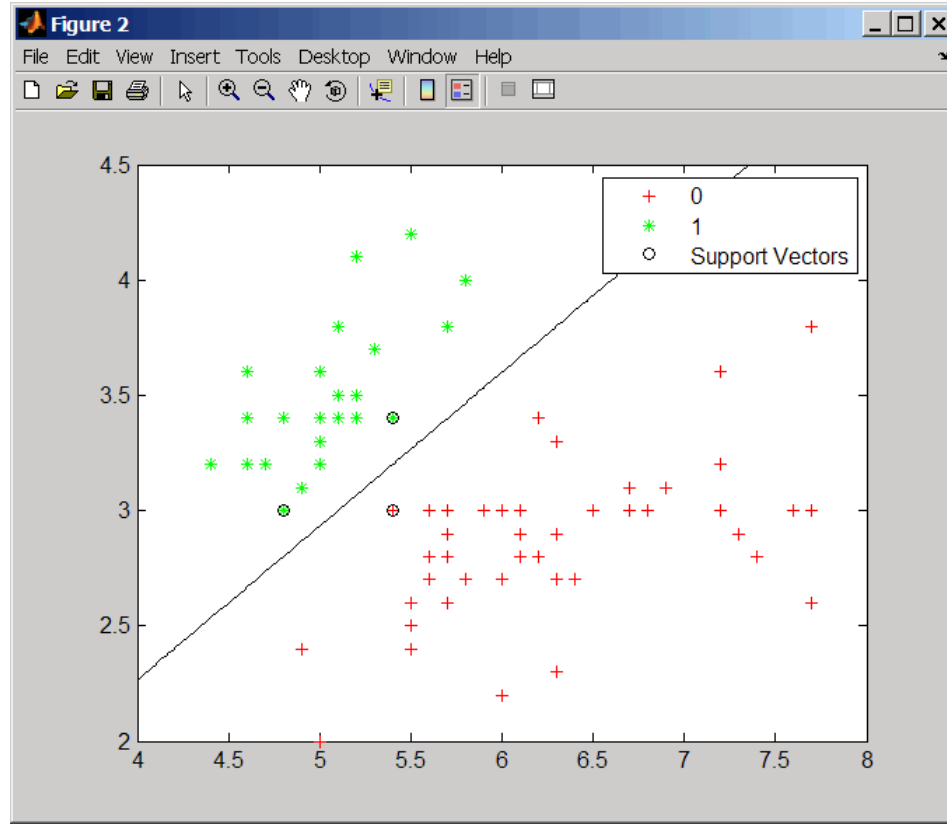


8 Evaluate the performance of the classifier.

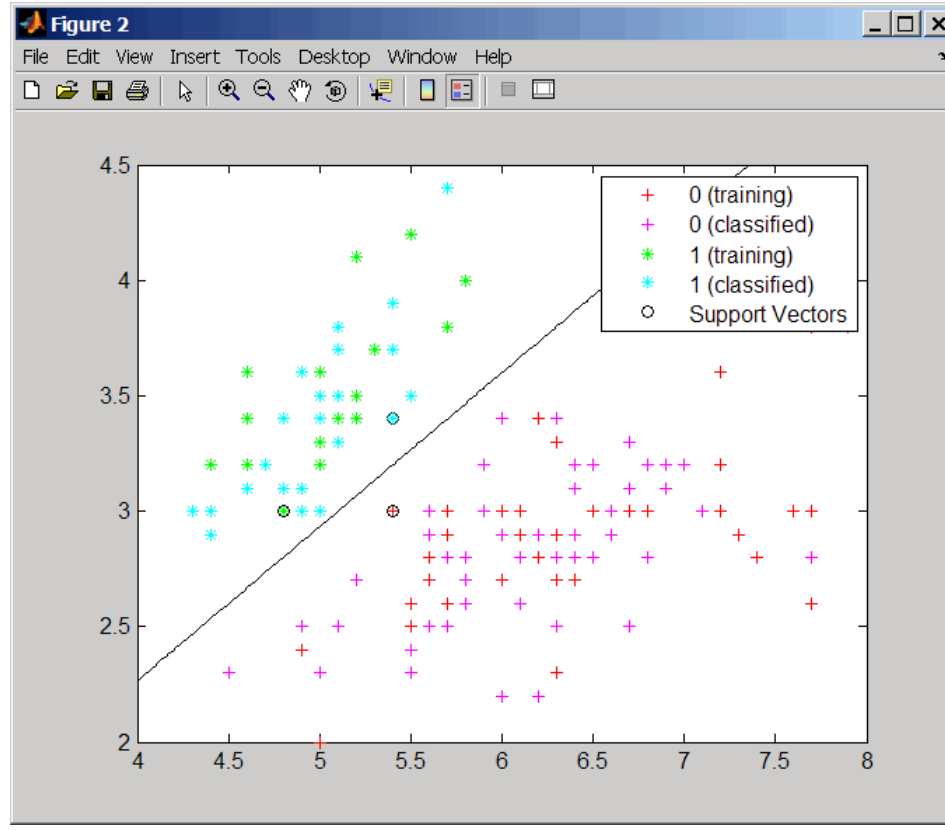
```
classperf(cp,classes,test);
cp.CorrectRate

ans =

    0.9867
```

9 Use a one-norm, hard margin support vector machine classifier by changing the `boxconstraint` property.

```
figure
svmStruct = svmtrain(data(train,:),groups(train),...
                     'showplot',true,'boxconstraint',1e6);
```




```
classes = svmclassify(svmStruct,data(test,:),'showplot',true);
```



10 Evaluate the performance of the classifier.

```
classperf(cp,classes,test);
cp.CorrectRate

ans =

    0.9867
```

References

[1] Kecman, V., Learning and Soft Computing, MIT Press, Cambridge, MA. 2001.

[2] Suykens, J.A.K., Van Gestel, T., De Brabanter, J., De Moor, B., and Vandewalle, J., Least Squares Support Vector Machines, World Scientific, Singapore, 2002.

[3] Scholkopf, B., and Smola, A.J., Learning with Kernels, MIT Press, Cambridge, MA. 2002.

[4] Cristianini, N., and Shawe-Taylor, J. (2000). An Introduction to Support Vector Machines and Other Kernel-based Learning Methods, First Edition (Cambridge: Cambridge University Press). `http://www.support-vector.net/`

See Also

Bioinformatics Toolbox functions: `classperf`, `crossvalind`, `knnclassify`, `svmtrain`

Statistics Toolbox function: `classify`

Optimization Toolbox™ function: `quadprog`

Purpose

Create or edit Sequential Minimal Optimization (SMO) options structure

Syntax

```
SMO_OptsStruct = svmsmoset('Property1Name', Property1Value,
   'Property2Name', Property2Value, ...)
SMO_OptsStruct = svmsmoset(OldOpts, 'Property1Name',
   Property1Value, 'Property2Name', Property2Value, ...)
SMO_OptsStruct = svmsmoset(OldOpts, NewOpts)
```

Arguments

OldOpts	Structure that specifies options used by the `SMO` method of the `svmtrain` function.
NewOpts	Structure that specifies options used by the `SMO` method of the `svmtrain` function.

PropertyName	Description of *PropertyValue*
`TolKKT`	Value that specifies the tolerance with which the KKT conditions are checked. KKT conditions are Karush-Kuhn-Tucker conditions. Default is `1.0000e-003`.
`MaxIter`	Integer that specifies the maximum number of iterations of the main loop. If this limit is exceeded before the algorithm converges, then the algorithm stops and returns an error. Default is `15000`.

PropertyName	Description of *PropertyValue*
`Display`	String that specifies the level of information about the optimization iterations that is displayed as the algorithm runs. Choices are: • `off` — Default. Reports nothing. • `iter` — Reports every 500 iterations. • `final` — Reports only when the algorithm finishes.
`KKTViolationLevel`	Value that specifies the fraction of variables allowed to violate the KKT conditions. Choices are any value ≥ `0` and `< 1`. Default is `0`. For example, if you set `KKTViolationLevel` to `0.05`, then 5% of the variables are allowed to violate the KKT conditions. **Tip** Set this option to a positive value to help the algorithm converge if it is fluctuating near a good solution. For more information on KKT conditions, see Cristianini, et al. 2000.
`KernelCacheLimit`	Value that specifies the size of the kernel matrix cache. The algorithm keeps a matrix with up to `KernelCacheLimit` × `KernelCacheLimit` double-precision, floating-point numbers in memory. Default is `5000`.

Return Values

`SMO_OptsStruct` Structure that specifies options used by the `SMO` method used by the `svmtrain` function.

Description

SMO_OptsStruct = svmsmoset(*'Property1Name'*, *Property1Value*, *'Property2Name'*, *Property2Value*, ...) creates *SMO_OptsStruct*, an SMO options structure from the specified inputs. This structure can be used as input for the svmtrain function.

SMO_OptsStruct = svmsmoset(*OldOpts*, *'Property1Name'*, *Property1Value*, *'Property2Name'*, *Property2Value*, ...) alters the options in *OldOpts*, an existing SMO options structure, with the specified inputs, creating a new output options structure.

SMO_OptsStruct = svmsmoset(*OldOpts*, *NewOpts*) alters the options in *OldOpts*, an existing SMO options structure, with the options specified in *NewOpts*, another SMO options structure, creating a new output options structure.

Examples

1. Create an SMO options structure and specify the Display, MaxIter, and KernelCacheLimit properties.

```
opts = svmsmoset('Display','final','MaxIter',20000,...
                 'KernelCacheLimit',1000)

opts =

             Display: 'final'
              TolKKT: 1.0000e-003
             MaxIter: 20000
    KKTViolationLevel: 0
     KernelCacheLimit: 1000
```

2. Create an alternate SMO options structure from the previous structure. Specify different Display and KKTViolationLevel properties.

```
alt_opts = svmsmoset(opts,'Display','iter','KKTViolationLevel',.05)

alt_opts =

             Display: 'iter'
```

```
                    TolKKT: 1.0000e-003
                   MaxIter: 20000
        KKTViolationLevel: 0.0500
         KernelCacheLimit: 1000
```

References

[1] Cristianini, N., and Shawe-Taylor, J. (2000). An Introduction to Support Vector Machines and Other Kernel-based Learning Methods, First Edition (Cambridge: Cambridge University Press). http://www.support-vector.net/

[2] Platt, J.C. (1999). Sequential Minimal Optimization: A Fast Algorithm for Training Support Vector Machines. In Advances in Kernel Methods - Support Vector Learning, B. Scholkopf, J.C. Burges, and A.J. Smola, eds. (Cambridge MA: MIT Press), pp. 185–208.

[3] Fan, R.E., Chen, P.H., and Lin, C.J. (2005). Working Set Selection Using Second Order Information for Training SVM. Journal of Machine Learning Research *6*, 1889–1918.

[4] Bottou, L. and Lin, C.J. (2006). Support Vector Machine Solvers. http://www.csie.ntu.edu.tw/~cjlin/papers.html

See Also

Bioinformatics Toolbox functions: `svmclassify`, `svmtrain`

Optimization Toolbox function: `optimset`

Purpose

Train support vector machine classifier

Syntax

```
SVMStruct = svmtrain(Training, Group)
SVMStruct = svmtrain(..., 'Kernel_Function',
Kernel_FunctionValue, ...)
SVMStruct = svmtrain(..., 'RBF_Sigma', RBFSigmaValue, ...)
SVMStruct = svmtrain(..., 'Polyorder', PolyorderValue, ...)
SVMStruct = svmtrain(..., 'Mlp_Params',
Mlp_ParamsValue, ...)
SVMStruct = svmtrain(..., 'Method', MethodValue, ...)
SVMStruct = svmtrain(..., 'QuadProg_Opts',
   QuadProg_OptsValue, ...)
SVMStruct = svmtrain(..., 'SMO_Opts', SMO_OptsValue, ...)
SVMStruct = svmtrain(..., 'BoxConstraint',
   BoxConstraintValue, ...)
SVMStruct = svmtrain(..., 'Autoscale', AutoscaleValue, ...)
SVMStruct = svmtrain(..., 'Showplot', ShowplotValue, ...)
```

Arguments

Training	Matrix of training data, where each row corresponds to an observation or replicate, and each column corresponds to a feature or variable.
Group	Column vector, character array, or cell array of strings for classifying data in *Training* into two groups. It has the same number of elements as there are rows in *Training*. Each element specifies the group to which the corresponding row in *Training* belongs.

Kernel_FunctionValue String or function handle specifying the kernel function that maps the training data into kernel space. Choices are:

- `linear` — Default. Linear kernel or dot product.
- `quadratic` — Quadratic kernel.
- `rbf` — Gaussian Radial Basis Function kernel with a default scaling factor, sigma, of `1`.
- `polynomial` — Polynomial kernel with a default order of `3`.
- `mlp` — Multilayer Perceptron kernel with default scale and bias parameters of `[1, -1]`.
- `@functionname` — Handle to a kernel function specified using `@`and the `functionname`. For example, `@kfun`, or an anonymous function.

RBFSigmaValue Positive number that specifies the scaling factor, sigma, in the radial basis function kernel. Default is `1`.

PolyorderValue Positive number that specifies the order of a polynomial kernel. Default is `3`.

Mlp_ParamsValue Two-element vector, `[p1, p2]`, that specifies the scale and bias parameters of the multilayer perceptron (mlp) kernel. `K = tanh(p1*U*V' + p2)`. `p1` must be `> 0`, and `p2` must be `< 0`. Default is `[1, -1]`.

MethodValue

String specifying the method to find the separating hyperplane. Choices are:

- `QP` — Quadratic Programming (requires the Optimization Toolbox software). The classifier is a two-norm, soft-margin support vector machine.
- `SMO` — Sequential Minimal Optimization. The classifier is a one-norm, soft-margin support vector machine.
- `LS` — Least-Squares.

If you installed the Optimization Toolbox software, the `QP` method is the default. Otherwise, the `SMO` method is the default.

QuadProg_OptsValue

An options structure created by the `optimset` function (Optimization Toolbox software). This structure specifies options used by the `QP` method. For more information on creating this structure, see the `optimset` and `quadprog` reference pages.

SMO_OptsValue

An options structure created by the `svmsmoset` function. This structure specifies options used by the `SMO` method. For more information on creating this structure, see the `svmsmoset` function.

BoxConstraintValue	Box constraints for the soft margin. Choices are: • Strictly positive numeric scalar. • Array of strictly positive values with the number of elements equal to the number of rows in the *Training* matrix. If *BoxConstraintValue* is a scalar, it is automatically rescaled by N/(2*N1) for the data points of group one and by N/(2*N2) for the data points of group two. N1 is the number of elements in group one, N2 is the number of elements in group two, and N = N1 + N2. This rescaling is done to take into account unbalanced groups, that is cases where N1 and N2 have very different values. If *BoxConstraintValue* is an array, then each array element is taken as a box constraint for the data point with the same index. Default is a scalar value of 1.
AutoscaleValue	Controls the shifting and scaling of data points before training. When *AutoscaleValue* is true, the columns of the input data matrix *Training* are shifted to zero mean and scaled to unit variance. Default is true.
ShowplotValue	Controls the display of a plot of the grouped data, including the separating line for the classifier, when using two-dimensional data. Choices are true or false (default).

