

# Bioinformatics Toolbox

For Use with **MATLAB**<sup>®</sup>

- Computation
- Visualization
- Programming

Reference

*Version 2*



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### *Bioinformatics Toolbox Reference*

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**Revision History**

May 2005 Online only  
September 2005 Online only  
November 2005 Online only  
March 2006 Online only  
May 2006 Online only

New for Version 2.1 (Release 14SP2+)  
Updated for Version 2.1.1 (Release 14SP3)  
Updated for Version 2.2 (Release 14SP3+)  
Updated for Version 2.2.1 (Release 2006a)  
Updated for Version 2.3 (Release 2006a+)



## Functions – By Category

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## **Functions — Alphabetical List**

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# Functions – By Category

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Data Formats and Databases (p. 1-3)	Get data into MATLAB® from Web databases. Read and write to files using specific sequence data formats.
Trace Tools (p. 1-5)	Read data from a SCF file and draw nucleotide trace plots.
Sequence Conversion (p. 1-5)	Convert nucleotide and amino acid sequences between character and integer formats, reverse and complement the order of nucleotide bases, and translate nucleotides codons to amino acids.
Sequence Utilities (p. 1-6)	Calculate a consensus sequence from a set of multiply aligned sequences, run a BLAST search from MATLAB, and search sequences using regular expressions.
Sequence Statistics (p. 1-8)	Determine base counts, nucleotide density, codon bias, and CpG islands. Search for words and identify open reading frames (ORFs).
Sequence Visualization (p. 1-9)	Visualize sequence data.
Pairwise Sequence Alignment (p. 1-9)	Compare nucleotide or amino acid sequences using pairwise sequence alignment functions.

Multiple Sequence Alignment (p. 1-9)	Compare sets of nucleotide or amino acid sequences. Progressively align sequences using a phylogenetic tree for guidance.
Scoring Matrices (p. 1-10)	Standard scoring matrices such as the PAM and BLOSUM families of matrices that alignment functions use.
Phylogenetic Tree Tools (p. 1-10)	Read phylogenetic tree files, calculate pairwise distances between sequences and build a phylogenetic tree.
Phylogenetic Tree Methods (p. 1-11)	Select, modify, and plot phylogenetic trees using phytree object methods.
Graph Visualization Methods (p. 1-12)	View relationships between data visually with interactive maps, hierarchy plots, and pathways.
Gene Ontology Functions (p. 1-12)	Read Gene Ontology formatted files.
Gene Ontology Methods (p. 1-13)	Import the Gene Ontology database from the Web and get a subset of the ontology.
Protein Analysis (p. 1-13)	Determine protein characteristics and simulate enzyme cleavage reactions.
Profile Hidden Markov Models (p. 1-14)	Get profile hidden Markov model data from the PFAM database or create your own profiles from a set of sequences.
Microarray File Formats (p. 1-15)	Read data from common microarray file formats including Affymetrix GeneChip, ImaGene results, and SPOT files. Read GenePix GPR and GAL files.



Microarray Utility Functions (p. 1-15)	Using Affymetrix and GeneChip data sets, get library information for a probe, gene information from a probe set, and probe set values from CEL and CDF information. Show probe set information from NetAffx and plot probe set values.
Microarray Data Analysis and Visualization (p. 1-16)	Analyze and visualize microarray data with t tests, spatial plots, box plots, loglog plots, and intensity-ratio plots.
Microarray Normalization and Filtering (p. 1-17)	Normalize microarray data with lowess and mean normalization functions. Filter raw data for cleanup before analysis.
Statistical Learning (p. 1-18)	Classify and identify features in data sets, set up cross-validation experiments, and compare different classification methods.
Mass Spectrometry Preprocessing and Visualization (p. 1-19)	Preprocess raw data mass spectrometry data from instruments, and analyze spectra to identify patterns and compounds.

## Data Formats and Databases

affyread	Read microarray data from Affymetrix GeneChip file (Windows 32)
agferead	Read Agilent Feature Extraction Software file
blastread	Read data from NCBI BLAST report file

celintensityread	Read probe intensities from Affymetrix CEL files (Windows 32)
emblread	Read data from EMBL file
fastaread	Read data from FASTA file
fastawrite	Write to file with FASTA format
galread	Read microarray data from GenePix array list file
genbankread	Read data from GenBank file
genpeptread	Read data from GenPept file
geosoftread	Read data from Gene Expression Omnibus (GEO) SOFT Sample (GSM) file
getblast	BLAST report from NCBI Web site
getembl	Sequence information from EMBL database
getgenbank	Sequence information from GenBank database
getgenpept	Sequence information from GenPept database
getgeodata	Retrieve Gene Expression Omnibus (GEO) Sample (GSM) data
gethmmalignment	Multiple aligned sequences from PFAM database
gethmmprof	Profile Hidden Markov Models (HMM) from PFAM database
gethmmtree	Phylogenetic tree data from PFAM database
getpdb	Protein structure data from Protein Data Bank (PDB) database
gprread	Read microarray data from GenePix Results (GPR) file

imageneread	Read microarray data from ImaGene Results file
jcampread	Read JCAMP-DX formatted files
multialignread	Read multiple-sequence alignment file
pdbread	Read data from Protein Data Bank (PDB) file
pfamhmmread	Read data from PFAM-HMM file
phytreeread	Read phylogenetic tree file
scfread	Read trace data from SCF file
sptread	Read data from SPOT file

## 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	Amino acid codes, abbreviations, names, and codons
baselookup	Nucleotide codes, abbreviations, and names

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 of nucleotides to DNA sequence
seq2regex	Convert sequence with ambiguous characters to regular expression
seqcomplement	Calculate complementary strand of nucleotide sequence
seqrcomplement	Calculate reverse complement of nucleotide sequence
seqreverse	Reverse the letters or numbers in nucleotide sequence

## Sequence Utilities

aminolookup	Amino acid codes, abbreviations, names, and codons
baselookup	Nucleotide codes, abbreviations, and names
blastncbi	Generate remote BLAST request
cleave	Cleave amino acid sequence with enzyme

geneticcode	Nucleotide codon to amino acid mapping
joinseq	Join two sequences to produce shortest supersequence
oligoprop	Calculate nucleotide DNA sequence properties
palindromes	Find palindromes in sequence
pdbdistplot	Visualize intermolecular distances in Protein Data Bank (PDB) file
pdbplot	Plot 3-D protein structure
proteinplot	Characteristics for amino acid sequences
ramachandran	Draw Ramachandran plot for Protein Data Bank (PDB) data
randseq	Generate random sequence from finite alphabet
rebasecuts	Find restriction enzymes that cut protein sequence
restrict	Split nucleotide sequence at restriction site
revgeneticcode	Reverse mapping for genetic code
seqconsensus	Calculate consensus sequence
seqdisp	Format long sequence output for easy viewing
seqlogo	Sequence logo for nucleotide and 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

aaccount	Count amino acids in sequence
aminolookup	Amino acid codes, abbreviations, names, and codons
basecount	Count nucleotides in sequence
baselookup	Nucleotide codes, abbreviations, and names
codonbias	Calculate codon frequency for each amino acid in DNA sequence
codoncount	Count codons in nucleotide sequence
cpgisland	Locate CpG islands in DNA sequence
dimercount	Count dimers in sequence
isoelectric	Estimate isoelectric point for amino acid sequence
molweight	Calculate molecular weight of amino acid sequence
nmercount	Count number of 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

seqtool

Open interactive tool to explore biological sequences

## Pairwise Sequence Alignment

fastaread

Read data from FASTA file

nwalign

Globally align two sequences using Needleman-Wunsch algorithm

seqdotplot

Create dot plot of two sequences

showalignment

Sequence alignment with color

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

Open viewer for multiple sequence alignments

profalign	Align two profiles using Needleman-Wunsch global alignment
showalignment	Sequence alignment with color

## Scoring Matrices

blosum	BLOSUM scoring matrix
dayhoff	Dayhoff scoring matrix
gonnet	Gonnet scoring matrix
nuc44	NUC44 scoring matrix for nucleotide sequences
pam	PAM scoring matrix

## Phylogenetic Tree Tools

dnds	Estimate synonymous and nonsynonymous substitution rates
dndsml	Estimate synonymous-nonsynonymous substitution rates by the maximum likelihood method
gethmmtree	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
seqlinkage	Construct phylogenetic tree from pairwise distances
seqneighjoin	Neighbor-joining method for phylogenetic tree reconstruction
seqpdist	Calculate pairwise distance between sequences

## Phylogenetic Tree Methods

get (phytree)	Information about phylogenetic tree object
getbyname (phytree)	Branches and leaves from phytree object
getcanonical (phytree)	Calculate canonical form of phylogenetic tree
getnewickstr (phytree)	Create Newick-formatted string
pdist (phytree)	Calculate pairwise patristic distances in phytree object
phytree	Create phytree object
plot (phytree)	Draw phylogenetic tree
prune (phytree)	Remove branch nodes from 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 Visualization Methods

biograph

Create biograph object

dolayout (biograph)

Calculate node positions and edge trajectories

getancestors (biograph)

Find ancestors in biograph object

getdescendants (biograph)

Find descendants in biograph object

getedgesbynodeid (biograph)

Handles to edges in biograph object

getnodesbyid (biograph)

Handles to nodes

getrelatives (biograph)

Find relatives in biograph object

view (biograph)

Draw figure from biograph object

## Gene Ontology Functions

goannotread

Annotations from Gene Ontology annotated file

num2goid

Convert numbers to Gene Ontology IDs

## Gene Ontology Methods

geneont	Create geneont object
getancestors (geneont)	Numeric IDs for ancestors of Gene Ontology term
getdescendants (geneont)	Numeric IDs for descendants of Gene Ontology term
getmatrix (geneont)	Convert geneont object into relationship matrix
getrelatives (geneont)	Numeric IDs for relatives of Gene Ontology term

## Protein Analysis

aaccount	Count amino acids in sequence
aminolookup	Amino acid codes, abbreviations, names, and codons
atomiccomp	Calculate atomic composition of protein
cleave	Cleave amino acid sequence with enzyme
isoelectric	Estimate isoelectric point for amino acid sequence
molweight	Calculate molecular weight of amino acid sequence
pdbdistplot	Visualize intermolecular distances in Protein Data Bank (PDB) file
pdbplot	Plot 3-D protein structure
proteinplot	Characteristics for amino acid sequences

ramachandran	Draw Ramachandran plot for Protein Data Bank (PDB) data
rebasecuts	Find restriction enzymes that cut protein sequence

## Profile Hidden Markov Models

gethmmalignment	Multiple aligned sequences from PFAM database
gethmmprof	Profile Hidden Markov Models (HMM) from PFAM database
gethmmtree	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 profile Hidden Markov Model (HMM) structure
pfamhmmread	Read data from PFAM-HMM file
showhmmprof	Plot Hidden Markov Model (HMM) profile

## Microarray File Formats

affyread	Read microarray data from Affymetrix GeneChip file (Windows 32)
agferead	Read Agilent Feature Extraction Software file
celintensityread	Read probe intensities from Affymetrix CEL files (Windows 32)
galread	Read microarray data from GenePix array list file
geosoftread	Read data from Gene Expression Omnibus (GEO) SOFT Sample (GSM) file
getgeodata	Retrieve Gene Expression Omnibus (GEO) Sample (GSM) data
gprread	Read microarray data from GenePix Results (GPR) file
imageneread	Read microarray data from ImaGene Results file
sptread	Read data from SPOT file

## Microarray Utility Functions

magetfield	Extract data from a microarray structure
probelibraryinfo	Probe set library information for probe results
probesetlink	Link to NetAffx Web site
probesetlookup	Gene name for probe set

probesetplot	Plot values for Affymetrix CHP file probe set
probesetvalues	Probe set values from probe results

## **Microarray Data Analysis and Visualization**

clustergram	Create dendrogram and heat map
maboxplot	Box plot for microarray data
maimage	Spatial image for microarray data
mairplot	Intensity versus ratio scatter plot for microarray signals
maloglog	Create loglog plot of microarray data
mapcaplot	Create Principal Component plot of expression profile data
mattest	Perform two-sample, two-tailed 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
redgreencmap	Red and green colormap

## Microarray Normalization and Filtering

affyinvvarsetnorm	Perform rank invariant set normalization on probe intensities from multiple Affymetrix CEL or DAT files
exprprofrange	Calculate range of gene expression profiles
exprprofvar	Calculate variance of gene expression profiles
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

<code>rmabackadj</code>	Perform background adjustment on Affymetrix microarray probe-level data using Robust Multi-array Average (RMA) procedure
<code>rmasummary</code>	Calculate gene (probe set) expression values from Affymetrix microarray probe-level data using Robust Multi-array Average (RMA) procedure

## Statistical Learning

<code>classperf</code>	Evaluate performance of classifier
<code>crossvalind</code>	Generate cross-validation indices
<code>knnclassify</code>	Classify data using nearest neighbor method
<code>knnimpute</code>	Impute missing data using nearest-neighbor method
<code>randfeatures</code>	Generate randomized subset of features
<code>rankfeatures</code>	Rank key features by class separability criteria
<code>svmclassify</code>	Classify data using support vector machine
<code>svmtrain</code>	Train support vector machine classifier



## Mass Spectrometry Preprocessing and Visualization

<code>jcampread</code>	Read JCAMP-DX formatted files
<code>msalign</code>	Align peaks in mass spectrum to reference peaks
<code>msbackadj</code>	Correct baseline of mass spectrum
<code>msheatmap</code>	Color image for set of spectra
<code>mslowess</code>	Smooth mass spectrum using nonparametric method
<code>msnorm</code>	Normalize set of mass spectra
<code>msresample</code>	Resample mass spectrometry signal
<code>mssgolay</code>	Smooth mass spectrum with least-squares polynomial
<code>msviewer</code>	Explore MS spectrum or set of spectra



# Functions — Alphabetical List

---

# aa2int

---

**Purpose** Convert amino acid sequence from letter to integer representation

**Syntax** `SeqInt = aa2int(SeqChar)`

## Arguments

*SeqChar* Amino acid sequence represented with letters. Enter a character string with characters from the table Mapping Amino Acid Letters to Integers (unknown characters are mapped to 0). Integers are arbitrarily assigned to IUB/IUPAC letters. You can also enter a structure with the field Sequence.

*SeqInt* Amino acid sequence represented with numbers.

## Mapping Amino Acid Letters to Integers

Amino Acid	Code	Amino Acid	Code
Alanine	A1	Phenylalanine	F14
Arginine	R2	Proline	P15
Asparagine	N3	Serine	S-16
Aspartic acid (Aspartate)	D4	Threonine	T-17
Cysteine	C5	Tryptophan	W18
Glutamine	Q6	Tyrosine	Y19
Glutamic acid (Glutamate)	E7	Valine	V20
Glycine	G8	Aspartic acid or Asparagine	B21
Histidine	H9	Glutamic acid or glutamine	Z22
Isoleucine	I10	Unknown or any amino acid	X23

Amino Acid	Code	Amino Acid	Code
Leucine	L11	Translation stop	*24
Lysine	K12	Gap of indeterminate length	- 25
Methionine	M13	Any character or symbol not in table	?0

## Description

*SeqInt* = aa2int(*SeqChar*) converts a character string of amino acids (*SeqChar*) to a 1-by-N array of integers (*SeqInt*) using the table Mapping Amino Acid Letter to Integers.

## Examples

### Converting a simple sequence

Convert a sequence of letters to integers.

1 Enter the character string MATLAB.

```
SeqInt = aa2int('MATLAB')
```

```
SeqInt =
    13     1    17    11     1    21
```

### Converting a random sequence

Convert a random amino acid sequence of letters to integers.

1 Create a random character string with amino acid characters.

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

```
SeqChar =
    dwcztecakfuecvifchds
```

**2** Convert the character representation to integers.

```
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)
aa2nt(..., 'PropertyName', PropertyValue,...)
aa2nt(..., 'GeneticCode', GeneticCodeValue)
aa2nt(..., 'Alphabet', AlphabetValue)
```

## Arguments

<i>SeqAA</i>	Amino acid sequence. Enter a character string or a vector of integers from the table . Examples: 'ARN' or [1 2 3]
<i>GeneticCodeValue</i>	Property to select a genetic code. Enter a code number or code name from the table Genetic Code below. If you use a code name, you can truncate the name to the first two characters of the name.
<i>AlphabetValue</i>	Property to select a nucleotide alphabet. Enter either 'DNA' or 'RNA'. The default value is 'DNA', which uses the symbols A, C, T, G. The value 'RNA' uses the symbols A, C, U, G.

## Genetic Code

Code Number	Code Name	Code Number	Code Name
1	Standard	12	Alternative Yeast Nuclear
2	Vertebrate Mitochondrial	13	Ascidian Mitochondrial
3	Yeast Mitochondrial	14	Flatworm Mitochondrial

Code Number	Code Name	Code Number	Code Name
4	Mold, Protozoan, Coelenterate Mitochondrial, and Mycoplasma /Spiroplasma	15	Blepharisma Nuclear
5	Invertebrate Mitochondrial	16	Chlorophycean Mitochondrial
6	Ciliate, Dasycladacean, and Hexamita Nuclear	21	Trematode Mitochondrial
9	Echinoderm Mitochondrial	22	Scenedesmus Obliquus Mitochondrial
10	Euplotid Nuclear	23	Thraustochytrium Mitochondrial
11	Bacterial and Plant Plastid		

## Description

*SeqNT* = *aa2nt(SeqAA)* converts an amino acid sequence (*SeqAA*) to a nucleotide sequence (*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 more than one possible nucleotide codon, this function selects randomly 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.



`aa2nt(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`aa2nt(..., 'GeneticCode', GeneticCodeValue)` selects a genetic code (*GeneticCodeValue*) to use when converting an amino acid sequence (*SeqAA*) to a nucleotide sequence (*SeqNT*).

`aa2nt(..., 'Alphabet', AlphabetValue)` selects a nucleotide alphabet (*AlphabetValue*).

### Standard Genetic Code

Amino Acid		Amino Acid	
Alanine (A)	GCT, GCC, GCA, GCG	Phenylalanine (F)	TTT, TTC
Arginine (R)	CGT, CGC, CGA, CGG, AGA, AGG	Proline (P)	CCT, CCC, CCA, CCG
Asparagine (N)	ATT, AAC	Serine (S)	TCT, TCC, TCA, TCG, AGT, AGC
Aspartic acid (Aspartate, D)	GAT, GAC	Threonine (T)	ACT, ACC, ACA, ACG
Cysteine (C)	TGT, TGC	Tryptophan (W)	TGG
Glutamine (Q)	CAA, CAG	Tyrosine (Y)	TAT, TAC
Glutamic acid (Glutamate, E)	GAA, GAG	Valine (V)	GTT, GTC, GTA, GTG

Amino Acid		Amino Acid	
Glycine (G)	GGT, GGC, GGA, GGG	Aspartic acid or Asparagine	B—random codon from D and N
Histidine (H)	CAT, CAC	Glutamic acid or Glutamine	Z—random codon from E and Q
Isoleucine (I)	ATT, ATC, ATA	Unknown or any amino acid	Xrandom codon
Leucine (L)	TTA, TTG, CTT, CTC, CTA, CTG	Translation stop (*)	TAA, TAG, TGA
Lysine (K)	AAA, AAG	Gap of indeterminate length (-)	- - -
Methionine (M)	ATG	Any character or any symbol not in table (?)	???

## Examples

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

```
aa2nt('MATLAB')
```

```
Warning: The sequence contains ambiguous characters.
ans =
ATGGCAACCCTGGCGAAT
```

- 2 Use the Vertebrate Mitochondrial genetic code.

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

```
ans =
ATGGCAACTCTAGCGCCT
```

- 3** Use the genetic code for the Echinoderm Mitochondrial RNA alphabet.

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

```
Warning: The sequence contains ambiguous characters.  
ans =  
AUGGCUACAUUGGCUGAU
```

- 4** Convert a sequence with the ambiguous amino acid characters B.

```
aa2nt('abcd')
```

```
Warning: The sequence contains ambiguous characters.  
ans =  
GCCACATGCGAC
```

## See Also

Bioinformatics Toolbox functions `geneticcode`, `nt2aa`, `revgeneticcode`, `seqtool`  
MATLAB function `rand`

# aaccount

---

**Purpose** Count amino acids in sequence

**Syntax**

```
Amino = aaccount(SeqAA)  
aaccount(..., 'PropertyName', PropertyValue,...)  
aaccount(..., 'Chart', ChartValue)  
aaccount(..., 'Others', OthersValue)  
aaccount(..., 'Structure', StructureValue)
```

## Arguments

<i>SeqAA</i>	Amino acid sequence. Enter a character string or vector of integers from the table . Examples: 'ARN' or [1 2 3]. You can also enter a structure with the field Sequence.
<i>ChartValue</i>	Property to select a type of plot. Enter either 'pie' or 'bar'.
<i>OthersValue</i>	Property to control the counting of ambiguous characters individually. Enter either 'full' or 'bundle'(default).
<i>StructureValue</i>	Property to control blocking the unknown characters warning and to not count unknown characters.

## Description

*Amino* = aaccount(*SeqAA*) counts the type and number of amino acids in an amino acid sequence (*SeqAA*) and returns the counts in a 1-by-1 structure (*Amino*) with 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 V).

- If a sequence contains amino acids with ambiguous characters (B, Z, X), the stop character (\*), or gaps indicated with a hyphen (-), the field Others is added to the structure and a warning message is displayed.

Warning: Symbols other than the standard 20 amino acids appear in the sequence

- If a sequence contains any characters other than the 20 standard amino acids, ambiguous characters, stop, and gap characters, the characters are counted in the field `Others` and a warning message is displayed.

Warning: Sequence contains unknown characters. These will be ignored.

- If the property `Others = 'full'`, this function lists the ambiguous characters separately, asterisks are counted in a new field (`Stop`), and hyphens are counted in a new field, (`Gap`).

`aaccount(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`aaccount(..., 'Chart', ChartValue)` creates a chart showing the relative proportions of the amino acids.

`aaccount(..., 'Others', OthersValue)`, when `OthersValue` is `'full'`, counts the ambiguous amino acid characters individually instead of adding them together in the field `Others`.

`aaccount(..., 'Structure', StructureValue)` when `StructureValue` is `'full'`, blocks the unknown characters warning and ignores counting unknown characters.

- `aaccount(SeqAA)` — Display 20 amino acids, and only if there are ambiguous and unknown characters, add an `Others` field with the counts.
- `aaccount(SeqAA, 'Others', 'full')` — Display 20 amino acids, 3 ambiguous amino acids, stops, gaps, and only if there are unknown characters, add an `Others` field with the unknown counts.
- `aaccount(SeqAA, 'Structure', 'full')` — Display 20 amino acids and always display an `Others` field. If there are ambiguous and unknown characters, adds counts to the `Others` field otherwise display 0.

# aaccount

---

- `aaccount(SeqAA, 'Others', 'full', 'Structure', 'full')` — Display 20 amino acids, 3 ambiguous amino acids, stops, gaps, and Others field. If there are unknown characters, add counts to the Others field otherwise display 0.

## Examples

- 1 Create a sequence.

```
Seq = aaccount('MATLAB')
```

- 2 Count the amino acids in the sequence.

```
AA = aaccount(Seq)
```

```
Warning: Symbols other than the standard 20 amino acids appear  
in the sequence.
```

```
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
```

**See Also**

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

# affyinvvarsetnorm

---

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

**Syntax**

```
NormData = affyinvvarsetnorm(Data)
[NormData, MedStructure] = affyinvvarsetnorm(Data)
... affyinvvarsetnorm(..., 'Baseline', BaselineValue, ...)
... affyinvvarsetnorm(..., 'Thresholds', ThresholdsValue, ...)
... affyinvvarsetnorm(..., 'StopPrctile',
StopPrctileValue, ...)
... affyinvvarsetnorm(..., 'RayPrctile', RayPrctileValue, ...)
... affyinvvarsetnorm(..., 'Method', MethodValue, ...)
... affyinvvarsetnorm(..., 'Showplot', ShowplotValue, ...)
```

## Arguments

<i>Data</i>	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.)
<i>MedStructure</i>	Structure of each column's intensity median before and after normalization, and the index of the column chosen as the baseline.
<i>BaselineValue</i>	Property to control the selection of the column index <i>N</i> from <i>Data</i> 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  $[0.05, 0.005]$ .

*StopPrctileValue* 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.

---

*RayPrctileValue* 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 piece-wise linear curve. Default is 1.5.

# affyinvarsetnorm

---

<i>MethodValue</i>	Property to select the smoothing method used to normalize the data. Enter 'lowess' or 'runmedian'. Default is 'lowess'.
<i>ShowplotValue</i>	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 <i>Data</i> . 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.

$$prd = \text{abs}(\text{RankX} - \text{RankY})$$

- 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, ...)` defines optional properties that use property name/value pairs in any order. These property name/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

---

`... 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(..., 'StopPrctile', StopPrctileValue, ...)` 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(..., 'RayPrctile', RayPrctileValue, ...)` 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 piece-wise 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'.

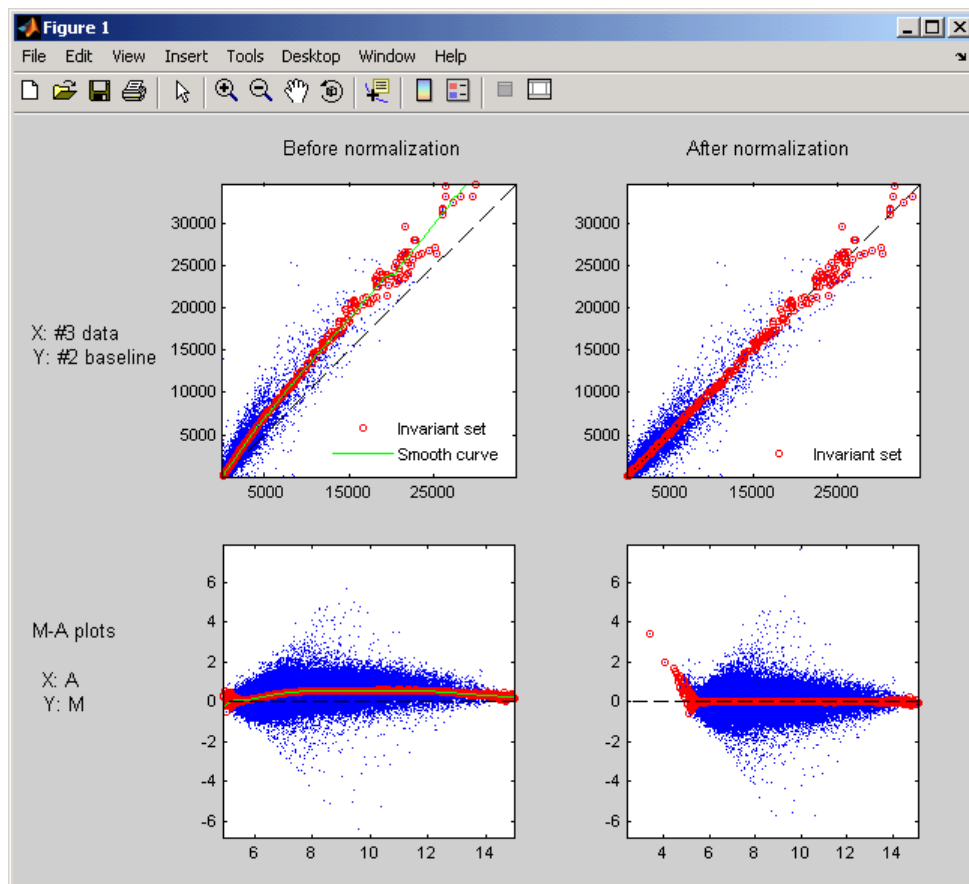
`... affyinvarsetnorm(..., 'Showplot', ShowplotValue, ...)` plots two pairs of scatter plots (before and after normalization). The first pair plots baseline data versus data from a specified column

(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', *affyinvaretnorm* plots a pair of scatter plots for each column or chip. When *ShowplotValue* is a number(s) or range of numbers, *affyinvaretnorm* 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*.

# affyinvarsetnorm



## Examples

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

```
load prostatecancerpdata
```

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

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

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

## References

[1] Li, C., and Wong, W.H. (2001). Model-based analysis of oligonucleotide arrays: model validation, design issues and standard error application. *Genome Biology* 2(8): research0032.1-0032.11.

[2] <http://biosun1.harvard.edu/complab/dchip/normalizing20arrays.htm#isn>

[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

affyread, celintensityread, mainvarsetnorm, malowess, manorm, quantilenorm, rmabackadj, rmasummary

# affyread

---

**Purpose** Read microarray data from Affymetrix GeneChip file (Windows 32)

**Syntax**  
`AFFYData = affyread(File)`  
`AFFYData = affyread(File, LibraryDir)`

## Arguments

<i>File</i>	Enter a filename, or a path and filename supported by your computer. Supported file formats are DAT, EXP, CEL, CHP and, CDF. If the file cannot be located on the Web, it needs to be stored locally.
<i>LibraryDir</i>	Enter the path and directory where the library file (CDF) is stored.

## Description

---

**Note** This function is supported on the Windows 32 platform only.

---

The function `affyread` can read four types of Affymetrix data files. These are

- DAT files which contain raw image data
- CEL files that contain information about the expression levels of the individual probes
- CHP files that contain information about probe sets,
- EXP files which contain information about experimental conditions and protocols

`affyread` can also read CDF and GIN library files. The CDF file contains information about which probes belong to which probe set and the GIN file contains information about the probe sets such as the gene name with which the probe set is associated. To learn more about the actual files, you can download sample data files from:



[http://www.affymetrix.com/support/technical/sample\\_data/demo\\_data.af](http://www.affymetrix.com/support/technical/sample_data/demo_data.af)

`AFFYData = affyread(File)` reads an Affymetrix data file (*File*) and creates a MATLAB structure (*AFFYDdata*).

`AFFYData = affyread(File, LibraryDir)` specifies the directory where the library files (CDF) are stored.

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When reading a CHP file, the Affymetrix GDAC Runtime Libraries look for the associated CEL file in the directory that it was in when the CHP file was created. If the CEL file is not found, then `affyread` does not read probe set values.

If you encounter errors reading files, then check that the Affymetrix GDAC Runtime Libraries are correctly installed. You can reinstall the libraries by running the installer from the Windows Explorer:

```
$MATLAB$\toolbox\bioinfo\microarray\lib\...
GdacFilesRuntimeInstall-v4.exe
```

## Example

- 1 Read a CEL file.

```
celStruct = affyread('Drosophila.CEL')
```

- 2 Display a spatial plot of probe intensities

```
mimage(celStruct, 'Intensity')
```

- 3 Read in a DAT file and display the raw image data

```
datStruct = affyread('Drosophila.data')
imagesc(datStruct.Image);
axis image;
```

- 4 Read a CHP file and plot the probe values for a probe set. The CHP files require the library files. Your file may be in a different location than this example.

# affyread

---

```
chpStruct = affyread('Drosophila.chp',...  
  'D:\Affymetrix\LibFiles\DrosGenome1')  
geneName = probesetlookup(chpStruct, '14317_at')  
probesetplot(chpStruct, '142417_at');
```

Sample data files are available from

[http://www.affymetrix.com/support/technical/sample\\_data/demo\\_data.affx](http://www.affymetrix.com/support/technical/sample_data/demo_data.affx)

## See Also

Bioinformatics Toolbox functions `agferead`, `celintensityread`, `gprread`, `probelibraryinfo`, `probesetlink`, `probesetlookup`, `probesetplot`, `probesetvalues`, `sptread`

**Purpose** Read Agilent Feature Extraction Software file

**Syntax** `AGFEData = agferead(File)`

**Arguments**

*File* Microarray data file generated with Agilent's Feature Extraction Software.

**Description**

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

Field
Header
Stats
Columns
Rows
Names
IDs
Data
ColumnNames
TextData
TextColumnNames

Feature Extraction Software takes an image from a Agilent microarray scanner and generates raw intensity data for each spot on the plate. For more information about this software, see a description on their Web site at

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

**Example**

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

# agferead

---

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

**2** Plot the median foreground.

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

## See Also

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

**Purpose** Amino acid codes, abbreviations, names, and codons

**Syntax**

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

## Arguments

<i>SeqAA</i>	Amino acid sequence. Enter a character string of single-letter codes or three-letter abbreviations from the Amino Acid Lookup Table below.
<i>CodeValue</i>	Amino acid single-letter code. Enter a single character from the Amino Acid Lookup Table below.
<i>IntegerValue</i>	
<i>AbbreviationValue</i>	Amino acid three-letter abbreviation. Enter a three-letter abbreviation from the Amino Acid Lookup Table below.
<i>NameValue</i>	Amino acid name. Enter an amino acid name from the Amino Acid Lookup Table below.

## Amino Acid Lookup Table

Code	Integer	Abbreviation	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

# aminolookup

---

Code	Integer	Abbreviation	Name	Codons
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
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

Code	Integer	Abbreviation	Name	Codons
B	21	Asx	Aspartic acid or Asparagine	AAU AAC GAU GAC
Z	22	Glx	Glutamic acid or Glutamine	CAA CAG GAA GAG
X	23	Xaa	Any amino acid	All codons
*	24	END	Termination (translation stop)	UAA UAG UGA
-	25	GAP	Gap of unknown length	- - -
?	0	???	Unknown amino acid	

## Description

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

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

If you enter one of the ambiguous characters B, Z, X, this function displays the 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

---

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

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

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

## Examples

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

```
aminolookup('Name', 'proline')  
  
ans =  
    P  Pro
```

- 2 Convert a single-letter amino acid sequence to a three-letter sequence.

```
aminolookup('MWKQAEDIRDIYDF')  
  
ans =  
    MetTrpLysGlnAlaGluAspIleArgAspIleTyrAspPhe
```

- 3 Convert a three-letter amino acid sequence to a single-letter sequence.

```
aminolookup('MetTrpLysGlnAlaGluAspIleArgAspIleTyrAspPhe')  
  
ans =  
    MWKQAEDIRDIYDF
```

- 4 Display the single-letter code, three-letter abbreviation, and name for an integer.

```
aminolookup('integer', 1)
```



```
ans =  
A Ala Alanine
```

## See Also

Bioinformatics Toolbox functions `aa2int`, `aacount`, `geneticcode`, `int2aa`, `nt2aa`, `revgeneticcode`

# atomiccomp

---

**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 Letters to Integers on page 2-2. 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** Get an amino acid sequence from the NCBI Genpept Database

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

**2** Count the atoms in a sequence.

```
rhodopsinAC = atomiccomp(rhodopsin)
```

```
rhodopsinAC =
```

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

**3** Retrieve the number of carbon atoms in the sequence.

```
rhodopsinAC.C
```

```
ans =
```

```
    1814
```

**See Also** Bioinformatics Toolbox functions `aaccount`, `molweight`, `proteinplot`

# basecount

---

**Purpose** Count nucleotides in sequence

**Syntax**

```
NumberBases = basecount(SeqNT)
basecount(..., 'PropertyName', PropertyValue,...)
basecount(..., 'Chart', ChartValue)
basecount(..., 'Others', OthersValue)
basecount(..., 'Structure', StructureValue)
```

## Arguments

<i>SeqNT</i>	Nucleotide sequence. Enter a character string with the letters A, T, U, C, and G. The count for U characters is included with the count for T characters. . You can also enter a structure with the field Sequence.
<i>ChartValue</i>	Property to select a type of plot. Enter either 'pie' or 'bar'.
<i>OthersValue</i>	Property to control counting ambiguous characters individually. Enter either full' or 'bundle' (default).

## Description

*NumberBases* = basecount(*SeqNT*) counts the number of bases in a nucleotide sequence (*SeqNT*) and returns the base counts in a 1-by-1 structure (*Bases*) with the fields A, C, G, T.

- For sequences with the character U, the number of U characters is added to the number of T characters.
- If the sequence contains ambiguous nucleotide characters (R, Y, K, M, S, W, B, D, H, V, N), or gaps indicated with a hyphen (-), this function creates a field *Others* and displays a warning message.

```
Warning: Ambiguous symbols 'symbol list' 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 Z), the characters are counted in the field `Others` and a warning message is displayed.

```
Warning: Unknown symbols 'symbol list' appear
in the sequence.
These will be ignored.
```

- If `Others = 'full'`, ambiguous characters are listed separately and hyphens are counted in a new field (`Gaps`).

`basecount(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`basecount(..., 'Chart', ChartValue)` creates a chart showing the relative proportions of the nucleotides.

`basecount(..., 'Others', OthersValue)`, when `OthersValue` is `'full'`, counts all the ambiguous nucleotide symbols individually instead of bundling them together into the `Others` field of the output structure.

`basecount(..., 'Structure', StructureValue)` when `StructureValue` is `'full'`, blocks the unknown characters warning and ignores counting unknown characters.

- `basecount(SeqNT)` — Display 4 nucleotides, and only if there are ambiguous and unknown characters, add an `Others` field with the counts.
- `basecount(SeqNT, 'Others', 'full')` — Display 4 nucleotides, 11 ambiguous nucleotides, gaps, and only if there are unknown characters, add an `Others` field with the unknown counts.
- `basecount(SeqNT, 'Structure', 'full')` — Display 4 nucleotides and always display an `Others` field. If there are ambiguous and unknown characters, adds counts to the `Others` field otherwise display 0.

# basecount

---

- `basecount(SeqNT, 'Others', 'full', 'Structure', 'full')`  
— Display 4 nucleotides, 11 ambiguous nucleotides, gaps, and Others field. If there are unknown characters, add counts to the Others field otherwise display 0.

## Examples

- 1 Count the number of bases in a DNA sequence.