Return Values

SVMStruct

Structure containing information about the trained SVM classifier, including the following fields:

- `SupportVectors`
- `Alpha`
- `Bias`
- `KernelFunction`
- `KernelFunctionArgs`
- `GroupNames`
- `SupportVectorIndices`
- `ScaleData`
- `FigureHandles`

Note The sign of the values in the `Alpha` field indicates group membership only, and not positive or negative value; all values are actually positive.

Tip You can use *`SVMStruct`* as input to the `svmclassify` function, to use for classification.

Description

`SVMStruct` = `svmtrain(`*`Training`*`, `*`Group`*`)` trains a support vector machine (SVM) classifier using *`Training`*, a matrix of training data taken from two groups, specified by *`Group`*. `svmtrain` treats NaNs or empty strings in *`Group`* as missing values and ignores the corresponding

rows of *Training*. Information about the trained SVM classifier is returned in *SVMStruct*, a structure with the following fields.

- SupportVectors
- Alpha
- Bias
- KernelFunction
- KernelFunctionArgs
- GroupNames
- SupportVectorIndices
- ScaleData
- FigureHandles

SVMStruct = svmtrain(*Training*, *Group*, ...'*PropertyName*', *PropertyValue*, ...) calls svmtrain with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

SVMStruct = svmtrain(..., 'Kernel_Function', *Kernel_FunctionValue*, ...) specifies the kernel function (*Kernel_FunctionValue*) that maps the training data into kernel space. *Kernel_FunctionValue* can be one of the following strings or a function handle:

- linear — Default. Linear kernel or dot product.
- quadratic — Quadratic kernel.
- rbf — Gaussian Radial Basis Function kernel with a default scaling factor, sigma, of 1.
- polynomial — Polynomial kernel with a default order of 3.

- `mlp` — Multilayer Perceptron kernel with default scale and bias parameters of `[1, -1]`.
- `@functionname` — Handle to a kernel function specified using `@`and the `functionname`. For example, `@kfun`, or an anonymous function.

A kernel function must be of the following form:

```
function K = kfun(U, V)
```

Input arguments `U` and `V` are matrices with `m` and `n` rows respectively. Return value `K` is an `m`-by-`n` matrix. If `kfun` is parameterized, you can use anonymous functions to capture the problem-dependent parameters. For example, suppose that your kernel function is:

```
function K = kfun(U,V,P1,P2)
K = tanh(P1*(U*V')+P2);
```

You can set values for `P1` and `P2` and then use an anonymous function as follows:

```
@(U,V) kfun(U,V,P1,P2)
```

For more information on the types of functions that can be used as kernel functions, see Cristianini and Shawe-Taylor, 2000.

`SVMStruct` `= svmtrain(..., 'RBF_Sigma',` *`RBFSigmaValue`*`, ...)` specifies the scaling factor, sigma, in the radial basis function kernel. *`RBFSigmaValue`* must be a positive number. Default is `1`.

`SVMStruct` `= svmtrain(..., 'Polyorder',` *`PolyorderValue`*`, ...)` specifies the order of a polynomial kernel. *`PolyorderValue`* must be a positive number. Default is `3`.

`SVMStruct` `= svmtrain(..., 'Mlp_Params',` *`Mlp_ParamsValue`*`, ...)` specifies the scale and bias parameters of the multilayer perceptron (mlp) kernel as a two-element vector, `[p1, p2]`. `K = tanh(p1*U*V' + p2)`, `p1 > 0`, and `p2 < 0`. `p1` must be `> 0`, and `p2` must be `< 0`. Default is `[1, -1]`.

SVMStruct = svmtrain(..., 'Method', *MethodValue*, ...) specifies the method to find the separating hyperplane. Choices are:

- QP — Quadratic Programming (requires the Optimization Toolbox software). The classifier is a two-norm, soft-margin support vector machine.
- SMO — Sequential Minimal Optimization. The classifier is a one-norm, soft-margin support vector machine.
- LS — Least-Squares.

If you installed the Optimization Toolbox software, the QP method is the default. Otherwise, the SMO method is the default.

Note If you specify the QP method, the classifier is a two-norm, soft-margin support vector machine.

SVMStruct = svmtrain(..., 'QuadProg_Opts', *QuadProg_OptsValue*, ...) specifies an options structure created by the optimset function (Optimization Toolbox software). This structure specifies options used by the QP method. For more information on creating this structure, see the optimset and quadprog functions.

SVMStruct = svmtrain(..., 'SMO_Opts', *SMO_OptsValue*, ...) specifies an options structure created by svmsmoset function. This structure specifies options used by the SMO method. For more information on creating this structure, see the svmsmoset function.

SVMStruct = svmtrain(..., 'BoxConstraint', *BoxConstraintValue*, ...) specifies box constraints for the soft margin. *BoxConstraintValue* can be either of the following:

- Strictly positive numeric scalar
- Array of strictly positive values with the number of elements equal to the number of rows in the *Training* matrix

If *BoxConstraintValue* is a scalar, it is automatically rescaled by N/(2*N1) for the data points of group one and by N/(2*N2) for the data points of group two. N1 is the number of elements in group one, N2 is the number of elements in group two, and N = N1 + N2. This rescaling is done to take into account unbalanced groups, that is cases where N1 and N2 have very different values.

If *BoxConstraintValue* is an array, then each array element is taken as a box constraint for the data point with the same index.

Default is a scalar value of `1`.

SVMStruct = `svmtrain(..., 'Autoscale', AutoscaleValue, ...)` controls the shifting and scaling of data points before training. When *AutoscaleValue* is `true`, the columns of the input data matrix *Training* are shifted to zero mean and scaled to unit variance. Default is `true`.

SVMStruct = `svmtrain(..., 'Showplot', ShowplotValue, ...)`, controls the display of a plot of the grouped data , including the separating line for the classifier, when using two-dimensional data. Choices are `true` or `false` (default).

Memory Usage and Out of Memory Error

When you set `'Method'` to `'QP'`, the `svmtrain` function operates on a data set containing `N` elements, it creates an `(N+1)`-by-`(N+1)` matrix to find the separating hyperplane. This matrix needs at least `8*(n+1)^2` bytes of contiguous memory. If this size of contiguous memory is not available, the software displays an “out of memory” message.

When you set `'Method'` to `'SMO'`, memory consumption is controlled by the SMO option `KernelCacheLimit`. For more information on the `KernelCacheLimit` option, see the `svmsmoset` function. The SMO algorithm stores only a submatrix of the kernel matrix, limited by the size specified by the `KernelCacheLimit` option. However, if the number of data points exceeds the size specified by the `KernelCacheLimit` option, the SMO algorithm slows down because it has to recalculate the kernel matrix elements.

When using `svmtrain` on large data sets, and you run out of memory or the optimization step is very time consuming, try either of the following:

- Use a smaller number of samples and use cross validation to test the performance of the classifier.
- Set `'Method'` to `'SMO'`, and set the `KernelCacheLimit` option as large as your system permits. For information on setting the `KernelCacheLimit` option, see the `svmsmoset` function.

Tip If you set `'Method'` to `'SMO'`, setting the `'BoxConstraint'` property as small as possible will help the SMO algorithm run faster.

Examples

1. Load the sample data, which includes Fisher's iris data of 5 measurements on a sample of 150 irises.

   ```
   load fisheriris
   ```

2. Create `data`, a two-column matrix containing sepal length and sepal width measurements for 150 irises.

   ```
   data = [meas(:,1), meas(:,2)];
   ```

3. From the `species` vector, create a new column vector, `groups`, to classify data into two groups: Setosa and non-Setosa.

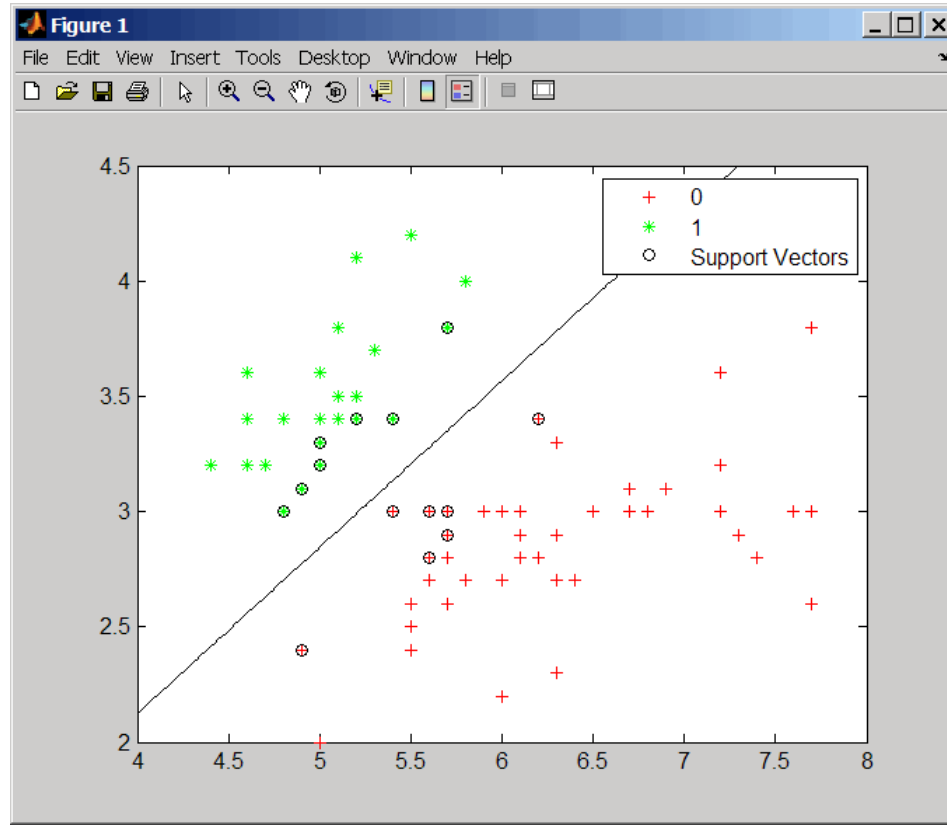
   ```
   groups = ismember(species,'setosa');
   ```

4. Randomly select training and test sets.

   ```
   [train, test] = crossvalind('holdOut',groups);
   cp = classperf(groups);
   ```

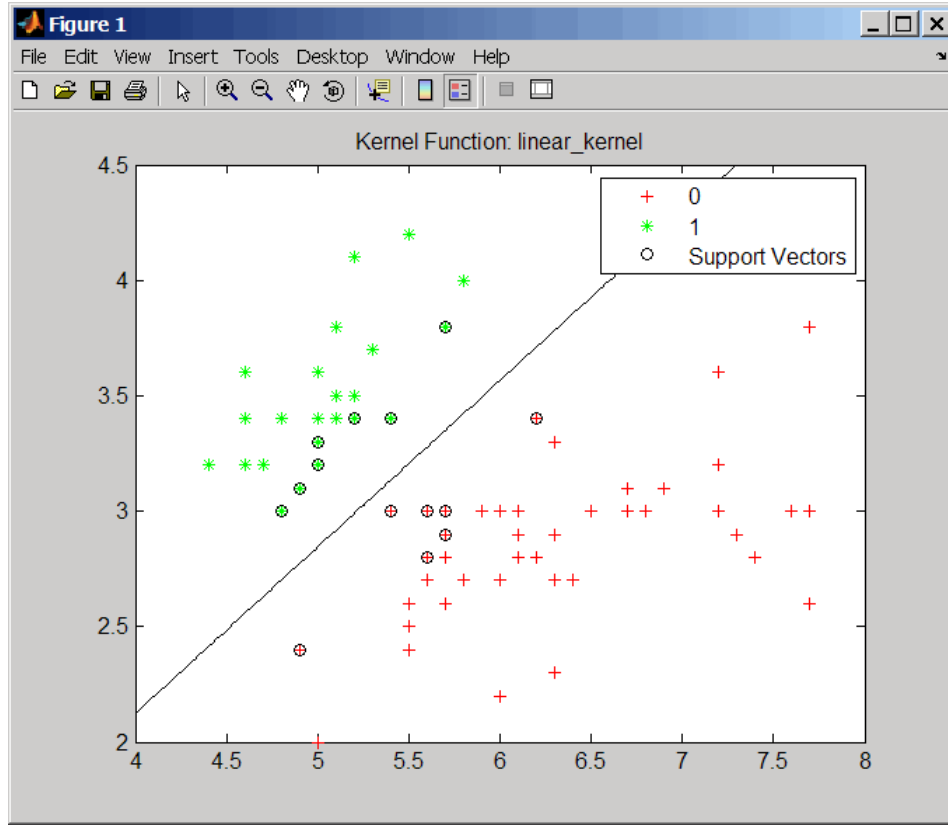
5. Train an SVM classifier using a linear kernel function and plot the grouped data.

   ```
   svmStruct = svmtrain(data(train,:),groups(train),'showplot',true);
   ```



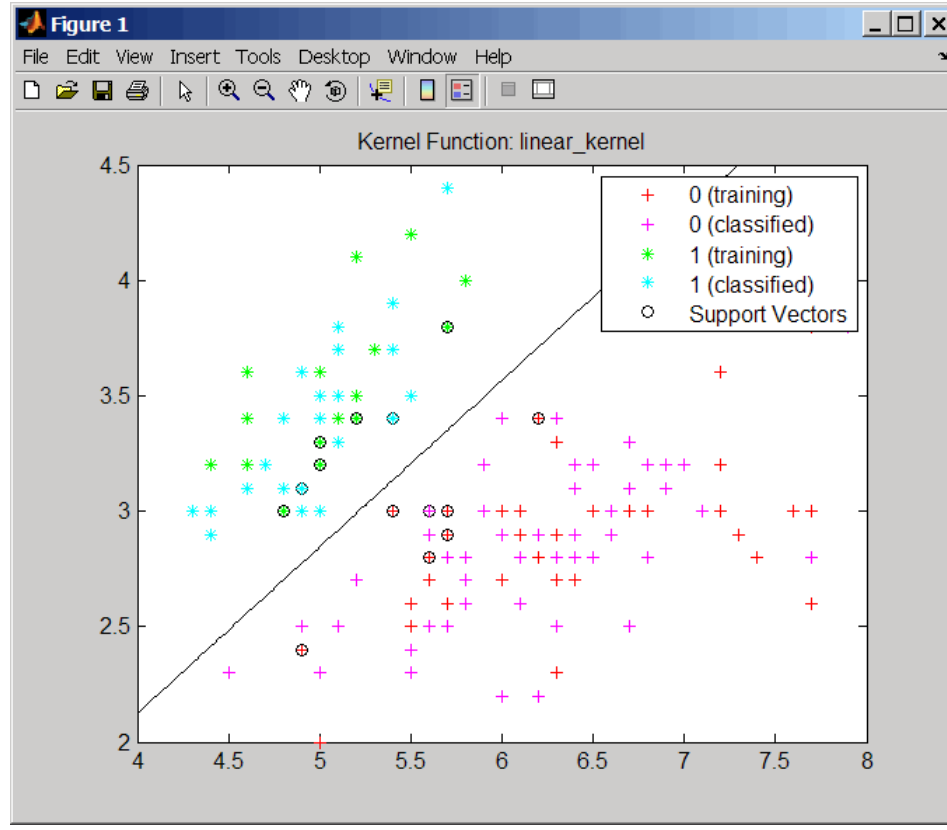
6 Add a title to the plot, using the `KernelFunction` field from the `svmStruct` structure as the title.

```
title(sprintf('Kernel Function: %s',...
              func2str(svmStruct.KernelFunction)),...
              'interpreter','none');
```



7 Use the `svmclassify` function to classify the test set.

```
classes = svmclassify(svmStruct,data(test,:),'showplot',true);
```

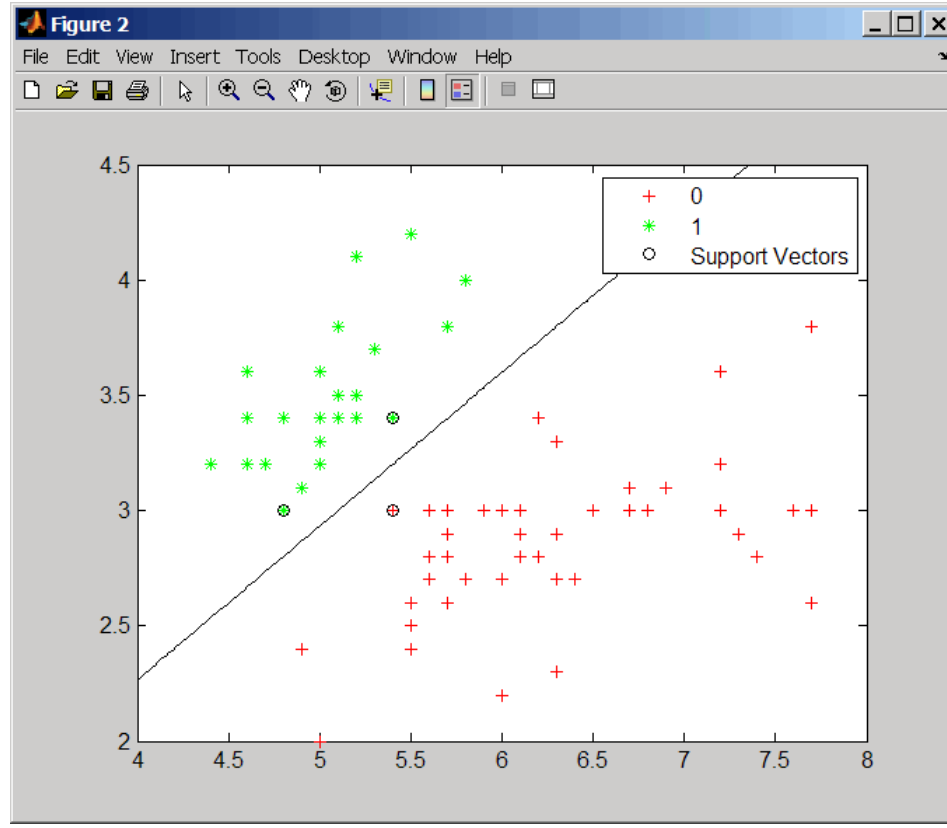


8 Evaluate the performance of the classifier.

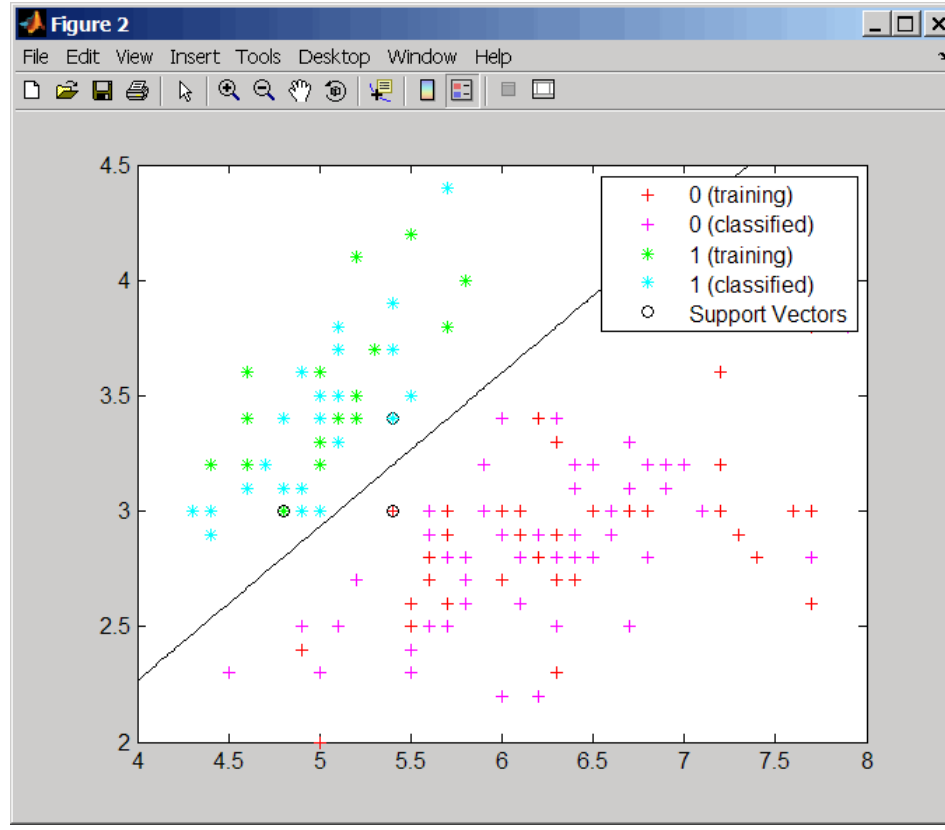
```
classperf(cp,classes,test);
cp.CorrectRate

ans =

    0.9867
```

9 Use a one-norm, hard margin support vector machine classifier by changing the `boxconstraint` property.

```
figure
svmStruct = svmtrain(data(train,:),groups(train),...
                     'showplot',true,'boxconstraint',1e6);
```




```
classes = svmclassify(svmStruct,data(test,:),'showplot',true);
```



10 Evaluate the performance of the classifier.

```
classperf(cp,classes,test);
cp.CorrectRate

ans =

    0.9867
```

References

[1] Kecman, V. (2001). Learning and Soft Computing (Cambridge, MA: MIT Press).

[2] Suykens, J.A.K., Van Gestel, T., De Brabanter, J., De Moor, B., and Vandewalle, J. (2002). Least Squares Support Vector Machines (Singapore: World Scientific).

[3] Scholkopf, B., and Smola, A.J. (2002). Learning with Kernels (Cambridge, MA: MIT Press).

[4] Cristianini, N. and Shawe-Taylor, J. (2000). An Introduction to Support Vector Machines and Other Kernel-based Learning Methods, First Edition (Cambridge: Cambridge University Press). `http://www.support-vector.net/`

See Also

Bioinformatics Toolbox functions: `knnclassify`, `svmclassify`, `svmsmoset`

Statistics Toolbox function: `classify`

Optimization Toolbox function: `quadprog`

MATLAB function: `optimset`

Purpose

Locally align two sequences using Smith-Waterman algorithm

Syntax

```
Score = swalign(Seq1, Seq2)
[Score, Alignment] = swalign(Seq1, Seq2)
[Score, Alignment, Start] = swalign(Seq1, Seq2)
... = swalign(Seq1,Seq2, ...'Alphabet', AlphabetValue)
... = swalign(Seq1,Seq2, ...'ScoringMatrix',
   ScoringMatrixValue, ...)
... = swalign(Seq1,Seq2, ...'Scale', ScaleValue, ...)
... = swalign(Seq1,Seq2, ...'GapOpen', GapOpenValue, ...)
... = swalign(Seq1,Seq2, ...'ExtendGap',
ExtendGapValue, ...)
... = swalign(Seq1,Seq2, ...'Showscore',
ShowscoreValue, ...)
```

Arguments

Seq1, *Seq2*

Amino acid or nucleotide sequences. Enter any of the following:

- Character string of letters representing amino acids or nucleotides, such as returned by `int2aa` or `int2nt`
- Vector of integers representing amino acids or nucleotides, such as returned by `aa2int` or `nt2int`
- Structure containing a `Sequence` field

Tip For help with letter and integer representations of amino acids and nucleotides, see Amino Acid Lookup on page 3-111 or Nucleotide Lookup on page 3-122.

AlphabetValue

String specifying the type of sequence. Choices are `'AA'` (default) or `'NT'`.

ScoringMatrixValue Either of the following:

- String specifying the scoring matrix to use for the local alignment. Choices for amino acid sequences are:
  - `'BLOSUM62'`
  - `'BLOSUM30'` increasing by `5` up to `'BLOSUM90'`
  - `'BLOSUM100'`
  - `'PAM10'` increasing by `10` up to `'PAM500'`
  - `'DAYHOFF'`
  - `'GONNET'`

  Default is:
  - `'BLOSUM50'` — When *`AlphabetValue`* equals `'AA'`
  - `'NUC44'` — When *`AlphabetValue`* equals `'NT'`

  Note The above scoring matrices, provided with the software, also include a structure containing a scale factor that converts the units of the output score to bits. You can also use the `'Scale'` property to specify an additional scale factor to convert the output score from bits to another unit.

- Matrix representing the scoring matrix to use for the local alignment, such as returned by the `blosum`, `pam`, `dayhoff`, `gonnet`, or `nuc44` function.

Note If you use a scoring matrix that you created or was created by one of the above functions, the matrix does not include a scale factor. The output score will be returned in the same units as the scoring matrix. You can use the `'Scale'` property to specify a scale factor to convert the output score to another unit.

`ScaleValue`

Positive value that specifies a scale factor that is applied to the output score.

For example, if the output score is initially determined in bits, and you enter `log(2)` for *`ScaleValue`*, then `swalign` returns *`Score`* in nats.

Default is `1`, which does not change the units of the output score.

Note If the `'ScoringMatrix'` property also specifies a scale factor, then `swalign` uses it first to scale the output score, then applies the scale factor specified by *`ScaleValue`* to rescale the output score.

Tip Before comparing alignment scores from multiple alignments, ensure the scores are in the same units. You can use the `'Scale'` property to control the units of the output scores.

GapOpenValue	Positive value specifying the penalty for opening a gap in the alignment. Default is `8`.
ExtendGapValue	Positive value specifying the penalty for extending a gap. Default is equal to *GapOpenValue*.
ShowscoreValue	Controls the display of the scoring space and the winning path of the alignment. Choices are `true` or `false` (default).

Return Values

Score	Optimal local alignment score in bits.
Alignment	3-by-N character array showing the two sequences, *Seq1* and *Seq2*, in the first and third rows, and symbols representing the optimal local alignment between them in the second row.
Start	2-by-1 vector of indices indicating the starting point in each sequence for the alignment.

Description

Score = swalign(*Seq1*, *Seq2*) returns the optimal local alignment score in bits. The scale factor used to calculate the score is provided by the scoring matrix.

[*Score*, *Alignment*] = swalign(*Seq1*, *Seq2*) returns a 3-by-N character array showing the two sequences, *Seq1* and *Seq2*, in the first and third rows, and symbols representing the optimal local alignment between them in the second row. The symbol | indicates amino acids or nucleotides that match exactly. The symbol : indicates amino acids or nucleotides that are related as defined by the scoring matrix (nonmatches with a zero or positive scoring matrix value).

`[Score, Alignment, Start] = swalign(Seq1, Seq2)` returns a 2-by-1 vector of indices indicating the starting point in each sequence for the alignment.

`... = swalign(Seq1,Seq2, ...'PropertyName', PropertyValue, ...)` calls `swalign` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

`... = swalign(Seq1,Seq2, ...'Alphabet', AlphabetValue)` specifies the type of sequences. Choices are `'AA'` (default) or `'NT'`.

`... = swalign(Seq1,Seq2, ...'ScoringMatrix', ScoringMatrixValue, ...)` specifies the scoring matrix to use for the local alignment. Default is:

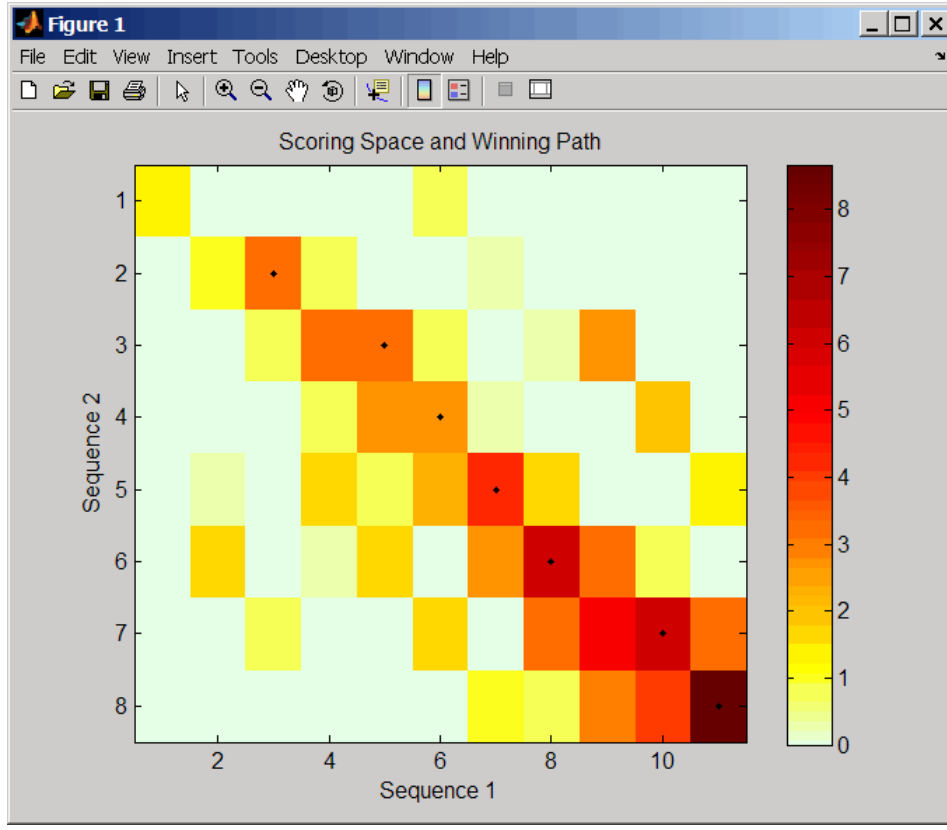
- `'BLOSUM50'` — When *`AlphabetValue`* equals `'AA'`
- `'NUC44'` — When *`AlphabetValue`* equals `'NT'`

`... = swalign(Seq1,Seq2, ...'Scale', ScaleValue, ...)` specifies a scale factor that is applied to the output score, thereby controlling the units of the output score. Choices are any positive value.