```
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 with ambiguous characters.

```
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  
Gaps: 0

## See Also

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

# baselookup

---

**Purpose** Nucleotide codes, abbreviations, and names

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

## Arguments

<i>SeqNT</i>	Nucleotide sequence. Enter a character string of single-letter codes from the Nucleotide Lookup Table below.  In addition to a single nucleotide sequence, <i>SeqNT</i> can be a cell array of sequences, or a two-dimensional character array of sequences. The complement for each sequence is determined independently
<i>CodeValue</i>	Nucleotide letter code. Enter a single character from the Nucleotide Lookup Table below. Code can also be a cell array or a two-dimensional character array.
<i>IntegerValue</i>	Nucleotide integer. Enter an integer from the Nucleotide Lookup Table below. Integers are arbitrarily assigned to IUB/IUPAC letters.
<i>NameValue</i>	Nucleotide name. Enter a nucleotide name from the Nucleotide Lookup Table below. <i>NameValue</i> can also be a single name, a cell array, or a two-dimensional character array.

## Nucleotide Lookup Table

Code	Integer	Base Name	Meaning	Complement
A	1	Adenine	A	T
C	2	Cytosine	C	G



Code	Integer	Base Name	Meaning	Complement
G	3	Guanine	G	C
T	4	Thymine	T	A
U	4	Uracil	U	A
R	5	(PuRine)	G A	Y
Y	6	(PYrimidine)	T C	R
K	7	(Keto)	G T	M
M	8	(AMino)	A C	K
S	9	Strong interaction (3 H bonds)	G C	S
W	10	Weak interaction (2 H bonds)	A T	W
B	11	Not-A (B follows A)	G T C	V
D	12	Not-C (D follows C)	G A T	H
H	13	Not-G (H follows G)	A T C	D
V	14	Not-T (or U) (V follows U)	G A C	B
N,X	15	ANy nucleotide	G A T C	N
-	16	Gap of indeterminate length	Gap	-

## Description

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

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

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

# baselookup

---

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

## Examples

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

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

## See Also

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

**Purpose** Create biograph object

**Syntax**  
*BGobj* = biograph(*CMatrix*)  
*BGobj* = biograph(*CMatrix*, *NodeIDs*)

## Arguments

<i>CMatrix</i>	Connection matrix. Enter a square matrix that is full or sparse. For a square matrix the number of rows is equal to the number of nodes. A value of 1 indicates a connection to a node while a 0 indicates no connection.
<i>NodeIDs</i>	Node identification strings. Enter a cell array of strings with the same number of strings as the number of rows/columns in the connection matrix ( <i>CMatrix</i> ). Default values are the row/column numbers.

## Description

*BGobj* = biograph(*CMatrix*) creates a graph 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.

A biograph object (*BGobj*) has two properties (Nodes, Edges) that have their own properties. For a list of the Nodes and Edges properties, see the tables below.

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

Access properties of a biograph object with *BGobj.propertyname*, *BGobj.propertyname.propertyname*, or with the get and set commands.

## Method Summary

biograph	Create biograph object
dolayout (biograph)	Calculate node positions and edge trajectories

# biograph

---

getancestors (biograph)	Find ancestors in biograph object
getdescendants (biograph)	Find descendants in biograph object
getedgesbynodeid (biograph)	Handles to edges in biograph object
getnodesbyid (biograph)	Handles to nodes
getrelatives (biograph)	Find relatives in biograph object
view (biograph)	Draw figure from biograph object

## Property Summary

### Properties for a biograph Object

Property	Description
ID	Enter a character string.
Label	Enter a character string.
Description	Description of the graph. Enter text.
LayoutType	Algorithm for the layout engine. Enter 'hierarchical'(default), 'equilibrium', 'radial'.
EdgeType	Enter 'straight', 'curved'(default), 'segmented'. Curved or segmented edges occur only when necessary to avoid obstruction by nodes. Graphs with LayoutType equal to 'equilibrium' or 'Radial' cannot produce curved or segmented edges.

Property	Description
Scale	Property to post-scale the node coordinates. Enter a positive number.
LayoutScale	Property to scale the size of the nodes before calling the layout engine. Enter a positive number.
ShowArrows	Property to control showing arrows with the edges. Enter either 'on' (default) or 'off'.
NodeAutoSize	Property to control precalculating the node size before calling the layout engine. Enter either 'on' or 'off'.
NodeCallback	User callback for all nodes. Enter the name of a function or a function handle. Default is 'display'.
EdgeCallback	User callback for all edges. Enter the name of a function or function handle. Default is 'display'.
Nodes	Column vector with handles to nodes. Size of vector is <code>NumberOfNodes x 1</code> . For properties of the Nodes property, see the table below.
Edges	Column vector with handles to edges. Size of vector is <code>NumberOfEdges x 1</code> . For properties of the Edges property, see the table below.

## Properties of the Nodes Property

Property	Description
ID	Character string defined when the biograph object is created. Node IDs must be unique. Read-only.
Label	User defined label for a node on a graph. Enter a character string. The default value is the ID property.
Description	Description of the node. Enter text.
Position	Two element numeric vector of x and y coordinates computed by the layout engine. The default is []. For example, [150 150].
Shape	Enter 'box'(default), 'ellipse', 'circle', 'rect', 'rectangle', 'diamond', 'trapezium', 'house', 'invtrapezium', 'inverse', 'parallelogram'.
Size	Two element numeric vector calculated before calling the layout engine using the actual font size and shape of the node. The default value is [10 10].
Color	RGB three element numeric vector. Default is [1 1 0.7].
LineWidth	Positive number. Default is 1.
LineColor	RGB three element numeric vector. Default is [0.3 0.3 1].
FontSize	Positive number. Default is 8 pts.
TextColor	RGB three element numeric vector. Default is [0 0 0].

## Properties of the Edge Property

Property	Description
ID	Character string defined when the biograph object is created. Edge IDs must be unique. Read-only.
Label	Label for a node on a graph. Enter a string.
Description	Description for a node. Enter a text.
LineWidth	Positive number. Default is 1.
LineColor	RGB three element numeric vector. Default is [0.5 0.5 0.5].

## Example

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];
bg1 = biograph(cm)
get(bg1.nodes, 'ID')

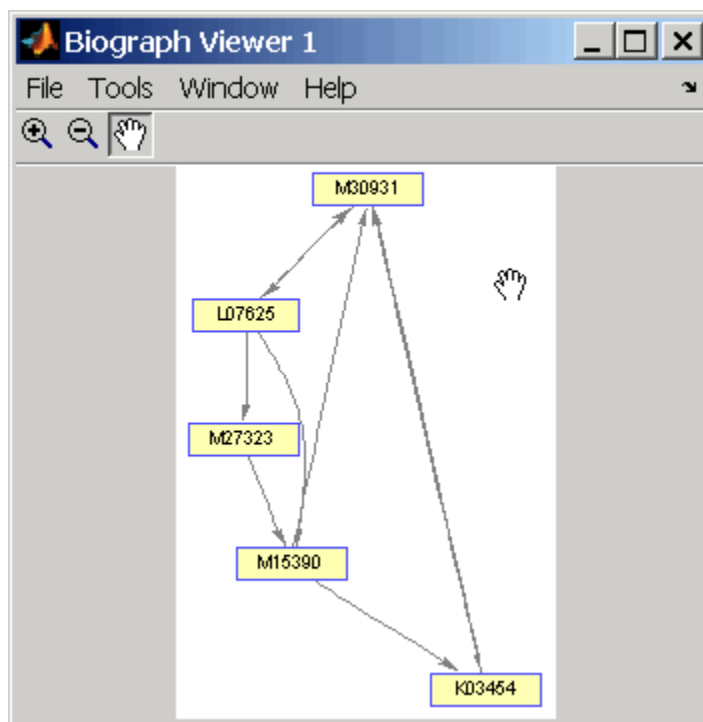
ans =
    'Node 1'
    'Node 2'
    'Node 3'
    'Node 4'
    'Node 5'
```

2 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'};
bg2 = biograph(cm,ids);
get(bg2.nodes, 'ID');

view(bg2);
```

# biograph



In `bg1.Node`, the properties `ID` and `Label` are set to the same value. However, you can only modify the **Label** field. `Node.ID` is used internally to identify the nodes.

## See Also

Bioinformatics Toolbox

- `function` — `biograph` (object constructor)
- `biograph` object methods — `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `view`

MATLAB



- functions — get, set

# blastncbi

---

**Purpose** Generate remote BLAST request

**Syntax**

```
blastncbi(Seq, Program)
RID = blastncbi(Seq, Program)
[RID, RTOE] = blastncbi(Seq, Program)
blastncbi(..., 'PropertyName', PropertyValue,...)
blastncbi(..., 'Database', DatabaseValue)
blastncbi(..., 'Descriptions', DescriptionsValue)
blastncbi(..., 'Alignments', AlignmentsValue)
blastncbi(..., 'Filter', FilterValue)
blastncbi(..., 'Expect', ExpectValue)
blastncbi(..., 'Word', WordValue)
blastncbi(..., 'Matrix', MatrixValue)
blastncbi(..., 'GapOpen', GapOpenValue)
blastncbi(..., 'ExtendGap', ExtendGapValue)
blastncbi(..., 'Inclusion', InclusionValue)
blastncbi(..., 'Pct', PctValue)
```

## Arguments

<i>Seq</i>	Nucleotide or amino acid sequence. Enter a GenBank or RefSeq accession number, GI, FASTA file, URL, string, character array, or a MATLAB structure that contains the field Sequence. You can also enter a structure with the field Sequence.
<i>Program</i>	BLAST program. Enter 'blastn', 'blastp', 'pciblast', 'blastx', 'tblastn', 'tblastx', or 'megablast'.

<i>Database</i>	<p>Property to select a database. Compatible databases depend upon the type of sequence submitted and program selected. The nonredundant database, 'nr', is the default value for both nucleotide and amino acid sequences.</p> <p>For nucleotide sequences, enter 'nr', 'est', 'est_human', 'est_mouse', 'est_others', 'gss', 'htgs', 'pat', 'pdb', 'month', 'alu_repeats', 'dbsts', 'chromosome', 'wgs', 'refseq_rna', 'refseq_genomic', or 'env_nt'. The default value is 'nr'.</p> <p>For amino acid sequences, enter 'nr', 'swissprot', 'pat', 'pdb', 'month', 'refseq_protein', or 'env_nr'. The default value is 'nr'.</p>
<i>Description</i>	<p>Property to specify the number of short descriptions. The default value is normally 100, and for Program = pciblast, the default value is 500.</p>
<i>Alignment</i>	<p>Property to specify the number of sequences to report high-scoring segment pairs (HSP). The default value is normally 100, and for Program = pciblast, the default value is 500.</p>
<i>Filter</i>	<p>Property to select a filter. Enter 'L' (low-complexity), 'R' (human repeats), 'm' (mask for lookup table), or 'lcase' (to turn on the lowercase mask). The default value is 'L'.</p>
<i>Expect</i>	<p>Property to select the statistical significance threshold. Enter a real number. The default value is 10.</p>
<i>Word</i>	<p>Property to select a word length. For amino acid sequences, Word can be 2 or 3 (3 is the default value), and for nucleotide sequences, Word can be 7, 11, or 15 (11 is the default value). If Program = 'MegaBlast', Word can be 11, 12, 16, 20, 24, 28, 32, 48, or 64, with a default value of 28</p>

# blastncbi

---

<i>Matrix</i>	Property to select a substitution matrix for amino acid sequences. Enter 'PAM30', 'PAM70', 'BLOSUM80', 'BLOSUM62', or 'BLOSUM45'. The default value is 'BLOSUM62'.
<i>Inclusion</i>	Property for PCI-BLAST searches to define the statistical significance threshold. The default value is 0.005.
<i>Pct</i>	Property to select the percent identity. Enter None, 99, 98, 95, 90, 85, 80, 75, or 60. Match and mismatch scores are automatically selected. The default value is 99 (99, 1, -3)

## Description

The Basic Local Alignment Search Tool (BLAST) offers a fast and powerful comparative analysis of interesting protein and nucleotide sequences against known structures in existing online databases.

`blastncbi(Seq, Program)` sends a BLAST request against a sequence (*Seq*) to NCBI using a specified program (*Program*). With no output arguments, `blastncbi` returns a command window link to the actual NCBI report.

`RID = blastncbi(Seq, Program)` calls with one output argument and returns the Report ID (*RID*).

`[RID, RTOE] = blastncbi(Seq, Program)` calls with two output arguments and returns both the report ID (*RID*) and the Request Time Of Execution (*RTOE*) which is an estimate of the time until completion.

`blastncbi` uses the NCBI default values for the optional arguments: 'nr' for the database, 'L' for the filter, and '10' for the expectation threshold. The default values for the remaining optional arguments depend on which program is used. For help in selecting an appropriate BLAST program, visit

<http://www.ncbi.nlm.nih.gov/BLAST/producttable.shtml>

Information for all of the optional parameters can be found at

[http://www.ncbi.nlm.nih.gov/staff/tao/URLAPI/blastcgihelp\\_new.html](http://www.ncbi.nlm.nih.gov/staff/tao/URLAPI/blastcgihelp_new.html)

`blastncbi(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`blastncbi(..., 'Database', DatabaseValue)` selects a database for the alignment search.

`blastncbi(..., 'Descriptions', DescriptionsValue)`, when the function is called without output arguments, specifies the numbers of short descriptions returned to the quantity specified.

`blastncbi(..., 'Alignments', AlignmentsValue)`, when the function is called without output arguments, specifies the number of sequences for which high-scoring segment pairs (HSPs) are reported.

`blastncbi(..., 'Filter', FilterValue)` selects the filter to applied to the query sequence.

`blastncbi(..., 'Expect', ExpectValue)` provides a statistical significance threshold for matches against database sequences. You can learn more about the statistics of local sequence comparison at

<http://www.ncbi.nlm.nih.gov/BLAST/tutorial/Altschul-1.html#head2>

`blastncbi(..., 'Word', WordValue)` selects a word size for amino acid sequences.

`blastncbi(..., 'Matrix', MatrixValue)` selects the substitution matrix for amino acid sequences only. This matrix assigns the score for a possible alignment of two amino acid residues.

`blastncbi(..., 'GapOpen', GapOpenValue)` selects a gap penalty for amino acid sequences. Allowable values for a gap penalty vary with the selected substitution matrix. For information about allowed gap penalties for matrixes other than the BLOSUM62 matrix, see

[http://www.ncbi.nlm.nih.gov/staff/tao/URLAPI/blastcgihelp\\_new.html](http://www.ncbi.nlm.nih.gov/staff/tao/URLAPI/blastcgihelp_new.html)

`blastncbi(..., 'ExtendGap', ExtendGapValue)` defines the penalty for extending a gap greater than one space.

## blastncbi

---

`blastncbi(..., 'Inclusion', InclusionValue)` for PSI-BLAST only, defines the statistical significance threshold (*InclusionValue*) for including a sequence in the Position Specific Score Matrix (PSSm) created by PSI-BLAST for the subsequent iteration. The default value is 0.005.

`blastncbi(..., 'Pct', PctValue)`, when *ProgramValue* is 'Megablast', selects the percent identity and the corresponding match and mismatch score for matching existing sequences in a public database.

## Values by Program

	<b>BLASTN</b>	<b>BLASTP</b>	<b>BLASTX</b>	<b>TBLASTN</b>	<b>TBLASTX</b>	<b>MEGA</b>
<b>Database</b>	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	nr(default), swissprot, pat, pdb, month, refseq_protein, env_nr	values same as BLASTP	values same as BLASTN	values same as BLASTN	values same as BLASTN
<b>Filter</b>	low(default), human, table, lower	low(default), table, lower	low(default), table, lower	low(default), table, lower	low(default), human, table, lower	low
<b>Expect</b>	10(default)	10(default)	10(default)	10(default)	10(default)	10
<b>Word</b>	7 11 (default) 15	2 3 (default)	2 3 (default)	2 3 (default)	2 3 (default)	11, 12, 16, 20, 24, 28(def), 32, 48, 64
<b>Matrix</b>	x	PAM30 PAM70 BLOSUM45 BLOSUM80 BLOSUM62 (default)	PAM30 PAM70 BLOSUM45 BLOSUM80 BLOSUM62 (default)	PAM30 PAM70 BLOSUM45 BLOSUM80 BLOSUM62 (default)	PAM30 PAM70 BLOSUM45 BLOSUM80 BLOSUM62 (default)	x

	<b>BLASTN</b>	<b>BLASTP</b>	<b>BLASTX</b>	<b>TBLASTN</b>	<b>TBLASTX</b>	<b>MEGA</b>
<b>2-54</b> GAP	x	[9 2], [8 2], [7 2], [12 1], [11 1](default), [10 1]	[9 2], [8 2], [7 2], [12 1], [11 1](default), [10 1]	[9 2], [8 2], [7 2], [12 1], [11 1](default), [10 1]	[9 2], [8 2], [7 2], [12 1], [11 1](default), [10 1]	x
Pct	x	x	x	x	x	79, 80, 88, 95, 98, 99(def)



**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 try a search directly with an accession
% number and an alternative scoring matrix.
RID = blastncbi('AAA59174','blastp','matrix','PAM70','...
                'expect',1e-10)

% The results based on the RID are at
http://www.ncbi.nlm.nih.gov/BLAST/Blast.cgi

% or pass the RID to BLASTREAD to parse the report and
% load it into a MATLAB structure.
blastread(RID)
```

**See Also**

Bioinformatics Toolbox function `blastread`, `getblast`

# blastread

---

**Purpose** Read data from NCBI BLAST report file

**Syntax** `Data = blastread(File)`

## Arguments

*File* NCBI BLAST formatted report file. Enter a filename, a path and filename, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text for a NCBI BLAST report.

## Description

BLAST (**B**asic **L**ocal **A**lignment **S**earch **T**ool) reports offer a fast and powerful comparative analysis of interesting protein and nucleotide sequences against known structures in existing online databases. BLAST reports can be lengthy, and parsing the data from the various formats can be cumbersome.

`Data = blastread(File)` reads a BLAST report from an NCBI formatted file (*File*) and returns a data structure (*Data*) 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
RID
Algorithm
Query
Database
Hits.Name
Hits.Length
Hits.HSP.Score
Hits.HSP.Expect

Field
Hits.HSP.Identities
Hits.HSP.Positives
Hits.HSP.Gaps
Hits.HSP.Frame
Hits.HSP.Strand
Hits.HSP.Alignment
Hits.HSPs.QueryIndices
Hits.HSPs.SubjectIndices
Statistics

## References

For more information about reading and interpreting BLAST reports, see

[http://www.ncbi.nlm.nih.gov/Education/BLASTinfo/Blast\\_output.html](http://www.ncbi.nlm.nih.gov/Education/BLASTinfo/Blast_output.html)

## Examples

- 1 Create a BLAST request with a GenPept accession number.

```
RID = blastncbi('AAA59174', 'blastp', 'expect', 1e-10)
```

- 2 Pass the RID to getblast, download the report and save the report to a text file.

```
getblast(RID, 'ToFile' , 'AAA59174_BLAST.rpt')
```

- 3 Using the saved file, read the results into a MATLAB structure.

```
results = blastread('AAA59174_BLAST.rpt')
```

## See Also

Bioinformatics Toolbox functions `blastncbi`, `getblast`

# blosum

---

**Purpose** BLOSUM scoring matrix

**Syntax**

```
Matrix = blosum(Identity)
[Matrix, MatrixInfo] = blosum(Identity)
blosum(..., 'PropertyName', PropertyValue, ...)
blosum(..., 'Extended', ExtendedValue)
blosum(..., 'Order', OrderValue)
```

## Arguments

<i>Identity</i>	Percent identity level. Enter values from 30 to 90 in increments of 5, enter 62, or enter 100.
<i>ExtendedValue</i>	Property to control the listing of extended amino acid codes. Enter either true (default) or false.
<i>OrderValue</i>	Property to specify the order amino acids are listed in the matrix. Enter a character string of legal amino acid characters. The length is 20 or 24 characters.

## Description

*Matrix* = blosum(*Identity*) returns a BLOSUM (**B**locks **S**ubstitution **M**atrix) 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 a structure of information (*MatrixInfo*) about a BLOSUM matrix (*Matrix*) with the fields Name, Scale, Entropy, ExpectedScore, HighestScore, LowestScore, and Order.

blosum(..., 'PropertyName', PropertyValue, ...) defines optional properties using property name/value pairs.

`blosum(..., 'Extended', ExtendedValue)`, if `Extended` is false, returns the scoring matrix for the standard 20 amino acids. Ordering of the output when `Extended` is false is

A R N D C Q E G H I L K M F P S T W Y V

`blosum(..., 'Order', OrderValue)` returns a BLOSUM matrix ordered by an amino acid sequence (*OrderString*).

**Examples**

Return a BLOSUM matrix with a value of 50.

`B50 = blosum(50)`

Return a BLOSUM matrix with the amino acids in a specific order.

`B75 = blosum(75, 'Order', 'CSTPAGNDEQHRKMILVFW')`

**See Also**

Bioinformatics Toolbox functions `dayhoff`, `gonnet`, `nalign`, `pam`, `swalign`

# celintensityread

---

**Purpose** Read probe intensities from Affymetrix CEL files (Windows 32)

**Syntax**

```
ProbeStructure = celintensityread(CELFiles, CDFFile)
ProbeStructure = celintensityread(..., 'CELPath',
CELPathValue, ...)
ProbeStructure = celintensityread(..., 'CDFPath',
CDFPathValue, ...)
ProbeStructure = celintensityread(..., 'PMOnly',
PMOnlyValue, ...)
```

## Arguments

<i>CELFiles</i>	Cell array of CEL filenames. If you set <i>CELFiles</i> to '*', then it reads all CEL files in the current directory. If you set <i>CELFiles</i> 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 <b>Ctrl</b> or <b>Shift</b> while clicking to select multiple CEL files.
<i>CDFFile</i>	String of the CDF filename. If you set <i>CDFFile</i> to ' ', then it opens the Select CDF File dialog box from which you select the CDF file.
<i>CELPathValue</i>	String of the path and directory where the files specified in <i>CELFiles</i> are stored.
<i>CDFPathValue</i>	String of the path and directory where the file specified in <i>CDFFile</i> is stored.
<i>PMOnlyValue</i>	Property to include or exclude the mismatch (MM) probe intensity values in the returned structure. Enter <code>true</code> to return only perfect match (PM) probe intensities. Enter <code>false</code> to return both PM and MM probe intensities. Default is <code>true</code> .

## Description

---

**Note** This function is supported on the Windows 32 platform only.

---

*ProbeStructure* = celintensityread(*CELFiles*, *CDFFile*) reads the specified Affymetrix CEL files and the associated CDF library file, and then creates a structure (*ProbeStructure*) containing probe intensities, probe indices, and probe set IDs. *CELFiles* is a cell array of CEL filenames. *CDFFile* is a string of a CDF filename.

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*, ...) defines optional properties that use property name/value pairs in any order. These property name/value pairs are as follows:

*ProbeStructure* = celintensityread(..., 'CELPath', *CELPathValue*, ...) lets you specify a path and directory where the files specified in *CELFiles* are stored.

*ProbeStructure* = celintensityread(..., 'CDFPath', *CDFFileValue*, ...) lets you specify a path and directory where the file specified in *CDFFile* is stored.

*ProbeStructure* = celintensityread(..., 'PMOnly', *PMOnlyValue*, ...) lets you include or exclude 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.

*ProbeStructure* contains the following fields:

# celintensityread

---

Field	Description
CDFName	Path and filename of the Affymetrix library CDF file.
CELNames	Cell array of names of the Affymetrix CEL files.
NumProbeSets	Number of probe sets in each CEL file.
ProbeSetIDs	Cell array of the probe set IDs from the Affymetrix CDF library file.
GenBankIDs	Cell array of the probe set IDs from the Affymetrix GIN library file, if available.
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.
PMIntensities	Matrix containing PM probe intensity values. Each row corresponds to a probe, and each column corresponds to a CEL file, generated from a single chip.
MMIntensities	Matrix containing MM probe intensity values. Each row corresponds to a probe, and each column corresponds to a CEL file, generated from a single chip.

## Examples

In the following 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

affyread, agferead, gprread, probelibraryinfo, probesetlink, probesetlookup, probesetplot, probesetvalues, sptread

# classperf

---

**Purpose** Evaluate performance of classifier

**Syntax**

```
classperf
cp = classperf(groundtruth)
classperf(cp, classout)
classperf(cp, classout, testidx)
cp = classperf(groundtruth, classout,...)
cp = classperf(..., 'Positive', PositiveValue,
'Negative', NegativeValue)
```

**Description** classperf provides an interface to keep track of the performance during the validation of classifiers. classperf creates and updates a classifier performance object (CP) that accumulates the results of the classifier. Later, classification standard performance parameters can be accessed using the function get or as fields in structures. Some of these performance parameters are ErrorRate, CorrectRate, ErrorDistributionByClass, Sensitivity and Specificity. classperf, without input arguments, displays all the available performance parameters.

cp = classperf(groundtruth) creates and initializes an empty object. CP is the handle to the object. groundtruth is a vector containing the true class labels for every observation. groundtruth can be a numeric vector or a cell array of strings. When used in a cross-validation design experiment, groundtruth should have the same size as the total number of observations.

classperf(cp, classout) updates the CP object with the classifier output classout. classout is the same size and type as groundtruth. When classout is numeric and groundtruth is a cell array of strings, the function grp2idx is used to create the index vector that links classout to the class labels. 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 the CP object with the classifier output classout. classout has smaller size than groundtruth, and testidx is an index vector or a logical index vector of

the same size as `groundtruth`, which indicates the observations that were used in the current validation.

`cp = classperf(groundtruth, classout, ...)` creates and updates the `CP` object with the first validation. This form is useful when you want to know the performance of a single validation.

`cp = classperf(..., 'Positive', PositiveValue, 'Negative', NegativeValue)` sets the 'positive' and 'negative' labels to identify the target disorder and the control classes. These labels are used to compute clinical diagnostic test performance. `p` and `n` must consist of disjoint sets of the labels used in `groundtruth`. For example, if

```
groundtruth = [1 2 2 1 3 4 4 1 3 3 3 2]
```

you could set

```
p = [1 2];
n = [3 4];
```

If `groundtruth` is a cell array of strings, `p` and `n` can either be cell arrays of strings or numeric vectors whose entries are subsets of `grp2idx(groundtruth)`. `PositiveValue` defaults to the first class returned by `grp2idx(groundtruth)`, while `NegativeValue` defaults to all the others. In clinical tests, inconclusive values (' ' 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 true class 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 `groundtruth` are counted as inconclusive.

## 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)
```

# classperf

---

```
% 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}
          GroundTruth: [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 `knnclassify`, `svmclassify`, `crossvalind`

Statistics Toolbox functions `grp2idx`, `classify`

# cleave

---

**Purpose** Cleave amino acid sequence with enzyme

**Syntax**

```
Fragments = cleave(SeqAA, PeptidePattern, Position)  
[Fragments, CuttingSites] = cleave(...)  
[Fragments, CuttingSites, Lengths] = cleave(...)  
cleave(..., 'PropertyName', PropertyValue,...)  
cleave(..., 'PartialDigest', PartialDigestValue)
```

## Arguments

<i>SeqAA</i>	Amino acid sequence. Enter a character string or a vector of integers from the table Mapping Amino Acid Letters to Integers on page 2-2.  Examples: 'ARN' or [1 2 3]. You can also enter a structure with the field Sequence.
<i>PeptidePattern</i>	Short amino acid sequence to search in a larger sequence. Enter a character string, vector of integers, or a regular expression.
<i>Position</i>	Position on the <i>PeptidePattern</i> where the sequence is cleaved. Enter a position within the <i>PeptidePattern</i> . Position 0 corresponds to the N terminal end of the <i>PeptidePattern</i> .
<i>PartialDigestValue</i>	Property to specify the probability that a cleavage site will be cleaved. Enter a value from 0 to 1 (default).

## Description

*Fragments* = cleave(*SeqAA*, *PeptidePattern*, *Position*) cuts an amino acid sequence (*SeqAA*) into parts at the specified cleavage site specified by a peptide pattern and position.

[*Fragments*, *CuttingSites*] = cleave(...) returns a numeric vector with the indices representing the cleave sites. A 0 (zero) is added to the list, so numel(*Fragments*)==numel(*CuttingSites*). You can

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 with the lengths of every fragment.

`cleave(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`cleave(..., 'PartialDigest', PartialDigestValue)` simulates a partial digestion where `PartialDigest` is the probability of a cleavage site being cut.

The following table lists some common proteases and their cleavage sites.

Protease	Peptide Pattern	Position
Trypsin	[KR](?!P)	1
Chymotrypsin	[WYF](?!P)	1
Glutamine C	[ED](?!P)	1
Lysine C	[K](?!P)	1
Aspartic acid N	D	1

## Example

- 1 Get a protein sequence from the GenPept database.

```
S = getgenpept('AAA59174')
```

- 2 Cleave the sequence using trypsin. Trypsin cleaves after K or R when the next residue is not P.

```
[parts, sites, lengths] = cleave(S.Sequence, '[KR](?!P)', 1);
for i=1:10
    fprintf('%5d%5d  %s\n', sites(i), lengths(i), parts{i})
end

0    6  MGTGGR
6    1   R
```

# cleave

---

```
    7  34  GAAAAPLLVAVAALLLGAAGHLYPGEVCPGMDIR
   41   5  NNLTR
   46  21  LHELENCVIEGHLQILLMFK
   67   7  TRPEDFR
   74   6  DLSFPK
   80  12  LIMITDYLLLFR
   92   8  VYGLESK
  100  10  DLFPNLTVIR
```

## See Also

Bioinformatics Toolbox functions `restrict`, `rebasecuts`, `seqshowwords`  
MATLAB function `regexp`



**Purpose** Create dendrogram and heat map

**Syntax**

```
clustergram(Data)
clustergram(..., 'PropertyName', PropertyValue,...)
clustergram(..., 'RowLabels', RowLabelsValue)
clustergram(..., 'ColumnLabels', ColumnLabelsValue)
clustergram(..., 'Pdist', PdistValue)
clustergram(..., 'Linkage', LinkageValue)
clustergram(..., 'Dendrogram', DendrogramValue)
clustergram(..., 'ColorMap', ColorMapValue)
clustergram(..., 'SymmetricRange', SymmetricRangeValue)
clustergram(..., 'Dimension', DimensionValue)
clustergram(..., 'Ratio', RatioValue)
```

## Arguments

<i>Data</i>	Matrix where each row corresponds to a gene. Each column is the result from one experiment.
<i>RowLabelsValue</i>	Property to label the rows in Data.Collabels Enter a cell array of text strings.
<i>ColumnLabelsValue</i>	Property to label the columns in Data. For example, you can enter the names of the genes. Enter a cell array of text strings.
<i>PdistValue</i>	Property to select the distance metric and pass arguments to the function pdist. The default distance metric for a clustergram is 'correlation'.
<i>LinkageValue</i>	Property to select the linkage method and pass arguments to the function linkage. The default linkage method is 'average'
<i>DendrogramValue</i>	Property to pass arguments to the function dendrogram.

# clustergram

---

<i>ColorMapValue</i>	Property to select a colormap. Enter the name or function handle of a function that returns a colormap, or an M-by-3 array containing RGB values. The default value is REDGREENCMAP.
<i>SymmetricRangValue</i>	Property to force the color range to be symmetric around zero. Enter either true (default) or false.
<i>DimensionValue</i>	Property to select either a one-dimensional or two-dimensional clustergram. Enter either 1 (default) or 2.
<i>RatioValue</i>	Property to specify the ratio of the space that the dendrogram(s) uses.

## Description

`clustergram(Data)` creates a dendrogram and heat map from gene expression data (*Data*) using hierarchical clustering with correlation as the distance metric and using average linkage to generate the hierarchical tree. The clustering is performed on the rows of data (*Data*). The rows are typically genes and the columns are the results from different microarrays. To cluster the columns instead of the rows, transpose the data using the transpose (') operator.

`clustergram(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`clustergram(..., 'RowLabels', RowLabelsValue)` uses the contents of a cell array (*RowLabelsValue*) as labels for the rows in *Data*.

`clustergram(..., 'ColumnLabels', ColumnLabelsValue)` uses the contents of a cell array (*ColumnLabelsValue*) as labels for the columns in *Data*.

`clustergram(..., 'Pdist', PdistValue)` sets the distance metric the function `pdist` uses to calculate the pairwise distances between observations. If the distance metric requires extra arguments, then pass the arguments as a cell array. For example, to use the Minkowski distance with exponent *P* you would use {'minkowski', *P*}. For

information about the available options, see the help for Statistical Toolbox function `pdist`.

`clustergram(..., 'Linkage', LinkageValue)` selects the linkage method the function `linkage` uses to create the hierarchical cluster tree. For more information about the available options, see the help for the Statistical Toolbox function `linkage`.

`clustergram(..., 'Dendrogram', DendrogramValue)` passes arguments the function `dendrogram` uses to create a dendrogram. `Dendrogram` should be a cell array of parameter name/value pairs that can be passed to `dendrogram`. For more information about the available options, see the help for the Statistical Toolbox function `dendrogram`.

`clustergram(..., 'ColorMap', ColorMapValue)` specifies the colormap (*ColorMapValue*) for the figure containing the clustergram. This controls the colors used to display the heat map.

`clustergram(..., 'SymmetricRange', SymmetricRangeValue)`, when *SymmetricRangeValue* is `false`, disables the default behavior of forcing the color scale of the heat map to be symmetric about zero.

`clustergram(..., 'Dimension', DimensionValue)` specifies whether to create a one-dimensional or two-dimensional clustergram. The one-dimensional clustergram clusters the rows of the data. The two-dimensional clustergram creates the one-dimensional clustergram, and then clusters the columns of the row-clustered data.

`clustergram(..., 'Ratio', RatioValue)` specifies the ratio of the space that the dendrogram(s) uses, relative to the size of the heat map, in the X and Y directions. If *RatioValue* is a single scalar value, it is used as the ratio for both directions. If *RatioValue* is a two-element vector, the first element is used for the X ratio, and the second element is used for the Y ratio. The Y ratio is ignored for one-dimensional clustergrams. The default ratio is 1/5.

Hold the mouse button down over the image to see the exact values at a particular point.

# clustergram

---

## Example

**1** Load filtered yeast data.

```
load filteredyeastdata;  
clustergram(yeastvalues);
```

**2** Add labels.

```
clustergram(yeastvalues, 'ROWLABELS', genes, ...  
            'COLUMNLABELS', times);
```

**3** Change the clustering parameters.

```
clustergram(yeastvalues, 'PDIST', 'euclidean', ...  
            'LINKAGE', 'complete');
```

**4** Change the dendrogram color parameter.

```
clustergram(yeastvalues, 'ROWLABELS', genes, ...  
            'DENDROGRAM', {'color', 5});
```

## See Also

Statistics Toolbox functions `cluster`, `dendrogram`, `linkage`, `pdist`

**Purpose** Calculate codon frequency for each amino acid in DNA sequence

**Syntax**

```
codonbias(SeqDNA)
codonbias(..., 'PropertyName', PropertyValue,...)
codonbias(..., 'GeneticCode', GeneticCodeValue)
codonbias(..., 'Frame', FrameValue)
codonbias(..., 'Reverse', ReverseValue)
codonbias(..., 'Pie', PieValue)
```

### Arguments

*SeqDNA* Nucleotide sequence (DNA or RNA). Enter a character string with the letters A, T or U, C, and G or a vector of integers. You can also enter a structure with the field *Sequence*. *codonbias* does not count ambiguous bases or gaps.

### Description

Many amino acids are coded by two or more nucleic acid codons. However, the probability that a codon (from the various possible codons for an amino acid) is used to code an amino acid is different between sequences. Knowing the frequency of each codon in a protein coding sequence for each amino acid is a useful statistic.

*codonbias(SeqDNA)* calculates the codon frequency in percent for each amino acid in a DNA sequence (*SeqDNA*).

*codonbias(..., 'PropertyName', PropertyValue,...)* defines optional properties using property name/value pairs.

*codonbias(..., 'GeneticCode', GeneticCodeValue)* selects an alternative genetic code (*GeneticCodeValue*). The default value is 'Standard' or 1. For a list of genetic codes, see Genetic Code on page 2-133.

*codonbias(..., 'Frame', FrameValue)* selects a reading frame (*FrameValue*). *FrameValue* can be 1 (default), 2, or 3.

# codonbias

---

`codonbias(..., 'Reverse', ReverseValue)`, when *ReverseValue* is true, returns the codon frequency for the reverse complement of the DNA sequence (*SeqDNA*).

`codonbias(..., 'Pie', PieValue)`, when *PieValue* is true, creates a figure of 20 pie charts for each amino acid.

## Example

- 1 Import a nucleotide sequence from GenBank to MATLAB. For example, get the DNA sequence that codes for a human insulin receptor.

```
S = getgenbank('M10051');
```

- 2 Calculate the codon frequency for each amino acid and plot the results.

```
cb = codonbias(S.Sequence, 'PIE', true)
```

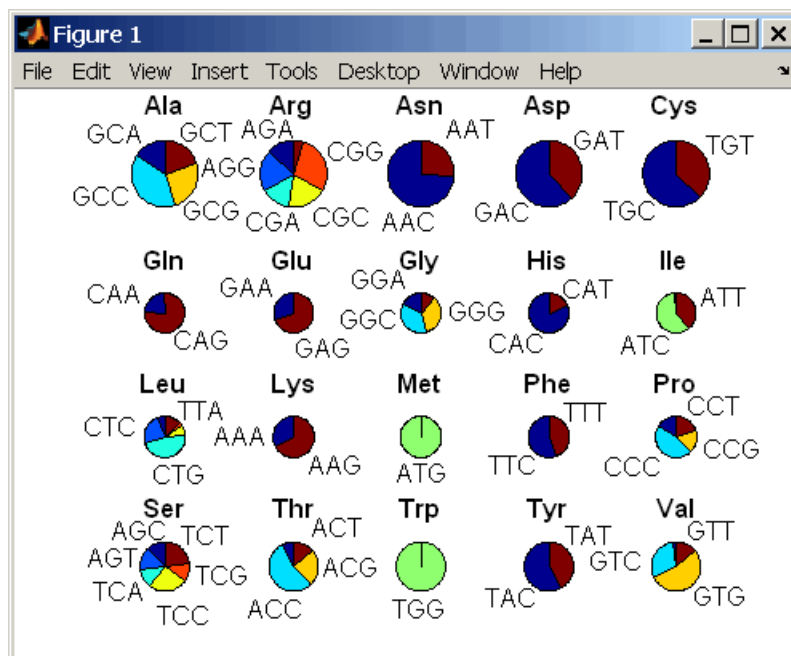
```
cb.Ala
```

```
ans =
```

```
    Codon: {'GCA' "GCC' "GCG' 'GCT'}
```

```
    Freq: [0.1600 0.3867 0.2533 0.2000]
```

MATLAB draws a figure with 20 pie charts for the 20 amino acids.



**See Also**

Bioinformatics Toolbox functions aminolookup, codoncount, geneticcode, nt2aa

# codoncount

---

**Purpose** Count codons in nucleotide sequence

**Syntax**

```
Codons = codoncount(SeqNT)
codoncount(..., 'PropertyName', PropertyValue, ...)
codoncount(..., 'Frame', FrameValue)
codoncount(..., 'Reverse', ReverseValue)
codoncount(..., 'Figure', FigureValue)
```

**Arguments**

<i>SeqNT</i>	Nucleotide sequence. Enter a character string or vector of integers. You can also enter a structure with the field Sequence.
<i>FrameValue</i>	Property to select a reading frame. Enter 1 (default), 2, or 3.
<i>ReverseValue</i>	Property to control returning the complement sequence. Enter true or false (default).
<i>FigureValue</i>	Property to control plotting a heat map. Enter either true or false (default).

**Description** *Codons = codoncount(SeqNT)* counts the number of codon in a sequence (*SeqNT*) and returns the codon counts in a structure with the fields AAA, AAC, AAG, ..., TTG, TTT.

- For sequences that have codons with the character U, the U characters are added to codons with T characters.
- If the sequence contains ambiguous nucleotide characters (R Y K M S W B D H V N), or gaps indicated with a hyphen (-), this function creates a field Others and displays a warning message.

```
Warning: Ambiguous symbols 'symbol' 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 Z), codoncount ignores the characters and displays a warning message.