`... = swalign(Seq1,Seq2, ...'GapOpen', GapOpenValue, ...)` specifies the penalty for opening a gap in the alignment. Choices are any positive value. Default is `8`.

`... = swalign(Seq1,Seq2, ...'ExtendGap', ExtendGapValue, ...)` specifies the penalty for extending a gap in the alignment. Choices are any positive value. Default is equal to *`GapOpenValue`*.

`... = swalign(Seq1,Seq2, ...'Showscore', ShowscoreValue, ...)` controls the display of the scoring space and winning path of the alignment. Choices are `true` or `false` (default).



The scoring space is a heat map displaying the best scores for all the partial alignments of two sequences. The color of each (`n1,n2`) coordinate in the scoring space represents the best score for the pairing of subsequences `Seq1(s1:n1)` and `Seq2(s2:n2)`, where `n1` is a position in `Seq1`, `n2` is a position in `Seq2`, `s1` is any position in `Seq1` between `1:n1`, and `s2` is any position in `Seq2` between `1:n2`. The best score for a pairing of specific subsequences is determined by scoring all possible alignments of the subsequences by summing matches and gap penalties.

The winning path is represented by black dots in the scoring space, and it illustrates the pairing of positions in the optimal local alignment. The

color of the last point (lower right) of the winning path represents the optimal local alignment score for the two sequences and is the *Score* output returned by swalign.

Note The scoring space visually shows tandem repeats, small segments that potentially align, and partial alignments of domains from rearranged sequences.

Examples

1 Locally align two amino acid sequences using the BLOSUM50 (default) scoring matrix and the default values for the GapOpen and ExtendGap properties. Return the optimal local alignment score in bits and the alignment character array.

```
[Score, Alignment] = swalign('VSPAGMASGYD','IPGKASYD')

Score =

     8.6667

Alignment =

PAGMASGYD
| | || ||
P-GKAS-YD
```

2 Locally align two amino acid sequences specifying the PAM250 scoring matrix and a gap open penalty of 5.

```
[Score, Alignment] = swalign('HEAGAWGHEE','PAWHEAE',...
                             'ScoringMatrix', 'pam250',...
                             'GapOpen',5)

Score =

     8
```

```
Alignment =

GAWGHE
:|| ||
PAW-HE
```

3 Locally align two amino acid sequences returning the *Score* in nat units (nats) by specifying a scale factor of `log(2)`.

```
[Score, Alignment] = swalign('HEAGAWGHEE','PAWHEAE','Scale',log(2))

Score =

    6.4694

Alignment =

AWGHE
|| ||
AW-HE
```

References

[1] Durbin, R., Eddy, S., Krogh, A., and Mitchison, G. (1998). Biological Sequence Analysis (Cambridge University Press).

[2] Smith, T., and Waterman, M. (1981). Identification of common molecular subsequences. Journal of Molecular Biology *147*, 195–197.

See Also

Bioinformatics Toolbox functions: `aa2int`, `aminolookup`, `baselookup`, `blosum`, `dayhoff`, `gonnet`, `int2aa`, `int2nt`, `localalign`, `multialign`, `nt2aa`, `nt2int`, `nuc44`, `nwalign`, `pam`, `pdbsuperpose`, `seqdotplot`, `showalignment`

Purpose

Data structure containing information about Gene Ontology (GO) term

Description

A term object is a data structure containing information about a Gene Ontology (GO) term. You can explore and traverse Gene Ontology terms using “is_a” and “part_of” relationships.

Construction

geneont	Create geneont object and term objects

Properties

definition	Read-only string that defines GO term
id	Read-only numeric value that corresponds to GO identifier of GO term
is_a	Read-only numeric array containing GO identifiers of GO terms that have an “is a” relationship with this GO term
name	Read-only string representing name of GO term
obsolete	Read-only Boolean value that indicates whether a GO term is obsolete
ontology	Read-only string describing the ontology of GO term

part_of	Read-only numeric array containing GO identifiers of GO terms that have a “part of” relationship with this GO term
synonym	Read-only array containing GO terms that are synonyms of this GO term

Instance Hierarchy

A geneont object contains term objects.

Copy Semantics

Handle. To learn how this affects your use of the class, see Copying Objects in the MATLAB Programming Fundamentals documentation.

Indexing

You can use parenthesis () indexing to access the terms in an array of handles to term objects. See “Examples” on page 3-1546 below.

Examples

1 Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

```
GeneontObj = geneont('LIVE', true)
```

The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

```
Gene Ontology object with 27827 Terms.
```

2 Use the `terms` property to create a variable containing an array of handles to the term objects of the geneont object.

```
array_of_terms = GeneontObj.terms

27827x1 struct array with fields:
    id
    name
    ontology
```

```
definition
comment
synonym
is_a
part_of
obsolete
```

Note Although the `terms` property is an array of handles to term objects, in the MATLAB Command Window, it displays as a structure array, with one structure for each GO term in the geneont object.

3 Return the fifth term (term object) of the geneont object.

```
fifth_term = array_of_terms(5)

            id: 6
          name: [1x60 char]
      ontology: 'molecular function'
    definition: [1x321 char]
       comment: ''
       synonym: []
          is_a: 5385
       part_of: [0x1 double]
      obsolete: 0
```

See Also

Bioinformatics Toolbox class: `geneont`

tgspcinfo

Purpose

Return information about SPC file

Syntax

```
InfoStruct = tgspcinfo(File)
```

Description

`InfoStruct = tgspcinfo(File)` returns a MATLAB structure containing summary information about a Galactic SPC file from Thermo Scientific®.

Inputs

`File`

String specifying a file name or path and file name of an SPC file. If you specify only a file name, that file must be on the MATLAB search path or in the current folder.

Outputs

`InfoStruct`

MATLAB structure containing the following fields:

Field	Description
`Filename`	Name of the SPC file.
`FileSize`	Size of the SPC file in bytes.
`ExperimentType`	Experimental technique used to create the data.
`NumDataPoints`	Number of data points (*y* data values) in the SPC file.
`XFirst`	First *x* data value in the SPC file.
`XLast`	Last *x* data value in the SPC file.
`NumScans`	Number of scans or subfiles in the SPC file.
`XLabel`	Label for the *x* data values.
`YLabel`	Label for the *y* data values.
`ZLabel`	Label for the *z* data values.

Field	Description
`CollectionTime`	Date and time the scans were collected.
`CollectionTimeDatenum`	Date and time the scans were collected in serial date number format. For more information, see `datenum`.
`Resolution`	Instrument resolution.
`SourceInstrument`	Name or model of the instrument used to collect data.
`InterferogramPeakPointNumber`	Peak point number for interferograms. It is `0` for scans that are not interferograms.
`Comment`	User-provided comments.
`CustomAxisUnitLabel`	User-provided labels for the axis units.
`SubScanHeaders`	Header information for subfiles or scans, including scan index, next scan index, and *w* data value.
`ZValues`	Vector containing the *z* data values of all scans in the SPC file.

Examples

The SPC file, `sample.spc`, used in the following example is not provided with the Bioinformatics Toolbox software. You can download sample files from:

```
https://ftirsearch.com/default3.htm
```

Return information about an SPC file:

```
% Return information about an SPC file named sample.spc
info = tgspcinfo('sample.spc')

Reading header for file: SAMPLE.SPC
File contains 1 scans

info =

                        Filename: 'SAMPLE.SPC'
                        FileSize: 48380
                  ExperimentType: 'General SPC'
                   NumDataPoints: 12031
                          XFirst: 6.2998e+003
                           XLast: 499.9531
                        NumScans: 1
                          XLabel: 'Wavenumber (cm-1)'
                          YLabel: 'Absorbance'
                          ZLabel: 'Arbitrary'
                  CollectionTime: '08-Mar-1993 15:13:00'
            CollectionTimeDatenum: 7.2800e+005
                      Resolution: '  .00   '
                SourceInstrument: ''
    InterferogramPeakPointNumber: 0
                         Comment: [1x74 char]
             CustomAxisUnitLabel: ''
                  SubScanHeaders: [1x1 struct]
                         ZValues: 0
```

See Also

tgspcread | datenum

Related Links

Purpose

Read data from SPC file

Syntax

```
SPCStruct = tgspcread(File)
tgspcread(..., 'ZRange', ZRangeValue, ...)
tgspcread(..., 'ScanIndices', ScanIndicesValue, ...)
tgspcread(..., 'Verbose', VerboseValue, ...)
```

Description

`SPCStruct = tgspcread(File)` reads a Galactic SPC file from Thermo Scientific, and returns the data in a MATLAB structure.

`tgspcread(..., 'PropertyName', PropertyValue, ...)` calls `tgspcread` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Enclose each *`PropertyName`* in single quotation marks. Each *`PropertyName`* is case insensitive. These property name/property value pairs are as follows:

`tgspcread(..., 'ZRange', ZRangeValue, ...)` specifies a range of *z* data values in the SPC file from which to extract scans.

`tgspcread(..., 'ScanIndices', ScanIndicesValue, ...)` specifies a scan, multiple scans, or range of scans in the SPC file to read.

`tgspcread(..., 'Verbose', VerboseValue, ...)` controls the display of the progress of the reading of the SPC file. Choices are `true` or `false` (default).

Inputs

`File`

String specifying a file name or path and file name of an SPC file that conforms to the Thermo Scientific Universal Data Format Specification. If you specify only a file name, that file must be on the MATLAB search path or in the current directory.

`ZRangeValue`

Two-element numeric array `[Start End]` that specifies the range of *z* data values in *`File`* to read. *`Start`* and *`End`* must be positive scalars, and *`Start`* must be less than *`End`*. Default is to extract all scans.

Tip For summary information about the *z* data values in an SPC file, use the `tgspcinfo` function.

Note If you specify a *`ZRangeValue`*, you cannot specify a *`ScanIndicesValue`*.

`ScanIndicesValue`

Positive integer, vector of integers, or a two-element numeric array `[`*`Start_Ind`*`:  `*`End_Ind`*`]` that specifies a scan, multiple scans, or a range of scans in *`File`* to read. *`Start_Ind`* and *`End_Ind`* are each positive integers indicating a scan index. *`Start_Ind`* must be less than *`End_Ind`*. Default is to read all scans.

Tip For summary information about the scan indices in an SPC file, check the `NumScans` field in the structure returned by the `tgspcinfo` function.

Note If you specify a *`ScanIndicesValue`*, you cannot specify a *`ZRangeValue`*.

`VerboseValue`

Controls the display of the progress of the reading of *`File`*. Choices are `true` or `false` (default).

Outputs

`SPCStruct`

Structure containing information from an SPC file. The structure contains the following fields.

Field	Description
`Header`	Structure containing the following fields: • `Filename` — Name of the SPC file. • `FileSize` — Size of the SPC file in bytes. • `ExperimentType` — Experimental technique used to create the data. • `NumDataPoints` — Number of data points (*y* data values) in the SPC file. • `XFirst` — First *x* data value in the SPC file. • `XLast` — Last *x* data value in the SPC file. • `NumScans` — Number of scans or subfiles in the SPC file. • `XLabel` — Label for the *x* data values. • `YLabel` — Label for the *y* data values. • `ZLabel` — Label for the *z* data values. • `CollectionTime` — Date and time the scan data were collected. • `CollectionTimeDatenum` — Date and time the scan data were collected in serial date number format. For more information, see `datenum`. • `Resolution` — Instrument resolution. • `SourceInstrument` — Name or model of instrument used to collect data. • `InterferogramPeakPointNumber` — Peak point number for interferograms. It is `0` for scans that are not interferograms. • `Comment` — User-provided comments.

Field	Description
	• `CustomAxisUnitLabel` — User-provided labels for the axis units. • `SubScanHeaders` — Header information for subfiles or scans, including scan index, next scan index, and *w* data value. • `ZValues` — Vector containing the *z* data values of all scans in the SPC file.
`X`	Vector or cell array containing the *x* data values. If all scans share the same *x* data values, then `X` is a vector. If scans have different *x* data values, then `X` is a cell array.
`Y`	Vector, matrix, or cell array containing the *y* data values. If there is only one scan, then `Y` is a vector. If there are multiple scans that share the same *x* data values, then `Y` is a matrix. If there are multiple scans having different *x* data values, then `Y` is a cell array.
`Z`	Vector containing the *z* data values of scans read from the SPC file

Examples

The SPC file, `results.spc`, used in the following example is not provided with the Bioinformatics Toolbox software. You can download sample files from:

```
https://ftirsearch.com/default3.htm
```

Read an SPC file:

```
% Read the contents of an SPC file into a MATLAB structure
```

```
out = tgspcread('results.spc')

File contains 1 scans

out =

    Header: [1x1 struct]
         X: [12031x1 single]
         Y: [12031x1 double]
         Z: 0
```

Plot an SPC file:

```
% Plot the first scan in the SPC file:
plot(out.X,out.Y(:,1));
```

See Also

tgspcinfo | jcampread | mzcdfinfo | mzcdf2peaks | mzcdfread | mzxmlread | mzxml2peaks | mzxmlinfo | datenum

Related Links

-
-
-

times (DataMatrix)

Purpose

Multiply DataMatrix objects

Syntax

```
DMObjNew = times(DMObj1, DMObj2)
DMObjNew = DMObj1 .* DMObj2
DMObjNew = times(DMObj1, B)
DMObjNew = DMObj1 .* B
DMObjNew = times(B, DMObj1)
DMObjNew = B .* DMObj1
```

Arguments

DMObj1, *DMObj2*	DataMatrix objects, such as created by `DataMatrix` (object constructor).
B	MATLAB numeric or logical array.

Return Values

DMObjNew	DataMatrix object created by multiplication.

Description

DMObjNew = `times(`*DMObj1*`, `*DMObj2*`)` or the equivalent *DMObjNew* = *DMObj1* `.*` *DMObj2* performs an element-by-element multiplication of the DataMatrix objects *DMObj1* and *DMObj2* and places the results in *DMObjNew*, another DataMatrix object. *DMObj1* and *DMObj2* must have the same size (number of rows and columns), unless one is a scalar (1-by-1 DataMatrix object). The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*, unless *DMObj1* is a scalar; then they are the same as *DMObj2*.

DMObjNew = `times(`*DMObj1*`, `*B*`)` or the equivalent *DMObjNew* = *DMObj1* `.*` *B* performs an element-by-element multiplication of the DataMatrix object *DMObj1* and *B*, a numeric or logical array, and places the results in *DMObjNew*, another DataMatrix object. *DMObj1* and *B* must have the same size (number of rows and columns), unless *B* is a scalar. The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*.

DMObjNew = `times(`*B*`, `*DMObj1*`)` or the equivalent *DMObjNew* = *B* `.*` *DMObj1* performs an element-by-element multiplication of *B*, a numeric or logical array, and the DataMatrix object *DMObj1*, and places the results in *DMObjNew*, another DataMatrix object. *DMObj1* and *B* must have the same size (number of rows and columns), unless *B* is a scalar. The size (number of rows and columns), row names, and column names for *DMObjNew* are the same as *DMObj1*.

Note Arithmetic operations between a scalar DataMatrix object and a nonscalar array are not supported.

MATLAB calls *DMObjNew* = `times(`*X*`, `*Y*`)` for the syntax *DMObjNew* = *X* `.*` *Y* when *X* or *Y* is a DataMatrix object.

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox methods of a DataMatrix object: `minus`, `plus`

MATLAB functions: `Arithmetic Operators + - * / \ ^ '`

topoorder (biograph)

Purpose

Perform topological sort of directed acyclic graph extracted from biograph object

Syntax

```
order = topoorder(BGObj)
```

Arguments

BGObj	Biograph object created by `biograph` (object constructor).

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

order = `topoorder(`*BGObj*`)` returns an index vector with the order of the nodes sorted topologically. In topological order, an edge can exist between a source node `u` and a destination node `v`, if and only if `u` appears before `v` in the vector *order*. *BGObj* is a biograph object from which an N-by-N adjacency matrix is extracted and represents a directed acyclic graph (DAG). In the N-by-N sparse matrix, all nonzero entries indicate the presence of an edge.

References

[1] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphtopoorder`

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `isdag`, `isomorphism`, `isspantree`, `maxflow`, `minspantree`, `shortestpath`, `traverse`

Purpose

Draw nucleotide trace plots

Syntax

```
traceplot(TraceStructure)
traceplot(A, C, G, T)
h = traceplot(...)
```

Description

`traceplot(TraceStructure)` creates a trace plot from data in a structure with fields `A`, `C`, `G`, and `T`.

`traceplot(A, C, G, T)` creates a trace plot from data in vectors *A*, *C*, *G*, and *T*.

`h = traceplot(...)` returns a structure with the handles of the lines corresponding to `A`, `C`, `G`, `T`.

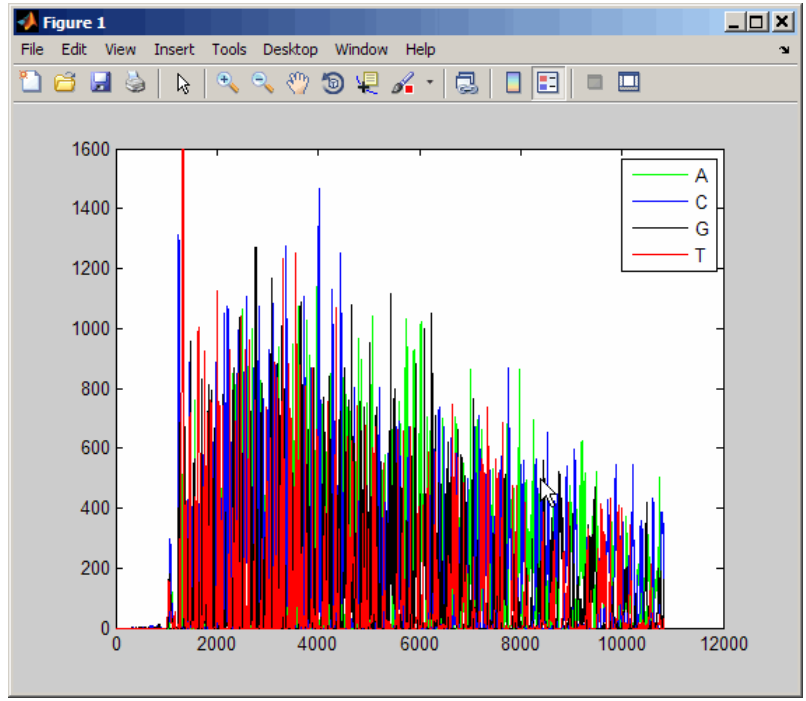
Examples

1 Read trace data from an SCF-formatted file into a MATLAB structure.

```
tstruct = scfread('sample.scf')

tstruct =

    A: [10827x1 double]
    C: [10827x1 double]
    G: [10827x1 double]
    T: [10827x1 double]
```

2 Draw a nucleotide trace plot of the data.

```
traceplot(tstruct)
```



See Also

Bioinformatics Toolbox function: `scfread`

Purpose

Traverse biograph object by following adjacent nodes

Syntax

```
[disc, pred, closed] = traverse(BGObj, S)
[...] = traverse(BGObj, S, ...'Depth', DepthValue, ...)
[...] = traverse(BGObj, S, ...'Directed', DirectedValue, ...)
[...] = traverse(BGObj, S, ...'Method', MethodValue, ...)
```

Arguments

BGObj	Biograph object created by `biograph` (object constructor).
S	Integer that indicates the source node in *BGObj*.
DepthValue	Integer that indicates a node in *BGObj* that specifies the depth of the search. Default is `Inf` (infinity).
DirectedValue	Property that indicates whether graph represented by an N-by-N adjacency matrix extracted from a biograph object, *BGObj* is directed or undirected. Enter `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.
MethodValue	String that specifies the algorithm used to traverse the graph. Choices are: • `'BFS'` — Breadth-first search. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively. • `'DFS'` — Default algorithm. Depth-first search. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.

Description

Tip For introductory information on graph theory functions, see "Graph Theory Functions" in the *Bioinformatics Toolbox User's Guide*.

`[disc, pred, closed] = traverse(BGObj, S)` traverses the directed graph represented by an N-by-N adjacency matrix extracted from a biograph object, *`BGObj`*, starting from the node indicated by integer `S`. In the N-by-N sparse matrix, all nonzero entries indicate the presence of an edge. *`disc`* is a vector of node indices in the order in which they are discovered. *`pred`* is a vector of predecessor node indices (listed in the order of the node indices) of the resulting spanning tree. *`closed`* is a vector of node indices in the order in which they are closed.

`[...] = traverse(BGObj, S, ...'PropertyName', PropertyValue, ...)` calls `traverse` with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *`PropertyName`* must be enclosed in single quotes and is case insensitive. These property name/property value pairs are as follows:

`[...] = traverse(BGObj, S, ...'Depth', DepthValue, ...)` specifies the depth of the search. *`DepthValue`* is an integer indicating a node in the graph represented by the N-by-N adjacency matrix extracted from a biograph object, *`BGObj`*. Default is `Inf` (infinity).

`[...] = traverse(BGObj, S, ...'Directed', DirectedValue, ...)` indicates whether the graph represented by the N-by-N adjacency matrix extracted from a biograph object, *`BGObj`* is directed or undirected. Set *`DirectedValue`* to `false` for an undirected graph. This results in the upper triangle of the sparse matrix being ignored. Default is `true`.

`[...] = traverse(BGObj, S, ...'Method', MethodValue, ...)` lets you specify the algorithm used to traverse the graph represented by the N-by-N adjacency matrix extracted from a biograph object, *`BGObj`*. Choices are:

- `'BFS'` — Breadth-first search. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.
- `'DFS'` — Default algorithm. Depth-first search. Time complexity is `O(N+E)`, where `N` and `E` are number of nodes and edges respectively.

References

[1] Sedgewick, R., (2002). Algorithms in C++, Part 5 Graph Algorithms (Addison-Wesley).

[2] Siek, J.G., Lee, L-Q, and Lumsdaine, A. (2002). The Boost Graph Library User Guide and Reference Manual, (Upper Saddle River, NJ:Pearson Education).

See Also

Bioinformatics Toolbox functions: `biograph` (object constructor), `graphtraverse`

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: `allshortestpaths`, `conncomp`, `isdag`, `isomorphism`, `isspantree`, `maxflow`, `minspantree`, `shortestpath`, `topoorder`

var (DataMatrix)

Purpose

Return variance values in DataMatrix object

Syntax

```
V = var(DMObj)
V = var(DMObj, Flag)
V = var(DMObj, Wgt)
V = var(..., Dim)
V = var(..., Dim, IgnoreNaN)
```

Arguments

DMObj	DataMatrix object, such as created by `DataMatrix` (object constructor).
Flag	Scalar specifying how to normalize the data. Choices are: • `0` — Default. Normalizes using a sample size of $N - 1$, unless $N = 1$, in which case, normalizes using a sample size of `1`. • `1` — Normalizes using a sample size of N. N = the number of elements in each column or row, as specified by *Dim*. For more information on the normalization equations, see the MATLAB function `std`.
Wgt	Weight vector equal in length to the dimension over which `var` operates (specified by *Dim*. It is used to compute the variance.

Dim	Scalar specifying the dimension of *DMObj* to calculate the variances. Choices are: • 1 — Default. Returns variance values for elements in each column. • 2 — Returns variance values for elements in each row.
IgnoreNaN	Specifies if NaNs should be ignored. Choices are `true` (default) or `false`.

Return Values

V	An unbiased estimator of the variance within the columns or rows of a DataMatrix object. It can be either of the following: • Row vector containing the variance values from elements in each column in *DMObj* (when *Dim* = 1) • Column vector containing the variance values from elements in each row in *DMObj* (when *Dim* = 2)

Description

V = var(*DMObj*) returns the variance values of the elements in the columns of a DataMatrix object, treating NaNs as missing values. The data is normalized using a sample size of $N - 1$, where N = the number of elements in each column. *V* is a row vector containing the variance values for elements in each column in *DMObj*. The variance is the square of the standard deviation.

V = var(*DMObj*, *Flag*) specifies how to normalize the data. If *Flag* = 0, normalizes using a sample size of $N - 1$. If *Flag* = 1, normalizes using a sample size of N. N = the number of elements in each column or row, as specified by *Dim*. For more information on the normalization equations, see the MATLAB function `std`. Default *Flag* = 0.

`V = var(DMObj, Wgt)` computes the variance using `Wgt`, a weight vector whose length must equal the length of the dimension over which `var` operates (specified by `Dim`). All elements in `Wgt` must be nonnegative. The `var` function normalizes `Wgt` to sum of `1`.

`V = var(..., Dim)` returns the variance values of the elements in the columns or rows of a DataMatrix object, as specified by `Dim`. If `Dim = 1`, returns `V`, a row vector containing the variance values for elements in each column in `DMObj`. If `Dim = 2`, returns `V`, a column vector containing the variance values for elements in each row in `DMObj`. Default `Dim = 1`.

`V = var(..., Dim, IgnoreNaN)` specifies if NaNs should be ignored. `IgnoreNaN` can be `true` (default) or `false`.

See Also

Bioinformatics Toolbox function: `DataMatrix` (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox methods of a DataMatrix object: `mean`, `median`, `std`

Purpose

Retrieve or set variable descriptions for samples in MetaData object

Syntax

```
DSVarDescriptions = variableDesc(MDObj)
NewMDObj = variableDesc(MDObj, NewDSVarDescriptions)
```

Description

`DSVarDescriptions = variableDesc(MDObj)` returns a dataset array containing the variable names and descriptions for samples from a MetaData object.

`NewMDObj = variableDesc(MDObj, NewDSVarDescriptions)` replaces the sample variable descriptions in *`MDObj`*, a MetaData object, with *`NewDSVarDescriptions`*, and returns *`NewMDObj`*, a new MetaData object.

Inputs

`MDObj`

Object of the `bioma.data.MetaData` class.

`NewDSVarDescriptions`

Descriptions of the sample variable names, specified by one of the following:

- A new dataset array containing the variable names and descriptions for samples. In this dataset array, each row corresponds to a variable. The first column contains the variable name, and the second column (`VariableDescription`) contains a description of the variable. The row names (variable names) must match the row names (variable names) in *`DSVarDescriptions`*, the dataset array being replaced in the MetaData object, *`MDObj`*.
- Cell array of strings containing descriptions of the variables. The number of elements in *`VarDesc`* must equal the number of row names (variable names) in *`DSVarDescriptions`*, the dataset array being replaced in the MetaData object, *`MDObj`*.

Outputs

DSVarDescriptions

A dataset array containing the variable names and descriptions from a MetaData object. In this dataset array, each row corresponds to a sample variable. The first column contains the variable name, and the second column (`VariableDescription`) contains a description of the variable.

NewMDObj

Object of the `bioma.data.MetaData` class, returned after replacing the dataset array containing the sample variable descriptions.

Examples

Construct a MetaData object, and then retrieve the sample variable descriptions from it:

```
% Import bioma.data package to make constructor function
% available
import bioma.data.*
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Retrieve the sample variable descriptions
VarDescriptions = variableDesc(MDObj2)
```

See Also

`bioma.data.MetaData` | `sampleNames` | `variableValues` | `variableNames`

How To

- "Working with MetaData Objects"

Purpose

Retrieve or set variable names for samples in MetaData object

Syntax

```
VarNames = variableNames(MDObj)
VarNames = variableNames(MDObj, Subset)
NewMDObj = variableNames(MDObj, Subset, NewVarNames)
```

Description

`VarNames = variableNames(MDObj)` returns a cell array of strings specifying all variable names in a MetaData object.

`VarNames = variableNames(MDObj, Subset)` returns a cell array of strings specifying a subset the variable names in a MetaData object.

`NewMDObj = variableNames(MDObj, Subset, NewVarNames)` replaces the variable names specified by `Subset` in `MDObj`, a MetaData object, with `NewVarNames`, and returns `NewMDObj`, a new MetaData object.

Inputs

MDObj

Object of the `bioma.data.MetaData` class.

Subset

One of the following to specify a subset of the variable names in a MetaData object:

- String specifying a variable name
- Cell array of strings specifying variable names
- Positive integer
- Vector of positive integers
- Logical vector

NewVarNames

New variable names for specific sample or feature variable names within a MetaData object, specified by one of the following:

- Numeric vector

- String or cell array of strings
- String, which `variableNames` uses as a prefix for the variable names, with variable numbers appended to the prefix
- Logical `true` or `false` (default). If `true`, `variableNames` assigns unique variable names using the format `Var1`, `Var2`, etc.

The number of variable names in *`NewVarNames`* must equal the number of variable names specified by *`Subset`*.

Outputs

`VarNames`

Cell array of strings specifying all variable names in a MetaData object.

`NewMDObj`

Object of the `bioma.data.MetaData` class, returned after replacing the variable names.

Examples

Construct a MetaData object, and then retrieve the sample variable names from it:

```
% Import bioma.data package to make constructor function
% available
import bioma.data.*
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Retrieve the sample variable names
VNames = variableNames(MDObj2)
```

See Also

`bioma.data.MetaData` | `sampleNames` | `variableValues` | `variableDesc`

How To

- "Working with MetaData Objects"

Purpose

Retrieve or set variable values for samples in MetaData object

Syntax

```
DSVarValues = variableValues(MDObj)
NewMDObj = variableValues(MDObj, NewDSVarValues)
```

Description

`DSVarValues = variableValues(MDObj)` returns a dataset array containing the measured value of each variable per sample from a MetaData object.