```
Warning: Unknown symbols 'symbol' appear
in the sequence.
These will be ignored.
```

`[Codons, CodonArray] = codoncount(SeqNT)` returns a 4x4x4 array (*CodonArray*) with the raw count data for each codon. The three dimensions correspond to the three positions in the codon. For example, the element (2,3,4) of the array gives the number of CGT codons where A <=> 1, C <=> 2, G <=> 3, and T <=> 4.

`codoncount(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`codoncount(..., 'Frame', FrameValue)` counts the codons in a specific reading frame.

`codoncount(..., 'Reverse', ReverseValue)`, when *ReverseValue* is true, counts the codons for the reverse complement of the sequence.

`codoncount(..., 'Figure', FigureValue)`, when *FigureValue* is true displays a figure showing a heat map of the codon counts.

## Examples

Count the number of standard 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
```

## codoncount

---

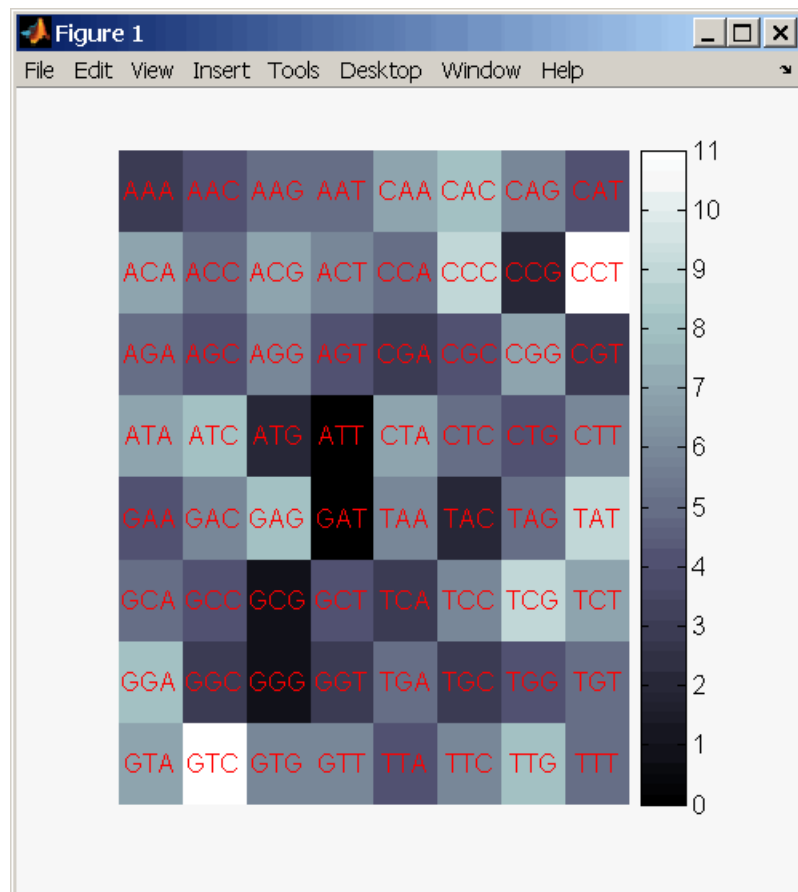
```
AGA: 0 CCC: 0 GAG: 0 GTT: 0 TTA: 0
AGC: 0 CCG: 0 GAT: 0 TAA: 0 TTC: 0
AGG: 0 CCT: 0 GCA: 0 TAC: 0 TTG: 0
AGT: 0 CGA: 0 GCC: 0 TAG: 0 TTT: 0
ATA: 0 CGC: 0 GCG: 0 TAT: 0
```

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 for the codons in a nucleotide sequence.

```
a = randseq(1000);
codoncount(a,'Figure', true);
```

**See Also**

Bioinformatics Toolbox functions `aaccount`, `basecount`, `baselookup`, `codonbias`, `dimercount`, `nmercount`, `ntdensity`, `seqrcomplement`, `seqwordcount`

# cpgisland

---

**Purpose** Locate CpG islands in DNA sequence

**Syntax**

```
cpgisland(SeqDNA)
cpgisland(..., 'PropertyName', PropertyValue,...)
cpgisland(..., 'Window', WindowValue)
cpgisland(..., 'MinIsland', MinIslandValue)
cpgisland(..., 'CpGoe', CpGoeValue)
cpgisland(..., 'GCmin', GCminValue)
cpgisland(..., 'Plot', PlotValue)
```

## Arguments

<i>SeqDNA</i>	DNA nucleotide sequence. Enter a character string with the letters A, T, C, and G. You can also enter a structure with the field <i>Sequence</i> . <i>cpgisland</i> does not count ambiguous bases or gaps.
---------------	---

## Description

*cpgisland(SeqDNA)* finds CpG islands by marking bases within a moving window of 100 DNA bases with a GC content greater than 50% and a CpGobserved/CpGexpected ratio greater than 60%.

*cpgisland(..., 'PropertyName', PropertyValue,...)* defines optional properties using property name/value pairs.

*cpgisland(..., 'Window', WindowValue)* specifies the window size for calculating GC percent and CpGobserved/CpGexpected ratios for a sequence. The default value is 100 bases. A smaller window size increases the noise in a plot.

*cpgisland(..., 'MinIsland', MinIslandValue)* specifies the minimum number of consecutive marked bases to report. The default value is 200 bases.

*cpgisland(..., 'CpGoe', CpGoeValue)* specifies the minimum CpGobserved/CpGexpected ratio in each window needed to mark a base. Enter a value between 0 and 1. The default value is 0.6. This ratio is defined as

$$\text{CPGobs/CpGexp} = (\text{NumCpGs} * \text{Length}) / (\text{NumGs} * \text{NumCs})$$

`cpgisland(..., 'GCmin', GCminValue)` specifies the minimum GC percent in a window needed to mark a base. Enter a value between 0 and 1. The default value is 0.5.

`cpgisland(..., 'Plot', PlotValue)`, when `Plot` is true, plots GC content, CpGoe content, CpG islands greater than the minimum island size, and all potential CpG islands for the specified criteria.

## Example

- 1 Import a nucleotide sequence from GenBank. For example, get a sequence from Homo Sapiens chromosome 12.

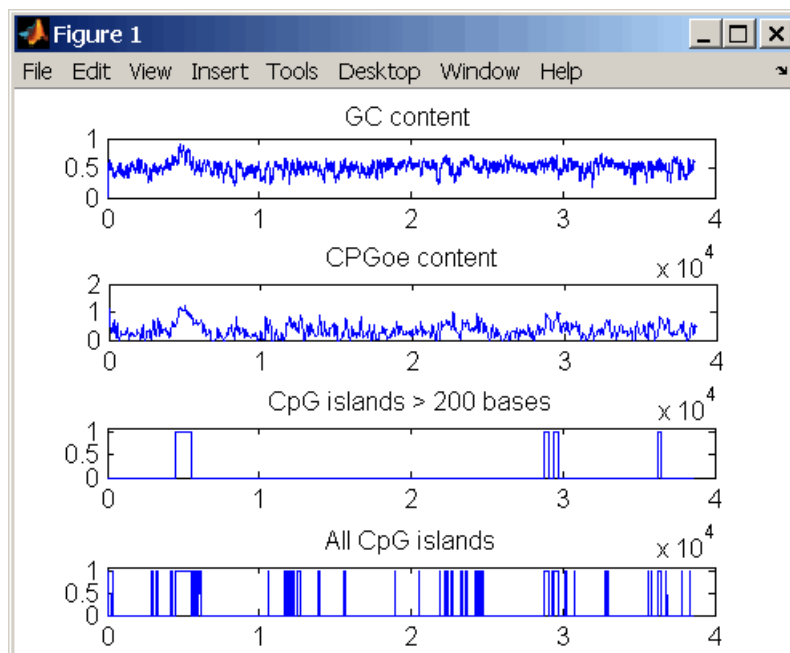
```
S = getgenbank('AC156455');
```

- 2 Calculate the CpG islands in the sequence and plot the results.

```
cpgisland(S.Sequence, 'PLOT', true)
```

MATLAB lists the CpG islands greater than 200 bases and draws a figure.

```
ans =  
Starts: [4470 28753 29347 36229]  
Stops: [5555 29064 29676 36450]
```



## 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  $Q \cdot N$  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  $(100 \cdot P)\%$ , 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.

## Example 1

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

# dayhoff

---

**Purpose** 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, pam.

**Purpose** Count dimers in sequence

**Syntax**

```
Dimers = dimercount(SeqNT)
[Dimers, Percent] = dimercount(SeqNT)
dimercount(..., 'PropertyName', PropertyValue, ...)
dimercount(..., 'Chart', ChartStyle)
```

## Arguments

<i>SeqNT</i>	Nucleotide sequence. Enter a character string or vector of integers.  Examples: 'ACGT' and [1 2 3 4]. You can also enter a structure with the field Sequence.
<i>ChartStyleValue</i>	Property to select the type of plot. Enter 'pie' or 'bar'.

## Description

*Dimers* = dimercount(*SeqNT*) counts the number of nucleotide dimers in a 1-by-1 sequence and returns the dimer counts in a structure with the fields AA, AC, AG, AT, CA, CC, CG, CT, GA, GC, GG, GT, TA, TC, TG, TT.

- For sequences that have dimers with the character U, the U characters are added to dimers with T characters.
- If the sequence contains ambiguous nucleotide characters (R Y K M S W B D H V N), or gaps indicated with a hyphen (-), this function creates a field Others and displays a warning message.

Warning: Ambiguous symbols '*symbol list*' 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 Z), codoncount ignores the characters and displays a warning message.

# dimercount

---

Warning: Unknown symbols '*symbol list*' appear in the sequence.  
These will be ignored.

`[Dimers, Percent] = dimercount(SeqNT)` returns 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.

`dimercount(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`dimercount(..., 'Chart', ChartStyle)` creates a chart showing the relative proportions of the dimers.

## Examples

Count the number of dimers in a nucleotide sequence.

```
dimercount('TAGCTGGCCAAGCGAGCTTG')
```

```
ans =  
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
```

### **See Also**

Bioinformatics Toolbox functions `aaccount`, `basecount`, `baselookup`, `codoncount`, `nmercount`, `ntdensity`

# dna2rna

---

**Purpose** Convert DNA sequence to RNA sequence

**Syntax** `SeqRNA = dna2rna(SeqDNA)`

## Arguments

*SeqDNA* DNA sequence. Enter either a character string with the characters A, T, G, C, and ambiguous characters R, Y, K, M, S, W, B, D, H, V, N, or a vector of integers from the table Mapping Nucleotide Letters to Integers on page 2-329. You can also enter a structure with the field Sequence.

*SeqRNA* RNA sequence.

**Description** `SeqRNA = dna2rna(SeqDNA)` converts a DNA sequence to an RNA sequence by converting any thymine nucleotides (T) in the DNA sequence to uracil (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** Calculate node positions and edge trajectories

**Syntax**  
`dolayout(BGobj)`  
`dolayout(..., 'PropertyName', PropertyValue, ...)`  
`dolayout(..., 'OnlyPaths', OnlyPathsValue)`

## Arguments

<i>BGobj</i>	Biograph object.
<i>OnlyPathsValue</i>	Property to control the calculation of node position and edge paths. Enter 'true' to calculate only the edge paths.

## Description

`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 following biograph object properties interact with the layout engine:

- `LayoutType` — Selects 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` — When `NodeAutoSize` is 'on', the layout engine uses the node properties `FontSize`, `Shape`, and `LayoutScale` to precalculate the actual size of every node. When `NodeAutoSize` is 'off', the layout engine uses the node property `Size`.

`dolayout(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`dolayout(..., 'OnlyPaths', OnlyPathsValue)`, when `OnlyPathsValue` is 'true', leaves the nodes at their current positions and calculates new curves for the edges.

# dolayout (biograph)

---

## Example

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)  
bg.nodes(1).Position
```

Nodes do not have a position yet.

2 Call the layout engine and render the graph.

```
dolayout(bg)  
bg.nodes(1).Position  
view(bg)
```

3 Manually modify a node position and recalculate the paths.

```
bg.nodes(1).Position = [150 150];  
dolayout(bg, 'Onlypaths', true)  
view(bg)
```

## See Also

Bioinformatics Toolbox

- `function` — `biograph` (object constructor)
- `biograph` object methods — `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `view`

MATLAB

- functions — `get`, `set`



**Purpose** Estimate synonymous and nonsynonymous substitution rates

**Syntax**

```
[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2)
dnds(..., 'PropertyName', PropertyValue,...)
dnds(..., 'GeneticCode', GeneticCodeValue)
dnds(..., 'Method', MethodValue)
```

## Arguments

<i>SeqNT1, SeqNT2</i>	Nucleotide sequences. Enter a character string or a structure with the field Sequence.
<i>GeneticCodeValue</i>	Property to select a genetic code. Enter a code number or code name from the table Genetic Code on page 2-133. If you use a code name, you can truncate the name to the first two characters of the name.
<i>MethodValue</i>	Property to select the method for calculating substitution rates. Enter 'NG', 'LWL', or 'PBL'.

## Description

`[Dn, Ds, Vardn, Vards] = dnds(SeqNT1, SeqNT2)` estimates the synonymous and nonsynonymous substitution rate per site between two homologous nucleotide sequences (*SeqNT1*, *SeqNT2*) by comparing codons using the Nei-Gojobori method. This function returns the nonsynonymous substitution rate (*Dn*), the synonymous substitution rate (*Ds*), the variance for the nonsynonymous substitution rate (*Vardn*), and the variance for the synonymous substitutions per site (*Vards*). Any codons that include gaps are excluded from calculation. This analysis considers the number of codons in the shortest sequence.

`dnds(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`dnds(..., 'GeneticCode', GeneticCodeValue)` calculates synonymous and nonsynonymous substitution rates using the specified genetic code. The default is 'Standard' or 1.

`dnds(..., 'Method', MethodValue)` allows you to calculate synonymous and nonsynonymous substitution rates using the following approaches:

'NG' — uses the Nei-Gojobori method '86 (default)

'LWL' — uses the Li-Wu-Luo method '85

'PBL' — uses the Pamilo-Bianchi-Li method '93

## References

[1] Li W, Wu C, Luo C (1984), “A new method for estimating synonymous and aonsynonymous rates of nucleotide substitution considering the relative likelihood of nucleotide and codon changes”, *Molecular Biology and Evolution*, 2(2):150-174.

[2] Nei M, 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, 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, Kumar S (2000), “Synomymous and nonsymonymous nucleotide substitutions” in *Molecular Evolution and Phylogenetics*, Oxford University Press.

[5] Pamilo P, Bianchi N (1993), “Evolution of the Zfx And Zfy genes: rates and interdependence between the genes”, *Molecular Biology and Evolution*, 10(2): 271-281.

## Example

1 Get two sequences from Genbank for the human immunodeficiency virus.

```
gag1 = getgenbank('L11768')
gag2 = getgenbank('L11770')
```

- 2 Pairwise align the sequences using the Needleman-Wunsch algorithm.

```
[sc,al]= nwalign(gag1,gag2,'alpha','nt');
```

- 3 Calculate synonymous and nonsynonymous substitution rates.

```
[dn ds vardn vards] = dnds(al(1,:), al(3,:))
```

```
dn =  
    0.0240  
ds =  
    0.0739  
vardn =  
    2.2745e-005  
vards =  
    2.6447e-004
```

## See Also

Bioinformatics Toolbox functions `dndsm1`, `geneticcode`, `nt2aa`, `seqpdist`

# dndsm1

---

**Purpose** Estimate synonymous-nonsynonymous substitution rates by the maximum likelihood method

**Syntax**  
`[Dn, Ds, Like] = dndsm1(SeqNT1, SeqNT2)`  
`dndsm1(..., 'PropertyName', PropertyValue, ...)`  
`dndsm1(..., 'GeneticCode', GeneticCodeValue)`

## Arguments

*SeqNT1, SeqNT2* Nucleotide sequences. Enter a character string or a structure with the field `Sequence`.

*GeneticCodeValue* Property to select a genetic code. Enter a code number or code name from the table Genetic Code on page 2-133. If you use a code name, you can truncate the name to the first two characters of the name.

## Description

`[Dn, Ds, Like] = dndsm1(SeqNT1, SeqNT2)` estimates synonymous and nonsynonymous substitution rates between two homologous sequences (*SeqNT1*, *SeqNT2*) by the maximum likelihood method. `dndsm1` returns the nonsynonymous substitution rate (*Dn*), the synonymous substitution rate (*Ds*), and the likelihood of this estimate (*Like*). The maximum likelihood method is best suited for sequences larger than 100 bases. Gaps are ignored in this analysis. This analysis considers the number of codons in the shortest sequence.

`dndsm1(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`dndsm1(..., 'GeneticCode', GeneticCodeValue)` calculates synonymous and nonsynonymous substitution rates using the specified genetic code. The default value is 'Standard' or 1.

## Examples

**1** Get two sequences from Genbank for the human immunodeficiency virus.

```
gag1 = getgenbank('L11768')
gag2 = getgenbank('L11770')
```

- 2** Pairwise align the sequences using the Needleman-Wunsch algorithm.

```
[sc,al]= nwalign(gag1,gag2,'alpha','nt');
```

- 3** Calculate synonymous and nonsynonymous substitution rates.

```
[dn ds like] = dndsml(al(1,:), al(3,:))
```

```
dn =  
    0.0259  
ds =  
    0.0624  
like =  
-2.1864e+003
```

## References

- [1] Tamura K, 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, Nielsen R (2000), “Estimating synonymous and nonsynonymous substitution rates under realistic evolutionary models”, *Molecular Biology and Evolution*, 17:32–43.

## See Also

Bioinformatics Toolbox functions `dnds`, `geneticcode`, `nt2aa`, `seqpdist`

# emblread

---

**Purpose** Read data from EMBL file

**Syntax**

```
EMBLData = emblread('File')  
EMBLSeq = emblread('File',  
SequenceOnly', SequenceOnlyValue)
```

## Arguments

<i>File</i>	EMBL formatted file (ASCII text file). Enter a filename, a path and filename, or a URL pointing to a file. <i>File</i> can also be a MATLAB character array that contains the text for a filename.
<i>SequenceOnlyValue</i>	Property to control reading EMBL file information. If <i>SequenceOnlyValue</i> is true, <code>emblread</code> returns only the sequence ( <i>EMBLSeq</i> ).
<i>EMBLData</i>	MATLAB structure with fields corresponding to EMBL data.
<i>EMBLSeq</i>	MATLAB character string without metadata for the sequence.

## Description

`EMBLData = emblread('File')` reads data from an EMBL formatted file (*File*) and creates a MATLAB structure (*EMBLData*) 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 for the 137.0 version contains the following fields:

Field
Comments
Identification
Accession
SequenceVersion

Field
Datecreated
Dateupdated
Description
Keyword
OrganismSpecies
OrganismClassification
Organelle
Reference.Number
Reference.Comment
Reference.Position
Reference{#}.MedLine
Referemce{#}.PubMed
Reference.Authors
Reference.Title
Reference.Location
DatabaseCrossReference
Feature
Basecount
Sequence

*EMBLSeq* = emblread ('File', SequenceOnly', *SequenceOnlyValue*),  
 when *SequenceOnlyValue* is true, reads only the sequence information.

## Examples

Get sequence information from the Web, save to a file, and then read back into MATLAB.

```
getembl('X00558','ToFile','rat_protein.txt');
EMBLData = emblread('rat_protein.txt')
```

# emblread

---

## **See Also**

Bioinformatics Toolbox functions `fastaread`, `genbankread`, `getembl`, `seqtool`



**Purpose** Calculate range of gene expression profiles

**Syntax**

```

Range = exprprofrange(Data)
[Range, LogRange] = exprprofrange(Data)
exprprofrange(..., 'PropertyName', PropertyValue,...)
exprprofrange(..., 'ShowHist', ShowHistValue)

```

## Arguments

*Data* Matrix where each row corresponds to a gene.

*ShowHistValue* Property to control displaying a histogram with range data. Enter either true (include range data) or false. The default value is false.

## Description

*Range* = `exprprofrange(Data)` calculates the range of each expression profile in a data set (*Data*).

`[Range, LogRange] = exprprofrange(Data)` returns the log range, that is,  $\log(\max(\text{prof})) - \log(\min(\text{prof}))$ , of each expression profile. If you do not specify output arguments, `exprprofrange` displays a histogram bar plot of the range.

`exprprofrange(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`exprprofrange(..., 'ShowHist', ShowHistValue)`, when *ShowHistValue* is true, displays a histogram of the range data.

## Examples

Calculate the range of expression profiles for yeast data as gene expression changes during the metabolic shift from fermentation to respiration.

```

load yeastdata
range = exprprofrange(yeastvalues, 'ShowHist', true);

```

## See Also

Bioinformatics Toolbox function `exprprofvar`, `generangefilter`

# exprprofvar

---

**Purpose** Calculate variance of gene expression profiles

**Syntax**  
*Variance* = exprprofvar(*Data*)  
exprprofvar(..., 'PropertyName', PropertyValue,...)  
exprprofvar(..., 'ShowHist', ShowHistValue)

**Arguments**

*Data* Matrix 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 a data set (*Data*). 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** Calculate the variance of expression profiles for yeast data as gene expression changes during the metabolic shift from fermentation to respiration.

```
load yeastdata  
datavar = exprprofvar(yeastvalues, 'ShowHist', true);
```

**See Also** Bioinformatics Toolbox functions exprprofrange, generangefilter, genevarfilter

**Purpose** Read data from FASTA file

**Syntax**

```
FASTAData = fastaread('File')
[Header, Sequence] = fastaread('File')
multialignread(..., 'PropertyName', PropertyValue,...)
multialignread(..., 'IgnoreGaps', IgnoreGapsValue)
```

## Arguments

<i>File</i>	FASTA formatted file (ASCII text file). Enter a filename, a path and filename, or a URL pointing to a file. <i>File</i> can also be a MATLAB character array that contains the text for a filename.
<i>IgnoreGapsValue</i>	Property to control removing gap symbols. Enter either true or false (default).
<i>FASTAData</i>	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

# fastaread

---

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.

`multialignread(..., 'PropertyName', PropertyValue, ...)` defines optional properties. 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).

`multialignread(..., 'IgnoreGaps', IgnoreGapsValue)`, when `IgnoreGapsValue` is true, removes any gap symbol ('-' or '.') from the sequences. Default is false.

## 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 function `emblread`, `fastawrite`, `genbankread`, `genpeptread`, `multialignread`, `seqprofile`, `seqtool`

<b>Purpose</b>	Write to file with FASTA format								
<b>Syntax</b>	<pre>fastawrite('File', Data) fastawrite('File', Header, Sequence)</pre>								
<b>Arguments</b>	<table><tr><td><i>File</i></td><td>Enter either a filename or a path and filename supported by your operating system. (ASCII text file).</td></tr><tr><td><i>Data</i></td><td>Enter a character string with a FASTA format, a sequence object, a structure containing the fields Sequence and Header, or a GenBank/GenPept structure.</td></tr><tr><td><i>Header</i></td><td>Information about the sequence.</td></tr><tr><td><i>Sequence</i></td><td>Nucleotide or amino acid sequence using the standard IUB/IUPAC codes. For a list of valid characters, see Mapping Amino Acid Letters to Integers on page 2-2 and Mapping Nucleotide Letters to Integers on page 2-329.</td></tr></table>	<i>File</i>	Enter either a filename or a path and filename supported by your operating system. (ASCII text file).	<i>Data</i>	Enter a character string with a FASTA format, a sequence object, a structure containing the fields Sequence and Header, or a GenBank/GenPept structure.	<i>Header</i>	Information about the sequence.	<i>Sequence</i>	Nucleotide or amino acid sequence using the standard IUB/IUPAC codes. For a list of valid characters, see Mapping Amino Acid Letters to Integers on page 2-2 and Mapping Nucleotide Letters to Integers on page 2-329.
<i>File</i>	Enter either a filename or a path and filename supported by your operating system. (ASCII text file).								
<i>Data</i>	Enter a character string with a FASTA format, a sequence object, a structure containing the fields Sequence and Header, or a GenBank/GenPept structure.								
<i>Header</i>	Information about the sequence.								
<i>Sequence</i>	Nucleotide or amino acid sequence using the standard IUB/IUPAC codes. For a list of valid characters, see Mapping Amino Acid Letters to Integers on page 2-2 and Mapping Nucleotide Letters to Integers on page 2-329.								
<b>Description</b>	<p><code>fastawrite('File', Data)</code> writes the contents of <code>Data</code> to a file with a FASTA format.</p> <p><code>fastawrite('File', Header, Sequence)</code> writes header and sequence information to a file with a FASTA format.</p>								
<b>Examples</b>	<pre>%get the sequence for the human p53 gene from GenBank. seq = getgenbank('NM_000546')  %find the CDS line in the FEATURES information. cdsline = strmatch('CDS',seq.Features)  %read the coordinates of the coding region.</pre>								

# fastawrite

---

```
[start,stop] = stread(seq.Features(cdsline,:), '%*s%d..%d')

%extract the coding region.
codingSeq = seq.Sequence(start:stop)

%write just the coding region to a FASTA file.
fastawrite('p53coding.txt', 'Coding region for p53', codingSeq);
```

Save multiple sequences.

```
data(1).Sequence = 'ACACAGGAAA'
data(1).Header = 'First sequence'
data(2).Sequence = 'ACGTCAGGTC'
data(2).Header = 'Second sequence'

fastawrite('my_sequences.txt', data)
type('my_sequences.txt')

>First sequence
ACACAGGAAA

>Second sequence
ACGTCAGGTC
```

## See Also

Bioinformatics Toolbox function `fastaread`, `seqtool`

**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.

# featuresmap

---

<i>Levels</i>	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 <i>Levels</i> = [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, <i>Levels</i> = [1:N].
<i>FontSizeValue</i>	Scalar that sets the font size (points) for the annotations of the features. Default is 9.
<i>ColorMapValue</i>	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.
<i>QualifiersValue</i>	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, <i>QualifiersValue</i> = {'gene', 'product', 'locus_tag', 'note', 'db_xref', 'protein_id'}. Provide your own <i>QualifiersValue</i> 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 2-117.
- 

*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.

# featuresmap

---

- 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.

---

# featuresmap

---

---

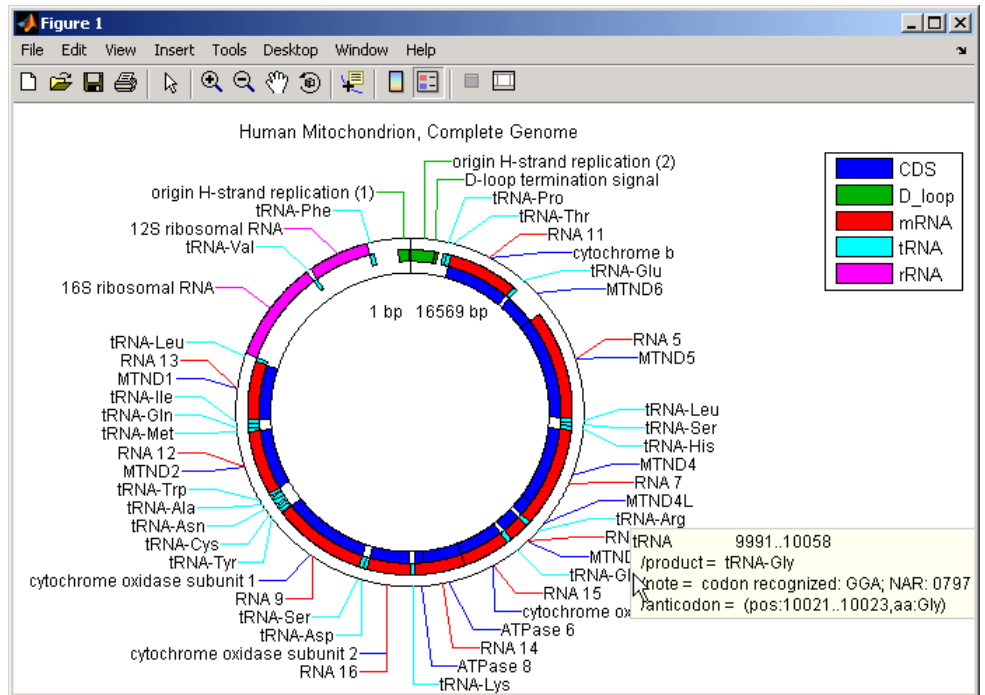
## Tip

To determine all qualifiers available for a given feature, do either of the following:

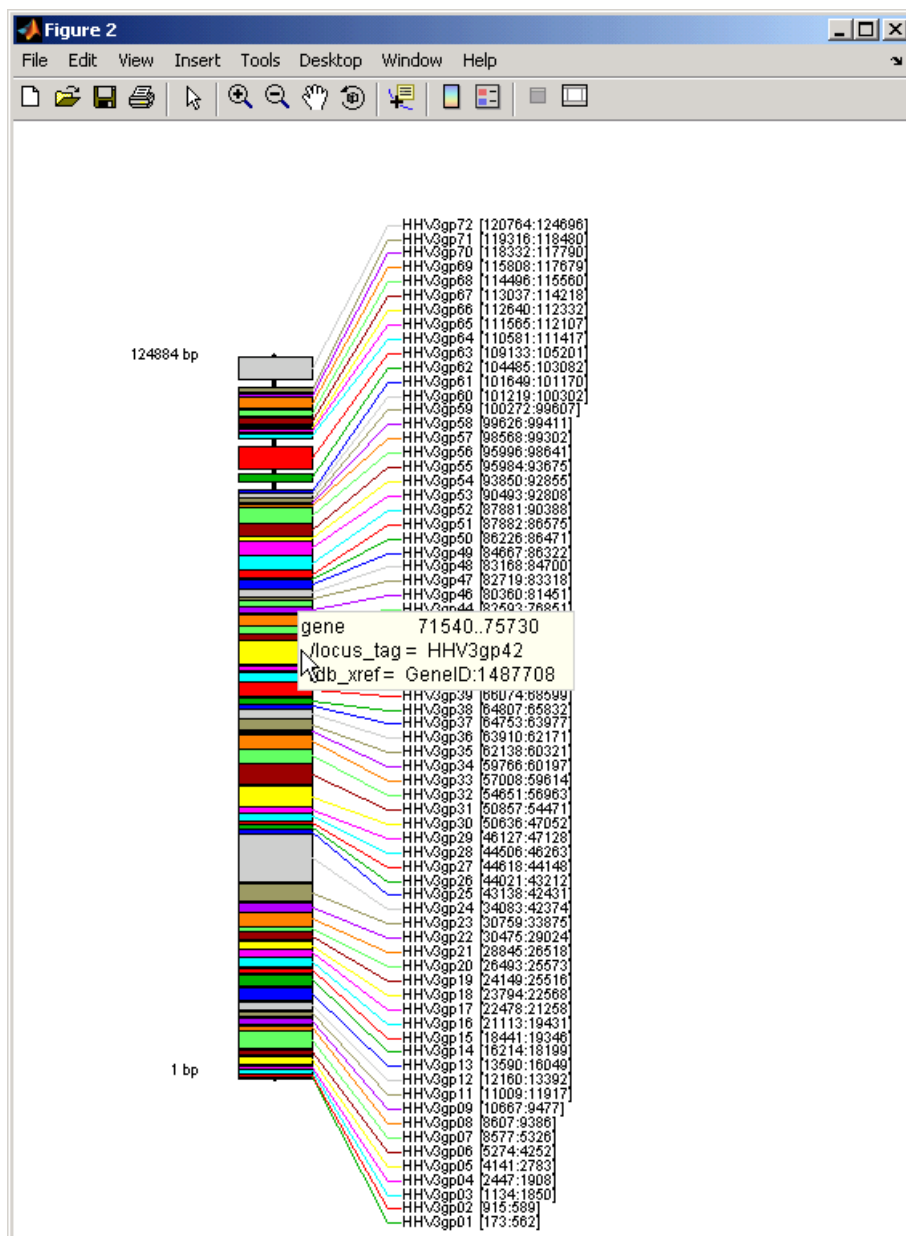
- Create the map, and then click a feature or its annotation to list all qualifiers for that feature.
- Use the `featuresparse` command to parse all the features into a new structure, and then use the `fieldnames` command to list the qualifiers for a specific feature. See [Determining Qualifiers for a Specific Feature](#) on page 2-117.

---

`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.



# featuresmap



After creating a map:

- Click a feature or annotation to display a list of all qualifiers for that feature.
- Zoom the plot by using the following buttons



## Examples

### Creating a Circular Map with 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

# featuresmap

---

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



**Purpose** Read microarray data from GenePix array list file

**Syntax** `GALData = galread('File')`

**Arguments**

*File* GenePix Array List formatted file (GAL). Enter a filename, or enter a path and filename.

**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](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](http://www.moleculardevices.com/pages/software/gn_genepix_file_formats.html)

GenePix is a registered trademark of Molecular Devices Corporation.

**See Also**

Bioinformatics Toolbox functions `affyread`, `geosoftread`, `gprread`, `imageneread`, `sptread`

# genbankread

---

**Purpose** Read data from GenBank file

**Syntax** `GenBankData = genbankread('File')`

## Arguments

<i>File</i>	GenBank formatted file (ASCII text file). Enter a filename, a path and filename, or a URL pointing to a file. <i>File</i> can also be a MATLAB character array that contains the text of a GenBank formatted file.
<i>GenBankData</i>	MATLAB structure with fields corresponding to GenBank data.

## Discussion

`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 Get sequence information for a gene (HEXA), store data in a file, and then read back into MATLAB.

```
getgenbank('nm_000520', 'ToFile', 'TaySachs_Gene.txt')
s = genbankread('TaySachs_Gene.txt')
```

```
s =
      LocusName: "NM_000520"
  LocusSequenceLength: '2255'
  LocusNumberofStrands: ''
      LocusTopology: 'linear'
   LocusMoleculeType: 'mRNA'
  LocusGenBankDivision: 'PRI'
LocusModificationDate: '23-SEP-2005'
      Definition: [1x63 char]
      Accession: 'NM_00520'
      Version: 'NM_000520.2'
```

```
GI: '13128865'  
Keywords: []  
Segment: []  
Source: [1x20 char]  
SourceOrganism: [4x65 char]  
Reference: {1x14 cell}  
Comment: [15x67 char]  
Features: [77x74 char]  
CDS: [1x1 struct]  
Sequence: [1x2255 char]
```

**2** Display the source organism for this sequence.

```
s.SourceOrganism
```

```
ans =
```

```
Homo sapiens  
Eukaryota; Metazoa; Chordata; Craniata; Vertebrata;  
Euteleostomi; Mammalia; Eutheria; Euarchontoglires;  
Primates; Catarrhini; Hominidae; Homo
```

## See Also

Bioinformatics Toolbox functions `emblread`, `fastaread`, `genpeptread`, `getgenbank`, `scfread`, `seqtool`

# geneentropyfilter

---

**Purpose** Remove genes with low entropy expression values

**Syntax**

```
Mask = geneentropyfilter(Data)
[Masks, FData] = geneentropyfilter(Data)
[Mask, FData, FNames] = geneentropyfilter(Data,Names)
geneentropyfilter(..., 'PropertyName', PropertyValue,...)
geneentropyfilter(..., 'Percentile', PercentileValue)
```

## Arguments

<i>Data</i>	Matrix where each row corresponds to the experimental results for one gene. Each column is the results for all genes from one experiment.
<i>Names</i>	Cell array with the name of a gene for each row of experimental data. <i>Names</i> has same number of rows as <i>Data</i> with each row containing the name or ID of the gene in the data set.
<i>Percentile</i>	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 than the threshold are 0.

[*Masks*, *FData*] = geneentropyfilter(*Data*) returns a filtered data matrix (*FData*). *FData* can also be created using *FData* = *Data*(find(*I*),:).

[*Mask*, *FData*, *FNames*] = geneentropyfilter(*Data*,*Names*) returns a filtered names array (*FNames*). You can also create *FNames* using *FNames* = *Names*(*I*).

geneentropyfilter(..., 'PropertyName', PropertyValue,...) defines optional properties using property name/value pairs.

`geneentropyfilter(..., 'Percentile', PercentileValue)` removes from the experimental data (*Data*) gene expression profiles with entropy values less than a given percentile (*PercentileValue*).

## References

[1] Kohane I.S., Kho A.T., Butte A.J. (2003), Microarrays for an Integrative Genomics, Cambridge, MA:MIT Press.

## Examples

```
load yeastdata
[fyeastvalues, fgenes] = geneentropyfilter(yeastvalues,genes);
```

## See Also

Bioinformatics Toolbox functions `exprprofrange`, `exprprofvar`, `genelowvalfilter`, `generangefilter`, `genevarfilter`

# genelowvalfilter

---

**Purpose** Remove gene profiles with low absolute values

**Syntax**

```
Mask = genelowvalfilter(Data)
[Mask, FData] = genelowvalfilter(Data)
[Mask, FData, FNames] = genelowvalfilter(Data, Names)
genelowvalfilter(..., 'PropertyName', PropertyValue,...)
genelowvalfilter(..., 'Prctile', PrctileValue)
genelowvalfilter(..., 'AbsValue', AbsValueValue)
genelowvalfilter(..., 'AnyVal', AnyValValue)
```

## Arguments

<i>Data</i>	Matrix where each row corresponds to the experimental results for one gene. Each column is the results for all genes from one experiment.
<i>Names</i>	Cell array with the same number of rows as <i>Data</i> . Each row contains the name or ID of the gene in the data set.
<i>PrctileValue</i>	Property to specify a percentile below which gene expression profiles are removed. Enter a value from 0 to 100.
<i>AbsValueValue</i>	Property to specify an absolute value below which gene expression profiles are removed.
<i>AnyValValue</i>	Property to select the minimum or maximum absolute value for comparison with <i>AbsValueValue</i> . If <i>AnyValValue</i> is true, selects the minimum absolute value. If <i>AnyValValue</i> 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 than the threshold are 0.

`[Mask, FData] = genelowvalfilter(Data)` returns a filtered data matrix (*FData*). You can create *FData* using `FData = Data(find(I),:)`.

`[Mask, FData, FNames] = genelowvalfilter(Data, Names)` returns a filtered names array (*FNames*), 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(I)`.

`genelowvalfilter(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`genelowvalfilter(..., 'Prctile', PrctileValue)` removes from the experimental data (*Data*) gene expression profiles with all absolute values less than a specified percentile (*Percentile*).

`genelowvalfilter(..., 'AbsValue', AbsValueValue)` calculates the maximum absolute value for each gene expression profile and removes the profiles with maximum absolute values less than *AbsValueValue*.

`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*.

## References

[1] Kohane I.S., Kho A.T., Butte A.J. (2003), *Microarrays for an Integrative Genomics*, Cambridge, MA:MIT Press.

## Examples

```
[data, labels, I, FI] = genelowvalfilter(data, labels, 'AbsValue', 5);
```

## See Also

Bioinformatics Toolbox functions `exprprofrange`, `exprprofvar`, `geneentropyfilter`, `generangefilter`, `genevarfilter`

# geneont

---

**Purpose** Create geneont object

**Syntax**

```
GeneontObj = geneont
GeneontObj = geneont('File', 'FileValue')
GeneontObj = geneont('Live',
LiveValue)
GeneontObj = geneont('Live', LiveValue, 'ToFile',
ToFileValue)
```

## Arguments

<i>FileValue</i>	Filename of an OBO formatted file that is on the MATLAB search path.
<i>LiveValue</i>	Property to create the most up-to-date geneont object. Enter true to create a geneont object ( <i>GeneontObj</i> ) from the most recent version of the Gene Ontology database. Default is false.
<i>ToFileValue</i>	Filename to which to save the geneont object from the Gene Ontology database.

## Description

*GeneontObj* = geneont searches for the file `gene_ontology.obo` in the MATLAB Current Directory and creates a geneont object.

*GeneontObj* = geneont('File', 'FileValue') creates a geneont object (*GeneontObj*) from an OBO formatted file that is on the MATLAB search path.

*GeneontObj* = geneont('Live', *LiveValue*), when *LiveValue* is true, creates a geneont object (*GeneontObj*) from the most recent version of the Gene Ontology database, which is the file at

[http://www.geneontology.org/ontology/gene\\_ontology.obo](http://www.geneontology.org/ontology/gene_ontology.obo)

---

**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 a *geneont* object (*GeneontObj*) from the file at

`http://www.geneontology.org/ontology/gene_ontology.obo`

and saves the file to a local file (*ToFileValue*).

## Method Summary

<code>geneont</code>	Create <i>geneont</i> object
<code>getancestors (geneont)</code>	Numeric IDs for ancestors of Gene Ontology term
<code>getdescendants (geneont)</code>	Numeric IDs for descendants of Gene Ontology term
<code>getmatrix (geneont)</code>	Convert <i>geneont</i> object into relationship matrix
<code>getrelatives (geneont)</code>	Numeric IDs for relatives of Gene Ontology term

## Property Summary

Property	Of Object Type	Description
<code>default_namespace</code>	<code>geneont.geneont</code>	string
<code>format_version</code>	<code>geneont.geneont</code>	string
<code>date</code>	<code>geneont.geneont</code>	string
<code>Terms</code>	<code>geneont.geneont</code>	array that contains objects of type <code>geneont.term</code>

Property	Of Object Type	Description
id	geneont.term	numeric value that corresponds to the GO ID of the GO term  <b>Tip</b> You can use the num2goid function to convert id to a GO ID string.
name	geneont.term	string representing the name of the GO term
ontology	geneont.term	string limited to 'molecular function', 'biological process', or 'cellular component'
definition	geneont.term	string that defines the GO term
synonym	geneont.term	numeric array containing GO IDs of GO terms that are synonyms of this GO term
is_a	geneont.term	numeric array containing GO IDs of GO terms that have an "is_a" relationship with this GO term
part_of	geneont.term	numeric array containing GO IDs that of GO terms that have a "part_of" relationship with this GO term
obsolete	geneont.term	Boolean value that indicates if the GO term is obsolete (1 or not obsolete (0))

## Examples

- 1 Download the Gene Ontology database from the Web into MATLAB.