`NewMDObj = variableValues(MDObj, NewDSVarValues)` replaces the sample variable values in *`MDObj`*, a MetaData object, with *`NewDSVarValues`*, and returns *`NewMDObj`*, a new MetaData object.

Inputs

`MDObj`

Object of the `bioma.data.MetaData` class.

`NewDSVarValues`

A new dataset array containing a value for each variable per sample. In this dataset array, the columns correspond to variables and rows correspond to samples. The row names (sample names) must match the row names (sample names) in *`DSVarValues`*, the dataset array being replaced in the MetaData object, *`MDObj`*.

Outputs

`DSVarValues`

A dataset array containing the measured value of each variable per sample from a MetaData object. In this dataset array, the columns correspond to variables and rows correspond to samples.

`NewMDObj`

Object of the `bioma.data.MetaData` class, returned after replacing the dataset array containing the sample variable values.

Examples

Construct a MetaData object, and then retrieve the sample variable values from it:

```
% Import bioma.data package to make constructor function
```

```
% available
import bioma.data.*
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Retrieve the sample variable values
VarValues = variableValues(MDObj2)
```

See Also

bioma.data.MetaData | sampleNames | variableNames | variableDesc

How To

- "Working with MetaData Objects"

Purpose

Create 2-D graphic table GUI of variable values in MetaData object

Syntax

```
Handle = varValuesTable(MDObj)
Handle = varValuesTable(MDObj, ParentHandle)
```

Description

`Handle = varValuesTable(MDObj)` creates a 2-D graphic table containing variable data from a MetaData object and returns a uitable handle to the table.

`Handle = varValuesTable(MDObj, ParentHandle)` specifies the parent handle to the table. The parent can be a figure or uipanel handle.

Inputs

`MDObj`

Object of the `bioma.data.MetaData` class.

`ParentHandle`

Figure or uipanel handle to be the parent handle to the table.

Examples

Construct a MetaData object, and then create a 2-D table of the variable values from it:

```
% Import bioma.data package to make constructor function
% available
import bioma.data.*
% Construct MetaData object from .txt file
MDObj2 = MetaData('File', 'mouseSampleData.txt', 'VarDescChar', '#');
% Retrieve the sample variable values in a table
handle = varValuesTable(MDObj2)
```

MetaData 1

File Edit View Insert Tools Desktop Window Help

	Gender	Age	Type	Strain	Source
A	Male	8	Wild type	129S6/SvEv...	amygdala
B	Male	8	Wild type	129S6/SvEv...	amygdala
C	Male	8	Wild type	129S6/SvEv...	amygdala
D	Male	8	Wild type	A/J	amygdala
E	Male	8	Wild type	A/J	amygdala
F	Male	8	Wild type	C57BL/6J	amygdala
G	Male	8	Wild type	C57BL/6J	amygdala
H	Male	8	Wild type	129S6/SvEv...	cingulate cor...
I	Male	8	Wild type	129S6/SvEv...	cingulate cor...
J	Male	8	Wild type	A/J	cingulate cor...
K	Male	8	Wild type	A/J	cingulate cor...
L	Male	8	Wild type	A/J	cingulate cor...
M	Male	8	Wild type	C57BL/6J	cingulate cor...
N	Male	8	Wild type	C57BL/6J	cingulate cor...
O	Male	8	Wild type	129S6/SvEv...	hippocampus
P	Male	8	Wild type	129S6/SvEv...	hippocampus
Q	Male	8	Wild type	A/J	hippocampus
R	Male	8	Wild type	A/J	hippocampus
S	Male	8	Wild type	C57BL/6J	hippocampus
T	Male	8	Wild type	C57BL/6J4	hippocampus
U	Male	8	Wild type	129S6/SvEv...	hypothalamus
V	Male	8	Wild type	129S6/SvEv...	hypothalamus
W	Male	8	Wild type	A/J	hypothalamus
X	Male	8	Wild type	A/J	hypothalamus
Y	Male	8	Wild type	C57BL/6J	hypothalamus
Z	Male	8	Wild type	C57BL/6J	hypothalamus

See Also

`bioma.data.MetaData`

How To

- "Working with MetaData Objects"

vertcat (DataMatrix)

Purpose

Concatenate DataMatrix objects vertically

Syntax

```
DMObjNew = vertcat(DMObj1, DMObj2, ...)
DMObjNew = (DMObj1; DMObj2; ...)
DMObjNew = vertcat(DMObj1, B, ...)
DMObjNew = (DMObj1, B, ...)
```

Arguments

DMObj1, *DMObj2*	DataMatrix objects, such as created by `DataMatrix` (object constructor).
B	MATLAB numeric or logical array.

Return Values

DMObjNew	DataMatrix object created by vertical concatenation.

Description

DMObjNew = `vertcat(`*DMObj1*`, `*DMObj2*`, ...)` or the equivalent *DMObjNew* = `(`*DMObj1*`; `*DMObj2*`; ...)` vertically concatenates the DataMatrix objects *DMObj1* and *DMObj2* into *DMObjNew*, another DataMatrix object. *DMObj1* and *DMObj2* must have the same number of columns. The column names and the order of columns for *DMObjNew* are the same as *DMObj1*. The column names of *DMObj2* and any other DataMatrix object input arguments are not preserved. The row names for *DMObjNew* are the row names of *DMObj1*, *DMObj2*, and other DataMatrix object input arguments.

DMObjNew = `vertcat(`*DMObj1*`, `*B*`, ...)` or the equivalent *DMObjNew* = `(`*DMObj1*`, `*B*`, ...)` vertically concatenates the DataMatrix object *DMObj1* and a numeric or logical array *B* into *DMObjNew*, another DataMatrix object. *DMObj1* and *B* must have the same number of columns. The column names for *DMObjNew* are the same as *DMObj1*. The column names of *DMObj2* and any other DataMatrix object input arguments are not preserved. The row names for *DMObjNew* are the row names of *DMObj1* and empty for the rows from *B*.

MATLAB calls *DMObjNew* = vertcat(*X1*, *X2*, *X3*, ...) for the syntax *DMObjNew* = [*X1*; *X2*; *X3*; ...] when any one of *X1*, *X2*, *X3*, etc. is a DataMatrix object.

See Also

Bioinformatics Toolbox function: DataMatrix (object constructor)

Bioinformatics Toolbox object: DataMatrix object

Bioinformatics Toolbox methods of a DataMatrix object: horzcat

view (biograph)

Purpose

Draw figure from biograph object

Syntax

```
view(BGobj)
BGobjHandle = view(BGobj)
```

Arguments

BGobj	Biograph object created with the function `biograph`.

Description

`view(BGobj)` opens a Figure window and draws a graph represented by a biograph object (*BGobj*). When the biograph object is already drawn in the Figure window, this function only updates the graph properties.

BGobjHandle `= view(`*BGobj*`)` returns a handle to a deep copy of the biograph object (`BGobj`) in the Figure window. When updating an existing figure, you can use the returned handle to change object properties programmatically or from the command line. When you close the Figure window, the handle is no longer valid. The original biograph object (*BGobj*) is left unchanged.

Examples

1 Create a biograph object.

```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];
bg = biograph(cm)
```

2 Render the biograph object into a Handles Graphic figure and get back a handle.

```
h = view(bg)
```

3 Change the color of all nodes and edges.

```
set(h.Nodes,'Color',[.5 .7 1])
set(h.Edges,'LineColor',[0 0 0])
```

See Also

Bioinformatics Toolbox function: `biograph` (object constructor)

Bioinformatics Toolbox object: biograph object

Bioinformatics Toolbox methods of a biograph object: `dolayout`, `get`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `set`, `view`

view (clustergram)

Purpose

View clustergram and dendrograms of clustergram object

Syntax

```
view(CGObject)
```

Arguments

CGObject	Clustergram object created with the function `clustergram`.

Description

`view(CGObject)` opens a Clustergram window and draws a clustergram and dendrograms representing a clustergram object, *CGObject*. The clustergram shows hierarchical clustering using a heat map and dendrograms.

Note You can further explore the heat map and dendrograms using the mouse, toolbar buttons, and menu items in the Clustergram window. For more information, see the Examples section of the `clustergram` function.

Examples

View the clustergram object created in the Examples section of the `clustergram` function.

```
view(cgo)
```

See Also

Bioinformatics Toolbox function: `clustergram` (object constructor)

Bioinformatics Toolbox object: clustergram object

Bioinformatics Toolbox methods of a clustergram object: `get`, `plot`, `set`

Purpose

View heat map of HeatMap object

Syntax

```
view(HMObject)
```

Arguments

HMObject	HeatMap object created with the function `HeatMap`.

Description

`view(HMObject)` opens a HeatMap window and draws a heat map representing a HeatMap object, *`HMObject`*.

Examples

View the HeatMap object created in the Examples section of the `HeatMap` function.

```
view(hmo)
```

See Also

Bioinformatics Toolbox function: `HeatMap` (object constructor)

Bioinformatics Toolbox object: HeatMap object

Bioinformatics Toolbox method of a HeatMap object: `plot`

view (phytree)

Purpose

View phylogenetic tree

Syntax

```
view(Tree)
view(Tree, IntNodes)
```

Arguments

Tree	Phylogenetic tree (`phytree` object) created with the function `phytree`.
IntNodes	Nodes from the `phytree` object to initially display in the *Tree*.

Description

`view(Tree)` opens the Phylogenetic Tree Tool window and draws a tree from data in a `phytree` object (*Tree*). The significant distances between branches and nodes are in the horizontal direction. Vertical distances have no significance and are selected only for display purposes. You can access tools to edit and analyze the tree from the Phylogenetic Tree Tool menu bar or by using the left and right mouse buttons.

`view(Tree, IntNodes)` opens the Phylogenetic Tree Tool window with an initial selection of nodes specified by *IntNodes*. *IntNodes* can be a logical array of any of the following sizes: `NumLeaves + NumBranches x 1`, `NumLeaves x 1`, or `NumBranches x 1`. *IntNodes* can also be a list of indices.

Example

```
tree = phytreeread('pf00002.tree')
view(tree)
```

See Also

Bioinformatics Toolbox functions: `phytree` (object constructor), `phytreeread`, `phytreetool`, `seqlinkage`, `seqneighjoin`

Bioinformatics Toolbox object: phytree object

Bioinformatics Toolbox methods of phytree object: `cluster`, `plot`

Purpose

Calculate weights for phylogenetic tree

Syntax

```
W = weights(Tree)
```

Arguments

Tree	Phylogenetic tree (`phytree` object) created with the function `phytree`.

Description

`W = weights(Tree)` calculates branch proportional weights for every leaf in a tree (*Tree*) using the Thompson-Higgins-Gibson method. The distance of every segment of the tree is adjusted by dividing it by the number of leaves it contains. The sequence weights are the result of normalizing to unity the new patristic distances between every leaf and the root.

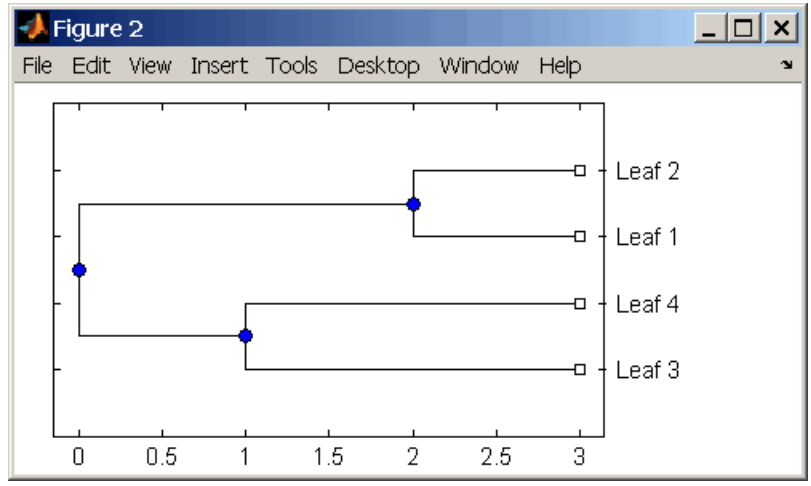
Examples

1 Create an ultrametric tree with specified branch distances.

```
bd = [1 2 3]';
tr_1 = phytree([1 2;3 4;5 6],bd)
```

2 View the tree.

```
view(tr_1)
```



3 Display the calculated weights.

```
weights(tr_1)

ans =

    1.0000
    1.0000
    0.8000
    0.8000
```

References

[1] Thompson JD, Higgins DG, Gibson TJ (1994), "CLUSTAL W: Improving the sensitivity of progressive multiple sequence alignment through sequence weighting, position-specific gap penalties and weight matrix choice," Nucleic Acids Research, 22(22):4673-4680.

[2] Henikoff S, Henikoff JG (1994), “Position-based sequence weights,” Journal Molecular Biology, 243(4):574-578.

See Also

Bioinformatics Toolbox functions: `multialign`, `phytree` (object constructor), `profalign`, `seqlinkage`

Bioinformatics Toolbox object: phytree object

zonebackadj

Purpose

Perform background adjustment on Affymetrix microarray probe-level data using zone-based method

Syntax

```
BackAdjustedData = zonebackadj(Data)
[BackAdjustedData, ZoneStruct] = zonebackadj(Data)
[BackAdjustedData, ZoneStruct,
   Background] = zonebackadj(Data)
... = zonebackadj(Data, ...'NumZones', NumZonesValue, ...)
... = zonebackadj(Data, ...'Percent', PercentValue, ...)
... = zonebackadj(Data, ...'SmoothFactor',
SmoothFactorValue,
   ...)
... = zonebackadj(Data, ...'NoiseFrac',
NoiseFracValue, ...)
... = zonebackadj(Data, ...'CDF', CDFValue, ...)
... = zonebackadj(Data, ...'Mask', MaskValue, ...)
... = zonebackadj(Data, ...'Showplot', ShowplotValue, ...)
```

Arguments

Data	Either of the following: • MATLAB structure containing probe intensities from an Affymetrix CEL file, such as returned by `affyread` when used to read a CEL file. • Array of MATLAB structures containing probe intensities from multiple Affymetrix CEL files.
NumZonesValue	Scalar or two-element vector that specifies the number of zones to use in the background adjustment. If a scalar, it must be a square number. If a two-element vector, the first element specifies the number of rows and the second element specifies the number of columns in a nonsquare grid. Default is 16.

PercentValue	Value that specifies a percentage, *P*, such that the lowest *P* percent of ranked intensity values from each zone is used to estimate the background for that zone. Default is `2`.
SmoothFactorValue	Value that specifies the smoothing factor used in the calculation of the weighted average of the contributions of each zone to the background of a point. Default is `100`.
NoiseFracValue	Value that specifies the noise fraction, `NF`, such that the background-adjusted value is given by `max((Intensity - WeightedBackground), NF*LocalNoiseEstimate)`. Default is `0.5`.
CDFValue	Either of the following: • String specifying a file name or path and file name of an Affymetrix CDF library file. If you specify only a file name, the file must be on the MATLAB search path or in the current directory. • MATLAB structure containing information from an Affymetrix CDF library file, such as returned by `affyread` when used to read a CDF file. The CDF library file or structure specifies control cells, which are not used in the background estimates.
MaskValue	Logical vector that specifies which cells to mask and not use in the background estimates. In the vector, `0 = not masked` and `1 = masked`. Defaults are the values in the `Masked` column of the `Probes` field of the CEL file.
ShowplotValue	Controls the plotting of an image of the background estimates. Choices are `true` or `false` (default).

Return Values

BackAdjustedData	Matrix or cell array of vectors containing background-adjusted probe intensity values.
ZoneStruct	MATLAB structure containing the centers of the zones used to perform the background adjustment and the estimates of the background values at the center of each zone.
Background	Matrix or cell array of vectors containing the estimated background values for each probe.

Description

BackAdjustedData = zonebackadj(*Data*) returns the background-adjusted probe intensities from *Data*, which contains probe intensities from Affymetrix CEL files. Details of the background adjustment are described in Statistical Algorithms Description Document.

[*BackAdjustedData*, *ZoneStruct*] = zonebackadj(*Data*) also returns a structure containing the centers of the zones used to perform the background adjustment and the estimates of the background values at the center of each zone.

[*BackAdjustedData*, *ZoneStruct*, *Background*] = zonebackadj(*Data*) also returns a matrix or cell array of vectors containing the estimated background values for each probe.

... = zonebackadj(*Data*, ...'*PropertyName*', *PropertyValue*, ...) calls zonebackadj with optional properties that use property name/property value pairs. You can specify one or more properties in any order. Each *PropertyName* must be enclosed in single quotation marks and is case insensitive. These property name/property value pairs are as follows:

... = zonebackadj(*Data*, ...'NumZones', *NumZonesValue*, ...) specifies the number of zones to use in the background adjustment.

NumZonesValue can be either a scalar that is a square number or a two-element array in which the first element specifies the number of rows and the second element specifies the number of columns in a nonsquare grid. Default is 16.

... = zonebackadj(*Data*, ...'Percent', *PercentValue*, ...) specifies a percentage, *P*, such that the lowest *P* percent of ranked intensity values from each zone is used to estimate the background for that zone. Default is 2.

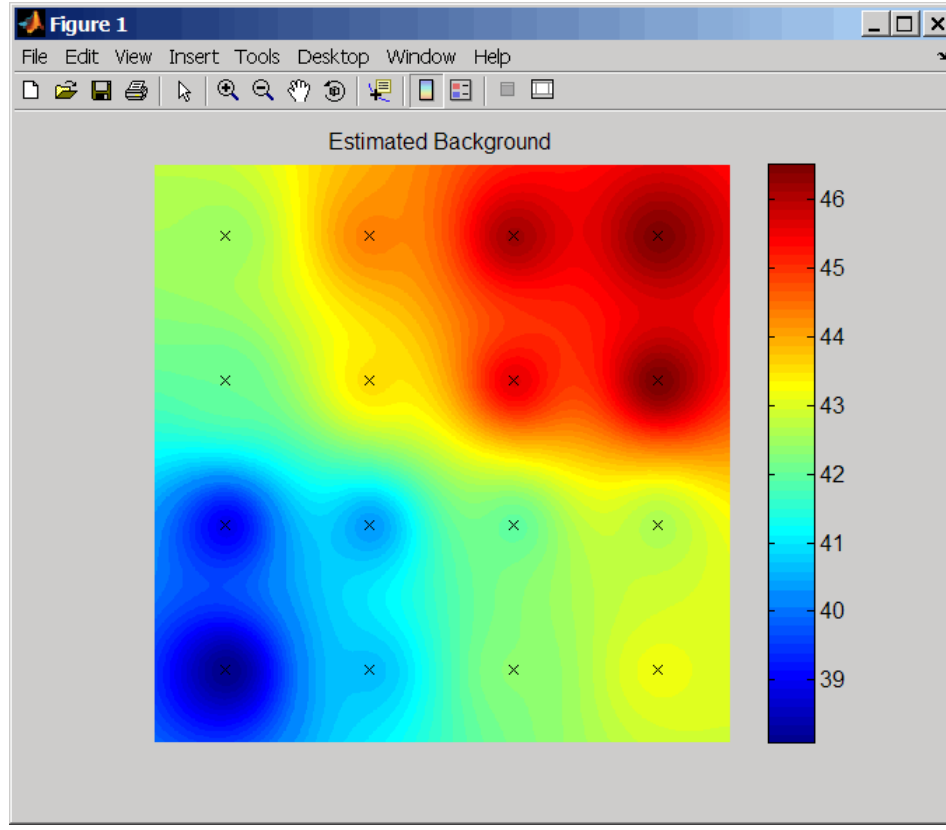
... = zonebackadj(*Data*, ...'SmoothFactor', *SmoothFactorValue*, ...) specifies the smoothing factor used in the calculation of the weighted average of the contributions of each zone to the background of a point, thus providing a smooth transition between zones. Default is 100.

... = zonebackadj(*Data*, ...'NoiseFrac', *NoiseFracValue*, ...) specifies the noise fraction, such that the background-adjusted value is given by max((Intensity - WeightedBackground), NF*LocalNoiseEstimate), where NF is *NoiseFracValue*. Default is 0.5.

... = zonebackadj(*Data*, ...'CDF', *CDFValue*, ...) specifies an Affymetrix CDF library file or structure, which specifies control cells, which are not used in the background estimates.

... = zonebackadj(*Data*, ...'Mask', *MaskValue*, ...) specifies a logical vector of that specifies which cells to mask and not use in the background estimates. In the vector, 0 = not masked and 1 = masked. Defaults are the values in the Masked column of the Probes field of the CEL file.

... = zonebackadj(*Data*, ...'Showplot', *ShowplotValue*, ...) plots an image of the background estimates. Choices are true or false (default).



Examples

The following example uses a sample CEL file and CDF library file from the *E. coli* Antisense Genome array, which you can download from:

```
http://www.affymetrix.com/support/technical/sample_data/demo_data.affx
```

After you download the demo data, you will need the Affymetrix Data Transfer Tool to extract the CEL file from a DTT file. You can download the Affymetrix Data Transfer Tool from:

```
http://www.affymetrix.com/products/software/specific/dtt.affx
```

The following example assumes that the `Ecoli-antisense-121502.CEL` file is stored on the MATLAB search path or in the current directory. It also assumes that the associated CDF library file, `Ecoli_ASv2.CDF`, is stored at `D:\Affymetrix\LibFiles\Ecoli`.

1. Use the `affyread` function to read an Affymetrix CEL file and create `celStruct`, a MATLAB structure containing probe intensities for a single Affymetrix GeneChip.

```
celStruct = affyread('Ecoli-antisense-121502.CEL');
```

2. Perform background adjustment on the probe intensities in the structure, excluding the probe intensities from the control cells on the chip.

```
BackAdjMatrix = zonebackadj(celStruct, 'cdf',...
                'D:\Affymetrix\LibFiles\Ecoli\Ecoli_ASv2.CDF');
```

References

[1] Statistical Algorithms Description Document, `http://www.affymetrix.com/support/technical/whitepapers/sadd_whitepaper.pdf`

See Also

Bioinformatics Toolbox functions: `affyinvarsetnorm`, `affyread`, `celintensityread`, `gcrma`, `gcrmabackadj`, `probelibraryinfo`, `probesetlink`, `probesetlookup`, `probesetvalues`, `quantilenorm`, `rmabackadj`, `rmasummary`

geneont.date property

Purpose

Read-only string containing date and time OBO file was last updated

Description

`date` is a read-only property of the geneont class. `date` is a string containing the date and time the OBO file was last updated. The OBO file is the Open Biomedical Ontology file from which the geneont object was created.

Values

Possible values are any date and time the OBO file was updated. Use this date information to compare the dates associated with ontologies used to create various geneont objects.

Examples

1. Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

   ```
   GeneontObj = geneont('LIVE', true)
   ```

   The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

   ```
   Gene Ontology object with 27769 Terms.
   ```

2. Display the date and time associated with the OBO file used to create the geneont object.

   ```
   GeneontObj.date

   ans =

   02:12:2008 19:30
   ```

See Also

Bioinformatics Toolbox property of geneont object: `geneont.format_version`

Purpose

Read-only string containing namespace to which GO terms are assigned

Description

`default_namespace` is a read-only property of the geneont class. `default_namespace` is a string containing the ontology namespace to which the GO terms are assigned.

Values

Currently, `gene_ontology` is the only possible namespace. However, other namespaces may be used in the future. Use this namespace information to determine the ontology namespace to which the GO terms in a geneont object are assigned.

Examples

1. Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

   ```
   GeneontObj = geneont('LIVE', true)
   ```

   The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

   ```
   Gene Ontology object with 27769 Terms.
   ```

2. Display the namespace associated with the GO terms of the geneont object.

   ```
   GeneontObj.default_namespace

   ans =

   gene_ontology
   ```

geneont.format_version property

Purpose

Read-only string containing version of encoding of OBO file

Description

`format_version` is a read-only property of the geneont class. `format_version` is a string containing the version of the encoding of the OBO file. The OBO file is the Open Biomedical Ontology file from which the geneont object was created.

Values

Possible values are the current or previous versions of the OBO file. Use this version information to compare the version associated with OBO file used to create various geneont objects.

Examples

1. Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

   ```
   GeneontObj = geneont('LIVE', true)
   ```

   The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

   ```
   Gene Ontology object with 27769 Terms.
   ```

2. Display the version of the OBO file used to create the geneont object.

   ```
   GeneontObj.format_version

   ans =

   1.0
   ```

Purpose

Read-only column vector with handles to term objects of geneont object

Description

`terms` is a read-only property of the geneont class. `terms` is a column vector with handles to the term objects of a geneont object.

Note Although `terms` is a column vector with handles to term objects, in the MATLAB Command Window, it displays as a structure array, with one structure for each GO term in the geneont object.

Values

Use the information in this structure to access (by GO ID) the terms of a geneont object and to view the properties of individual terms.

Examples

1. Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

   ```
   GeneontObj = geneont('LIVE', true)
   ```

   The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

   ```
   Gene Ontology object with 27786 Terms.
   ```

2. Use the `terms` property to display the MATLAB structure array containing 27,786 term objects associated with the geneont object.

   ```
   GeneontObj.terms

   27786x1 struct array with fields:
       id
       name
       ontology
       definition
       comment
       synonym
       is_a
   ```

```
part_of
obsolete
```

Note Although the `terms` property is an array of handles to term objects, in the MATLAB Command Window, it displays as a structure array, with one structure for each GO term in the geneont object.

3 Use the `terms` property to view the properties of the term object in the 14,723rd position in the geneont object.

```
GeneontObj.terms(14723)

           id: 31655
         name: 'negative regulation of heat dissipation'
     ontology: 'biological process'
   definition: [1x113 char]
      comment: ''
      synonym: {4x2 cell}
         is_a: [3x1 double]
      part_of: 31653
     obsolete: 0
```

4 Create a cell array of strings that list the `ontology` property for each term in the geneont object.

```
ontologies = get(GeneontObj.terms,'ontology');
```

5 Create a logical mask that identifies all the terms with an `ontology` property of `cellular component`.

```
mask = strcmp(ontologies,'cellular component');
```

6 Apply the logical mask to all the terms in the `GeneontObj` geneont object to return a MATLAB structure array of term objects, containing only terms with an `ontology` property of `cellular component`.

```
cell_comp_terms = GeneontObj.terms(mask)
2362x1 struct array with fields:
    id
    name
    ontology
    definition
    comment
    synonym
    is_a
    part_of
    obsolete
```

There are 2,362 terms with an `ontology` property of `cellular component`.

7 Create a subontology of all the cellular component terms by indexing into the `GeneontObj` geneont object with the masked term objects.

```
subontology = GeneontObj(cell_comp_terms)

Gene Ontology object with 2367 Terms.
```

See Also

Bioinformatics Toolbox class: `term`

term.definition property

Purpose

Read-only string that defines GO term

Description

`definition` is a read-only property of the term class. `definition` is a string that defines the GO term.

Values

Possible values are any definition used for a term in the Gene Ontology database. Use the `definition` property to determine definitions of term objects, or to access or filter term objects by definition.

Examples

Using the definition Property to Determine the Definition of a term Object

1 Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

```
GeneontObj = geneont('LIVE', true)
```

The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

```
Gene Ontology object with 27769 Terms.
```

2 Display the definition of the term object in the 287th position in the geneont object, `GeneontObj`.

```
GeneontObj.terms(287).name

ans =

"The smaller of the two subunits of an organellar ribosome." [GOC:mcc]
```

Tip If you know the GO identifier (for example, 314) of a term object, instead of its index or position number (for example, 287), you can use the following syntax to display the definition of a term object:

```
GeneontObj(314).terms.definition
```

For help converting the index or position number of a term object to its GO identifier, see the `term.id` property.

Filtering term Objects by Text in Their Definitions

1. Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

   ```
   GeneontObj = geneont('LIVE', true)
   ```

   The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

   ```
   Gene Ontology object with 27769 Terms.
   ```

2. Display the structure array containing 27,786 term objects associated with the geneont object.

   ```
   GeneontObj.terms

   27786x1 struct array with fields:
       id
       name
       ontology
       definition
       comment
       synonym
       is_a
       part_of
       obsolete
   ```

3. Find term objects whose definitions include the phrase "ceramide oligosaccharides" by first creating a cell array of strings that list the `definition` property for each term in the geneont object.

```
definitions = get(GeneontObj.terms,'definition');
```

4. Use the `regexpi` function to search these strings for `'ceramide oligosaccharides'`.

```
matches = regexpi(definitions,'ceramide oligosaccharides','once');
```

5. Create a logical mask that identifies all the terms with a `definition` property that includes the phrase "ceramide oligosaccharides."

```
mask = ~cellfun(@isempty,matches);
```

6. Apply the logical mask to all the terms in the `GeneontObj` geneont object to return a structure containing the GO identifiers of terms with a definition that includes the phrase "ceramide oligosaccharides."

```
get(GO.terms(mask),'id')

ans =

    [1573]
    [1574]
```

7. Apply the logical mask to all the terms in the `GeneontObj` geneont object to return a structure containing the full definitions of terms with a definition that includes the phrase "ceramide oligosaccharides."

```
char(get(GO.terms(mask),'definition'))
```

Purpose

Read-only numeric value that corresponds to GO identifier of GO term

Description

`id` is a property of the term class. `id` is a read-only numeric value that corresponds to the GO identifier of the GO term.