```
GO = geneont('LIVE', true);
```

MATLAB creates a geneont object and displays the number of terms in the database.

```
Gene Ontology object with 20005 Terms.
```

- 2 Display information about the geneont object.

```
get(GO)
```

```
default_namespace: 'gene_ontology'  
format_version: '1.0'  
date: '01:11:2005 16:51'  
Terms: [20005x1 geneont.term]
```

- 3 Search for all GO terms in the geneont object that contain the string ribosome in the property field name and create a structure of those terms.

```
comparison = regexp(get(GO.Terms,'name'),'ribosome');  
indices = find(~cellfun('isempty',comparison));  
terms_with_ribosome = GO.Term(indices)  
23x1 struct array with fields:  
id  
name  
ontology  
definition  
synonym  
is_a  
part_of  
obsolete
```

## See Also

Bioinformatics Toolbox

- functions — geneont (object constructor), goannotread, num2goid

## geneont

---

- geneont object methods — `getancestors`, `getdescendants`, `getmatrix`, `getrelatives`

**Purpose** Remove gene profiles with small profile ranges

**Syntax**

```
Mask = generangefilter(Data)
[Maks, FData] = generangefilter(Data)
[Maks, FData, FNames] = generangefilter(Data,Names)
generangefilter(..., 'PropertyName', PropertyValue,...)
generangefilter(..., 'Percentile', PercentileValue)
generangefilter(..., 'AbsValue', AbsValueValue)
generangefilter(..., 'LOGPercentile', LOGPercentileValue)
generangefilter(..., 'LOGValue', LOGValueValue)
```

## Arguments

<i>Data</i>	Matrix where each row corresponds to the experimental results for one gene. Each column is the results for all genes from one experiment.
<i>Names</i>	Cell array with the name of a gene for each row of experimental data. <i>Names</i> has same number of rows as <i>Data</i> with each row containing the name or ID of the gene in the data set.
<i>PercentileValue</i>	Property to specify a percentile below which gene expression profiles are removed. Enter a value from 0 to 100.
<i>AbsValueValue</i>	Property to specify an absolute value below which gene expression profiles are removed.
<i>LOGPercentileValue</i>	Property to specify the LOG of a percentile.
<i>LOGValueValue</i>	Property to specify the LOG of an absolute value.

**Description** *Mask* = generangefilter(*Data*) calculates the range for each gene expression profile in the experimental data (*Data*), and then identifies the expression profiles with ranges less than the 10th percentile.

# generangefilter

---

*Mask* is a logical vector with one element for each row in *Data*. The elements of *Mask* corresponding to rows with a range greater than the threshold have a value of 1, and those with a range less than the threshold are 0.

`[Maks, FData] = generangefilter(Data)` returns a filtered data matrix (*FData*). *FData* can also be created using `FData = Data(find(I),:)`.

`[Maks, FData, FNames] = generangefilter(Data,Names)` returns a filtered names array (*FNames*), where *Names* is a cell array with the names of the genes corresponding to each row in *Data*. You can also create *FNames* using `FNames = Names(I)`.

`generangefilter(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`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*.

## References

[1] Kohane I.S., Kho A.T., Butte A.J. (2003), Microarrays for an Integrative Genomics, Cambridge, MA:MIT Press.

## Examples

```
load yeastdata
[mask, fyeastvalues, fgenes] = generangefilter(yeastvalues,genes);
```

## See Also

Bioinformatics Toolbox functions `exprprofrange`, `exprprofvar`, `geneentropyfilter`, `genelowvalfilter`, `genevarfilter`

**Purpose** Nucleotide codon to amino acid mapping

**Syntax** `Map = geneticcode`  
`geneticcode(GeneticCode)`

**Arguments**

*GeneticCode* Enter a code number or code name from the table Genetic Code on page 2-133 below. If you use a code name, you can truncate the name to the first two characters of the name.

**Genetic Code**

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

# geneticcode

---

Code Number	Code Name	Code Number	Code Name
9	Echinoderm Mitochondrial	22	Scenedesmus Obliquus Mitochondrial
10	Euplotid Nuclear	23	Thraustochytrium Mitochondrial
11	Bacterial and Plant Plastid		

## Description

*Map* = geneticcode returns a structure with a mapping of nucleotide codons to amino acids for the standard genetic code.

geneticcode(*GeneticCode*) returns a structure of the mapping for alternate genetic codes, where *GeneticCode* is either the `transl_table` (code) number from the NCBI Genetics Web page (<http://www.ncbi.nlm.nih.gov/Taxonomy/Utils/wprintgc.cgi?mode=c>) or one of the supported names in the genetic code table above.

## Examples

List the mapping of nucleotide codons to amino acids for a specific genetic code.

```
wormcode = geneticcode('Flatworm Mitochondrial');
```

## See Also

Bioinformatics Toolbox functions `aa2nt`, `aminolookup`, `baselookup`, `codonbias`, `dnds`, `dndsml`, `nt2aa`, `revgeneticcode`, `seqshoworfs`, `seqtool`



**Purpose** Filter genes with small profile variance

**Syntax**

```
Mask = genevarfilter(Data)
[Mask, FData] = genevarfilter(Data)
[Mask, FData, FNames] = genevarfilter(Data,Names)
genevarfilter(..., 'PropertyName', PropertyValue,...)
genevarfilter(..., 'Percentile', PercentileValue)
genevarfilter(..., 'AbsValue', AbsValValue)
```

## Arguments

<i>Data</i>	Matrix where each row corresponds to a gene. The first column is the names of the genes, and each additional column is the results from an experiment.
<i>Names</i>	Cell array with the name of a gene for each row of experimental data. <i>Names</i> has same number of rows as <i>Data</i> with each row containing the name or ID of the gene in the data set.
<i>Percentile</i>	Property to specify a percentile below which gene expression profiles are removed. Enter a value from 0 to 100.
<i>AbsValue</i>	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.

# genevarfilter

---

`[Mask, FData] = genevarfilter(Data)` returns the filtered data matrix (*FData*). You can also create *FData* using `FData = Data(find(I),:)`.

`[Mask, FData, FNames] = genevarfilter(Data,Names)` returns a filtered names array (*FNames*). *Names* is a cell array of the names of the genes corresponding to each row of *Data*. *FNames* can also be created using `FNames = Names(I)`.

`genevarfilter(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`genevarfilter(..., 'Percentile', PercentileValue)` removes from the experimental data (*Data*) gene expression profiles with a variance less than the percentile (*Percentile*).

`genevarfilter(..., 'AbsValue', AbsValValue)` removes from *Data* gene expression profiles with a variance less than *AbsValue*.

## References

[1] Kohane I.S., Kho A.T., Butte A.J. (2003), *Microarrays for an Integrative Genomics*, Cambridge, MA:MIT Press.

## Examples

```
load yeastdata
[fyeastvalues, fgenes] = genevarfilter(yeastvalues,genes);
```

## 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 filename, a path and filename, 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 recently changed the name of their protein search engine from GenPept to Entrez Protein. However, the function names in the Bioinformatics Toolbox (getgenpept, 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

Get sequence information for the protein coded by the gene HEXA, save to a file, and then read back into MATLAB.

```
getgenpept('p06865', 'ToFile', 'TaySachs_Protein.txt')
genpeptread('TaySachs_Protein.txt')
```

## See Also

Bioinformatics Toolbox functions `fastaread`, `genbankread`, `getgenpept`, `pdbread`, `seqtool`

# geosoftread

---

**Purpose** Read data from Gene Expression Omnibus (GEO) SOFT Sample (GSM) file

**Syntax** `GEOSOFTData = geosoftread('File')`

**Arguments**

<i>File</i>	Gene Expression Omnibus (GEO) formatted file (ASCII text file). Enter a filename, a path and filename, or a URL pointing to a file. <i>File</i> can also be a MATLAB character array that contains the text of a GEO file.
-------------	--

**Description** `GEOSOFTData = geosoftread('File')` reads data from a Gene Expression Omnibus (GEO) SOFT formatted Sample (GSM) file (*File*), and creates a MATLAB structure (*GEOSOFTdata*) with the following fields:

Fields
Scope
Accession
Header
ColumnDescriptions
ColumnNames
Data

Fields correspond to the GenBank keywords. Each separate entry listed in *File* is stored as a separate element of the structure.

---

**Note** Currently, the Bioinformatics Toolbox supports only Sample (GSM) records.

---

## Examples

Get data from the GEO Web site and save it to a file.

```
geodata = getgeodata('GSM3258','ToFile','GSM3258.txt');
```

Use geosoftread to access a local copy from disk instead of accessing it from the GEO Web site.

```
geodata = geosoftread('GSM3258.txt')
```

## See Also

Bioinformatics Toolbox functions galread, getgeodata, gprread, sptread

# get (phytree)

---

**Purpose** 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 = phytread('pf00002.tree')
```

- 2 Get the names of the leafs.

```
protein_names = get(tr, 'LeafNames')
```

```
protein_names =
```

```
    'BAI2_HUMAN/917-1197'
```

```
    'BAI1_HUMAN/944-1191'
```

```
    '000406/622-883'
```

```
    ...
```

## See Also

Bioinformatics Toolbox

- functions — `phytree` (object constructor), `phytreeread`
- `phytree` object methods — `getbyname`, `select`

# getancestors (biograph)

---

**Purpose** Find ancestors in biograph object

**Syntax**  
`Nodes = getancestors(BiographNode)`  
`Nodes = getancestors(BiographNode, NumGenerations)`

## Arguments

<i>BiographNode</i>	Node in a biograph object.
<i>NumGenerations</i>	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*).

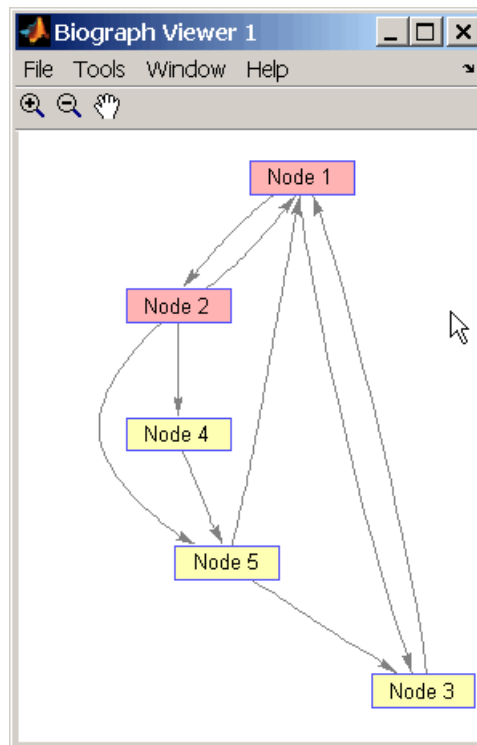
## Examples

**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;
```

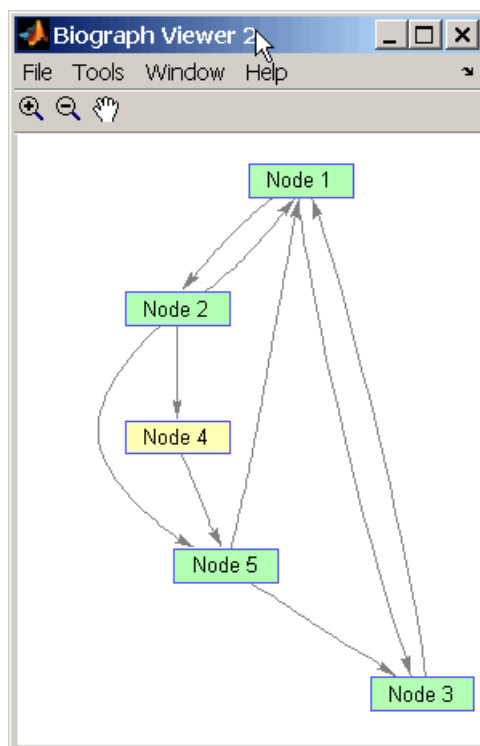


**3** Find two generations of ancestors for node 2.

```
ancNodes = getancestors(bg.nodes(2),2);  
set(ancNodes,'Color',[.7 1 .7]);  
bg.view;
```

# getancestors (biograph)

---



## See Also

Bioinformatics Toolbox

- `function` — `biograph` (object constructor)
- `biograph` object methods — `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `view`

MATLAB

- `functions` — `get`, `set`

## Purpose

Numeric IDs for ancestors of Gene Ontology term

## Syntax

```
AncestorIDs = getancestors(GeneontObj, ID)
AncestorIDs = getancestors(..., 'Height', HeightValue, ...)
```

## Description

*AncestorIDs* = `getancestors(GeneontObj, ID)` returns the numeric IDs (*AncestorIDs*) for the ancestors of a term (*ID*) including the ID for the term. *ID* is a nonnegative integer or a numeric vector with a set of IDs.

*AncestorIDs* = `getancestors(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

*AncestorIDs* = `getancestors(..., 'Height', HeightValue, ...)` searches up through a specified number of levels (*HeightValue*) in the Gene Ontology database. *HeightValue* is a positive integer. Default is Inf.

## Examples

- 1 Download the Gene Ontology database from the Web into MATLAB.

```
GO = geneont('LIVE', true);
```

MATLAB creates a `geneont` object and displays the number of terms in the database.

```
Gene Ontology object with 20005 Terms.
```

- 2 Get the ancestors for a Gene Ontology term.

```
ancestors = getancestors(GO,46680)
```

```
ancestors =
    8150
    9628
    9636
   17085
   42221
```

## getancestors (geneont)

---

```
46680  
50896
```

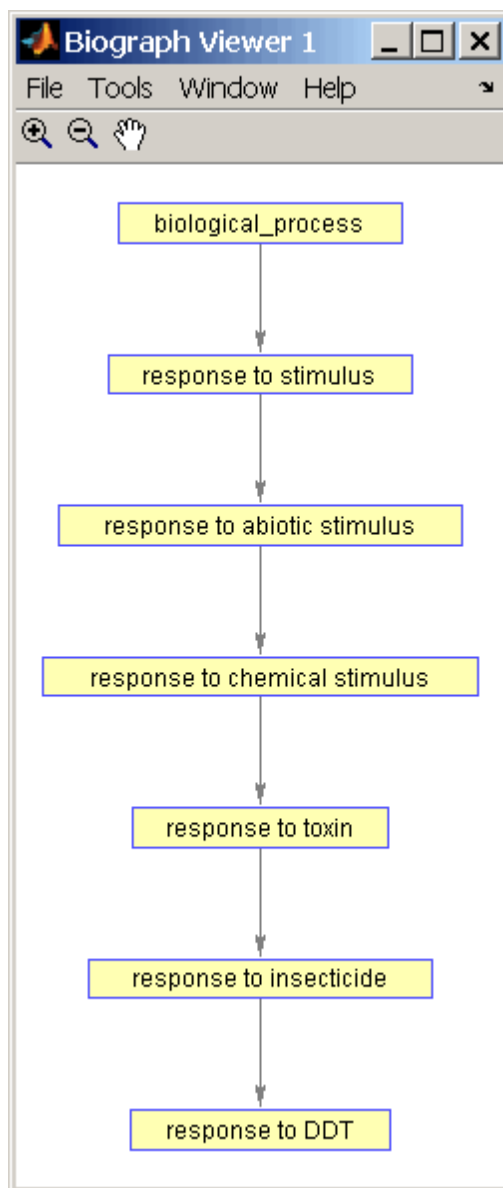
### 3 Create a sub Gene Ontology.

```
subontology = GO(ancestors)
```

Gene Ontology object with 7 Terms.

### 4 View relationships using the biograph functions.

```
[cm acc rels] = getmatrix(subontology);  
BG = biograph(cm, get(subontology.Terms, 'name'))  
view(BG)
```



## getancestors (geneont)

---

### See Also

Bioinformatics Toolbox

- functions — geneont (object constructor), goannotread, num2goid
- geneont object methods — getdescendants, getmatrix, getrelatives



**Purpose**

BLAST report from NCBI Web site

**Syntax**

```
Data = getblast(RID)
getblast(..., 'PropertyName', PropertyValue,...)
getblast(..., 'Descriptions', DescriptionsValue)
getblast(..., 'Alignments', AlignmentsValue)
getblast(..., 'ToFile', ToFileValue)
getblast(..., 'FileFormat', FileFormatValue)
getblast(..., 'WaitTilReady', WaitTilReadyValue)
```

**Arguments**

<i>RID</i>	BLAST Request ID ( <i>RID</i> ) from the function <code>blastncbi</code> .
<i>DescriptionsValue</i>	Property to specify the number of descriptions in a report.
<i>AlignmentsValue</i>	Property to select the number of alignments in a report. Enter values from 1 to 100. The default value is 50.
<i>ToFileValue</i>	Property to specify a filename for saving report data.
<i>FileFormatValue</i>	Property to select the format of the file named in <i>ToFileValue</i> . Enter either 'TEXT' or 'HTML'. The default value is 'TEXT'.

**Description**

BLAST (**B**asic **L**ocal **A**lignment **S**earch **T**ool) reports offer a fast and powerful comparative analysis of interesting protein and nucleotide sequences against known structures in existing online databases. `getblast` parses NCBI BLAST reports, including BLASTN, BLASTP, BLASTX, TBLASTN, TBLASTX, and psi-BLAST.

# getblast

---

`Data = getblast(RID)` reads a BLAST Request ID (*RID*) and returns the report data in a structure (*Data*). The NCBI Request ID (*RID*) must be a recently generated report because NCBI purges reports after 24 hours.

`getblast(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`getblast(..., 'Descriptions', DescriptionsValue)` includes the specified number of descriptions (*DescriptionsValue*) in the report.

`getblast(..., 'Alignments', AlignmentsValue)` includes the specified number of alignments in the report.

`getblast(..., 'ToFile', ToFileValue)` saves the data returned from the NCBI BLAST report to a file (*ToFileValue*). The default format for the file is text, but you can specify HTML with the property `FileFormat`.

`getblast(..., 'FileFormat', FileFormatValue)` returns the report in the specified format (*FileFormatValue*).

`getblast(..., 'WaitTilReady', WaitTilReadyValue)` pauses MATLAB and waits a specified time for a report from the NCBI Web site. If the report is still not available after the wait time (*WaitTilReadyValue*), `getblast` returns an error message. The default behavior is to not wait for a report.

For more information about reading and interpreting BLAST reports, see

<http://www.ncbi.nlm.nih.gov/Education/BLASTinfo/tut1.html>

## Example

- 1 Run a BLAST search with an NCBI accession number.

```
RID = blastncbi('AAA59174','blastp','expect',1e-10)
```

- 2 Pass the RID to GETBLAST to parse the report, load it into a MATLAB structure, and save a copy as a text file.

```
report = getblast(RID,'TOFILE','Report.txt')
```

**See Also**      Bioinformatics Toolbox functions `blastncbi`, `blastread`

# getbyname (phytree)

---

**Purpose** Branches and leaves from phytree object

**Syntax**  
`S = getbyname(Tree, Expression)`  
`S = getbyname(Tree, String,`  
`'Exact', true)`

## Arguments

<i>Tree</i>	Phytree object created with the function <code>phytree</code> .
<i>Expression</i>	Regular expression. When <i>Expression</i> is a cell array of strings, <code>getbyname</code> returns a matrix where every column corresponds to every query in <i>Expression</i> . For information about the symbols that you can use in a matching regular expression, see the MATLAB function <code>regexp</code> .
<i>String</i>	Char string or cell array of char strings.

## Description

`S = getbyname(Tree, Expression)` returns a logical vector (*S*) of size `NumNodes-by-1` with the node names of a phylogenetic tree (*Tree*) that match the regular expression (*Expression*) regardless of letter case.

`S = getbyname(Tree, String, 'Exact', true)` looks for exact string matches and ignores case. When *String* is a cell array of char strings, `getbyname` returns a vector with indices.

## Examples

**1** Load a phylogenetic tree created from a protein family.

```
tr = phytread('pf00002.tree');
```

**2** Select all the 'mouse' and 'human' proteins.

```
sel = getbyname(tr,{'mouse','human'});  
view(tr,any(sel,2));
```

## See Also

Bioinformatics Toolbox

- `function` — `phytree` (object constructor)

- phytree object methods — get, prune, select

# getcanonical (phytree)

---

**Purpose** Calculate canonical form of phylogenetic tree

**Syntax**  
`Pointers = getcanonical(Tree)`  
`[Pointers, Distances, Names] = getcanonical(Tree)`

## Arguments

*Tree* Phytree object created with the function `phytree`.

## 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`
- `phytree` object methods — `getbyname`, `select`, `subtree`

# getdescendants (biograph)

---

**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.

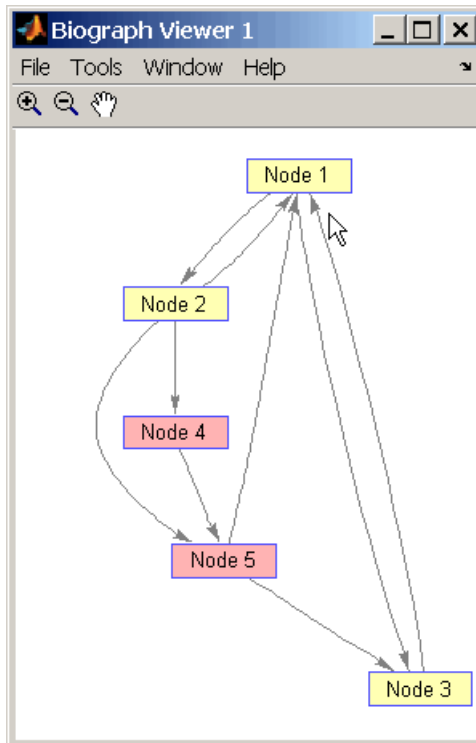
```
cm = [0 1 1 0 0;1 0 0 1 1;1 0 0 0 0;0 0 0 0 1;1 0 1 0 0];  
bg = biograph(cm)
```

**2** Find one generation of descendants for node 4.

```
desNodes = getdescendants(bg.nodes(4));  
set(desNodes, 'Color', [1 .7 .7]);  
bg.view;
```



# getdescendants (biograph)

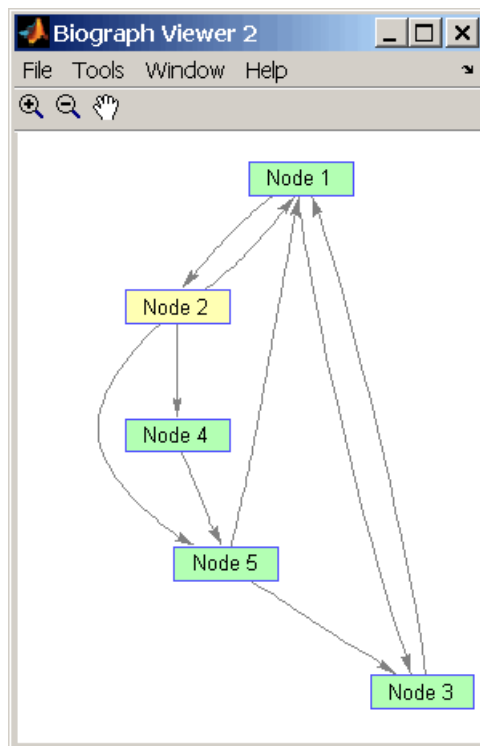


- 3** Find two generations of descendants for node 4.

```
desNodes = getdescendants(bg.nodes(4),2);  
set(desNodes,'Color',[.7 1 .7]);  
bg.view;
```

# getdescendants (biograph)

---



## See Also

Bioinformatics Toolbox

- `function` — `biograph` (object constructor)
- `biograph` object methods — `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `view`

MATLAB

- functions — `get`, `set`

**Purpose** Numeric IDs for descendants of Gene Ontology term

**Syntax**  
*DescendantIDs* = getdescendants(*GeneontObj*, *ID*)  
*DescendantIDs* = getdescendants(..., 'Depth', *DepthValue*,...)

**Description** *DescendantIDs* = getdescendants(*GeneontObj*, *ID*) returns the numeric IDs (*DescendantIDs*) for the descendants of a term (*ID*) including the ID for the term. *ID* is a nonnegative integer or a numeric vector with a set of IDs.

*DescendantIDs* = getdescendants(..., 'PropertyName', *PropertyValue*,...) defines optional properties using property name/value pairs.

*DescendantIDs* = getdescendants(..., 'Depth', *DepthValue*,...) searches down through a specified number of levels (*DepthValue*) in the Gene Ontology. *DepthValue* is a positive integer. Default is Inf.

**Examples** **1** Download the Gene Ontology database from the Web into MATLAB.

```
GO = geneont('LIVE', true);
```

MATLAB creates a geneont object and displays the number of terms in the database.

```
Gene Ontology object with 20005 Terms.
```

**2** Get the ancestors for a Gene Ontology term.

```
descendants = getdescendants(GO,5622, 'Depth', 5)
```

**3** Create a sub Gene Ontology.

```
subontology = GO(descendants)
```

```
Gene Ontology object with 1071 Terms.
```

## getdescendants (geneont)

---

### See Also

Bioinformatics Toolbox

- functions — geneont (object constructor), goannotread, num2goid
- geneont object methods — getancestors, getmatrix, getrelatives

**Purpose** Handles to edges in biograph object

**Syntax** `Edges = getedgesbynodeid(BGobj, SourceIDs, SinkIDs)`

## Arguments

<i>BGobj</i>	Biograph object.
<i>SourceIDs</i> , <i>SinkIDs</i>	Enter a cell string, or an empty cell array (gets all edges).

## Description

`Edges = getedgesbynodeid(BGobj, SourceIDs, SinkIDs)` gets the edge handles that connect the specified source nodes (*SourceIDs*) to the specified sink nodes (*SinkIDs*).

## Example

**1** Create a biograph object for the Hominidae family.

```
species = {'Homosapiens', '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 Homosapiens 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]);
```

## getedgesbynodeid (biograph)

---

```
bg.view;
```

### See Also

Bioinformatics Toolbox

- function — biograph (object constructor)
- biograph object methods — dolayout, getancestors, getdescendants, getedgesbynodeid, getnodesbyid, getrelatives, view

MATLAB

- functions — get, set

**Purpose** Sequence information from EMBL database

**Syntax**

```
Data = getembl('AccessionNumber')
getembl(..., 'PropertyName', PropertyValue,...)
getembl(..., 'ToFile', ToFileValue)
getembl(..., 'SequenceOnly', SequenceOnlyValue)
```

## Arguments

<i>AccessionNumber</i>	Unique identifier for a sequence record. Enter a unique combination of letters and numbers.
<i>ToFileValue</i>	Property to specify the location and filename for saving data. Enter either a filename or a path and filename supported by your system (ASCII text file).
<i>SequenceOnlyValue</i>	Property to control getting a sequence without the metadata. Enter either true or false (default).

## 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-Bank database, see

<http://www.ebi.ac.uk/embl/Documentation/index.html>

`Data = getembl('AccessionNumber')` searches for the accession number in the EMBL database (<http://www.ebi.ac.uk/embl>) and returns a MATLAB structure containing the following fields:

### Field

Comments
Identification
Accession

Field
SequenceVersion
DateCreated
DateUpdated
Description
Keyword
OrganismSpecies
OrganismClassification
Organelle
Reference
DatabaseCrossReference
Feature
BaseCount
Sequence

`getembl(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`getembl(..., 'ToFile', ToFileValue)` returns a structure containing information about the sequence and saves the information in a file using an EMBL data format. If you do not give a location or path to the file, the file is stored in the MATLAB current directory. Read an EMBL formatted file back into MATLAB using the function `emblread`.

`getembl(..., 'SequenceOnly', SequenceOnlyValue)`, if `SequenceOnlyValue` is true, returns the sequence information without the metadata.

## Examples

Retrieve data for the rat liver apolipoprotein A-I.

```
emblout = getembl('X00558')
```



Retrieve data for the rat liver apolipoprotein and save in the file `rat_protein`. If a filename is given without a path, the file is stored in the current directory.

```
Seq = getembl('X00558', 'ToFile', 'c:\project\rat_protein.txt')
```

Retrieve only the sequence for the rat liver apolipoprotein.

```
Seq = getembl('X00558', 'SequenceOnly', true)
```

**See Also**

Bioinformatics Toolbox functions `emblread`, `getgenbank`, `getgenpept`, `getpdb`, `seqtool`

# getgenbank

---

**Purpose** Sequence information from GenBank database

**Syntax**

```
Data = getgenbank('AccessionNumber')
getgenbank('AccessionNumber')
getgenbank(..., 'PropertyName', PropertyValue,...)
getgenbank(..., 'ToFile', ToFileValue)
getgenbank(..., 'FileFormat', FileFormatValue)
getgenbank(..., 'SequenceOnly', SequenceOnlyValue)
```

## Arguments

<i>AccessionNumber</i>	Unique identifier for a sequence record. Enter a unique combination of letters and numbers.
<i>ToFileValue</i>	Property to specify the location and filename for saving data. Enter either a filename or a path and filename supported by your system (ASCII text file).
<i>FileFormatValue</i>	Property to select the format for the file specified with the property <i>ToFileValue</i> . Enter either 'GenBank' or 'FASTA'.
<i>SequenceOnlyValue</i>	Property to control getting the sequence only. Enter either true or false.

**Description** getgenbank retrieves nucleotide and amino acid sequence 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. If an error occurs while retrieving the GenBank formatted information, then an attempt is made to retrieve the FASTA formatted data.

`getgenbank('AccessionNumber')` displays information in the MATLAB Command Window without returning data to a variable. The displayed information includes hyperlinks to the URLs for searching and retrieving data.

`getgenbank(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`getgenbank(..., 'ToFile', ToFileValue)` saves the data returned from GenBank in a file. If you do not give a location or path to the file, the file is stored in the MATLAB current directory. Read a GenBank formatted file back into MATLAB using the function `genbankread`.

`getgenbank(..., 'FileFormat', FileFormatValue)` returns the sequence in the specified format (*FileFormatValue*).

`getgenbank(..., 'SequenceOnly', SequenceOnlyValue)` when `SequenceOnly` is true, returns only the sequence as a character array. When the properties `SequenceOnly` and `ToFile` are used together, the output file is in the FASTA format.

## Examples

Retrieve the sequence from chromosome 19 that codes for the human insulin receptor and store it in a structure.

**1** 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 co
        Accession: 'M10051'
        Version: 'M10051.1'
```

# getgenbank

---

```
GI: '186439'  
Keywords: 'insulin receptor; tyrosine kinase.'  
Segment: []  
Source: 'Homo sapiens (human)'  
SourceOrganism: [3x65 char]  
Reference: {[1x1 struct]}  
Comment: [14x67 char]  
Features: [51x74 char]  
CDS: [139 4287]  
Sequence: [1x4723 char]  
SearchURL: [1x105 char]  
RetrieveURL: [1x95 char]
```

## See Also

Bioinformatics Toolbox functions `genbankread`, `getembl`, `getgenpept`, `getpdb`, `seqtool`

**Purpose** Sequence information from GenPept database

**Syntax**

```
Data = getgenpept('AccessionNumber')
getgenpept(...)
getgenpept(..., 'PropertyName', PropertyValue, ...)
getgenpept(..., 'ToFile', ToFileValue)
getgenpept(..., 'FileFormat', FileFormatValue)
getgenpept(..., 'SequenceOnly', SequenceOnlyValue)
```

## Arguments

<i>AccessionNumber</i>	Unique identifier for a sequence record. Enter a combination of letters and numbers.
<i>ToFileValue</i>	Property to specify the location and filename for saving data. Enter either a filename or a path and filename supported by your system (ASCII text file).
<i>FileFormatValue</i>	Property to select the format for the file specified with the property <i>ToFileValue</i> . Enter either 'GenBank' or 'FASTA'.
<i>SequenceOnlyValue</i>	Property to control getting the sequence without metadata. Enter either true or false.

## Description

getgenpept retrieves a protein (amino acid) sequence and sequence information from the database GenPept. This database is a translation of the nucleotide sequences in GenBank and is maintained by the National Center for Biotechnology Information (NCBI).

---

**Note** NCBI has recently changed the name of their protein search engine from GenPept to Entrez Protein. However, the function names in the Bioinformatics Toolbox (getgenpept, genpeptread) are unchanged representing the still-used GenPept report format.

---

For more details about the GenBank database, see

# getgenpept

---

<http://www.ncbi.nlm.nih.gov/Genbank/>

`Data = getgenpept('AccessionNumber')` searches for the accession number in the GenPept database and returns a MATLAB structure containing for the sequence. If an error occurs while retrieving the GenBank formatted information, then an attempt is made to retrieve the FASTA formatted data.

`getgenpept(...)` displays the information to the screen 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, ...)` defines optional properties using property name/value pairs.

`getgenpept(..., 'ToFile', ToFileValue)` saves the information in a file. If you do not give a location or path to the file, the file is stored in the MATLAB current directory. Read a GenPept formatted file back into MATLAB using the function `genpeptread`

`getgenpept(..., 'FileFormat', FileFormatValue)` returns the sequence in the specified format `FileFormatValue`.

`getgenpept(..., 'SequenceOnly', SequenceOnlyValue)` returns only the sequence information without the metadata if `SequenceOnlyValue` is true. When the properties `SequenceOnly` and `ToFile` are used together, the output file is in the FASTA format.

## Examples

Retrieve the sequence for the human insulin receptor and store it in structure `Seq`.

```
Seq = getgenpept('AAA59174')
```

## See Also

Bioinformatics Toolbox functions `genpeptread`, `getembl`, `getgenbank`, `getpdb`

**Purpose** Retrieve Gene Expression Omnibus (GEO) Sample (GSM) data

**Syntax**

```
Data = getgeodata('AccessionNumber')
getgeodata(..., 'PropertyName', PropertyValue,...)
getgeodata(..., 'ToFile', ToFileValue)
```

## Arguments

<i>AccessionNumber</i>	Unique identifier for a sequence record. Enter a combination of letters and numbers.
<i>ToFileValue</i>	Property to specify the location and filename for saving data. Enter either a filename, or a path and filename supported by your system (ASCII text file).

## Description

*Data = getgeodata('AccessionNumber')* searches for the accession number in the Gene Expression Omnibus database and returns a MATLAB structure containing the following fields:

Field
Scope
Accession
Header
ColumnDescriptions
ColumnNames
Data

*getgeodata(..., 'PropertyName', PropertyValue,...)* defines optional properties using property name/value pairs.

*getgeodata(..., 'ToFile', ToFileValue)* saves the data returned from the database to a file. Read a GenPept formatted file back into MATLAB using the function `gensoftread`.

---

**Note** Currently, the Bioinformatics Toolbox supports only Sample (GSM) records.

---

For more information, see

<http://www.ncbi.nlm.nih.gov/About/disclaimer.html>

## Examples

```
geoStruct = getgeodata('GSM1768')
```

## See Also

Bioinformatics Toolbox functions `geosoftread`, `getgenbank`, `getgenpept`



**Purpose** Multiple aligned sequences from PFAM database

**Syntax**

```
AlignData = gethmmalignment('PFAMKey')
gethmmalignment(..., 'PropertyName', PropertyValue,...)
gethmmalignment(..., 'ToFile', ToFileValue)
gethmmalignment(..., 'Type', TypeValue)
```

## Arguments

*PFAMKey* Unique identifier for a sequence record. Enter a unique combination of letters and numbers.

*ToFileValue* Property to specify the location and filename for saving data. Enter either a filename, or a path and filename supported by your system (ASCII text file).

*TypeValue* Property to select the set of alignments returned. Enter either 'seed' or 'full'.

## Description

`AlignData = gethmmalignment('PFAMKey')` retrieves multiple aligned sequences from a profile hidden Markov model stored in the PFAM database and returns a MATLAB structure containing the following fields:

Field
Header
Sequence

`gethmmalignment(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`gethmmalignment(..., 'ToFile', ToFileValue)` saves the data returned from the PFAM database to a file. Read a FASTA formatted file with PFAM data back into MATLAB using the function `fastaread`.

# gethmmalignment

---

`gethmmalignment(..., 'Type', TypeValue)`, if *TypeValue* equals 'seed', returns only the alignments used to generate the HMM model. If *TypeValue* equals 'full' (default), returns all alignments that fit the model.

## Examples

Retrieve a multiple alignment of the sequences used to train the HMM profile model for global alignment to the 7 transmembrane receptor protein in the secretin family (PFAMKey = PF00002).

```
pfamalign = gethmmalignment(2, 'Type', 'seed')
```

or

```
pfamalign = gethmmalignment('PF00002', 'Type', 'seed')
```

## See Also

Bioinformatics Toolbox function `fastaread`, `gethmmprof`, `gethmmtree`, `pfamhmmread`, `multialignread`

**Purpose** Profile Hidden Markov Models (HMM) from PFAM database

**Syntax**

```

Model = gethmmprof(FamilyNumber)
Model = gethmmprof('FamilyName')
Model = gethmmprof('AccessionNumber')
gethmmprof(..., 'PropertyName', PropertyValue, ...)
gethmmprof(..., 'ToFile', ToFileValue)
gethmmprof(..., 'Mode', ModeValue)
gethmmprof(..., 'Mirror', MirrorValue)

```

## Arguments

<i>FamilyNumber</i>	PFAM family number. For example, to retrieve the profile HMM model for the protein family PF0002, enter 2.
<i>FamilyName</i>	PFAM family name. For example, enter '7tm_2'.
<i>AccessionNumber</i>	PFAM family accession number. Enter a character string with a version number appended to an accession number. For example, enter 'PF0002.14'. Because of changing version numbers, this is not the recommend method for getting information from the database.
<i>ToFileValue</i>	Property to specify the location and filename for saving data. Enter either a filename or a path and filename supported by your computer system (ASCII text file).
<i>ModeValue</i>	Property to select returning the global or local alignment mode. Enter either 'ls' (default) for the global alignment mode or 'fs' for the local alignment mode.
<i>MirrorValue</i>	Property to select a Web database. Enter either 'Sanger' (default) or 'WUSTL'.

**Description** *Model = gethmmprof(FamilyNumber)* uses a numeric value (*Number*) to determine the PFAM accession number, queries the database, and

then retrieves the profile HMM model information into a structure with the following fields:

Field
Name
PfamAccessionNumber
ModelDescription
ModelLength
Alphabet
MatchEmission
InsertEmission
NullEmission
BeginX
MatchX
InsertX
DeleteX
FlankingInsertX

`Model = gethmmprof('FamilyName')` searches the PFAM database for a protein family name (*FamilyName*) and retrieves the information into a structure.

`Model = gethmmprof('AccessionNumber')` retrieves the information and the accession number into a structure. This is the most efficient method to query a database. However, you should be aware that the accession number can be different with different databases. For example, the Sanger database adds a version number to the accession number (PF00002.14)

`gethmmprof(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`gethmmprof(..., 'ToFile', ToFileValue)` saves data returned from the PFAM database in a file (*ToFileValue*). Read an hmmprof formatted file back into MATLAB using the function `pfamhmmread`.

`gethmmprof(..., 'Mode', ModeValue)` selects either the global alignment model or the local alignment model.

`gethmmprof(..., 'Mirror', MirrorValue)` selects a specific web database. You can reach other mirror sites by passing the complete URL to the function `pfamhmmread`. Note: these mirror sites are maintained separately and may have slight variations.

For more information about the PFAM database, see

<http://www.sanger.ac.uk/Software/Pfam/>  
<http://pfam.wustl.edu/>

## Examples

To retrieve an HMM profile model for global alignment to the 7-transmembrane receptor protein in the secretin family, enter one of the following

```
hmmmodel = gethmmprof(2)
```

```
hmmmodel = gethmmprof('7tm_2')
```

## See Also

Bioinformatics Toolbox functions `hmmprofalign`, `hmmprofstruct`, `pfamhmmread`, `showhmmprof`, `gethmmalignment`

# gethmmtree

---

**Purpose** Phylogenetic tree data from PFAM database

**Syntax**

```
Tree = gethmmtree(AccessionNumber)
gethmmtree(..., 'PropertyName', PropertyValue, ...)
gethmmtree(..., 'ToFile', ToFileValue)
gethmmtree(..., 'Type', TypeValue)
```

## Arguments

<i>AccessionNumber</i>	Accession number in the PFAM database.
<i>ToFileValue</i>	Property to specify the location and filename for saving data. Enter either a filename or a path and filename supported by your system (ASCII text file).
<i>TypeValue</i>	Property to control which alignments are included in the tree. Enter either 'seed' or 'full' (default).

## Description

`Tree = gethmmtree(AccessionNumber)` searches for the PFAM family accession number in the PFAM database and returns an object (*Tree*) containing a phylogenetic tree representative of the protein family.

`gethmmtree(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`gethmmtree(..., 'ToFile', ToFileValue)` saves the data returned from the PFAM database in the file *ToFileValue*.

`gethmmtree(..., 'Type', TypeValue)`, when *TypeValue* is 'seed', returns a tree with only the alignments used to generate the HMM model. When *TypeValue* is 'full', returns a tree with all of the alignments that match the model.

## Examples

Retrieve a phylogenetic tree built 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')
```

## See Also

Bioinformatics Toolbox functions `gethmmalignment`, `phytreeread`

# getmatrix (geneont)

---

**Purpose** Convert geneont object into relationship matrix

**Syntax** `[Matrix, ID, Relationship] = getmatrix(GeneontObj)`

**Arguments**  
*GeneontObj*

**Description** `[Matrix, ID, Relationship] = getmatrix(GeneontObj)` converts a geneont object (*GeneontObj*) into a matrix of relationship values. *ID* is a list of Gene Ontology IDs that correspond to the rows and columns of *Matrix*. The values in the matrix are indices of the relationship types in *Relationship* (usually 1 for 'is\_a' and 2 for 'part\_of').

**Examples** `[MATRIX ID REL] = getmatrix(GO);`

**See Also** Bioinformatics Toolbox

- functions — geneont (object constructor), goannotread, num2goid
- geneont object methods — getancestors, getdescendants, getrelatives



**Purpose** Create Newick-formatted string

**Syntax**

```
String = getnewickstr(Tree)
getnewickstr(..., 'PropertyName', PropertyValue,...)
getnewickstr(..., 'Distances', DistancesValue)
getnewickstr(..., 'BranchNames', BranchNamesValue)
```

## Arguments

<i>Tree</i>	Phytree object created with the function <code>phytree</code> .
<i>DistancesValue</i>	Property to control including or excluding distances in the output. Enter either <code>true</code> (include distances) or <code>false</code> (exclude distances). Default is <code>true</code> .
<i>BranchNamesValue</i>	Property to control including or excluding branch names in the output. Enter either <code>true</code> (include branch names) or <code>false</code> (exclude branch names). Default is <code>false</code> .

## 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>

# getnewickstr (phytree)

---

## 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
- phytree object methods — get, getbyname, getcanonical

**Purpose** 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 node handles for the specified nodes (*NodeIDs*).

## 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)
- biograph object methods — `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `view`

## getnodesbyid (biograph)

---

MATLAB

- functions — get, set

**Purpose** Protein structure data from Protein Data Bank (PDB) database

**Syntax**

```
Data = getpdb('PDBid')
getpdb(..., 'PropertyName', PropertyValue,...)
getpdb(..., 'ToFile', ToFileValue)
```

## Arguments

<i>PDBid</i>	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.
<i>ToFileValue</i>	Property to specify the location and filename for saving data. Enter either a filename or a path and filename supported by your system (ASCII text file).

## Description

getpdb retrieves sequence information from the Protein Data Bank. This database contains 3-D biological macromolecular structure data.

`Data = getpdb('PDBid')` searches for the ID in the PDB database and returns a MATLAB structure containing the following fields:

### Fields

- Header
- Title
- Compound
- Source
- Keywords
- ExperimentData
- Authors
- Journal

## Fields

Remark1  
Remark2  
Remark3  
Sequence  
HeterogenName  
HeterogenSynonym  
Formula  
Site  
Atom  
RevisionDate  
Superseded  
Remark4  
Remark5  
Heterogen  
Helix  
Turn  
Cryst1  
OriginX  
Scale  
Terminal  
HeterogenAtom  
Connectivity

`getpdb(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`getpdb(..., 'ToFile', ToFileValue)` saves the data returned from the database to a file (*ToFileValue*). Read a PDB formatted file back into MATLAB using the function `pdbread`.

**Examples**

Retrieve the structure information for the electron transport (heme protein) with PDB ID 5CYT.

```
pdbstruct = getpdb('5CYT')
```

**See Also**

Bioinformatics Toolbox functions `getembl`, `getgenbank`, `getgenpept`, `pdbdistplot`, `pdbplot`, `pdbread`

# getrelatives (biograph)

---

**Purpose** Find relatives in biograph object

**Syntax**  
`Nodes = getrelatives(BiographNode)`  
`Nodes = getrelatives(BiographNode, NumGenerations)`

## Arguments

<i>BiographNode</i>	Node in a biograph object.
<i>NumGenerations</i>	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)
- `biograph` object methods — `dolayout`, `getancestors`, `getdescendants`, `getedgesbynodeid`, `getnodesbyid`, `getrelatives`, `view`

MATLAB



- functions — get, set

# getrelatives (geneont)

---

**Purpose** Numeric IDs for relatives of Gene Ontology term

**Syntax**

```
RelativeIDs = getrelatives(GeneontObj, ID)
getrelatives(..., 'PropertyName', PropertyValue,...)
getrelatives(..., 'Height', HeightValue)
getrelatives(..., 'Depth', DepthValue)
```

## Arguments

*GeneontObj*  
*ID*

## Description

*RelativeIDs* = `getrelatives(GeneontObj, ID)` returns the numeric IDs (*RelativeIDs*) for the relatives of a term (*ID*) including the ID for the term. *ID* is a nonnegative integer or a numeric vector with a set of IDs.

`getrelatives(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`getrelatives(..., 'Height', HeightValue)` includes terms that are related up through a specified number of levels (*HeightValue*) in the Gene Ontology database. *HeightValue* is a positive integer. Default is 1.

`getrelatives(..., 'Depth', DepthValue)` includes terms that are related down through a specified number of levels (*DepthValue*) in the Gene Ontology database. *DepthValue* is a positive integer. Default is 1.

## Examples

**1** Download the Gene Ontology database from the Web into MATLAB.

```
GO = geneont('LIVE', true);
```

MATLAB creates a `geneont` object and displays the number of terms in the database.

```
Gene Ontology object with 20005 Terms.
```

**2** Get the relatives for a Gene Ontology term.

```
subontology = getrelatives(GO,46680)
```

### See Also

Bioinformatics Toolbox

- functions — `geneont` (object constructor), `goannotread`, `num2goid`
- `geneont` object methods — `getancestors`, `getdescendants`, `getmatrix`

# goannotread

---

**Purpose** Annotations from Gene Ontology annotated file

**Syntax** `Annotation = goannotread('File')`

**Arguments**  
*File*

**Description** `Annotation = goannotread('File')` converts the contents of a Gene Ontology annotated file (*File*) into an array of structs (*Annotation*). 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>

## Examples

**1** Open a Web browser to

<http://www.geneontology.org/GO.current.annotations.shtml>

**2** Download the file containing GO annotations for the gene products of *Saccharomyces cerevisiae* (`gene_association.sgd.gz`) to your MATLAB Current Directory.

**3** Uncompress the file using the `gunzip` function.

```
gunzip('gene_association.sgd.gz')
```

**4** Read the file into MATLAB.

```
SGDGenes = goannotread('gene_association.sgd');
```

**5** Create a structure with GO annotations and get a list of genes.

```
S = struct2cell(SGDGenes);  
genes = S(3,:);
```

## See Also

Bioinformatics Toolbox

- functions — `geneont` (object constructor), `num2goid`
- `geneont` object methods — `getancestors`, `getdescendants`, `getmatrix`, `getrelatives`

# gonnet

---

**Purpose** 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, Benner S (1992), "Exhaustive matching of the entire protein sequence database", Science, 256:1443-1445.

**See Also** Bioinformatics Toolbox functions blosum, dayhoff, pam

**Purpose** Read microarray data from GenePix Results (GPR) file

**Syntax**

```
GPRData = gprread('File')
gprread(..., 'PropertyName', PropertyValue,...)
gprread(..., 'CleanColNames', CleanColNamesValue)
```

## Arguments

<i>File</i>	GenePix Results formatted file (file extension GPR). Enter a filename or a path and filename.
<i>CleanColNamesValue</i>	Property to control creating column names that MATLAB can use 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)`. A GPR file may contain column names with spaces and some characters that MATLAB 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 MATLAB 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_genepix_file_formats.html#gpr)

[http://www.moleculardevices.com/pages/software/gn\\_gpr\\_format\\_history.html](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](http://www.moleculardevices.com/pages/software/gn_genepix_file_formats.html)

GenePix is a registered trademark of Molecular Devices Corporation.

## Examples

```
% Read in a sample GPR file and plot the median foreground
% intensity for the 635 nm channel.
gprStruct = gprread('mouse_a1pd.gpr')
mimage(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`, `geosoftread`, `imageneread`, `magetfield`, `sptread`

# hmmprofalign

---

**Purpose**                    Align query sequence to profile using hidden Markov model alignment

**Syntax**

```
Alignment = hmmprofalign(Model,Seq)
[Alignment, Score] = hmmprofalign(Model,Seq)
[Score, Alignment, Pointer] = hmmprofalign(Model,Seq)
hmmprofalign(..., 'PropertyName', PropertyValue,...)
hmmprofalign(..., 'ShowScore', ShowScoreValue)
hmmprofalign(..., 'Flanks', FlanksValue)
hmmprofalign(..., 'ScoreFlanks', ScoreFlanksValue)
hmmprofalign(..., 'ScoreNullTransitions',
ScoreNullTransitionValue)
```

## Arguments

<i>Model</i>	Hidden Markov model created with the function <code>hmmprofstruc</code> .
<i>Seq</i>	Amino acid or nucleotide sequence. You can also enter a structure with the field <code>Sequence</code> .
<i>ShowScoreValue</i>	Property to control displaying the scoring space and the winning path. Enter either true or false (default).
<i>FlanksValue</i>	Property to control including the symbols generated by the FLANKING INSERT states in the output sequence. Enter either true or false (default).
<i>ScoreFlanksValue</i>	Property to control including the transition probabilities for the flanking states in the raw score. Enter either true or false (default).
<i>ScoreNullTransValue</i>	Property to control adjusting the raw score using the null model for transitions ( <code>Model.NullX</code> ). Enter either true or false (default).

**Description**

*Alignment* = `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.

`[Alignment, Score] = hmmprofalign(Model,Seq)` 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, Prointer] = hmmprofalign(Model,Seq)` 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,...)` defines optional properties using property name/value pairs.

`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', ScoreNullTransitionValue)`, when *ScoreNullTransitionsValue* is true, adjusts the raw score using the null model for transitions (`Model.NullX`).

# hmmprofalign

---

---

**Note** Multiple target alignment is not supported in this implementation. All the Model.LoopX probabilities are ignored.

---

## Examples

```
load('hmm_model_examples','model_7tm_2') % load a model example
load('hmm_model_examples','sequences') % load a sequence example
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`

**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 <code>hmmprofstruct</code> .
MultipleAlignment	Array of sequences. Sequences can also be a structured array with the aligned sequences in a field <code>Aligned</code> or <code>Sequences</code> , and the optional names in a field <code>Header</code> or <code>Name</code> .
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 <code>Model.NullEmission</code> .
BMx	Property to set the background transition probabilities from any MATCH state ( <code>[M-&gt;M M-&gt;I M-&gt;D]</code> ). Default values are taken from <code>hmmprofstruct</code> .
BDx	Property to set the background transition probabilities from any DELETE state ( <code>[D-&gt;M D-&gt;D]</code> ). Default values are taken from <code>hmmprofstruct</code> .

# hmmprofestimate

---

## 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 ( $[M \rightarrow M \ M \rightarrow I \ M \rightarrow D]$ ). Default values are taken from `hmmprofstruct`.

`hmmprofestimate(..., 'BDx', BDxValue)` sets the background transition probabilities from any DELETE state ( $[D \rightarrow M \ D \rightarrow D]$ ). Default values are taken from `hmmprofstruct`.

**See Also**

Bioinformatics Toolbox functions `hmmprofalign`, `hmmprofstruct`, `showhmmprof`

# hmmprofgenerate

---

**Purpose** Generate random sequence drawn from profile Hidden Markov Model (HMM)

**Syntax**

```
Sequence = hmmprofgenerate(Model,  
'PropertyName', PropertyValue...)  
[Sequence, Profptr] = hmmprofgenerage(Model)  
hmmprofgenerate(..., 'Align', AlignValue)  
hmmprofgenerate(..., 'Flanks', FlanksValue)  
hmmprofgenerate(..., 'Signature', SignatureValue)
```

## Arguments

Model	Hidden Markov model created with the function <code>hmmprofstruc</code> .
Align	Property to control using uppercase letters for matches and lowercase letters for inserted letters. Enter either true or false. The default value is false.
Flanks	Property to control including the symbols generated by the FLANKING INSERT states in the output sequence. Enter either true or false. The default value is false.
Signature	Property to control returning the most likely path and symbols. Enter either true or false. Default value is false.

## Description

`Sequence = hmmprofgenerate(Model, 'PropertyName', PropertyValue...)` returns a string (Seq) 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 move information about this structure, see `hmmprofstruct`

`[Sequence, Profptr] = hmmprofgenerage(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(..., '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 `Align` is false, the output is a sequence of uppercase symbols. The default value is true.

`hmmprofgenerate(..., 'Flanks', FlanksValue)` if `Flanks` is true, the output sequence includes the symbols generated by the FLANKING INSERT states. The default value is false.

`hmmprofgenerate(..., 'Signature', SignatureValue)` if `Signature` 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`

# hmmprofmerge

---

**Purpose** Concatenate prealigned strings of several sequences to profile Hidden Markow Model (HMM)

**Syntax**  
A = 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 <code>Aligned</code> or <code>Sequences</code> , and the optional names in a field <code>Header</code> or <code>Name</code> .
Names	Names for the sequences. Enter a vector of names.
Scores	Pairwise alignment scores from the function <code>hmmprofalign</code> . Enter a vector of values with the same length as the number of sequences in <code>Sequences</code> .

## Description

`hmmprofmerge(Sequences)` displays a set of prealigned sequences to a 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`

# hmmprofstruct

---

**Purpose** Create profile Hidden Markov Model (HMM) structure

**Syntax**  
`Model = hmmprofstruct(Length)`  
`Model = hmmprofstruct(Length, 'Field1', FieldValues1,...)`  
`hmmprofstruct(Model, 'Field1', Field1Values1,...)`

## Arguments

<i>Length</i>	Number of match states in the model.
<i>Model</i>	Hidden Markov model created with the function <code>hmmprofstruct</code> .
<i>Field1</i>	Field name in the structure <i>Model</i> . Enter a name from the table below.

## Description

`Model = hmmprofstruct(Length)` returns a structure with the fields containing the required parameters of a profile HMM. *Length* specifies the number of match states in the model. All other mandatory model parameters are initialized to the default values.

`Model = hmmprofstruct(Length, 'Field1', FieldValues1, ...)` creates a profile HMM using the specified fields and parameters. All other mandatory model parameters are initialized to default values.

`hmmprofstruct(Model, 'Field1', Field1Values1, ...)` returns the updated profile HMM with the specified fields and parameters. All other mandatory model parameters are taken from the reference `MODEL`.

### HMM Profile Structure Format

Model parameters fields (mandatory). All probability values are in the [0 1] range.

Field Name	Description
<code>ModelLength</code>	Length of the profile (number of MATCH states)
<code>Alphabet</code>	'AA' or 'NT'. Default is 'AA'.

MatchEmission	<p>Symbol emission probabilities in the MATCH states.</p> <p>Size is [ModelLength x AlphaLength]. Defaults to uniform distributions. May accept a structure with residue counts (see aaccount or basecount).</p>
InsertEmission	<p>Symbol emission probabilities in the INSERT state.</p> <p>Size is [ModelLength x AlphaLength]. Defaults to uniform distributions. May accept a structure with residue counts (see aaccount or basecount).</p>
NullEmission	<p>Symbol emission probabilities in the MATCH and INSERT states for the NULL model. NULL model, size is [1 x AlphaLength]. Defaults to a uniform distribution. May accept a structure with residue counts (see aaccount or basecount). The NULL model is used to compute the log-odds ratio at every state and avoid overflow when propagating the probabilities through the model.</p>
BeginX	<p>BEGIN state transition probabilities.</p> <p>Format is</p> <p style="padding-left: 40px;">[B-&gt;D1 B-&gt;M1 B-&gt;M2 B-&gt;M3 . . . . B-&gt;Mend]</p> <p>Notes:</p> <p style="padding-left: 40px;"><math>\text{sum}(\text{S.BeginX}) = 1</math></p> <p>For fragment profiles</p> <p style="padding-left: 40px;"><math>\text{sum}(\text{S.BeginX}(3:\text{end})) = 0</math></p> <p>Default is [0.01 0.99 0 0 . . . 0].</p>

MatchX	<p>MATCH state transition probabilities</p> <p>Format is</p> <pre>[M1-&gt;M2 M2-&gt;M3 ... M[end-1]-&gt;Mend; M1-&gt;I1 M2-&gt;I2 ... M[end-1]-&gt;I[end-1]; M1-&gt;D2 M2-&gt;D3 ... M[end-1]-&gt;Dend; M1-&gt;E M2-&gt;E ... M[end-1]-&gt;E ]</pre> <p>Notes:</p> $\text{sum}(S.\text{MatchX}) = [ 1 \ 1 \ \dots \ 1 ]$ <p>For fragment profiles</p> $\text{sum}(S.\text{MatchX}(4,:)) = 0$ <p>Default is <code>repmat([0.998 0.001 0.001 0], profLength-1, 1)</code>.</p>
InsertX	<p>INSERT state transition probabilities</p> <p>Format is</p> <pre>[I1-&gt;M2 I2-&gt;M3 ... I[end-1]-&gt;Mend; [I1-&gt;I1 I2-&gt;I2 ... I[end-1]-&gt;I[end-1] ]</pre> <p>Note:</p> $\text{sum}(S.\text{InsertX}) = [ 1 \ 1 \ \dots \ 1 ]$ <p>Default is <code>repmat([0.5 0.5], profLength-1, 1)</code>.</p>

DeleteX	<p>DELETE state transition probabilities. The format is</p> <pre>[D1-&gt;M2 D2-&gt;M3 ... D[end-1]-&gt;Mend ;  [D1-&gt;D2 D2-&gt;D3 ... D[end-1]-&gt;Dend ]</pre> <p>Note: <math>\text{sum}(\text{S.DeleteX}) = [1 \ 1 \ \dots \ 1]</math></p> <p>Default is <code>repmat([0.5 0.5],profLength-1,1)</code>.</p>
FlankingInsertX	<p>Flanking insert states (N and C) used for LOCAL profile alignment. The format is</p> <pre>[N-&gt;B C-&gt;T ;  [N-&gt;N C-&gt;C ]</pre> <p>Note: <math>\text{sum}(\text{S.FlankingInsertsX}) = [1 \ 1]</math></p> <p>To force global alignment use</p> <pre>S.FlankingInsertsX = [1 1; 0 0]</pre> <p>Default is <code>[0.01 0.01; 0.99 0.99]</code>.</p>
LoopX	<p>Loop states transition probabilities used for multiple hits alignment. The format is</p> <pre>[E-&gt;C J-&gt;B ;  E-&gt;J J-&gt;J ]</pre> <p>Note: <math>\text{sum}(\text{S.LoopX}) = [1 \ 1]</math></p> <p>Default is <code>[0.5 0.01; 0.5 0.99]</code></p>
NullX	<p>Null transition probabilities used to provide scores with log-odds values also for state transitions. The format is</p> <pre>[G-&gt;F ; G-&gt;G]</pre> <p>Note: <math>\text{sum}(\text{S.NullX}) = 1</math></p>

# hmmprofstruct

---

	Default is [0.01; 0.99]
--	-------------------------

## Annotation fields (optional)

Name	Model Name
IDNumber	Identification Number
Description	Short description of the model

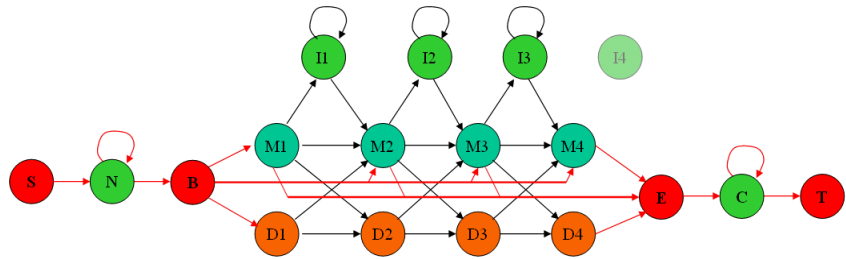
A profile Markov model is a common statistical tool for modeling structured sequences composed of symbols . These symbols include randomness in both the output (emission of symbols) and the state transitions of the process. Markov models are generally represented by state diagrams.

The figure shown below is a state diagram for a HMM profile of length 4. Insert, match, and delete states are in the regular part (middle section).

- 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 know as a silent state because it does not emit any symbol),
- Insert state represents the excess of one or more symbols in the target sequence that are not included in the profile.

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, N, E, and T are silent while N and C are used to insert symbols at the flanks.





## Examples

```
hmmprofstruct(100, 'Alphabet', 'AA')
```

## See Also

Bioinformatics Toolbox functions `gethmmprof`, `hmmprofalign`, `hmmprofestimate`, `hmmprofgenerate`, `hmmprofmerge`, `pfamhmmread`, `showhmmprof`, `aaccount`, `basecount`

# imageneread

---

**Purpose** Read microarray data from ImaGene Results file

**Syntax**

```
imagedata = imageneread('File')  
imagedata = imageneread(..., 'CleanColNames',  
CleanColNamesValue, ...)
```

## Arguments

<i>File</i>	ImaGene Results formatted file. Enter a filename or a path and filename.
<i>CleanColNameValue</i>	Property to control creating column names that MATLAB can use as variable names.

## Description

*imagedata* = 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

*imagedata* = imageneread(..., 'PropertyName', PropertyValue, ...) defines optional properties using property name/value pairs, described as follows:

`imagenedata = imageneread(..., 'CleanColNames', CleanColNamesValue, ...)`. An ImaGene file may contain column names with spaces and some characters that MATLAB cannot use in MATLAB variable names. If *CleanColNamesValue* is true, `imageneread` returns, in the field `ColumnNames`, names 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 not valid for MATLAB variable names.

The field `Indices` of the structure contains MATLAB 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 User Manual.

ImaGene is a registered trademark of BioDiscovery, Inc.

## Examples

- 1 Read in a sample ImaGene Results file. Note, the file `cy3.txt` is not provided with the Bioinformatics Toolbox.

```
cy3Data = imageneread('cy3.txt');
```

- 2 Plot the signal mean.

```
mimage(cy3Data, 'Signal Mean');
```

- 3 Read in a sample ImaGene Results file. Note, the file `cy5.txt` is not provided with the Bioinformatics Toolbox.

```
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');
```

# imageneread

---

## See Also

Bioinformatics Toolbox

- functions — `gprread`, `maboxplot`, `maimage`, `sptread`

**Purpose** Convert amino acid sequence from integer to letter representation

**Syntax**

```
SeqChar = int2aa(SeqInt)
int2aa(..., 'PropertyName', PropertyValue,...)
int2aa(..., 'Case', CaseValue)
```

## Arguments

*SeqInt* Amino acid sequence represented with integers. Enter a vector of integers from the table Mapping Amino Acid Integers to Letters below. The array does not have to be of type integer, but it does have to contain only integer numbers. Integers are arbitrarily assigned to IUB/IUPAC letters.

*Case* Property to select the case of the returned character string. Enter either 'upper' (default) or 'lower'.

### Mapping Amino Acid Integers to Letters

Amino Acid	Code	Amino Acid	Code	Amino Acid	
Alanine	A1	Isoleucine	I10	Tyrosine	Y19
Arginine	R2	Leucine	L11	Valine	V20
Asparagine	N3	Lysine	K12	Aspartic acid or Asparagine	B21
Aspartic acid (aspartate)	D4	Methionine	M13	Glutamic acid or Glutamine	Z22
Cystine	C5	Phenylalanine	F14	Any amino acid	X23
Glutamine	Q6	Proline	P15	Translation stop	*24

# int2aa

Amino Acid	Code	Amino Acid	Code	Amino Acid	
Glutamic acid (glutamate)	E7	Serine	S16	Gap of indeterminate length	- 25
Glycine	G8	Threonine	T17	Unknown or any integer not in table	?0
Histidine	H9	Tryptophan	W18		

## Description

*SeqChar* = `int2aa(SeqInt)` converts a 1-by-N array of integers to a character string using the table Mapping Amino Acid Integers to Letters above.

`int2aa(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`int2aa(..., 'Case', CaseValue)` sets the output case of the nucleotide string. Default is uppercase.

## Examples

```
s = int2aa([13 1 17 11 1 21])
```

```
s =  
MATLAB
```

## See Also

Bioinformatics Toolbox functions `aa2int`, `aminolookup`, `int2nt`, `nt2int`

**Purpose** Convert nucleotide sequence from integer to letter representation

**Syntax**

```
int2nt(SeqNT)
int2nt(..., 'PropertyName', PropertyValue,...)
int2nt(..., 'Alphabet', AlphabetValue)
int2nt(..., 'Unknown', UnknownValue)
int2nt(..., 'Case', CaseValue)
```

### Arguments

<i>SeqNT</i>	Nucleotide sequence represented by integers. Enter a vector of integers from the table Mapping Nucleotide Integers to Letters below. The array does not have to be of type integer, but it does have to contain only integer numbers. Integers are arbitrarily assigned to IUB/IUPAC letters.
<i>AlphabetValue</i>	Property to select the nucleotide alphabet. Enter either 'DNA' or 'RNA'.
<i>UnknownValue</i>	Property to select the integer value for the unknown character. Enter a character to map integers 16 or greater to an unknown character. The character must not be one of the nucleotide characters A, T, C, G or the ambiguous nucleotide characters N, R, Y, K, M, S, W, B, D, H, or V. The default character is *.
<i>CaseValue</i>	Property to select the letter case for the nucleotide sequence. Enter either 'upper' (default) or 'lower'.

### Mapping Nucleotide Integers to Letters

Base	Code	Base	Code	Base	Code
Adenosine	1—A	T, C (pyrimidine)	6—Y	A, T, G (not C)	12—D
Cytidine	2—C	G, T (keto)	7—K	A, T, C (not G)	13—H
Guanine	3—G	A, C (amino)	8—M	A, G, C (not T)	14—V
Thymidine	4—T	G, C (strong)	9—S	A, T, G, C (any)	15—N
Uridine (if 'Alphabet' = 'RNA')	4—U	A, T (weak)	10—W	Gap of indeterminate length	16 — -
A, G (purine)	5—R	T, G, C (not A)	11—B	Unknown (default)	0 and 17—*

### Description

`int2nt(SeqNT)` converts a 1-by-N array of integers to a character string using the table Mapping Nucleotide Letters to Integers above.

`int2nt(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`int2nt(..., 'Alphabet', AlphabetValue)` selects the nucleotide alphabet to use. The default value is 'DNA', which uses the symbols A, T, C, and G. If *AlphabetValue* is set to 'RNA', `int2nt` uses the symbols A, C, U, G instead.

`int2nt(..., 'Unknown', UnknownValue)` specifies the character to represent an unknown nucleotide base.



`int2nt(..., 'Case', CaseValue)` selects the output case of the nucleotide string.

## Examples

Enter a sequence of integers as a MATLAB vector (space or comma-separated list with square brackets).

```
s = int2nt([1 2 4 3 2 4 1 3 2])
```

```
s =  
ACTGCTAGC
```

Define a symbol for unknown numbers 16 and greater.

```
si = [1 2 4 20 2 4 40 3 2];  
s = int2nt(si, 'unknown', '#')
```

```
s =  
ACT#CT#GC
```

## See Also

Bioinformatics Toolbox function `aa2int`, `int2aa`, `nt2int`

# isoelectric

---

**Purpose** Estimate isoelectric point for amino acid sequence

**Syntax**

```
 $\rho I$  = isoelectric(SeqAA)
[ $\rho I$  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 . 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

$\rho I$  = isoelectric(SeqAA) returns the estimated isoelectric point ( $\rho I$ ) for an amino acid sequence. The isoelectric point is the pH at which the protein has a net charge of zero

[ $\rho I$  Charge] = isoelectric(SeqAA) returns the estimated isoelectric point ( $\rho I$ ) 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 `PKValsValues`. 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

---

`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('PQGGGGWGQPHGGGGWGQPHGGGGWGQGGSHSQ', '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 functions `aaccount`, `molweight`

**Purpose** Read JCAMP-DX formatted files

**Syntax** `JCAMPData = jcampread(File)`

**Arguments**

*File* JCAMP-DX formatted file (ASCII text file). Enter a filename, a path and filename, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text of 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 and 5 of the JCAMP-DX format. For more details, see

<http://www.jcamp.org/index.html>

`JCAMPData = jcampread(File)` reads data from a JCAMP-DX formatted file (*File*) and creates a MATLAB structure (*JCAMPData*) containing the following fields:

Field
Title
DataType
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

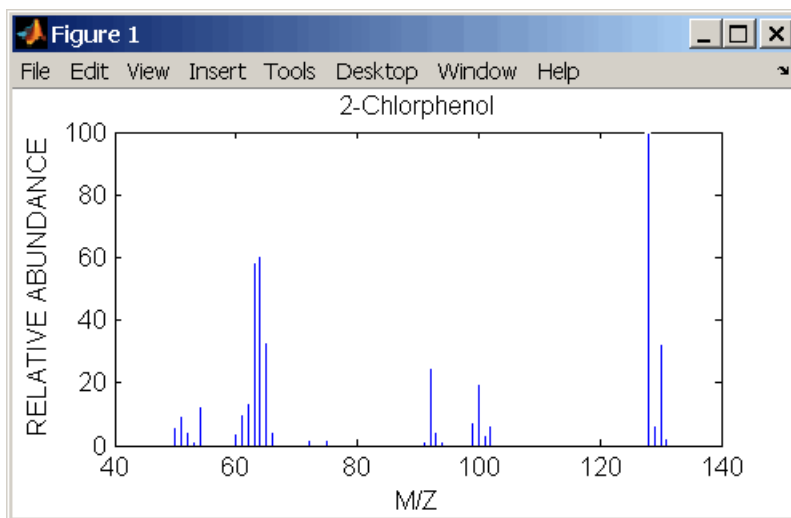
- 1 Download test data in the file isa\_ms1.dx from

<http://www.jcamp.org/testdata.html/testdata.zip>

- 2 Read a JCAMP-DX file (isas\_ms1.dx) into MATLAB 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`

# joinseq

---

**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**

```
seq1 = 'ACGTAAA';  
seq2 = 'AAATGCA';  
joined = joinseq(seq1,seq2)  
  
joined =  
    ACGTAAATGCA
```

**See Also** MATLAB functions `cat`, `strcat`, `strfind`



**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*

*Training*

*Group*

*k*

*distance*

*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. The default is 1.

`Class = knnclassify(Sample, Training, Group, k, distance)` enables you to specify the distance metric. The choices for `distance` are

# knnclassify

---

'euclidean'	Euclidean distance — the 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 (only suitable 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. The choices for rule are

'nearest'	Majority rule with nearest point tie-break — the 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.

## Example 1

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`.

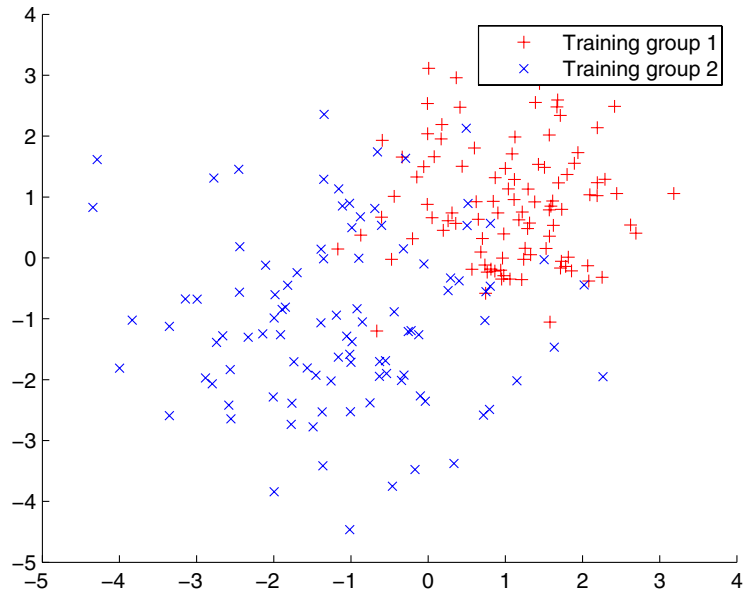
## Example 2

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); ...
```

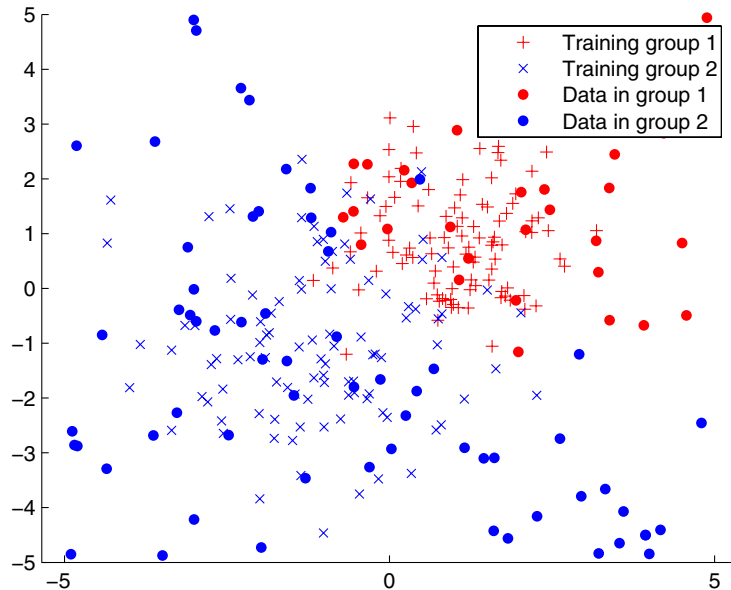
# knnclassify

```
        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;
```



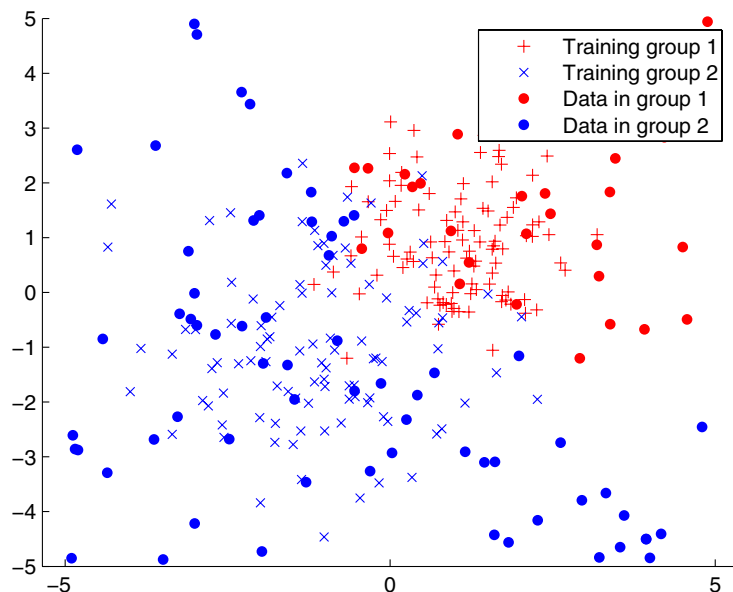
### Example 3

The following example uses the same data as in Example 2, 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');
```

# knnclassify

---



If you compare this plot with the one in Example 2, 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 `knnimpute`, `classperf`, `crossvalind`, `svmclassify`, `svmtrain`

Statistical Toolbox functions `classify`

**Purpose** Impute missing data using nearest-neighbor method

**Syntax**

```
knnimpute(Data)
knnimpute(Data, k)
knnimpute(..., 'PropertyName', PropertyValue, ...)
knnimpute(..., 'Distance', DistanceValue)
knnimpute(..., 'DistArgs', DistArgsValue)
knnimpute(..., 'Weights', WeightsValues)
knnimpute(..., 'Median', MedianValue)
```

## Arguments

*Data*

*k*

## Description

`knnimpute(Data)` replaces NaNs 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 NaNs 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, ...)` defines optional properties using property name/value pairs.