Tip You can use the `num2goid` function to convert `id` to a GO ID string formatted as a 7-digit number preceded by the prefix `GO:`, which is the standard used by the Gene Ontology database.

Values

Any value from `1` to *`N`*, where *`N`* is the largest value for an identifier of a term object in a geneont object. Use the `id` property to determine GO identifiers of term objects, or to access term objects by their GO identifier.

Tip You can use the `id` property for a GO term as input to methods of a geneont object, such as `geneont.getancestors`, `geneont.getdescendants`, and `geneont.getrelatives`.

Examples

Displaying and Formatting the GO Identifier of a term Object

1. Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

   ```
   GeneontObj = geneont('LIVE', true)
   ```

   The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

   ```
   Gene Ontology object with 27769 Terms.
   ```

2. Display the GO identifier of the term object in the 183rd position in the geneont object, `GeneontObj`.

   ```
   GeneontObj.terms(183).id
   ```

```
ans =

   207
```

Note The index or position (183 in this example) of the term object in the geneont object is not the same as the GO identifier (207 in this example) for the term object. This is because there are many terms that are obsolete and are not included as term objects in the geneont object.

3 Format the GO identifier into a character array.

```
num2goid(GeneontObj.terms(183).id)

ans =

    'GO:0000207'
```

Using the GO Identifier with Methods of a geneont Object

1 Find the index or position number of the term object whose `name` property is `'membrane'`.

```
membrane_index = find(strcmp(get(GeneontObj.terms,'name'),'membrane'))

membrane_index =

        9556
```

2 Use this index or position number and the `id` property to determine the GO identifier of the term object.

```
membrane_goid = GeneontObj.terms(membrane_index).id

membrane_goid =
```

```
        16020
```

3. Use this GO identifier as input to the `getrelatives` method to find the GO identifiers of other term objects that are immediate relatives of the term object whose `name` property is `'membrane'`.

```
relative_ids = getrelatives(GeneontObj,membrane_goid)

relative_ids =

         5628
         5886
        16020
        19867
        30673
        31090
        34045
        34357
        42175
        42622
        42734
        44464
        45211
        48475
        60342
```

4. List the `name` properties of these term objects.

```
get(GeneontObj(relative_ids).terms,'name')

ans =

    'prospore membrane'
    'plasma membrane'
    'membrane'
    'outer membrane'
    'axolemma'
```

```
'organelle membrane'
'pre-autophagosomal structure membrane'
'photosynthetic membrane'
'nuclear envelope-endoplasmic reticulum network'
'photoreceptor outer segment membrane'
'presynaptic membrane'
'cell part'
'postsynaptic membrane'
'coated membrane'
'photoreceptor inner segment membrane'
```

See Also

Bioinformatics Toolbox function: `num2goid`

Bioinformatics Toolbox methods of a geneont object: `geneont.getancestors`, `geneont.getdescendants`, `geneont.getrelatives`

Purpose

Read-only numeric array containing GO identifiers of GO terms that have an "is a" relationship with this GO term

Description

`is_a` is a read-only property of the term class. `is_a` is a column vector containing GO identifiers. These GO identifiers specify other term objects to which the term object has an "is a" relationship. The term object is an example of the term objects specified by its `is_a` property.

Values

Possible values are identifiers of GO terms from the Gene Ontology database. Use the `is_a` property to determine GO identifiers of GO terms that have an "is a" relationship with a specific GO term.

Examples

Using the is_a Property to Determine term Objects with an "is a" Relationship

1. Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

   ```
   GeneontObj = geneont('LIVE', true)
   ```

   The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

   ```
   Gene Ontology object with 27769 Terms.
   ```

2. Display the term objects to which the term object in the 18,703rd position has an "is a" relationship.

   ```
   GeneontObj.terms(18703).is_a

   ans =

          42754
          45187
          48521
          51241
   ```

Tip You can also use the `getancestors` method of a geneont object with the `'Relationtype'` property set to `'is_a'` to determine term objects with an "is a" relationship.

Tip If you know the GO identifier (for example, 42321) of a term object, instead of its index or position number (for example, 18703), you can use the following syntax to display the `is_a` property of a term object:

```
GeneontObj(42321).terms.is_a
```

For help converting the index or position number of a term object to its GO identifier, see the `term.id` property.

See Also

Bioinformatics Toolbox methods of a geneont object: `geneont.getancestors`, `geneont.getdescendants`, `geneont.getrelatives`

Purpose

Read-only string representing name of GO term

Description

`name` is a read-only property of the term class. `name` is a string representing the name of the GO term.

Values

Possible values are any name used for a term in the Gene Ontology database. Use the `name` property to determine names of term objects, or to access or filter term objects by name.

Examples

Using the name Property to Determine the Name of a term Object

1 Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

```
GeneontObj = geneont('LIVE', true)
```

The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

```
Gene Ontology object with 27769 Terms.
```

2 Display the name of the term object in the 157th position in the geneont object, `GeneontObj`.

```
GeneontObj.terms(157).name

ans =

  cytosolic small ribosomal subunit
```

Tip If you know the GO identifier (for example, 181) of a term object, instead of its index or position number (for example, 157), you can use the following syntax to display the name of a term object:

```
GeneontObj(181).terms.name
```

For help converting the index or position number of a term object to its GO identifier, see the `term.id` property.

Using the name Property to Find and Display Specific term Objects

1. Find the index or position number of the term object whose `name` property is `'membrane'`.

```
membrane_index = find(strcmp(get(GeneontObj.terms,'name'),'membrane'

membrane_index =

         9556
```

2. Use this index or position number and the `id` property to determine the GO identifier of the term object.

```
membrane_goid = GeneontObj.terms(membrane_index).id

membrane_goid =

        16020
```

3. Use this GO identifier as input to the `getrelatives` method to find the GO identifiers of other term objects that are immediate relatives of the term object whose `name` property is `'membrane'`.

```
relative_ids = getrelatives(GeneontObj,membrane_goid)
```

```
relative_ids =

        5628
        5886
       16020
       19867
       30673
       31090
       34045
       34357
       42175
       42622
       42734
       44464
       45211
       48475
       60342
```

4 List the `name` properties of these term objects.

```
get(GeneontObj(relative_ids).terms,'name')

ans =

    'prospore membrane'
    'plasma membrane'
    'membrane'
    'outer membrane'
    'axolemma'
    'organelle membrane'
    'pre-autophagosomal structure membrane'
    'photosynthetic membrane'
    'nuclear envelope-endoplasmic reticulum network'
    'photoreceptor outer segment membrane'
    'presynaptic membrane'
    'cell part'
    'postsynaptic membrane'
```

```
'coated membrane'
'photoreceptor inner segment membrane'
```

Purpose

Read-only Boolean value that indicates whether a GO term is obsolete

Description

`obsolete` is a read-only property of the term class. `obsolete` is a Boolean value that indicates if the GO term is obsolete (`1`) or not obsolete (`0`).

Values

`1` — Obsolete
`0` — Not obsolete

Use the `obsolete` property to determine whether a term object is obsolete, or to access or filter term objects by obsolete value.

Examples

Using the obsolete Property to Determine the Obsolete Status of a term Object

1 Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

```
GeneontObj = geneont('LIVE', true)
```

The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

```
Gene Ontology object with 27769 Terms.
```

2 Display the obsolete status of the term object in the third and seventh positions in the geneont object, `GO`

```
GeneontObj.terms(3).obsolete

ans =

     0

GeneontObj.terms(7).obsolete

ans =
```

```
1
```

Tip If you know the GO identifier (for example, 8) of a term object, instead of its index or position number (for example, 7), you can use the following syntax to display the obsolete status of a term object:

```
GeneontObj(8).terms.obsolete
```

For help converting the index or position number of a term object to its GO identifier, see the `term.id` property.

Filtering term Objects by Obsolete Status

1. Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

   ```
   GeneontObj = geneont('LIVE', true)
   ```

   The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

   ```
   Gene Ontology object with 27769 Terms.
   ```

2. Display the structure array containing 27,786 term objects associated with the geneont object.

   ```
   GeneontObj.terms

   27786x1 struct array with fields:
       id
       name
       ontology
       definition
       comment
       synonym
       is_a
       part_of
   ```

```
    obsolete
```

3. Create a cell array of logicals that list the `obsolete` property for each term in the geneont object.

```
obsolescence = get(GeneontObj.terms,'obsolete');
```

4. Create a logical mask from the cell array that identifies all the nonobsolete terms.

```
mask = ~cell2mat(obsolescence);
```

5. Apply the logical mask to all the terms in the `GeneontObj` geneont object to return a structure containing only terms that are not obsolete.

```
nonobsolete_terms = GeneontObj.terms(mask)

26424x1 struct array with fields:
    id
    name
    ontology
    definition
    comment
    synonym
    is_a
    part_of
    obsolete
```

There are 26,424 terms that are not obsolete.

term.ontology property

Purpose

Read-only string describing the ontology of GO term

Description

`ontology` is a read-only property of the term class. `ontology` is a string describing the ontology of the GO term.

Values

```
'molecular function'
'biological process'
'cellular component'
```

Use the `ontology` property to determine the ontology of term objects, or to access or filter term objects by ontology.

Examples

Using the ontology Property to Determine the Ontology of a term Object

1. Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

   ```
   GeneontObj = geneont('LIVE', true)
   ```

   The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

   ```
   Gene Ontology object with 27769 Terms.
   ```

2. Display the ontology of the term object in the 155th position in the geneont object, `GeneontObj`.

   ```
   GeneontObj.terms(155).ontology

   ans =

   molecular function
   ```

Tip If you know the GO identifier (for example, 179) of a term object, instead of its index or position number (for example, 155), you can use the following syntax to display the ontology of a term object:

```
GeneontObj(179).terms.ontology
```

For help converting the index or position number of a term object to its GO identifier, see the `term.id` property.

Filtering term Objects by Cellular Component Ontology

1. Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

   ```
   GeneontObj = geneont('LIVE', true)
   ```

   The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

   ```
   Gene Ontology object with 27769 Terms.
   ```

2. Display the structure array containing 27,786 term objects associated with the geneont object.

   ```
   GeneontObj.terms

   27786x1 struct array with fields:
       id
       name
       ontology
       definition
       comment
       synonym
       is_a
       part_of
       obsolete
   ```

3 View the properties of the term object in the 14,723rd position in the geneont object.

```
GeneontObj.terms(14723)

            id: 31655
          name: 'negative regulation of heat dissipation'
      ontology: 'biological process'
    definition: [1x113 char]
       comment: ''
       synonym: {4x2 cell}
          is_a: [3x1 double]
       part_of: 31653
      obsolete: 0
```

4 Create a cell array of strings that list the `ontology` property for each term in the geneont object.

```
ontologies = get(GeneontObj.terms,'ontology');
```

5 Create a logical mask that identifies all the terms with an `ontology` property of `cellular component`.

```
mask = strcmp(ontologies,'cellular component');
```

6 Apply the logical mask to all the terms in the `GeneontObj` geneont object to return a structure containing only terms with an `ontology` property of `cellular component`.

```
cell_comp_terms = GeneontObj.terms(mask)

2362x1 struct array with fields:
    id
    name
    ontology
    definition
    comment
```

```
synonym
is_a
part_of
obsolete
```

There are 2,362 terms with an `ontology` property of `cellular component`.

term.part_of property

Purpose

Read-only numeric array containing GO identifiers of GO terms that have a “part of” relationship with this GO term

Description

`part_of` is a read-only property of the term class. `part_of` is a column vector containing GO identifiers. These GO identifiers specify other term objects to which the term object has a “part_of” relationship. The term object is a subset of the term objects specified by its `part_of` property.

Values

Possible values are identifiers of GO terms from the Gene Ontology database. Use the `part_of` property to determine GO identifiers of GO terms that have a “part of” relationship with a specific GO term.

Examples

Using the part_of Property to Determine term Objects with a “part of” Relationship

1. Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

   ```
   GeneontObj = geneont('LIVE', true)
   ```

   The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

   ```
   Gene Ontology object with 27769 Terms.
   ```

2. Display the term objects to which the term object in the 18,703rd position has a “part of” relationship.

   ```
   GeneontObj.terms(18703).part_of

   ans =

          50802
   ```

Tip You can also use the `getancestors` method of a geneont object with the `'Relationtype'` property set to `'part_of'` to determine term objects with a "part of" relationship.

Tip If you know the GO identifier (for example, 42321) of a term object, instead of its index or position number (for example, 18703), you can use the following syntax to display the `part_of` property of a term object:

```
GeneontObj(42321).terms.part_of
```

For help converting the index or position number of a term object to its GO identifier, see the `term.id` property.

See Also

Bioinformatics Toolbox methods of a geneont object: `geneont.getancestors`, `geneont.getdescendants`, `geneont.getrelatives`

term.synonym property

Purpose

Read-only array containing GO terms that are synonyms of this GO term

Description

`synonym` is a read-only property of the term class. `synonym` is a two-column cell array containing GO terms that are synonyms of this GO term. The first column contains a string specifying the type of synonym, such as `'exact_synonym'`, `'related_synonym'`, `'broad_synonym'`, `'narrow_synonym'`, or `'alt_id'`. The second column contains the GO identifier of the synonymous term or a string describing the synonymous term.

Values

Possible values are identifiers of GO terms from the Gene Ontology database. Use the `synonym` property to determine GO identifiers of synonymous term objects.

Examples

Using the synonym Property to Determine Synonymous term Objects

1. Download the current version of the Gene Ontology database from the Web into a geneont object in the MATLAB software.

   ```
   GeneontObj = geneont('LIVE', true)
   ```

   The MATLAB software creates a geneont object and displays the number of term objects associated with the geneont object.

   ```
   Gene Ontology object with 27769 Terms.
   ```

2. Display the term objects that are synonymous to the term object in the third position in the geneont object, `GeneontObj`.

   ```
   synonyms = GeneontObj.terms(3).synonym

   synonyms =

       'alt_id'           'GO:0019952'
       'alt_id'           'GO:0050876'
   ```

```
    'exact_synonym'     [1x39 char]
```

3 Because the exact synonym does not have a GO identifier listed, display the text of this synonym.

```
synonyms(3,2)

ans =

    '"reproductive physiological process" []'
```

4 Display the term objects that are synonymous to the term object in the 352nd position in the geneont object, `GeneontObj`.

```
GeneontObj.terms(352).synonym

ans =

    'alt_id'             'GO:0006374'
    'alt_id'             'GO:0006375'
    'related_synonym'             [1x26 char]
    'related_synonym'             [1x26 char]
    'narrow_synonym'              [1x51 char]
    'narrow_synonym'              [1x50 char]
    'broad_synonym'      '"mRNA splicing" []'
    'broad_synonym'               [1x22 char]
```

Tip If you know the GO identifier (for example, 398) of a term object, instead of its index or position number (for example, 352), you can use the following syntax to display the synonym of a term object:

```
GeneontObj(398).terms.synonym
```

For help converting the index or position number of a term object to its GO identifier, see the `term.id` property.

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