`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.

# knnimpute

---

'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)` enables you to 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  $A(3,1) = \text{NaN}$ . 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, 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, Altman R (2001), "Missing value estimation methods for DNA microarrays", *Bioinformatics*, 17( 6)520-525.

# knnimpute

---

## See Also

Bioinformatics Toolbox function `knnclassify`

MATLAB function `isnan`

Statistics Toolbox functions `nanmean`, `nanmedian`, `pdist`

**Purpose** Box plot for microarray data

**Syntax**

```

maboxplot(MAData)
maboxplot(MAData, ColumnName)
maboxplot(MAStruct, FieldName)
H = maboxplot(...)
[H, HLines] = maboxplot(...)
maboxplot(..., 'PropertyName', PropertyValue, ...)
maboxplot(..., 'Title', TitleValue, ...)
maboxplot(..., 'Notch', NotchValue, ...)
maboxplot(..., 'Symbol', SymbolValue, ...)
maboxplot(..., 'Orientation', OrientationValue, ...)
maboxplot(..., 'WhiskerLength', WhiskerLengthValue, ...)

```

## Arguments

<i>MAData</i>	A numeric array or a structure containing a field called <i>Data</i> . The values in the columns of <i>MAData</i> will be used to create box plots.
<i>ColumnName</i>	An array of column names corresponding to the data in <i>MAData</i> .
<i>MAStruct</i>	A microarray data structure.
<i>FieldName</i>	A field within the microarray data structure, <i>MAStruct</i> . The values in the field <i>FieldName</i> will be used to create box plots.
<i>TitleValue</i>	A string to use as the title for the plot. The default title is <i>FieldName</i> .
<i>NotchValue</i>	Property to control the type of boxes drawn. Enter either <i>true</i> for notched boxes, or <i>false</i> , for square boxes. Default is <i>false</i> .

# maboxplot

---

<i>OrientationValue</i>	Property to specify the orientation of the box plot. Enter 'Vertical' or 'Horizontal'. Default is 'Horizontal'.
<i>WhiskerLengthValue</i>	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 <i>WhiskerLengthValue</i> *IQR of the box. Default = 1.5. If <i>WhiskerLengthValue</i> equals 0, then <code>maboxplot</code> displays all data values outside the box, using the plotting symbol <code>Symbol</code> .

## Description

`maboxplot(MAData)` displays a box plot of the values in the columns of data (*MAData*). *MAData* can be a numeric array or a structure containing a field called *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.

`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, ...)` defines optional properties using property name/value pairs in any order. These property name/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`.

## Examples

```
load yeastdata
maboxplot(yeastvalues,times);
xlabel('Sample Times');

% Using a structure
geoStruct = getgeodata('GSM1768');
maboxplot(geoStruct);

% For block-based data
madata = gprread('mouse_a1wt.gpr');
maboxplot(madata,'F635 Median');
figure
maboxplot(madata,'F635 Median - B635','TITLE',...
          'Cy5 Channel FG - BG');
```

## See Also

Bioinformatics Toolbox functions `magetfield`, `mimage`, `mairplot`, `maloglog`, `malowess`, `manorm`, `mavolcanoplot`

Statistics Toolbox function `boxplot`

# magetfield

---

**Purpose** Extract data from a microarray structure

**Syntax** `magetfield(MAStruct, FieldName)`

**Arguments**

*MAStruct*  
*FieldName*

**Description** `magetfield(MAStruct, FieldName)` extracts data for a column (*FieldName*) from a microarray structure (*MAStruct*).  
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`).

**Example**

```
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`, `imageneread`, `maboxplot`, `mairplot`, `maloglog`, `malowess`, `sptread`

**Purpose** Spatial image for microarray data

**Syntax**

```
mimage(X, FieldName)
H = mimage(...)
[H, HLines] = mimage(...)
mimage(..., 'PropertyName', PropertyValue,...)
mimage(..., 'Title', TitleValue)
mimage(..., 'ColorBar', ColorBarValue)
mimage(..., 'HandleGraphicsPropertyName' PropertyValue)
```

## Arguments

<i>X</i>	A microarray data structure.
<i>FieldName</i>	A field in the microarray data structure <i>X</i> .
<i>TitleValue</i>	A string to use as the title for the plot. The default title is <i>FieldName</i> .
<i>ColorBarValue</i>	Property to control displaying a colorbar in the figure window. Enter either true or false. The default value is false.

## Description

`mimage(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 = mimage(...)` returns the handle of the image.

`[H, HLines] = mimage(...)` returns the handles of the lines used to separate the different blocks in the image.

`mimage(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`mimage(..., 'Title', TitleValue)` allows you to specify the title of the plot. The default title is *FieldName*.

# mimage

---

`mimage(..., 'ColorBar', ColorBarValue)`, when *ColorBarValue* is true, a colorbar is shown. If *ColorBarValue* is false, no colorbar is shown. The default is for the colorbar to be shown.

`mimage(..., '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 `mimage(..., 'color' 'r')`.

## Examples

```
madata = gprread('mouse_a1wt.gpr');
mimage(madata,'F635 Median');
figure;
mimage(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(..., 'Prctile', PrctileValue, ...)
NormDataY = mainvarsetnorm(..., 'Iterate', IterateValue, ...)
NormDataY = mainvarsetnorm(..., 'Method', MethodValue, ...)
NormDataY = mainvarsetnorm(..., 'Span', SpanValue, ...)
NormDataY = mainvarsetnorm(..., 'Showplot',
ShowplotValue, ...)
```

## Arguments

<i>DataX</i>	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.
<i>DataY</i>	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.
<i>ThresholdsValue</i>	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.

## mainvarsetnorm

---

*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 [0.03, 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.

*PrctileValue* 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 (*StopPrctileValue*) 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.

---

<i>MethodValue</i>	Property to select the smoothing method used to normalize the data. Enter 'lowess' or 'runmedian'. Default is 'lowess'.
<i>SpanValue</i>	Property to set the window size for the smoothing method. If <i>SpanValue</i> is less than 1, the window size is that percentage of the number of data points. If <i>SpanValue</i> is equal to or greater than 1, the window size is of size <i>SpanValue</i> . Default is 0.05, which corresponds to a window size equal to 5% of the total number of data points in the invariant set.
<i>ShowplotValue</i>	Property to control the plotting of a pair of M-A scatter plots (before and after normalization). M is the ratio between <i>DataX</i> and <i>DataY</i> . A is the average of <i>DataX</i> and <i>DataY</i> . 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*.

$$prd = \text{abs}(\text{RankX} - \text{RankY})$$

- 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

## mainvarsetnorm

---

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 lowest 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*, ...) defines optional properties that use property name/value pairs in any order. These property name/value pairs are as follows:

*NormDataY* = *mainvarsetnorm*(..., '*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 [0.03, 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(..., 'Prctile', *PrctileValue*, ...) 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 (*PrctileValue*) 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'.

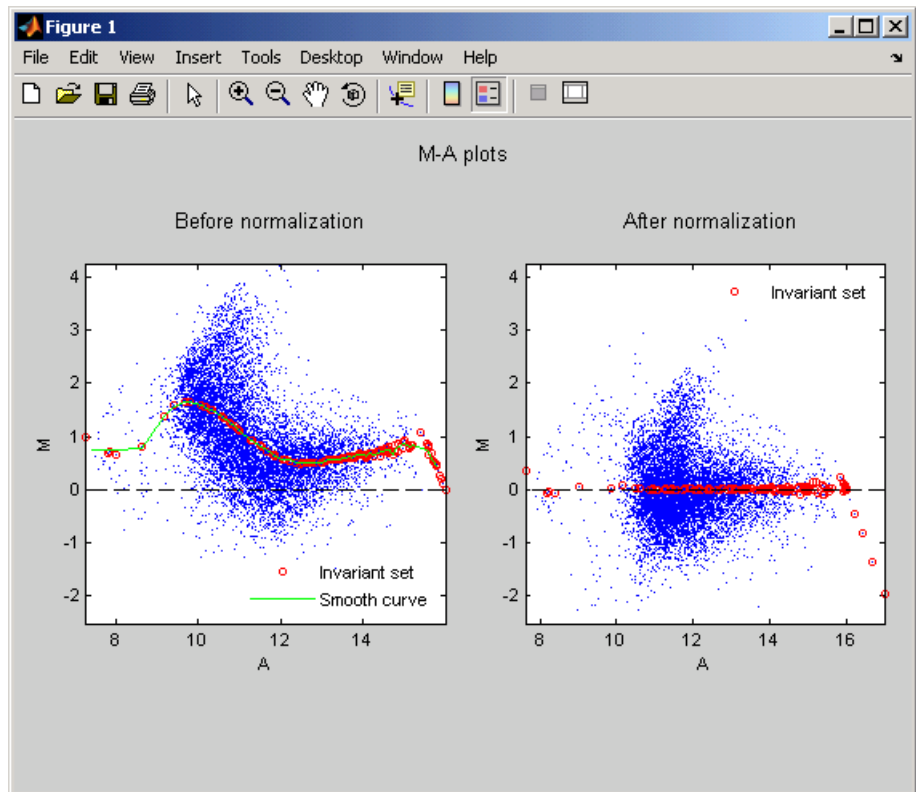
## mainvarsetnorm

---

*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

## mainvarsetnorm

---

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



**Purpose** Intensity versus ratio scatter plot for microarray signals

**Syntax**

```
mairplot(X, Y, 'PropertyName', PropertyValue...)
mairplot(..., 'FactorLines', FactorLinesValue)
mairplot(..., 'Title', TitleValue)
mairplot(..., 'Labels', LabelsValue)
mimage(..., 'HandleGraphicsPropertyName' PropertyValue)
[Intensity, Ratio] = mairplot(...)
[Intensity, Ratio, H] = mairplot(...)
```

## Arguments

X, Y	Gene expression data.
FactorLines	Property to specify a factor of change.
Title	Property to specify a title for the plot.
Labels	Property to specify labels for the plot.
HandleGraphics	Property to pass optional property name/value pairs from Handle Graphics.

## Description

`mairplot(X, Y, 'PropertyName', PropertyValue...)` creates an intensity versus ratio scatter plot of X versus Y.

`mairplot(..., 'FactorLines', FactorLinesValue)` adds lines showing a factor of *N* change.

`mairplot(..., 'Title', TitleValue)` allows you to specify a title for the plot.

`mairplot(..., 'Labels', LabelsValue)` allows you to specify 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.

`mimage(..., 'HandleGraphicsPropertyName' PropertyValue)` allows you to pass optional Handle Graphics property name/property value pairs to the function.

# mairplot

---

[Intensity, Ratio] = mairplot(...) returns the intensity and ratio values.

[Intensity, Ratio, H] = mairplot(...) returns the handle of the plot.

## 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')
% Add factor lines and labels
figure
names = maStruct.Names;
mairplot(cy3data,cy5data,'title','R vs G IR plot',...
% Normalize the plot using lowess normalization
figure
mairplot(cy3data,cy5data,'title','Normalized R vs G IR plot',...
          'Normalize',true,'Factorlines',2,...
          'Labels',maStruct.Names)
```

## See Also

Bioinformatics Toolbox functions `maboxplot`, `magetfield`, `maimage`, `mainvarsetnorm`, `maloglog`, `malowess`, `manorm`, `matteest`, `mavolcanoplot`

**Purpose** Create loglog plot of microarray data

**Syntax**

```
maloglog(X, Y, 'PropertyName', PropertyValue...)
maloglog(..., 'FactorLines', N)
maloglog(..., 'Title', TitleValue)
maloglog(..., 'Labels', LabelsValues)
maloglog(..., 'HandleGraphicsName', HGValue)
H = maloglog(...)
```

## Arguments

*X* A numeric array of microarray expression values from a single experimental condition.

*Y* A 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, 'PropertyName', PropertyValue...)` creates a loglog scatter plot of *X* versus *Y*. *X* and *Y* are numeric arrays of microarray expression values from two different experimental conditions.

`maloglog(..., 'FactorLines', N)` adds two lines to the plot showing a factor of *N* change.

`maloglog(..., 'Title', TitleValue)` allows you to specify a title for the plot.

`maloglog(..., '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(..., '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`, `mimage`, `mairplot`, `malowess`, `manorm`, `mattest`, `mavolcanoplot`

MATLAB function `loglog`

**Purpose** Smooth microarray data using Lowess method

**Syntax**

```
YSmooth = malowess(X, Y)
malowess(..., 'PropertyName', PropertyValue,...)
malowess(..., 'Order', OrderValue)
malowess(..., 'Robust', RobustValue)
malowess(..., 'Span', SpanValue)
```

## Arguments

<i>X, Y</i>	Scatter data.
<i>OrderValue</i>	Property to select the order of the algorithm. Enter either 1 (linear fit) or 2 (quadratic fit). The default order is 1.
<i>RobustValue</i>	Property to select a robust fit. Enter either true or false.
<i>SpanValue</i>	Property to specify the window size. The default value is 0.05 (5% of total points in <i>X</i> )

## Description

`YSmooth = malowess(X, Y)` smooths scatter data (*X, Y*) using the Lowess smoothing method. The default window size is 5% of the length of *X*.

`malowess(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`malowess(..., 'Order', OrderValue)` chooses the order of the algorithm. Note that the MATLAB Curve Fitting Toolbox refers to Lowess smoothing of order 2 as Loess smoothing.

`malowess(..., 'Robust', RobustValue)` uses a robust fit when *RobustValue* is set to true. This option can take a long time to calculate.

`malowess(..., '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*.

# malowess

---

## 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')
ymorm = 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)
```

**Description**

`XNorm = manorm(X)` scales the values in each column of microarray data (`X`) by dividing by the mean column intensity.

- `X` — Microarray data. Enter a vector or matrix.
- `XNorm` — Normalized microarray data.

`XNorm = manorm(MAstruct, FieldName)` scales the data for a field (`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.

- `MAstruct` — Microarray structure.

`[XNorm, ColVal] = manorm(...)` returns the values used to normalize the data.

`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 plot of expression profile data

**Syntax**  
`mapcaplot(Data)`  
`mapcaplot(Data,Label)`

**Arguments**

<code>Data</code>	Microarray data
<code>Label</code>	Data point labels.

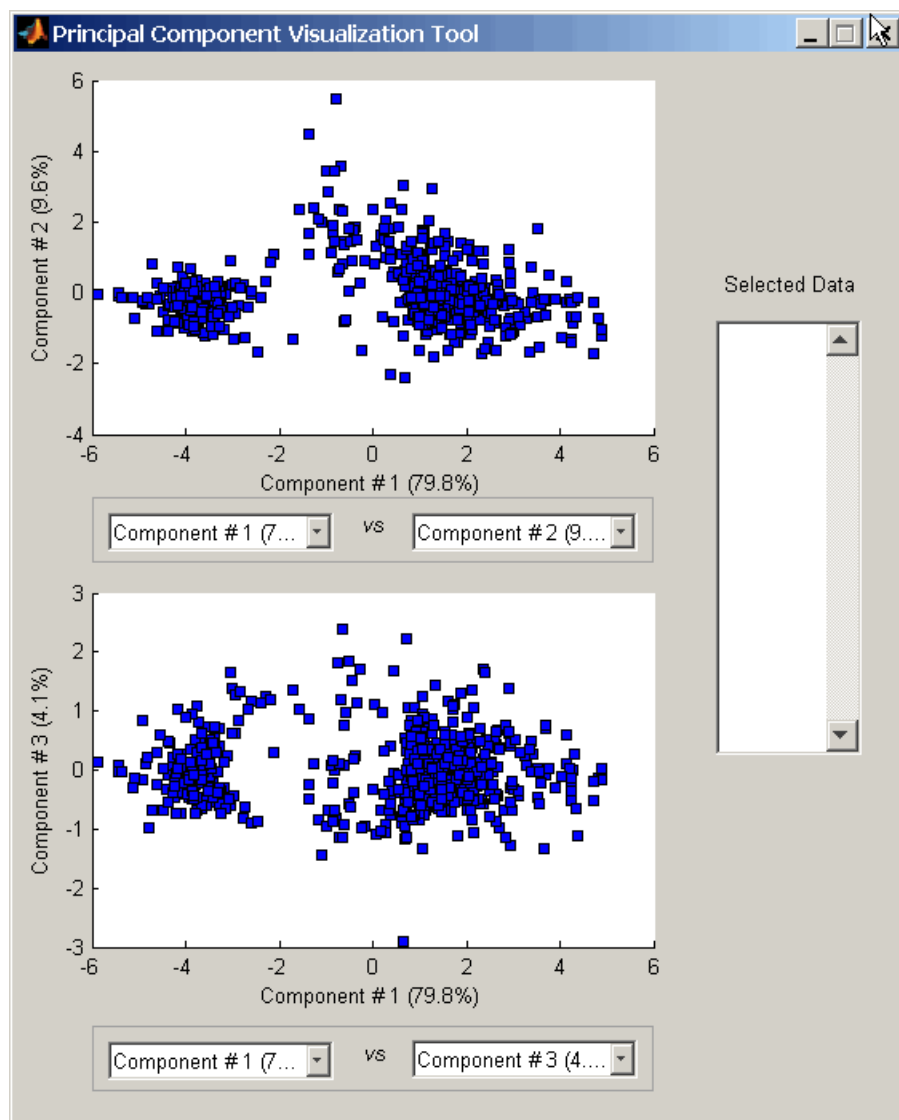
**Description** `mapcaplot(Data)` creates 2D scatter plots of principal components of the array DATA. The principal components used for the x and y data are selected from popup menus, below each scatter plot.

Once the principal components have been plotted, a region can be selected in either axes with the mouse. This will highlight the points in the selected region, and the corresponding points in the other axes. This will also display a list of the row numbers of the selected points in the list box. Selecting an entry in the list box will display a label with the row number in each axes, at the corresponding point. Clicking on a point in the scatter plot will display a label with its row number until the mouse is released.

`mapcaplot(Data,Label)` uses the elements of the cell array of strings Label, instead of the row numbers, to label the data points.

**Examples**

```
load filteredyeastdata
mapcaplot(yeastvalues,genes)
```

**See Also**

Bioinformatics Toolbox function `clustergram`, `mattest`, `mapvolcanoplot`

Statistical Toolbox function princomp

**Purpose** Perform two-sample, two-tailed 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, StdDevs] = mattest(DataX, DataY)
... = mattest(..., 'Showhist', ShowhistValue, ...)
... = mattest(..., 'Showplot', ShowplotValue, ...)
... = mattest(..., 'Labels', LabelsValue, ...)
```

## Arguments

<i>DataX</i>	Matrix of gene expression values (natural or log scale) where each row corresponds to a gene (probe set) and each column corresponds to expression values from a single experimental condition.
<i>DataY</i>	Matrix of gene expression values (natural or log scale) where each row corresponds to a gene (probe set) and each column corresponds to expression values from a single experimental condition.
<i>ShowhistValue</i>	Property to display histograms of t-score distributions and p-value distributions. Enter either true to display histograms or false. Default is false.
<i>ShowplotValue</i>	Property to display a normal t-score quantile plot. Enter true to display the plot, or false. Default is false. 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.
<i>LabelsValue</i>	Cell array of labels (typically gene names or probe set IDs) for each row in <i>DataX</i> and <i>DataY</i> . The labels display if you click a data point in the t-score quantile plot.

## Description

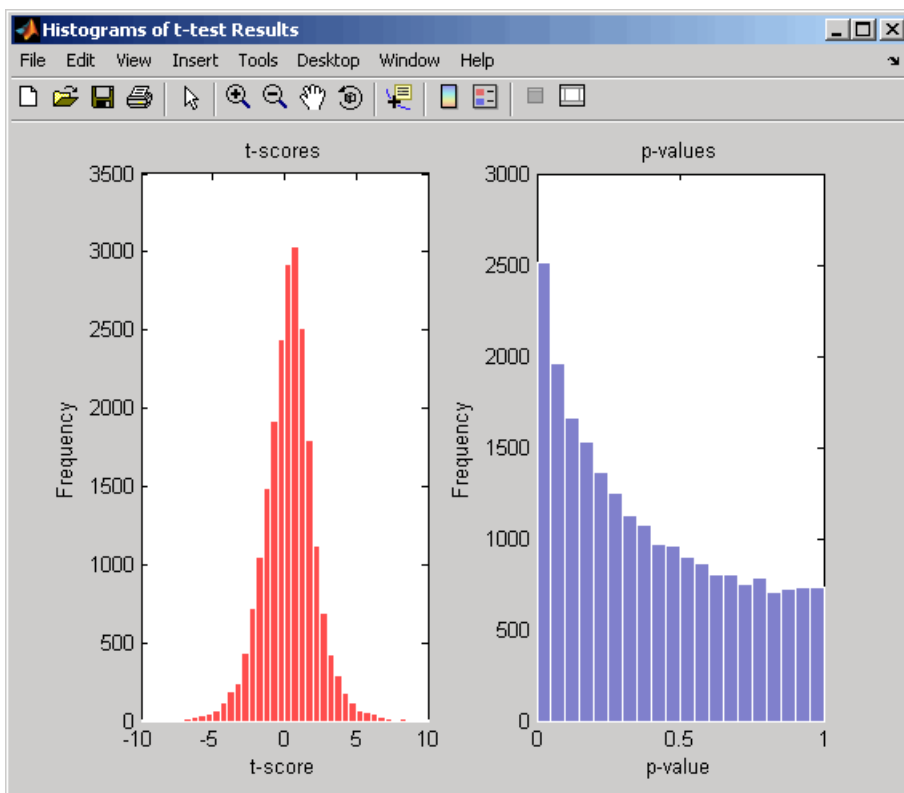
*PValues* = `mattest(DataX, DataY)` compares the gene expression profiles in *DataX* and *DataY* and returns a p-value for each gene. *DataX* and *DataY* are matrices of gene expression values, in which each row corresponds to a gene, and each column corresponds to expression values. *DataX* contains data from one experimental condition and *DataY* contains data from a different experimental condition. *DataX* and *DataY* must have the same number of rows and are assumed to be normally distributed in each class with equal variances. *PValues* is a column vector of p-values for each gene.

`[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.

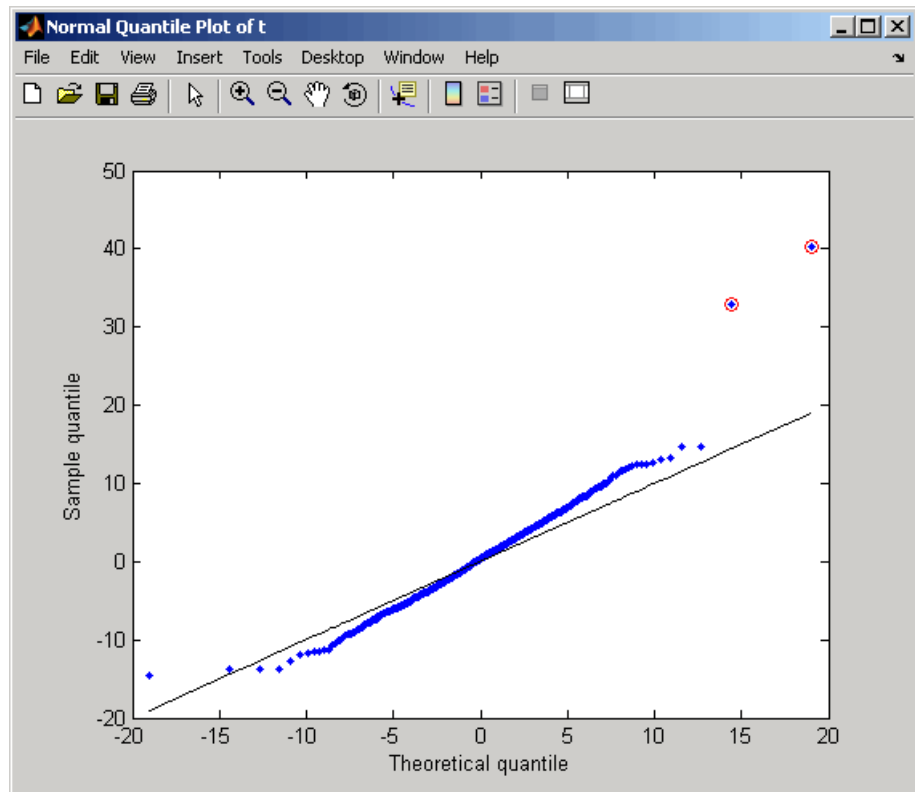
`[PValues, TScores, StdDevs]` = `mattest(DataX, DataY)` also returns the unpooled estimates of the population standard deviations for each gene in *DataX* and *DataY*. *StdDevs* is a column vector of standard deviations for each gene across both data sets.

`... = mattest(..., 'PropertyName', PropertyValue, ...)` defines optional properties that use property name/value pairs in any order. These property name/value pairs are as follows:

`... = 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 a MAT file, included with the Bioinformatics Toolbox, 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);
```

The `prostatecancerexpdata.mat` file used in the previous 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 Suppl1*, 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

`maboxplot`, `mainvarsetnorm`, `mairplot`, `maloglog`, `malowess`, `manorm`, `mavolcanoplot`, `rmasummary`

# mavolcanoplot

---

**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, ...)
```

## Arguments

*DataX* Matrix or vector of gene expression values from a single experimental condition. If *DataX* is 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* are natural scale, use the *LogTrans* property to convert them to log 2 scale.

---

*DataY* Matrix or vector of gene expression values from a single experimental condition. If 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 *DataY* are natural scale, use the *LogTrans* property to convert them to log 2 scale.

---

<i>PValues</i>	Vector of p-values for each gene in data sets from two different experimental conditions.
<i>LabelsValue</i>	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 <i>LabelsValue</i> , data points are labeled with row numbers from <i>DataX</i> and <i>DataY</i> .
<i>LogTransValue</i>	Property to control the conversion of data in <i>DataX</i> and <i>DataY</i> 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.
<i>PCutoffValue</i>	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.

---

<i>FoldchangeValue</i>	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.

---

## Description

`mavolcanoplot(DataX, DataY, PValues)` creates a scatter plot of gene expression data, plotting significance versus fold change of gene expression ratios. It uses the average gene expression values from two data sets, *DataX* and *DataY*, for each gene in the data sets. It plots significance as the  $-\log_{10}$  (p-value) from the vector, *PValues*. *DataX* and *DataY* can be vectors or matrices.

`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

`... 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 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.

---

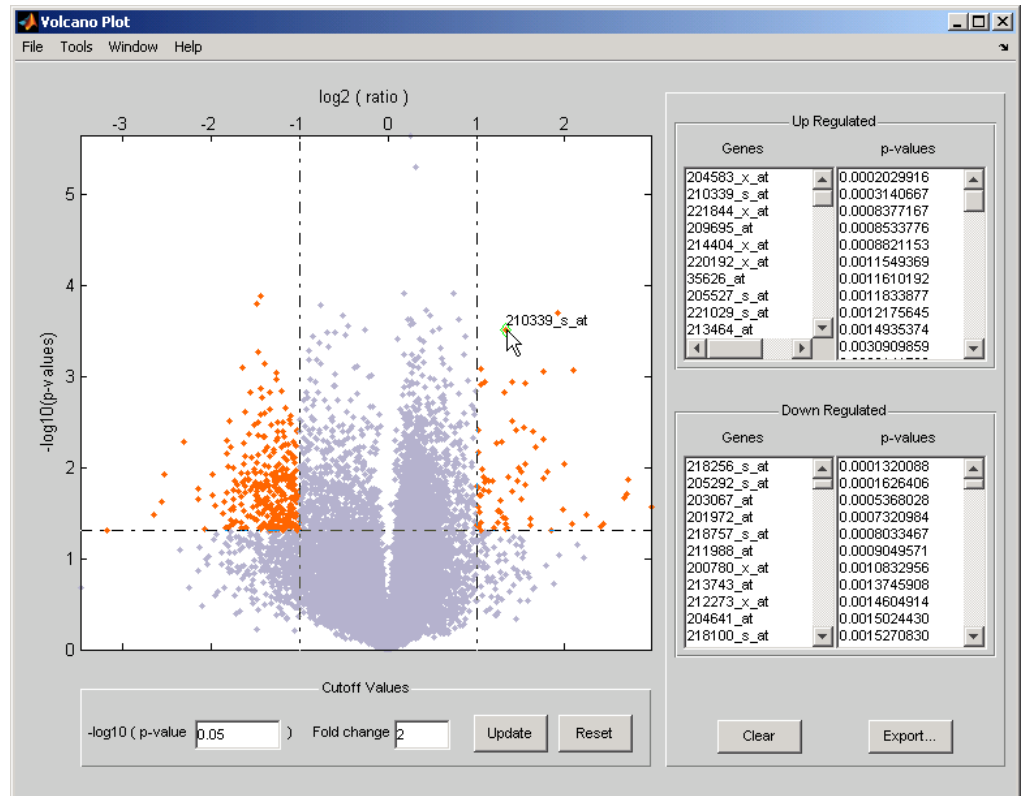
... `mavolcanoplot(..., 'Foldchange', FoldchangeValue, ...)` lets you specify a ratio fold change to define data points that are differentially expressed. Fold changes display graphically as two vertical lines on the plot. Default is 2, which corresponds to a ratio of 1 and  $-1$  on a  $\log_2$  (ratio) scale.

---

**Note** You can also change the fold change interactively after creating the plot.

---

# mavolcanoplot



The volcano plot displays the following:

- $-\log_{10}(\text{p-value})$  versus  $\log_2(\text{ratio})$  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  $\log_2(\text{ratio})$  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  $-\log_{10}(\text{p-value})$  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.

## Examples

- 1 Load a MAT file, included with the Bioinformatics Toolbox, 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);
```

# mavolcanoplot

---

- 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)
```

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

`maboxplot`, `maimage`, `mainvarsetnorm`, `mairplot`, `maloglog`, `malowess`, `manorm`, `mapcaplot`, `mattest`



**Purpose**

Align peaks in mass spectrum to reference peaks

**Syntax**

```
YOut = msalign(MZ, Y, R)  
msalign(..., 'PropertyName', PropertyValue,...)  
msalign(..., 'Weights', WeightsValue)  
msalign(..., 'Range', RangeValue)  
msalign(..., 'WidthOfPulses', WidthOfPulsesValue)  
msalign(..., 'WindowSizeRatio', WindowSizeRatioValue)  
msalign(..., 'Iterations', IterationsValue)  
msalign(..., 'GridSteps', GridStepsValue)  
msalign(..., 'SearchSpace', SearchSpaceValue)  
[YOut,ROut] = msalign(..., 'Group', GroupValue),  
msalign(..., 'ShowPlot', ShowPlotValue)
```

**Arguments**

<i>MZ</i>	Mass/charge vector with the range of ions in the spectra.
<i>Y</i>	Ion intensity vector with the same length as the mass/charge vector ( <i>MZ</i> ). <i>Y</i> can also be a matrix with several spectra that share the same mass/charge ( <i>MZ</i> ) range.
<i>R</i>	Reference mass vector with a list of known masses in the sample spectrum.

**Description**

*Y*Out = msalign(*MZ*, *Y*, *R*) aligns a raw mass spectrum (*Y*) by scaling and shifting the mass/charge scale (*MZ*) so that the cross-correlation between the spectrum (*Y*) and a synthetic spectrum is maximum. A synthetic spectrum is built with Gaussian pulses centered at the masses specified by the reference mass vector (*R*). Once the new mass/charge scale is determined, a new spectrum (*Y*Out) is calculated by piecewise cubic interpolating and shifting the new spectrum from the original mass/charge vector (*MZ*). This method preserves the shape of the peaks.

msalign uses an iterative grid search until it finds the best scale and shift factors for every spectrum.

---

**Note** The algorithm works best with three to five marker masses that you know will appear in the spectrum. If you use a single marker mass (a single internal standard), there is a possibility of picking a peak between the marker and sample peak for that marker as `msalign` scales and shifts the *MZ* vector. If you only require to shift the *MZ* vector, you may prefer to use `YOut = interp1(MZ, MZ - (MarkerMass - PeakPosition), Y)`.

---

`msalign(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`msalign(..., 'Weights', WeightsValue)` specifies the relative weights for every mass in the reference mass vector (*R*). The size of the weight vector (*WeightsValue*) must be the same as the reference mass vector (*R*). The default value is `ones(size(R))` with a range of 0 to 1, but you can use any range. If you have a small number of reference masses, you might want to change the weights.

`msalign(..., 'Range', RangeValue)` specifies the lower and upper bound for the allowable range in *m/z* units to shift any of the mass peaks. The default value is `[-100 100]`. Use these values to tune the robustness of the algorithm. Ideally, you should only try to correct small shifts by keeping the bounds small.

---

**Note** You can try to correct larger shifts by increasing the bounds, but you might also pick the wrong peaks to be aligned.

---

`msalign(..., 'WidthOfPulses', WidthOfPulsesValue)` specifies the width (*WidthOfPulsesValue*) in *m/z* units for all the Gaussian pulses used to build the correlating synthetic spectrum. *WidthOfPulsesValue* is at the point where the Gaussian pulse reaches 60.65% of its maximum. The default value is 10. *WidthOfPulsesValue* may also be a function handle. The function is evaluated at the respective *m/z* values and returns a variable width for the pulses. Its evaluation should give

reasonable values between 0 and  $\max(\text{abs}(\text{Range}))$ ; otherwise, the function errors out.

---

**Note** Tuning the spread of the Gaussian pulses controls a tradeoff between robustness (wider pulses) and precision (narrower pulses), but the spread is unrelated to the shape of the observed peaks in the spectrum.

---

`msalign(..., 'WindowSizeRatio', WindowSizeRatioValue)` specifies a scaling value that determines the size of the window around every alignment peak. The synthetic spectrum is correlated to the sample spectrum only within these regions, which saves computation time. Size of the window is given by  $\text{WidthOfPulsesValue} * \text{WindowSizeRatioValue}$  in m/z units. The default value 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. The default value is 5.

`msalign(..., 'GridSteps', GridStepsValue)` specifies the number of steps for the search grid. For example, at every iteration the search area is divided by  $\text{GridStepsValue}^2$ . The default value is 20.

`msalign(..., 'SearchSpace', SearchSpaceValue)` specifies the type of search space. Enter either 'regular' (evenly spaced lattice) or 'latin' (random latin hypercube with  $\text{GridStepsValue}^2$  samples). The default value is 'regular'.

`[YOut, ROut] = msalign(..., 'Group', GroupValue)`, when *GroupValue* is true and Y contains more than one spectrum, updates the original peak locations so that the actual movement of the peaks is minimized. *ROut* contains the reference masses with the updated ion peak locations. Use this property when you are uncertain about the values for the reference masses. The default value is false.

`msalign(..., 'ShowPlot', ShowPlotValue)` plots the original and the aligned spectrum over the reference masses (*R*). When `msalign` is called without output arguments, the spectra are plotted unless `ShowPlotValue` is false. When `ShowPlotValues` is true, only the first spectrum in *Y* is plotted. The default value is false.

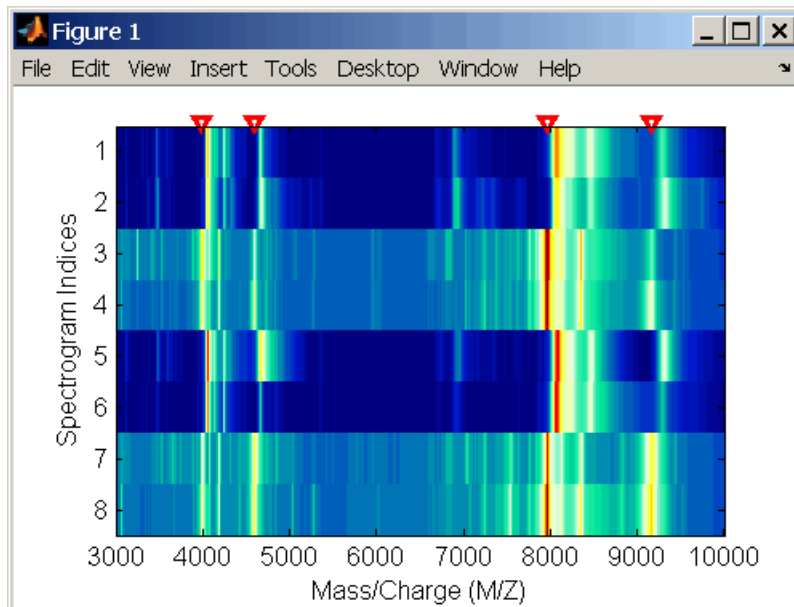
## Example 1

- 1 Load 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];
```

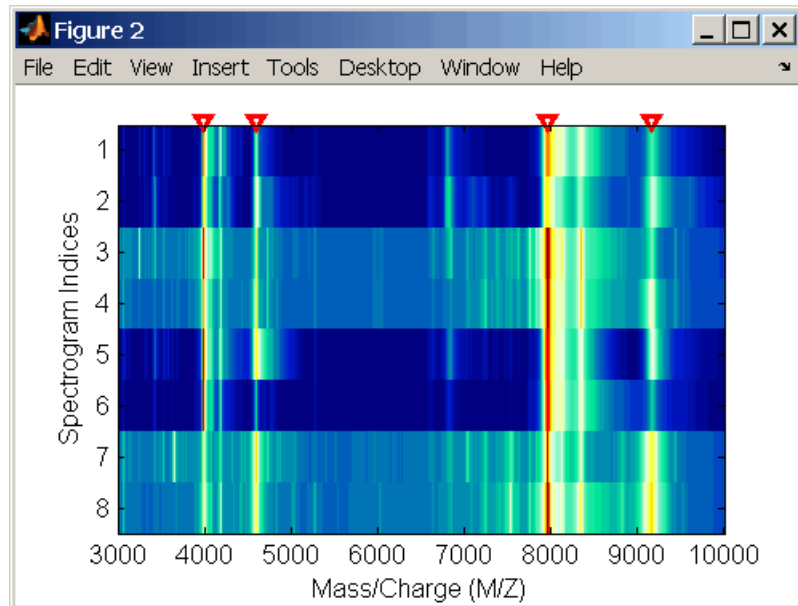
- 2 Display a color image of the mass spectra before alignment.

```
msheatmap(MZ_lo_res,Y_lo_res,'markers',R,'limit',[3000 10000])
title('before alignment')
```



- 3 Align spectra with reference masses and display a color image of mass spectra after alignment.

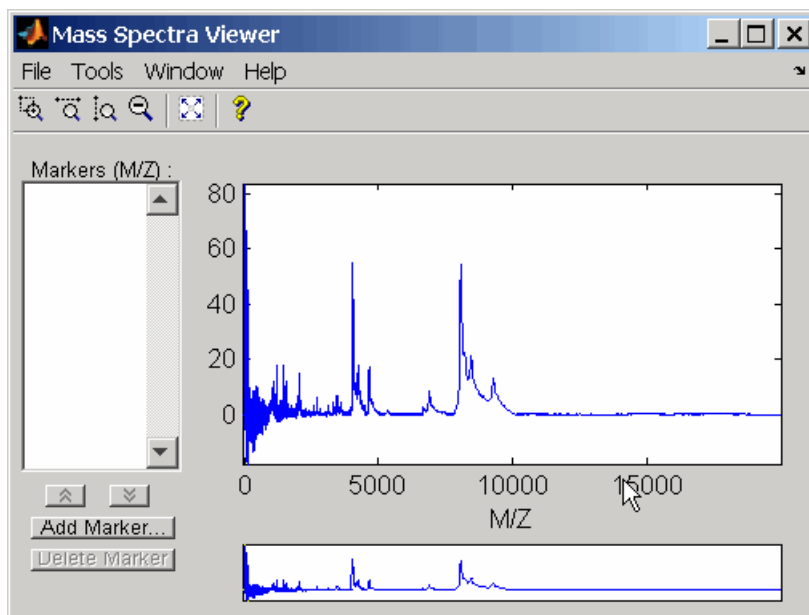
```
YA = msalign(MZ_lo_res,Y_lo_res,R,'weights',W);
msheatmap(MZ_lo_res,YA,'markers',R,'limit',[3000 10000])
title('after alignment')
```



## Example 2

- 1 Align a spectrum with a single reference peak. 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)
```

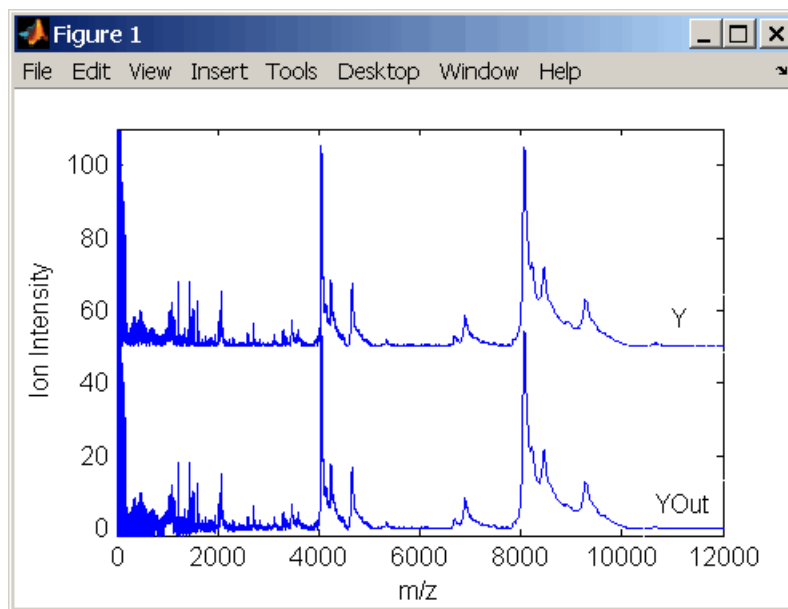


**2** Select a reference peak by zooming and right-clicking a peak.

**3** Shift a spectrum by the difference between the known reference mass (RP) and the experimental mass (SP).

```
RP = 4000;  
SP = 4050.33;  
YOut = interp1(MZ, MZ-(RP-SP), Y);
```

The plot below shows the original spectrum on top and the shifted spectrum on the bottom.

**See Also**

Bioinformatics Toolbox functions `msbackadj`, `msheatmap`, `mslowess`, `msnorm`, `msresample`, `mssgolay`, `msviewer`

# msbackadj

---

**Purpose** Correct baseline of mass spectrum

**Syntax**

```
Yout = msbackadj(MZ, Y)
msbackadj(..., 'PropertyName', PropertyValue,...)
msbackadj(..., 'WindowSize', WindowSizeValue)
msbackadj(..., 'StepSize', StepSizeValue)
msbackadj(..., 'RegressionMethod', RegressionMethodValue)
msbackadj(..., 'EstimationMethod', EstimationMethodValue)
msbackadj(..., 'SmoothMethod', SmoothMethodValue)
msbackadj(..., 'QuantileValue', QuantileValueValue)
msbackadj(..., 'PreserveHeights', PreserveHeightsValue)
msbackadj(..., 'ShowPlot', ShowPlotValue)
```

## Arguments

<i>MZ</i>	Range of mass/charge ions. Enter a vector with the range of ions in the spectra.
<i>Y</i>	Ion intensity vector with the same length as the mass/charge vector ( <i>MZ</i> ). <i>Y</i> can also be a matrix with several spectra that share the same mass/charge ( <i>MZ</i> ) range.

## Description

`Yout = msbackadj(MZ, Y)` adjusts the variable baseline of a raw mass spectrum by following three steps:

- 1** Estimates the baseline within multiple shifted windows of width 200 *m/z*
- 2** Regresses the varying baseline to the window points using a spline approximation
- 3** Adjusts the baseline of the spectrum (*Y*)

`msbackadj(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.



`msbackadj(..., 'WindowSize', WindowSizeValue)` specifies the width for the shifting window. *WindowSizeValue* can also be a function handler. The function is evaluated at the respective MZ 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 of the spectrogram. The default value is 200 (baseline point estimated for windows with a width of 200 m/z).

---

**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 spectrum and the presence of possible drifts. If you have wider peaks towards the end of the spectrum, you may want to use variable parameters.

---

`msbackadj(..., 'StepSize', StepSizeValue)` specifies the steps for the shifting window. The default value is 200 m/z (baseline point is estimated for windows placed every 200 m/z). *StepSizeValue* may also be a function handle. The function is evaluated at the respective m/z values and returns the distance between adjacent windows.

`msbackadj(..., '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'.

`msbackadj(..., '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.

`msbackadj(..., '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 value is 'none'.

`msbackadj(..., 'QuantileValue', QuantileValueValue)` specifies the quantile value. The default value is 0.10.

`msbackadj(..., '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.

`msbackadj(..., 'ShowPlot', ShowPlotValue)` plots the baseline estimated points, the regressed baseline, and the original spectrum. When `msbackadj` is called without output arguments, the spectra are plotted unless *ShowPlotValue* is false. When *ShowPlotValue* is true, only the first spectrum in *Y* is plotted. *ShowPlotValue* can also contain an index to one of the spectra in *Y*.

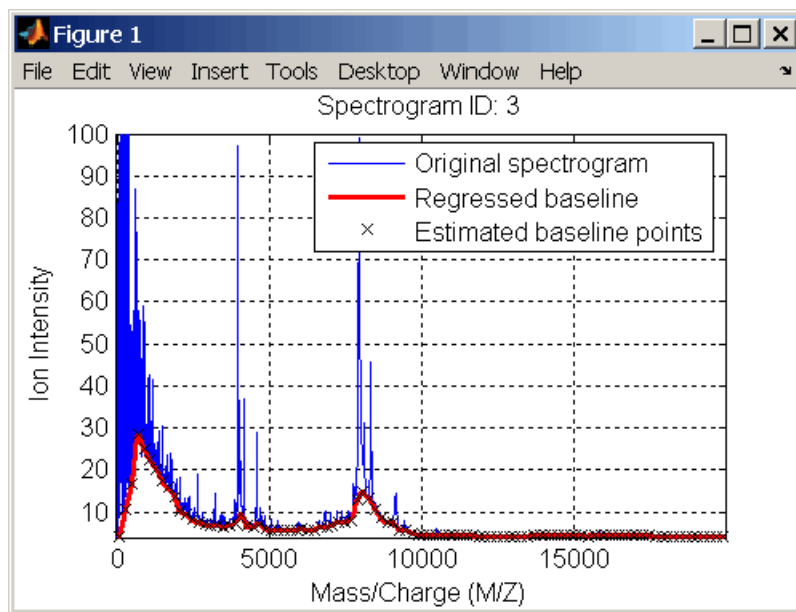
## Example

1 Load sample data.

```
load sample_lo_res
```

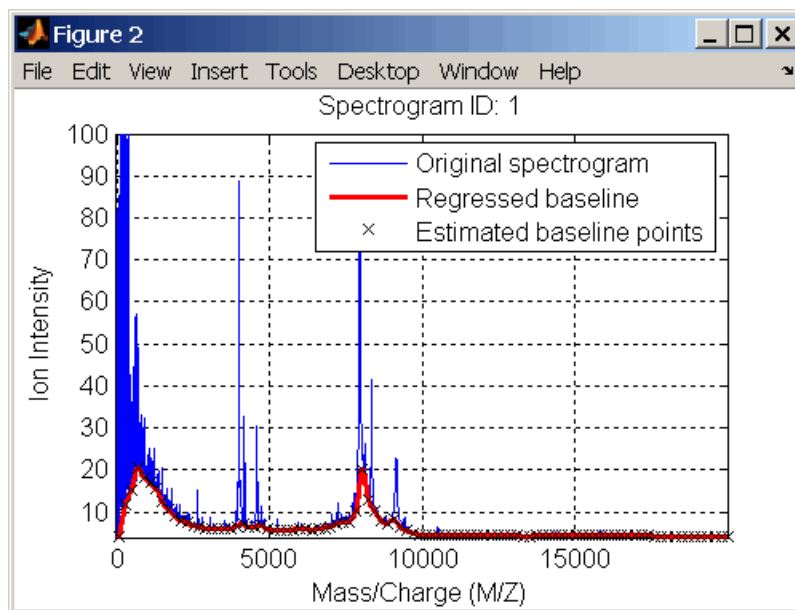
2 Adjust the baseline for a group of spectra and show only the third spectrum and its estimated background.

```
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`, `mslowess`, `msheatmap`, `msnorm`, `msresample`, `mssgolay`, `msviewer`

**Purpose** Smooth mass spectrum using nonparametric method

**Syntax**

```
Yout = mslowess(MZ, Y, 'PropertyName', PropertyValue...)
mslowess(..., 'Order', OrderValue)
mslowess(..., 'Span', SpanValue)
mslowess(..., 'Kernel', KernelValue)
mslowess(..., 'RobustIterations', RobustIterationsValue)
mslowess(..., 'ShowPlot', ShowPlotValue)
```

**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**

Yout = mslowess(MZ, Y, 'PropertyName', PropertyValue...) smoothes a mass spectrum (Y) using a locally weighted linear regression (lowess) method with a default span of 10 samples.

---

**Note** 1) mslowess assumes that a mass/charge vector (MZ) might not be uniformly spaced. Therefore, the sliding window for smoothing is centered using the closest samples in terms of the MZ value and not in terms of the MZ indices.

2) When the vector MZ does not have repeated values or NaNs, the algorithm is approximately twice as fast.

---

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** The MATLAB Curve Fitting Toolbox 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 mass/charge vector (MZ). 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 MZ.

`mslowess(..., 'Kernel', KernelValue)` selects the function (*KernelValue*) for weighting the observed ion intensities. Samples close to the MZ location being smoothed have the most weight in determining the estimate. Enter

'tricubic' (default)	$(1 - (\text{dist}/\text{dmax}))^3.^3$
'gaussian'	$\exp(-(2*\text{dist}/\text{dmax}).^2)$
'linear'	$1-\text{dist}/\text{dmax}$

`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 a uniformly spaced MZ vector, a nonrobust smoothing with Order equal to 0 is equivalent to filtering the signal with the kernel vector.

---

`mslowess(..., 'ShowPlot', ShowPlotValue)` plots the smoothed spectrum over the original spectrum. When `mslowess` is called without output arguments, the spectra are plotted unless *ShowPlotValue* is false. When *ShowPlotValue* is true, only the first spectrum in *Y* is plotted. *ShowPlotValue* can also contain an index to one of the spectra in *Y*.

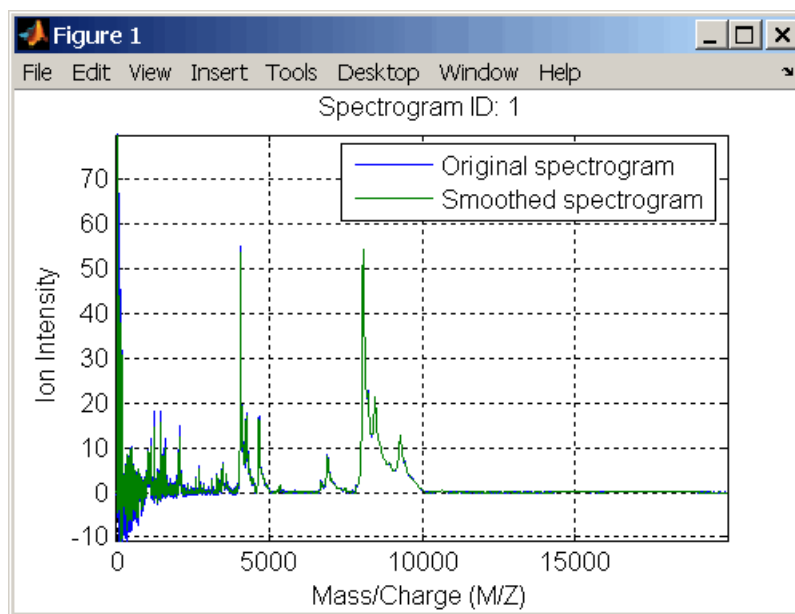
## Example

1 Load sample data.

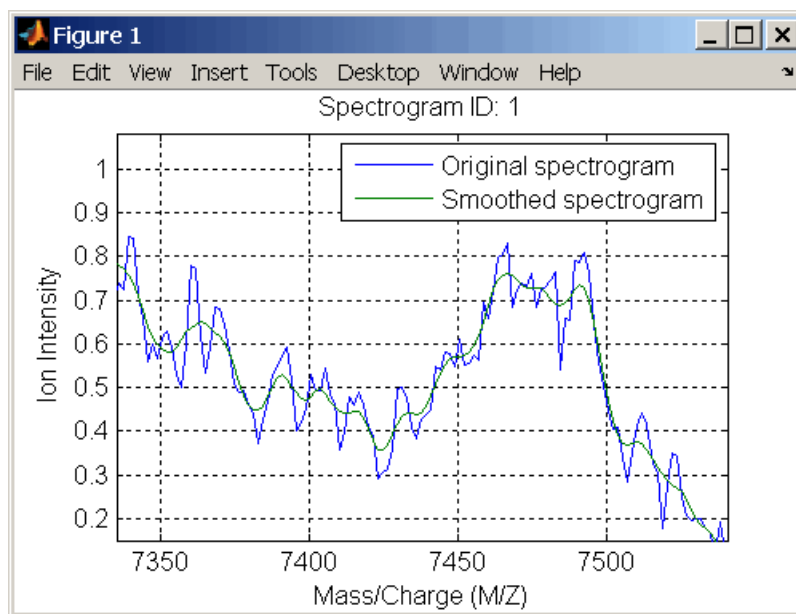
```
load sample_lo_res
```

2 Smooth spectrum and draw figure with unsmoothed and smoothed spectra.

```
YS = mslowess(MZ_lo_res, Y_lo_res(:,1), 'Showplot', true);
```





**See Also**

Bioinformatics Toolbox functions `msalign`, `msbackadj`, `msheatmap`, `msheatmap`, `msnorm`, `msresample`, `mssgolay`, `msviewer`

**Purpose** Normalize set of mass spectra

**Syntax**

```
Yout = msnorm(MZ, Y)  
[Yout, NormParameters]  
= msnorm(...)  
msnorm(MZ, NewY, NormParameters)  
msnorm(..., 'PropertyName', PropertyValue,...)  
msnorm(..., 'Quantile', QuantileValue)  
msnorm(..., 'Limits', LimitsValue)  
msnorm(..., 'Consensus', ConsensusValue)  
msnorm(..., 'Method', MethodValue)  
msnorm(..., 'Max', MaxValue)
```

## Arguments

<i>MZ</i>	Mass/charge vector with the range of ions in the spectra.
<i>Y</i>	Ion intensity vector with the same length as the mass/charge vector ( <i>MZ</i> ). <i>Y</i> can also be a matrix with several spectra that share the same mass/charge ( <i>MZ</i> ) range.

## Description

*Yout* = msnorm(*MZ*, *Y*) normalizes a group of mass spectra by standardizing the area under the curve (AUC) to the group median.

[*Yout*, *NormParameters*] = msnorm(...) returns a structure with the parameters to normalize another group of spectra.

msnorm(*MZ*, *NewY*, *NormParameters*) uses the parameter information from a previous normalization (*NormParameters*) to normalize a new set of spectra (*NewY*) with the *MZ* 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 *MZ* positions are selected, and normalization is performed using the same *MZ* positions.

msnorm(..., '*PropertyName*', *PropertyValue*,...) defines optional properties using property name/value pairs.

`msnorm(..., 'Quantile', QuantileValue)` specifies a 1-by-2 vector with the quantile limits for reducing the set of MZ values. For example, when *QuantileValue* is `[0.9 1]`, only the largest 10% of ion intensities in every spectrum 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 an MZ range for picking normalization points. This parameter is useful to eliminate low-mass noise from the AUC calculation. The default value is `[1, max(MZ)]`.

`msnorm(..., 'Consensus', ConsensusValue)` selects MZ positions with a consensus rule to include an MZ position into the AUC. Its ion intensity must be within the quantile limits of at least part (*ConsensusValue*) of the spectra in *Y*. The same MZ positions are used to normalize all the spectrums. Enter a scalar between 0 and 1.

Use the Consensus property to eliminate low-intensity peaks and noise from the normalization.

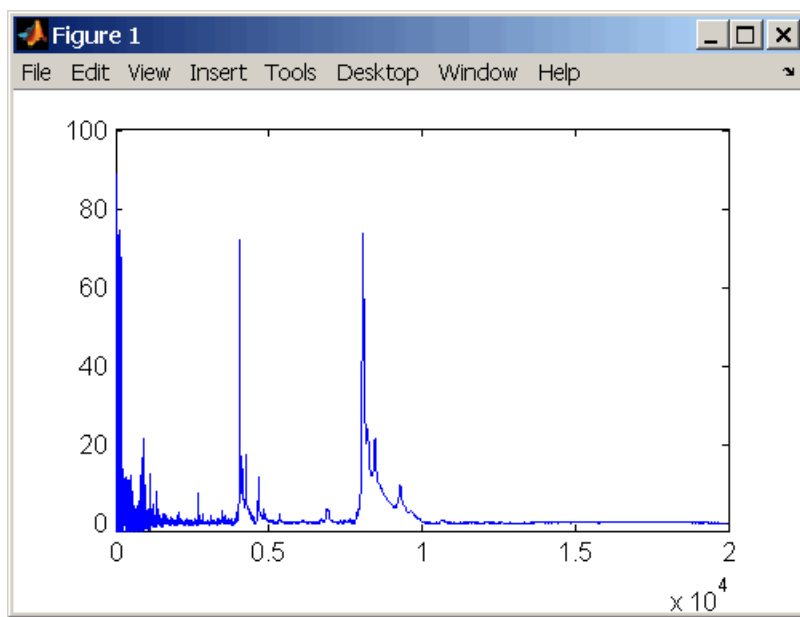
`msnorm(..., 'Method', MethodValue)` selects a method for normalizing the AUC of every spectrum. Enter either 'Median' (default) or 'Mean'.

`msnorm(..., 'Max', MaxValue)`, after individually normalizing every spectrum, scales each spectrum to an overall maximum intensity (Max). Max 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 Max.

## Example 1

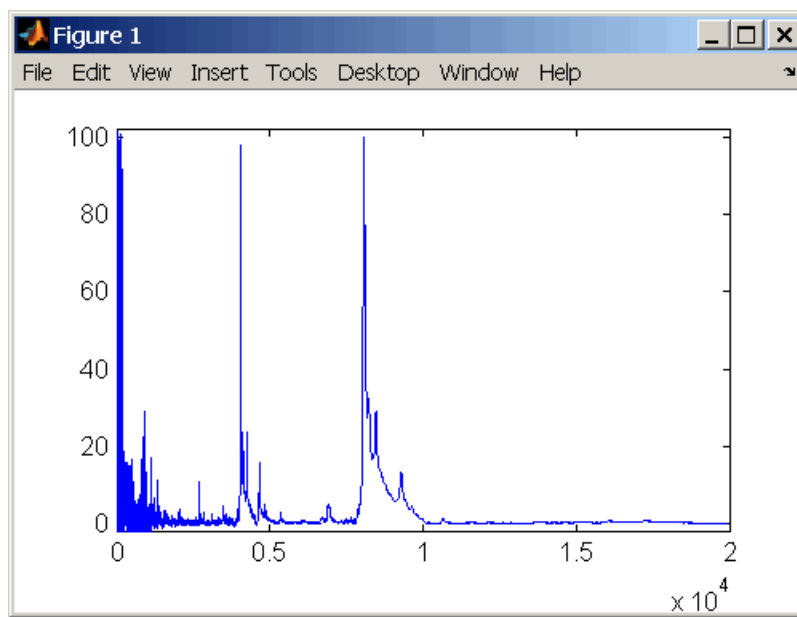
1 Load sample data and plot one of the spectra.

```
load sample_lo_res;
Y = Y_lo_res(:, [1 2 5 6]);
MZ = MZ_lo_res;
plot(MZ, Y(:, 4));
```



- 2 Normalize the AUC of every spectrum to its median, eliminating low-mass noise, and post-rescaling such that the maximum intensity is 100.

```
Y1 = msnorm(MZ,Y,'Limits',[1000 inf],'Max',100);  
plot(MZ, Y1(:, 4));
```



- 3 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 100 m/z.

```
Y2 = msnorm(MZ,Y,'QUANTILE',[1 1],'LIMITS',[1000 inf]);
```

## Example 2

- 1 Select MZ regions where the intensities are within the third quartile in at least 90% of the spectrograms.

```
[Y3,S] = msnorm(MZ,Y,'Quantile',[0.5 0.75],'Consensus',0.9);
```

- 2 Use the same MZ regions to normalize another set of spectrograms.

```
Y4 = msnorm(MZ,Y,S);
```

## See Also

Bioinformatics Toolbox functions `msalign`, `msbackadj`, `msheatmap`, `mslowess`, `msresample`, `mssgolay`, `msviewer`

# msheatmap

---

**Purpose** Color image for set of spectra

**Syntax**

```
msheatmap(MZ, Y)
msheatmap(..., 'PropertyName', PropertyValue,...)
msheatmap(..., 'Markers', MarkersValue)
msheatmap(..., 'Limits', LimitsValues)
msheatmap(..., 'Group', GroupValue)
```

## Arguments

<i>MZ</i>	Mass/charge vector with the range of ions in the spectra.
<i>Y</i>	Ion intensity vector with the same length as the mass/charge vector ( <i>MZ</i> ). <i>Y</i> can also be a matrix with several spectra that share the same mass/charge ( <i>MZ</i> ) range.

## Description

`msheatmap(MZ, Y)` shows a heatmap image of the spectra in *Y*.

`msheatmap(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`msheatmap(..., 'Markers', MarkersValue)` specifies a list of markers with positions marked along the top axis. The default value is `[]`.

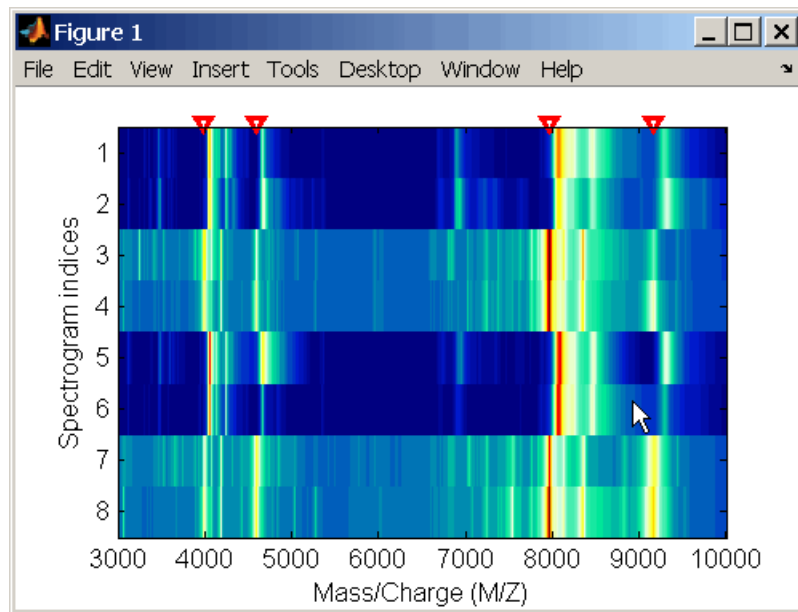
`msheatmap(..., 'Limits', LimitsValues)` specifies a `[2x1]` vector with the mass/charge range for the heatmap image.

`msheatmap(..., 'Group', GroupValue)` specifies the class label for every spectrum used to group the rows of the heatmap image. *GroupValue* can be a numeric vector or a cell array of strings with the same number of elements as there are spectra in *Y*.

## Examples

**1** Load sample data.

```
load sample_lo_res
M = [3991.4 4598 7964 9160];
msheatmap(MZ_lo_res,Y_lo_res,'markers',M,'limit',[3000 10000])
```



## 2 Plot heatmap.

```
msheatmap(MZ_lo_res,Y_lo_res,'markers',M,'group',[1 1 2 2 1 1 2 2])
```

## See Also

Bioinformatics Toolbox functions `msalign`, `msbackadj`, `mslowess`, `msnorm`, `msresample`, `mssgolay`, `msviewer`

# msresample

---

**Purpose** Resample mass spectrometry signal

**Syntax**

```
[MZout, Yout] = msresample(MZ, Y, N)
msresample(..., 'PropertyName', PropertyValue, ...)
msresample(..., 'Uniform', UniformValue)
msresample(..., 'Range', RangeValue)
msresample(..., 'Missing', MissingValue)
msresample(..., 'Window', WindowValue)
msresample(..., 'Cutoff', CutoffValue)
msresample(..., 'ShowPlot', ShowPlotValue)
```

## Arguments

<i>MZ</i>	Mass/charge vector with the range of ions in the spectra.
<i>Y</i>	Ion intensity vector with the same length as the mass/charge vector ( <i>MZ</i> ). <i>Y</i> can also be a matrix with several spectra that share the same mass/charge ( <i>MZ</i> ) range.
<i>N</i>	Total number of samples.

## Description

`[MZout, Yout] = msresample(MZ, Y, N)` resamples a raw mass spectrum (*Y*). The output spectrum will have *N* samples with a spacing that increases linearly within the range  $[\min(MZ) \text{ } \max(MZ)]$ . *MZ* can be a linear or a quadratic function of its index. When input arguments are set 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 cu-off frequency is set by the largest down-sampling ratio when comparing the same regions in the *MZ* and *MZout* vectors.

---

**Note** `msresample` is particularly useful when you have spectra with different mass/charge vectors and you want to match the scales.

---



`msresample(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`msresample(..., 'Uniform', UniformValue)`, when *UniformValue* is true, forces the vector *MZ* to be uniformly spaced. The default value is false.

`msresample(..., 'Range', RangeValue)` specifies a 1-by-2 vector with the mass/charge range for the output spectrum (*Yout*). *RangeValue* must be within  $[\min(MZ) \max(MZ)]$ . The default value is the full range  $[\min(MZ) \max(MZ)]$ .

`msresample(..., 'Missing', MissingValue)`, when *MissingValue* is true, analyzes the mass/charge vector (*MZ*) 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 *MZ* values follow a linear or a quadratic function of the *MZ* 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 between 0 and 1 (Nyquist frequency or half the sampling frequency). By default, `msresample` estimates the cutoff value by inspecting the mass/charge vectors (*MZ*, *MZout*). However, the cutoff frequency might be underestimated if *MZ* has anomalies.

`msresample(..., 'ShowPlot', ShowPlotValue)` plots the original and the resampled spectrum. When `msresample` is called without output arguments, the spectra are plotted unless *ShowPlotValue* is false. When *ShowPlotValue* is true, only the first spectrum in *Y* is plotted. *ShowPlotValue* can also contain an index to one of the spectra in *Y*.

## Examples

- 1 Load mass spectrometry data and extract m/z and intensity value vectors

```
load sample_hi_res;
```

# msresample

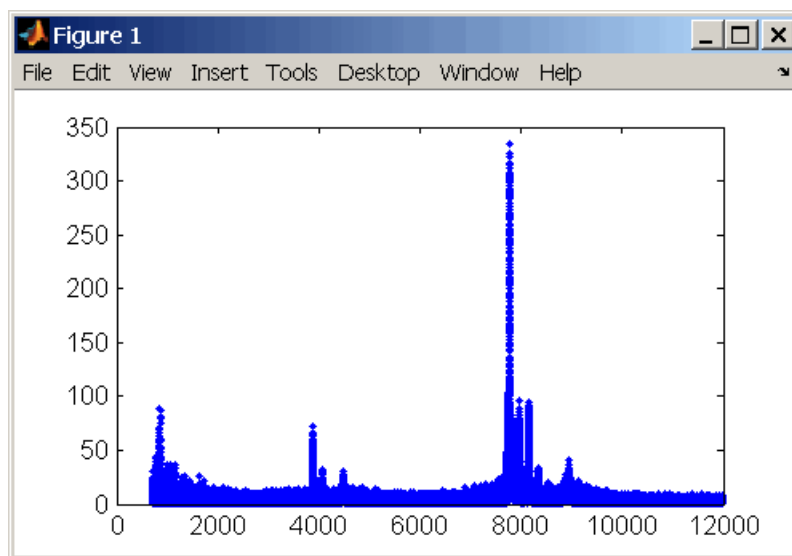
---

```
mz = MZ_hi_res;  
y = Y_hi_res;
```

**2** Plot original data to a lower resolution.

```
plot(mz, y, '.')
```

MATLAB draws a figure.



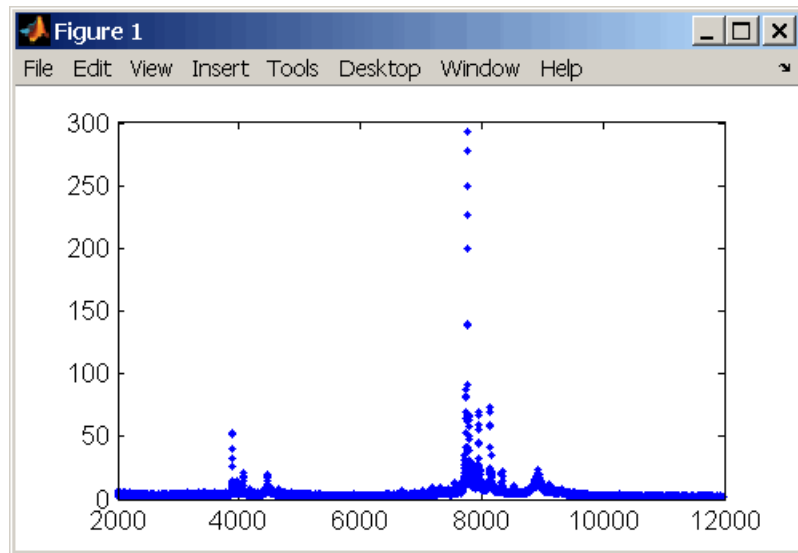
**3** Resample data

```
[mz1,y1] = msresample(mz, y, 10000, 'range',[2000 max(mz)]);
```

**4** Plot resampled data

```
plot(mz1,y1, '.')
```

MATLAB draws a figure with the down sampled data.



## See Also

The Bioinformatics Toolbox functions `msalign`, `msbackadj`, `msheatmap`, `mslowess`, `msnorm`, `mssgolay`, `msviewer`

# mssgolay

---

**Purpose** Smooth mass spectrum with least-squares polynomial

**Syntax**

```
Yout = mssgolay(MZ, Y)
mssgolay(..., 'PropertyName', PropertyValue, ...)
mssgolay(..., 'Span', SpanValue)
mssgolay(..., 'Degree', DegreeValue)
mssgolay(..., 'ShowPlot', ShowPlotValue)
```

## Arguments

<i>MZ</i>	Mass/charge vector with the range of ions in the spectrum.
<i>Y</i>	Ion intensity vector with the same length as the mass/charge vector ( <i>MZ</i> ). <i>Y</i> can also be a matrix with several spectra that share the same mass/charge ( <i>MZ</i> ) range.

## Description

`Yout = mssgolay(MZ, Y)` smoothes a raw mass spectrum (*Y*) using a least squares digital polynomial filter (Savitzky and Golay filters). The default span or frame is 15 samples.

`mssgolay(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`mssgolay(..., '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 *MZ* vector. Higher values will 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 data (*MZ*). For example, if *SpanValue* is 0.05, the window size is equal to 5% of the number of points in *MZ*.

---

**Note** 1) The original algorithm by Savitzky and Golay assumes a uniformly spaced mass/charge vector ( $MZ$ ), 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  $MZ$  value and not in terms of the  $MZ$  index.

2) When the vector  $MZ$  does not have repeated values or NaNs, the algorithm is approximately twice as fast.

3) When the vector  $MZ$  is evenly spaced, the least-squares fitting is performed once so that the spectrum is filtered with the same coefficients, and the speed of the algorithm increases considerably.

4) If the vector  $MZ$  is evenly spaced and `SpanValue` is even, `Span` is incremented by 1 to include both edge samples in the frame.

---

`mssgolay(..., '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(..., 'ShowPlot', ShowPlotValue)` plots smoothed spectra over the original. When `mssgolay` is called without output arguments, the spectra are plotted unless *ShowPlotValue* is false. When *ShowPlotValue* is true, only the first spectrum in  $Y$  is plotted. *ShowPlotValue* can also contain an index to one of the spectra in  $Y$ .

## Examples

```
load sample_lo_res
YS = mssgolay(MZ_low_res, Y_low_res(:,1));
plot(MZ,[Y(:,1) YS])
```

## See Also

Bioinformatics Toolbox functions `msalign`, `msbackadj`, `msheatmap`, `mslowess`, `msnorm`, `msresample`, `msviewer`

# msviewer

---

**Purpose** Explore MS spectrum or set of 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`



---

<b>Purpose</b>	Calculate molecular weight of amino acid sequence		
<b>Syntax</b>	<code>molweight(SeqAA)</code>		
<b>Arguments</b>	<table><tr><td><code>SeqAA</code></td><td>Amino acid sequence. Enter a character string or a vector of integers from the table Amino Acid Lookup Table on page 2-27. Examples: 'ARN', [1 2 3]. You can also enter a structure with the field <code>Sequence</code>.</td></tr></table>	<code>SeqAA</code>	Amino acid sequence. Enter a character string or a vector of integers from the table Amino Acid Lookup Table on page 2-27. Examples: 'ARN', [1 2 3]. You can also enter a structure with the field <code>Sequence</code> .
<code>SeqAA</code>	Amino acid sequence. Enter a character string or a vector of integers from the table Amino Acid Lookup Table on page 2-27. Examples: 'ARN', [1 2 3]. You can also enter a structure with the field <code>Sequence</code> .		
<b>Description</b>	<code>molweight(SeqAA)</code> calculates the molecular weight for the amino acid sequence <code>SeqAA</code> .		
<b>Examples</b>	<ol style="list-style-type: none"><li>1 Get an amino acid sequence from the NCBI Genpept Database <pre>rhodopsin = getgenpept('NP_000530');</pre></li><li>2 Calculate the molecular weight of the sequence. <pre>rhodopsinMW = molweight(rhodopsin)  rhodopsinMW =  3.8892e+004</pre></li></ol>		
<b>See Also</b>	Bioinformatics Toolbox functions <code>aaccount</code> , <code>atomiccomp</code> , <code>isoelectric</code> , <code>proteinplot</code>		

# multialign

---

**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(..., 'ExtendedGap', ExtendedGapValue)
multialign(..., 'DelayCutoff', DelayCutoffValue)
multialign(..., 'JobManager', JobManagerValue)
multialign(..., 'WaitInQueue', WaitInQueueValue)
multialign(..., 'Verbose', VerboseValue)
multialign(..., 'ExistingGapAdjust', ExistingGapAdjustValue)
multialign(..., 'TerminalGapAdjust', TerminalGapAdjustValue)
```

**Arguments**

<i>Seqs</i>	Vector of structures with the fields 'Sequence' for the residues and 'Header' or 'Name' for the labels.  <i>Seqs</i> may also be a cell array of strings or a char array.
<i>SeqsMultiAligned</i>	Vector of structures (same as <i>Seqs</i> ) but with the field 'Sequence' updated with the alignment.  When <i>Seqs</i> is a cell or char array, <i>SeqsMultiAligned</i> is a char array with the output alignment following the same order as the input.
<i>Tree</i>	Phylogenetic tree calculated with either of the functions <code>seqlinkage</code> or <code>seqneighjoin</code> .

<i>WeightsValue</i>	Property to select the sequence weighting method. Enter either 'THG' (default) or 'equal'.
<i>ScoringMatrixValue</i>	Property to select or specify the scoring matrix. Enter an [MxM] matrix or [MxMxN] array of matrixes with N user-defined scoring matrices. <i>ScoringMatrixValue</i> 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.
<i>SMInterpValue</i>	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.
<i>GapOpenValue</i>	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). Defaults value is @(sm, sx, len1, len2) 2*sm.

<i>ExtendedGapValue</i>	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 value is @(sm, sx, len1, len2) sm/20.
<i>DelayCutoffValue</i>	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.
<i>JobManagerValue</i>	JobManager object representing an available distributed MATLAB resource. Enter a jobmanager object returned by the Distributed Computing Toolbox function findResource.
<i>WaitInQueueValue</i>	Property to control waiting for a distributed MATLAB resource to be available. Enter either true or false. The default value is false.
<i>VerboseValue</i>	Property to control displaying the sequences with sequence information. Default value is false.

<i>ExistingGapAdjustValue</i>	Property to control automatic adjustment based on existing gaps. Default value is true.
<i>TerminalGapAdjustValue</i>	Property to adjust 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(..., 'ExtendedGap', ExtendedGapValue)` 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

$(\textit{DelayCutoffValue}) * (\text{median patristic distance between sequences})$

`multialign(..., 'JobManager', JobManagerValue)` distributes pairwise alignments into a cluster of computers using the Distributed Computing Toolbox.

`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 Distributed Computing Toolbox 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 `proalign` 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.

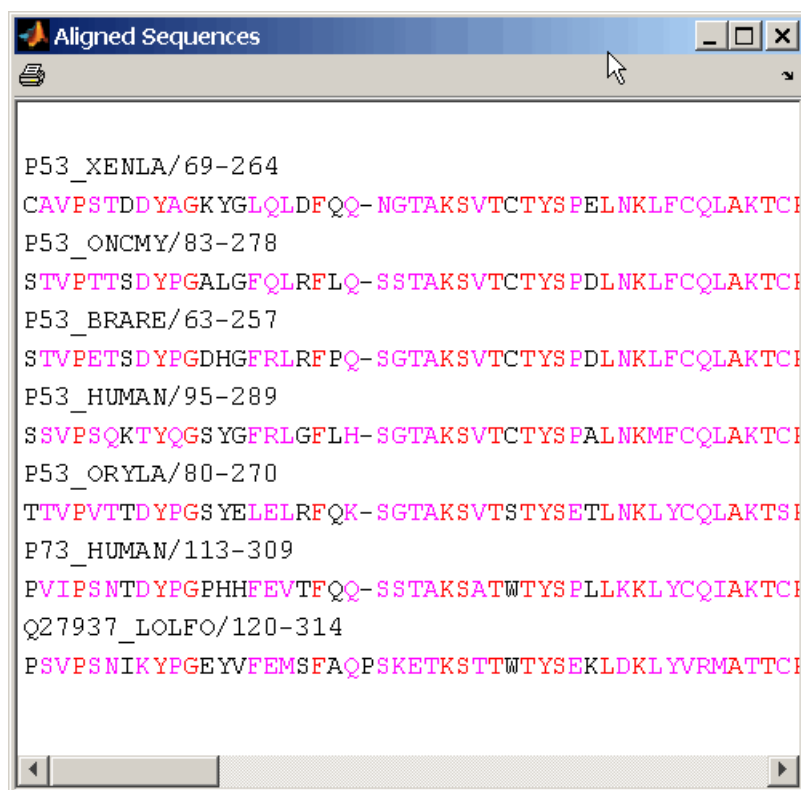
`multialign(..., 'TerminalGapAdjust', TerminalGapAdjustValue)`, when *TerminalGapAdjustValue* is true, adjusts the penalty for opening a gap at the ends of the sequence to be equal to the penalty for extending a gap.

## Example 1

1 Align seven cellular tumor antigen p53 sequences.

```
p53 = fastaread('p53samples.txt')
ma = multialign(p53, 'verbose', true)
showalignment(ma)
```

# multialign



2 Use an UPGMA phylogenetic tree instead as a guiding tree.

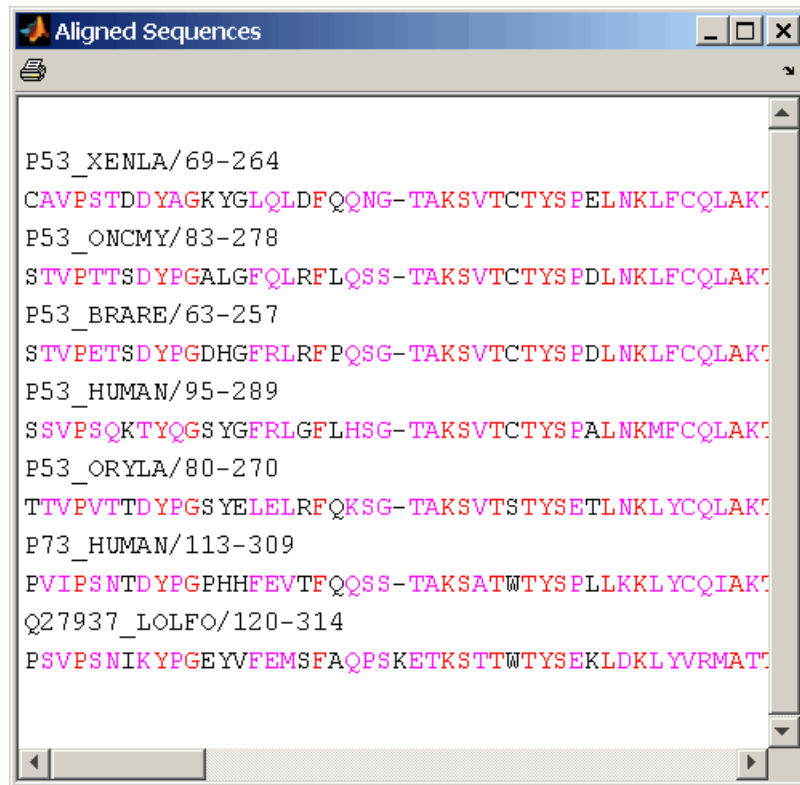
```
dist = seqpdist(p53, 'ScoringMatrix', gonnet);
tree = seqlinkage(dist, 'UPGMA', p53)
```

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
```

# multialign

---

```
-AAACGTAACATCTCGC
```

**3** Compare alignment without termination gap adjustment.

```
multialign(seqs)
```

```
ans =
```

```
CA--CGTAACATCT--C
```

```
ACGACGTAACATCTTCT
```

```
AA-ACGTAACATCTCGC
```

## See Also

Bioinformatics Toolbox functions `hmmprofalign`, `multialignread`, `nwalignment`, `profalign`, `seqprofile`, `seqconsensus`, `seqneighjoin`, `showalignment`

**Purpose** Read multiple-sequence alignment file

**Syntax**

```
S = multialignread(File)
[Headers, Sequences] = multialignread(File)
multialignread(..., 'PropertyName', PropertyValue,...)
multialignread(..., 'IgnoreGaps', IgnoreGapsValue)
```

## Arguments

<i>File</i>	Multiple sequence alignment file (ASCII text file). Enter a filename, a path and filename, or a URL pointing to a file. <i>File</i> can also be a MATLAB character array that contains the text of a multiple sequence alignment file. You can read common multiple alignment file types, such as ClustalW (.aln) and GCG (.msf).
<i>IgnoreGapsValue</i>	Property to control removing gap symbols.

## 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. (For an example, type `open aagag.aln`.) 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`.

`multialignread(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`multialignread(..., 'IgnoreGaps', IgnoreGapsValue)`, when *IgnoreGapsValue* is true, removes any gap symbol ('-' or '.') from the sequences. Default is false.

# multialignread

---

## Example

1 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`, `seqdisp`, `multialign`, `seqconsensus`, `seqprofile`

**Purpose** Open viewer for multiple sequence alignments

**Syntax**

```
multialignviewer(Alignment)  
multialignviewer(..., 'PropertyName', PropertyValue,...)  
multialignviewer(..., 'Alphabet', AlphabetValue)
```

**Description** The multialignviewer is an interactive graphical user interface (GUI) for viewing multiple sequence alignments.

multialignviewer(*Alignment*) loads a group of previously multiple aligned sequences into the viewer. *Alignment* is a structure with a field *Sequence*, a character array, or a filename.

multialignviewer(..., '*PropertyName*', *PropertyValue*,...) defines optional properties using property name/value pairs.

multialignviewer(..., '*Alphabet*', *AlphabetValue*) specifies the alphabet type for the sequences. *AlphabetValue* can be 'AA' for amino acids or 'NT' for nucleotides. The default value is 'AA'. If *AlphabetValue* is not specified, multialignviewer guesses the alphabet type.

**Examples**

```
multialignviewer('aagag.aln')
```

**See Also** Bioinformatics Toolbox functions fastaread, gethmmalignment, multialign, multialignread, seqtool

# nmercount

---

**Purpose** Count number of n-mers in nucleotide or amino acid sequence

**Syntax** `nmercount(Seq, Length)`  
`nmercount(Seq, Length, C)`

## Arguments

<i>Seq</i>	Nucleotide or amino acid sequence. Enter a character string or a structure with the field <code>Sequence</code> .
<i>Length</i>	Length of n-mer to count. Enter an integer.

## Description

`nmercount(Seq, Length)` counts the number of n-mers or patterns of a specific length in a sequence.

`nmercount(Seq, Length, C)` returns only the n-nmers with cardinality at least *C*.

## Examples

Count the number of n-mers in an amino acid sequence and display the first six rows in the cell array.

```
S = getgenpept('AAA59174','SequenceOnly',true)
nmers = nmercount(S,4);
nmers(1:6,:)

ans =
    'apes'    [2]
    'dfrd'    [2]
    'eslk'    [2]
    'frdl'    [2]
    'gnys'    [2]
    'lkel'    [2]
```

## See Also

Bioinformatics Toolbox functions `basecount`, `codoncount`, `dimercount`

**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: '.

**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` (constructor), `goannotread`
- `geneont` object methods — `getancestors`, `getdescendants`, `getmatrix`, `getrelatives`

**Purpose** Convert nucleotide sequence to amino acid sequence

**Syntax**

```
SeqAA = nt2aa(SeqNT, 'PropertyName', PropertyValue)
nt2aa(..., 'Frame', FrameValue)
nt2aa(..., 'GeneticCode', GeneticCodeValue)
nt2aa(..., 'AlternativeStartCodons', AlternativeValue)
```

## Arguments

<i>SeqNT</i>	DNA nucleotide sequence. Enter a character string with only the characters A, T, C, and G. You cannot use the character U, ambiguous characters, or a hyphen. You can also enter a structure with the field <i>Sequence</i> .
<i>FrameValue</i>	Property to select a frame. Enter 1, 2, 3, or 'ALL'. The default value is 1.
<i>GeneticCodeValue</i>	Property to select a genetic code. Enter a code number or code name from the table Genetic Code on page 2-326 below. If you use a code name, you can truncate the name to the first two characters of the name.
<i>AlternativeValue</i>	Property to control the use of alternative codons. Enter either true or false. The default value is true.

## Genetic Code

Code Number	Code Name	Code Number	Code Name
1	Standard	12	Alternative Yeast Nuclear
2	Vertebrate Mitochondrial	13	Ascidian Mitochondrial
3	Yeast Mitochondrial	14	Flatworm Mitochondrial



Code Number	Code Name	Code Number	Code Name
4	Mold, Protozoan, Coelenterate Mitochondrial, and Mycoplasma /Spiroplasma	15	Blepharisma Nuclear
5	Invertebrate Mitochondrial	16	Chlorophycean Mitochondrial
6	Ciliate, Dasycladacean, and Hexamita Nuclear	21	Trematode Mitochondrial
9	Echinoderm Mitochondrial	22	Scenedesmus Obliquus Mitochondrial
10	Euplotid Nuclear	23	Thraustochytrium Mitochondrial
11	Bacterial and Plant Plastid		

## Description

`SeqAA = nt2aa(SeqNT, 'PropertyName', PropertyValue)` converts a nucleotide sequence to an amino acid sequence using the standard genetic code.

`nt2aa(..., 'Frame', FrameValue)` converts a nucleotide sequence for a specific reading frame to an amino acid sequence. If `FrameValue` equals 'ALL', then the three reading frames are converted and the output is a 3-by-1 cell array.

`nt2aa(..., 'GeneticCode', GeneticCodeValue)` converts a nucleotide sequence to an amino acid sequence using a specific genetic code.

`nt2aa(..., 'AlternativeStartCodons', AlternativeValue)` controls the use of alternative start codons. By default, `AlternativeStartCodons` is set to `true`, and if the first codon of a sequence corresponds to a known alternative start codon, the codon is translated to methionine.

If this option is set to `false`, then alternative start codons at the start of a sequence are translated to their corresponding amino acids for the genetic code that you use, 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 details of alternative start codons, see

[www.ncbi.nlm.nih.gov/Taxonomy/Utils/wprintgc.cgi?mode=t#SG1](http://www.ncbi.nlm.nih.gov/Taxonomy/Utils/wprintgc.cgi?mode=t#SG1)

## Examples

Convert the gene ND1 on the human mitochondria genome.

```
mitochondria = getgenbank('NC_001807', 'SequenceOnly', true)
gene = mitochondria (3308;4264)
protein1 = nt2aa(gene, 'GeneticCode', 2)
protein2 = getgenpept('NP_536843', 'SequenceOnly', true)
```

Convert the gene ND2 on the human mitochondria genome. In this case, the first codon is `att`, which is converted to `M`, while the following `att` codons are converted to `I`. If you set `'AlternativeStartCodons'` to `false`, then the first codon `att` is converted to `I`.

```
mitochondria = getgenbank('NC_001807', 'SequenceOnly', true)
gene = mitochondria (3371:4264)
protein1 = nt2aa(gene, 'GeneticCode', 2)
protein2 = getgenpept('NP_536844', 'SequenceOnly', true)
```

## See Also

Bioinformatics Toolbox functions `aa2int`, `baselookup`, `geneticcode`, `revgeneticcode`, `aminolookup`, `baselookup`, `codonbias`, `dnds`, `dndsml`, `seqtool`

**Purpose** Convert nucleotide sequence from letter to integer representation

## Syntax

```
SeqInt =
nt2int(SeqChar, 'PropertyName', PropertyValue)
nt2int(..., 'Unknown', UnknownValue)
nt2int(..., 'ACGTONly', ACGTONlyValue)
```

## Arguments

<i>SeqChar</i>	Nucleotide sequence represented with letters. Enter a character string from the table Mapping Nucleotide Letters to Integers below. Integers are arbitrarily assigned to IUB/IUPAC letters. If the property <code>ACGTONly</code> is true, you can only enter the characters A, C, T, G, and U.
<i>UnknownValue</i>	Property to select the integer for unknown characters. Enter an integer. Maximum value is 255. Default value is 0.
<i>ACGTONlyValue</i>	Property to control the use of ambiguous nucleotides. Enter either true or false. Default value is false.

## Mapping Nucleotide Letters to Integers

Base	Code	Base	Code	Base	Code
Adenosine	A—1	T, C (pyrimidine)	Y—6	A, T, G (not C)	D—12
Cytidine	C—2	G, T (keto)	K—7	A, T, C (not G)	H—13
Guanine	G—3	A, C (amino)	M—8	A, G, C (not T)	V—14

Base	Code	Base	Code	Base	Code
Thymidine	T—4	G, C (strong)	S—9	A, T, G, C (any)	N—15
Uridine	U—4	A, T (weak)	W—10	Gap of indeterminate length	- —16
A, G (purine)	R—5	T, G, C (not A)	B—11	Unknown (default)	*—0 and ≥17

## Description

`SeqInt = nt2int(SeqChar, 'PropertyName', PropertyValue)` converts a character string of nucleotides to a 1-by-N array of integers using the table Mapping Nucleotide Letters to Integers above. Unknown characters (characters not in the table) are mapped to 0. Gaps represented with hyphens are mapped to 16.

`nt2int(..., 'Unknown', UnknownValue)` defines the number used to represent unknown nucleotides. The default value is 0.

`nt2int(..., 'ACGTOnly', ACGTOnlyValue)` if `ACGTOnly` is true, the ambiguous nucleotide characters (N, R, Y, K, M, S, W, B, D, H, and V) are represented by the unknown nucleotide number.

## Examples

Convert a nucleotide sequence with letters to integers.

```
s = nt2int('ACTGCTAGC')
```

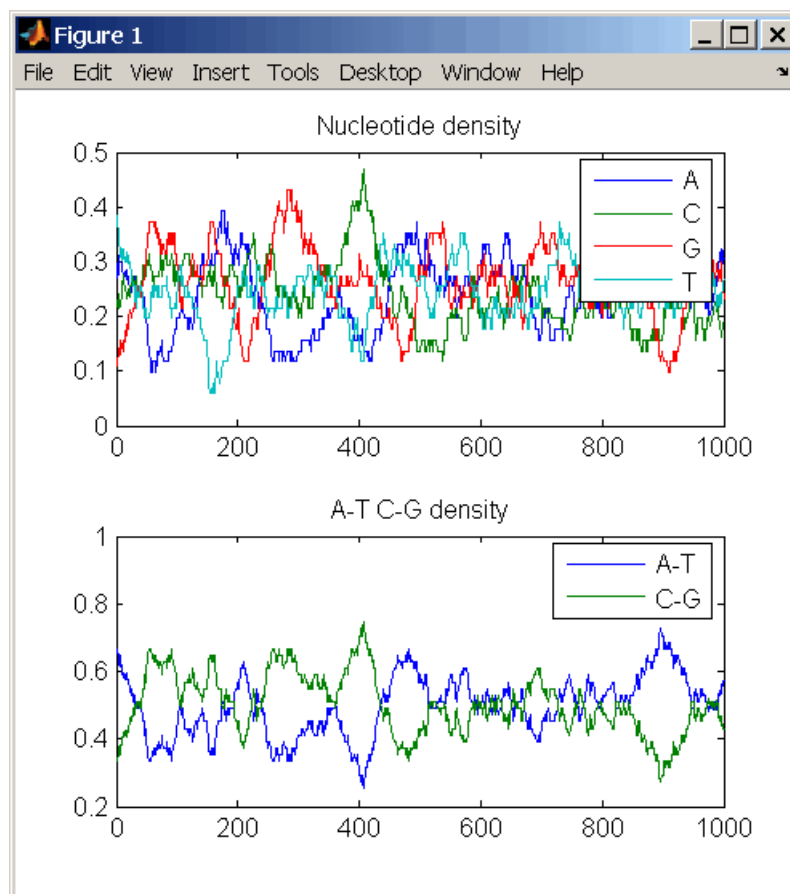
```
s =
     1     2     4     3     2     4     1     3     2
```

## See Also

Bioinformatics Toolbox function `aa2int`, `baselookup`, `int2aa`, `int2nt`

---

<b>Purpose</b>	Plot density of nucleotides along sequence
<b>Syntax</b>	<pre>Density = ntdensity(SeqNT, 'PropertyName', PropertyValue) ntdensity(..., 'Window', WindowValue) [Density, HighCG] = ntdensity(..., 'CGThreshold', CGThresholdValue)</pre>
<b>Description</b>	<p>ntdensity(SeqNT) plots the density of nucleotides A, T, C, G in sequence SeqNT.</p> <p>Density = ntdensity(SeqNT, 'PropertyName', PropertyValue) returns a MATLAB structure with the density of nucleotides A, C, G, and T.</p> <p>ntdensity(..., 'Window', WindowValue) uses a window of length Window for the density calculation. The default value is length(SeqNT)/20.</p> <p>[Density, HighCG] = ntdensity(..., 'CGThreshold', CGThresholdValue) returns indices for regions where the CG content of SeqNT is greater than CGThreshold. The default value for CGThreshold is 5.</p>
<b>Examples</b>	<pre>s = randseq(1000, 'alphabet', 'dna'); ndensity(s)</pre>



## See Also

Bioinformatics Toolbox functions `basecount`, `codoncount`, `cpgisland`, `dimercount`

MATLAB function `filter`

**Purpose** 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.

# nwalign

---

**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(..., 'PropertyName', PropertyValue,...)
nwalign(..., 'Alphabet', AlphabetValue)
nwalign(..., 'ScoringMatrix', ScoringMatirxValue)
nwalign(..., 'Scale', ScaleValue)
nwalign(..., 'GapOpen', GapOpenValue)
nwalign(..., 'Showscore', ShowscoreValue)
```

## Arguments

<i>Seq1, Seq2</i>	Nucleotide or amino acid sequences. Enter a character string or a structure with the field <i>Sequence</i> .
<i>AlphabetValue</i>	Property to select the type of sequence. Value is either 'AA'(default) or 'NT'.
<i>ScoringMatrixValue</i>	Enter the name of a scoring matrix. Values are 'PAM40', 'PAM250', DAYHOFF, GONNET, 'BLOSUM30' increasing by 5 to 'BLOSUM90', 'BLOSUM62', or 'BLOSUM100'.  The default value when <i>AlphabetValue</i> equals 'aa' is 'BLOSUM50', while the default value when <i>AlphabetValue</i> equals 'nt' is nuc44.
<i>ScaleValue</i>	Property to specify a scaling factor for a scoring matrix.
<i>GapOpenValue</i>	Property to specify the penalty for opening a gap. The default value is 8.



<i>ExtendedGapValue</i>	Property to specify the penalty for extending a gap. If <i>ExtendGapValue</i> is not specified, then the default value is equal to <i>GapOpenValue</i> .
<i>ShowscoreValue</i>	Property to control displaying the scoring space and the winning path. Enter either true or false. The default value is false.

## Description

`Score = nwalign(Seq1,Seq2)` returns the alignment score in bits for the optimal alignment. The scale factor used to calculate the score is provided by the scoring matrix information. If this is not defined, then `nwalign` returns the raw score.

`[Score, Alignment] = nwalign(Seq1,Seq2)` returns a string showing an optimal global alignment for the sequences. Amino acids that match are indicated with the symbol |, while related amino acids (nonmatches with a positive scoring matrix value) are indicated with the symbol :. Units for Score are bits.

`[Score, Alignment, Start] = nwalign(Seq1,Seq2)` returns a 2x1 vector with the starting point indices indicating the starting point of the alignment in the two sequences. Note: This output is for consistency with `nwalign`, but because this is a global alignment, the starting position is always [1;1].

`nwalign(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`nwalign(..., 'Alphabet', AlphabetValue)` selects the amino acid or nucleotide alphabet for sequences.

`nwalign(..., 'ScoringMatrix', ScoringMatirxValue)` selects the scoring matrix to use for the alignment.

`nwalign(..., 'Scale', ScaleValue)` specifies the scale factor of the scoring matrix to return the score using arbitrary units. If the scoring matrix also provides a scale factor, then both are used.

`nwalign(..., 'GapOpen', GapOpenValue)` specifies the penalty for opening a gap in the alignment.

`nwalign(..., 'ExtendGap', ExtendGapValue)` specifies the penalty for extending a gap in the alignment. If *ExtendGapValue* is not specified, then extensions to gaps are scored with the same value as *GapOpenValue*.

`nwalign(..., 'Showscore', ShowscoreValue)` displays the scoring space and the winning path.

## Examples

Globally align two amino acid sequences.

```
[Score, Alignment] = nwalign('VSPAGMASGYD','IPGKASYD')
```

```
Score =  
    7.3333
```

```
Alignment =  
VSPAGMASGYD  
: | | || | |  
I-P-GKAS-YD
```

Select scoring matrix and gap penalty.

```
[Score, Alignment] = nwalign('IGRHRYHIGG','SRYIGRG',...  
                             'scoringmatrix','pam250',...  
                             'gapopen',5)
```

```
Score =  
    2.3333
```

```
Alignment =
```

```
IGRHRYHIG-G  
:  || || |  
-S--RY-IGRG
```

## See Also

Bioinformatics Toolbox functions `blosum`, `multialign`, `nt2aa`, `pam`, `profalign`, `seqdotplot`, `showalignment`, `swalign`

**Purpose** Calculate nucleotide DNA sequence properties

**Syntax**

```
SeqProperties = oligoprop(SeqNT)
oligoprop(..., 'PropertyName', PropertyValue,...)
oligoprop(..., 'Salt', SaltValue)
oligoprop(..., 'Temp', TempValue)
oligoprop(..., 'Primerconc', PrimerconcValue)
oligoprop(..., 'HPBase', HPBaseValue)
oligoprop(..., 'HPLoop',HPLoopValue)
oligoprop(..., 'Dimerlength', DimerlengthValue)
```

## Arguments

<i>SeqNT</i>	DNA nucleotide sequence. Enter either a character string with the characters A, T, G, C, or a vector with the integers 1, 2, 3, 4. You can also enter a structure with the field Sequence.
--------------	--

## Description

`SeqProperties = oligoprop(SeqNT)` returns the properties for an oligonucleotide DNA sequence as a structure with the following fields:

GC	Percent GC content for the oligonucleotide
Hairpins	N-by-length(SEQ) matrix of characters where potential hairpin forming bases are in caps. Each row is a potential secondary structure (hairpin).
Dimers	N-by-length(SEQ) matrix of characters where potential self dimerizing bases are in caps. Each row is a potential dimer.
MolWeight	Molecular weight of the oligonucleotide.

Tm	A vector with melting temperature values. The values are listed in the following order: basic (Marmur 1962), salt adjusted (Howley 1979), nearest neighbor (Breslaur 1986), nearest neighbor (SantaLucia Jr 1996), nearest neighbor (SantaLucia Jr 1998), and nearest neighbor (Sugimoto 1996).
Thermo	4-by-3 matrix of thermodynamic calculations where the first column is delta H, the second column is delta S, and the third column is delta G at 37 degrees Celsius. The rows correspond to nearest-neighbor parameters from Breslaur 1986, SantaLucia Jr. 1996, SantaLucia Jr 1998, and Sugimoto 1996.

Unit labels for the thermodynamic and melting temp calculations:

- Tm — degrees Celsius, C
- delta H (enthalpy) — kilocalorie per mole, kcal/mol
- delta S (entropy) — calorie per mole-degrees Kelvin, (cal/(K)(mol)
- delta G (free energy) — kilocalorie per mole, kcal/mol

`oligoprop(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/property value pairs.

`oligoprop(..., 'Salt', SaltValue)` specifies a salt concentration in moles/liter for melting temperature calculations. The default value is 0.05 moles/liter.

`oligoprop(..., 'Temp', TempValue)` specifies the temperature for nearest neighbor calculations of free energy. The default value is 25 degrees Celsius.

`oligoprop(..., 'Primerconc', PrimerconcValue)` specifies the concentration for melting temperatures. The default value is 50e-6 moles/liter.

oligoprop(..., 'HPBase', HPBaseValue) specifies the minimum number of paired bases that form the neck of the hairpin. The default value is 4 bases.

oligoprop(..., 'HPLoop', HPLoopValue) specifies the minimum number of bases that form a hairpin. The default value is 2 bases.

oligoprop(..., 'Dimerlength', DimerlengthValue) specifies the minimum number of aligned bases between the sequence and its reverse. The default value is 4 bases.

## Example

- 1 Create a random sequence.

```
seq = randseq(25)
```

- 2 Calculate sequence properties.

```
S = oligoprop(seq)
```

MATLAB displays properties for the oligonucleotide sequence.

```
S =
      GC: 36
  Hairpins: [0x25 char]
    Dimers: 'tAGCTtcatcgttgacttctactaa'
MolWeight: 7.5820e+003
      Tm: [52.7640 60.8629 62.2493 55.2870 54.0293 61.0614]
  Thermo: [4x3 double]
```

- 3 List the thermodynamic calculations.

```
S.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
```

## References

- [1] Breslaur KJ, Frank R, Blöcker H, Marky LA (1986), "Predicting DNA duplex stability from the base sequence", *Proceedings National Academy of Science USA*, 83:3746-3750.
- [2] Chen S, Lin C, Cho C, Lo C, Hsiung C (2003), "Primer Design Assistant (PDA): A web-based primer design tool," *Nucleic Acids Research*, 31(13): 3751-3754.
- [3] Howley PM, Israel MF, Law M, Martin MA (1979), "A rapid method for detecting and mapping homology between heterologous DNAs. Evaluation of polyomavirus genomes," *The Journal of Biological Chemistry*, 254:4876-4883.
- [4] Marmur J, 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, Melo F (2005), "Comparison of different melting temperature calculation methods for short DNA sequences," *Bioinformatics*, 21( 6): 711-722.
- [6] SantaLucia Jr. J, Allawi HT, Seneviratne PA (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 National Academy of Science USA*, 95:1460-1465.
- [8] Sugimoto N, Nakano S, Yoneyama M, 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.nwu.edu/biotools/oligocalc.html> for weight calculations

## See Also

Bioinformatics Toolbox functions `isoelectric`, `molweight`, `ntdensity`, `palindromes`, `randseq`

# palindromes

---

**Purpose** Find palindromes in sequence

**Syntax**

```
[Position, Length] = palindromes(SeqNT,
'PropertyName', PropertyValue)
[Position, Length, Pal]
= palindromes(SeqNT)
palindromes(..., 'Length', LengthValue)
palindromes(..., 'Complement', ComplementValue)
```

**Description** [Position, Length] = palindromes(SeqNT, 'PropertyName', PropertyValue) 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(..., 'Length', LengthValue) finds all palindromes longer than or equal to Length. The default value is 6.

palindromes(..., 'Complement', ComplementValue) finds complementary palindromes if Complement is true, that is, where the elements match their complementary pairs A-T(or U) and C-G instead of an exact nucleotide match.

**Examples** [p,l,s] = palindromes('GCTAGTAACGTATATATAAT')

```
p =
    11
    12
l =
     7
     7
s =
    'TATATAT'
    'ATATATA'
```

```
[pc,lc,sc] = palindromes('GCTAGTAACGTATATATAAT',...
```



```
'Complement',true);
```

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 `seqrcomplement`, `seqshowwords`  
MATLAB functions `regexp`, `strfind`

**Purpose** PAM scoring matrix

**Syntax**

```
ScoringMatrix = pam(N,  
'PropertyName', PropertyValue)  
[ScoringMatrix, MatrixInfo] = pam(N)  
ScoringMatrix =  
pam(..., 'Extended', 'ExtendedValue')  
ScoringMatrix = pam(...,  
'Order', 'OrderValue')
```

## Arguments

N	Enter values 10:10:500. 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 *.  Entering a larger value for N to allow sequence alignments with larger evolutionary distances.
Extended	Property to add ambiguous characters to the scoring matrix. Enter either true or false. Default is false.
Order	Property to control the order of amino acids in the scoring matrix. Enter a string with at least the 20 standard amino acids.

## Description

`ScoringMatrix = pam(N, 'PropertyName', PropertyValue)` returns a PAM 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.

`ScoringMatrix = pam(..., 'Extended', 'ExtendedValue')` if `Extended` is true, returns a scoring matrix with the 20 amino acid characters, the ambiguous characters, and stop character (B, Z, X, \*), . If `Extended` is false, only the standard 20 amino acids are included in the matrix.

*ScoringMatrix* = pam(..., 'Order', 'OrderValue') returns a PAM matrix ordered by the amino acid sequence in Order. If Order 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

Get the PAM matrix with N = 50.

```
PAM50 = pam(50)
```

```
PAM250 = pam(250, 'Order', 'CSTPAGNDEQHRKMILVFW')
```

## See Also

Bioinformatics Toolbox functions `blosum`, `dayhoff`, `gonnet`, `nalign`, `swalign`

# pdbdistplot

---

**Purpose** Visualize intermolecular distances in Protein Data Bank (PDB) file

**Syntax**

```
pdbdistplot('PDBid')  
pdbdistplot('PDBid', Distance)
```

## Arguments

PDBid	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 value 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` can also be 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

Show spy plot at 7 Angstroms of the protein cytochrome C from albacore tuna.

```
pdbdistplot('5CYT');
```

Now take a look at 10 Angstroms.

```
pdbdistplot('5CYT',10);
```

## See Also

Bioinformatics Toolbox functions `getpdb`, `pdbread`, `pdbplot`, `pdbread`, `proteinplot`, `ramachandran`

# pdbplot

---

**Purpose** Plot 3-D protein structure

**Syntax**

```
pdbplot(PDBid, 'PropertyName', PropertyValue ...)  
pdbplot(..., 'Plotmode', PlotmodeValue)  
pdbplot(..., 'Colormode', ColormodeValue)  
pdbplot(..., 'Showlabel', ShowlabelValue)  
FigureHandle = pdbplot(...)
```

## Arguments

PDBid	PDBID can also be the name of a PDB structure or a file containing a PDB structure.
Plotmode	Property to select display backbone and side chains. Enter either 'backbone' or 'mainchain'. The default value is 'backbone' for the alpha carbon backbone.
Colormode	Property to select the color of atoms or folding patters. Enter 'atom', 'chain', or 'secondary'. The default is 'chain'.

## Description

`pdbplot(PDBid, 'PropertyName', PropertyValue ...)` retrieves 3D information from the Web for a protein (*PDBid*), and plots the backbone structure. Information for the protein is in the Protein Data Bank (PDB) database.

`pdbplot(..., 'Plotmode', PlotmodeValue)` selects a plot with only the alpha-carbon backbone or a plot with amino acid side-chains.

`pdbplot(..., 'Colormode', ColormodeValue)` selects the colors for a plot.

- If `Colormode` is 'atom' and `Plotmode` is 'mainchain', atoms and connections are colored green for carbon, blue for nitrogen, and red for oxygen.
- The `Colormode` is "chain", the entire structure is one color.

- If `Colormode` is 'secondary', alpha helix patterns are colored yellow, sheets are blue, turns are gray and, non alpha helix are cyan.

`pdbplot(..., 'Showlabel', ShowlabelValue)` when `Showlabel` is true, displays the labels that represent each amino acid name and sequence number in the protein. The default is false.

`FigureHandle = pdbplot(...)` returns the handle for the PDB plot figure.

For more on viewing PDB molecules in MATLAB, see the molecule viewer in MATLAB Central

[www.mathworks.com/matlabcentral/fileexchange/loadFile.do?objectId=808](http://www.mathworks.com/matlabcentral/fileexchange/loadFile.do?objectId=808)

## Examples

Plot the 3D backbone structure for the protein Insulin-Like-Growth-Factor-1. The identification number for this protein in the PDB database is 1B9G.

1. In the MATLAB Command Window, type

```
pdbplot('1B9G')
```

A figure window opens with the 3D structure for this protein. The figure title displays the identification number PDB Plot 1B9G while the bottom of the figure shows the protein title or compound name Title: INSULIN-LIKE-GROWTH-FACTOR-1.

3. Rotate, translate, and zoom the structure with the MATLAB camera toolbar.

4. From **File** menu, select

- **Save to Figure file** — Saves the plot to a MATLAB figure file
- **Print** - Prints the plot
- **Close** - Closes the current PDB plot figure window
- **Close All** - Closes all the opened PDB plot figure windows

5. Select the different view options from the **View** menu or navigation tool on the right side of the figure.

Select an Plot option button:

- **Backbone** - Plots c- alpha trace
- **Main Chain** - Plots main chain

Select a Color check box:

- **Atoms** - Color atoms based on predefined color code: Red = oxygen, Green = carbon, Blue = nitrogen
- **Secondary** - Color secondary structures based on predefined color code: yellow = a-helix, blue = beta-strand, gray = turn, cyan = helix (non-alpha), green = all other structures

Select the Show check box:

- **Labels** - Show amino acid sequence labels

6. From the **Help** menu, **Help** or **Demos** for Bioinformatics toolbox.

## See Also

Bioinformatics Toolbox functions `getpdb`, `pdbdistplot`, `pdbread`, `proteinplot`, `ramachandran`



**Purpose** Read data from Protein Data Bank (PDB) file

**Syntax** `PDBData = pdbread('File')`

**Arguments**

*File* Protein Data Bank (PDB) formatted file (ASCII text file). Enter a filename, a path and filename, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text for a PDB file.

**Description**

The Protein Data Bank (PDB) is an archive of experimentally determined three-dimensional protein structures. `pdbread` reads data from a PDB formatted file into MATLAB.

`PDBData = pdbread('File')` reads the data in PDB formatted text file *File* and stores the data in the MATLAB structure `PDBData`.

The data stored in each record of the PDB file is converted, where appropriate, to a MATLAB structure. For example, the `ATOM` records in a PDB file are converted to an array of structures with the following fields: `AtomSerNo`, `AtomName`, `altLoc`, `resName`, `chainID`, `resSeq`, `iCode`, `X`, `Y`, `Z`, `occupancy`, `tempFactor`, `segID`, `element`, and `charge`.

The sequence information from the PDB file is stored in the `Sequence` field of `PDBData`. The sequence information is itself a structure with the fields `NumOfResidues`, `ChainID`, `ResidueNames`, and `Sequence`. The field `ResidueNames` contains the three-letter codes for the sequence residues. The field `Sequence` contains the single-letter codes for the sequence. If the sequence has modified residues, then the `ResidueNames` might not correspond to the standard three-letter amino acid codes, in which case the field `Sequence` will contain a `?` in the position corresponding to the modified residue.

For more information about the PDB format, see

[http://www.rcsb.org/pdb/file\\_formats/pdb/pdbguide2.2/guide2.2\\_frame](http://www.rcsb.org/pdb/file_formats/pdb/pdbguide2.2/guide2.2_frame).

# pdbread

---

## Examples

Get information for the human hemoglobin protein with number 1A00 from the Protein Data Bank, store information in the file `collagen.pdb`, and then read the file back into MATLAB.

```
getpdb('1A00','ToFile','collagen.pdb')  
pdbdata = pdbread('collagen.pdb')
```

## See Also

Bioinformatics Toolbox functions `genpeptread`, `getpdb`, `pdbplot`, `pdbdistplot`

**Purpose** Calculate pairwise patristic distances in phytree object

**Syntax**

```
D = pdist(Tree)
[D,C] = pdist(Tree)
pdist(..., 'PropertyName', PropertyValue,...)
pdist(..., 'Nodes', NodeValue)
pdist(..., 'Squareform', SquareformValue)
pdist(..., 'Criteria', CriteriaValue)
```

## Arguments

Tree	Phylogenetic tree object created with the function <code>phytree</code> .
NodeValue	Property to select the nodes. Enter either 'leaves' (default) or 'all'.
SquareformValue	Property to control creating a square matrix.

## Description

`D = pdist(Tree)` returns a vector (*D*) containing the patristic distances between every possible pair of leaf nodes a phylogenetic tree object (*Tree*). The patristic distances are computed by following paths through the branches of the tree and adding the patristic branch distances originally created with `seqlinkage`.

The output vector *D* is arranged in the order  $((2,1), (3,1), \dots, (M,1), (3,2), \dots (M,3), \dots (M,M-1))$  (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,...)` defines optional properties using property name/value pairs.

`pdist(..., 'Nodes', NodeValue)` indicates the nodes included in the computation. When `Node='leaves'`, the output is ordered as before, but *M* is the total number of nodes in the tree (`NumLeaves+NumBranches`).

## pdist (phytree)

---

`pdist(... , Squareform', SquareformValue)`, when `Squareform` is true, 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. `C` can be 'distance' (default) or 'levels'.

### Examples

1 Get a phylogenetic tree from a file.

```
tr = phytread('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`

**Purpose** Read data from PFAM-HMM file

**Syntax** `Data = pfamhmmread('File')`

## Arguments

*File* PFAM-HMM formatted file. Enter a filename, a path and filename, or a URL pointing to a file. *File* can also be a MATLAB character array that contains the text of a PFAM-HMM file.

## Description

pfamhmmread reads data from a PFAM-HMM formatted file (file saved with the function gethmmprof) and creates a MATLAB structure.

`Data = pfamhmmread('File')` reads from *File* a Hidden Markov Model described by the PFAM format, and converts it to the MATLAB structure *Data*, containing fields corresponding to annotations and parameters of the model. For more information about the model structure format, see `hmmprofstruct`. *File* can also be a URL or a MATLAB cell array that contains the text of a PFAM formatted file.

pfamhmmread is based on the HMMER 2.0 file formats.

## Examples

```
pfamhmmread('pf00002.ls')  
  
site='http://www.sanger.ac.uk/';  
pfamhmmread([site 'cgi-bin/Pfam/download_hmm.pl?id=7tm_2'])
```

## See Also

Bioinformatics Toolbox functions `gethmmalignment`, `gethmmprof`, `hmmprofalign`, `hmmprofstruct`, `showhmmprof`

# phytree

---

**Purpose** Create phytree object

**Syntax**  
*Tree* = phytree(*B*)  
*Tree* = phytree(*B*, *D*)  
*Tree* = phytree(*B*, *C*)  
*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.

*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 branch or leaves, and distances of branches.

*N* Cell array with the names of leafs and branches.

## Description

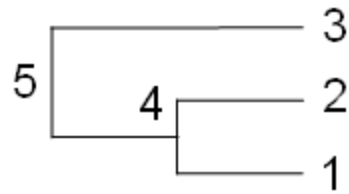
*Tree* = phytree(*B*) creates an ultrametric phylogenetic tree object.

*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,  $B(i, :) > \text{NUMLEAVES} + i$ ). 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.

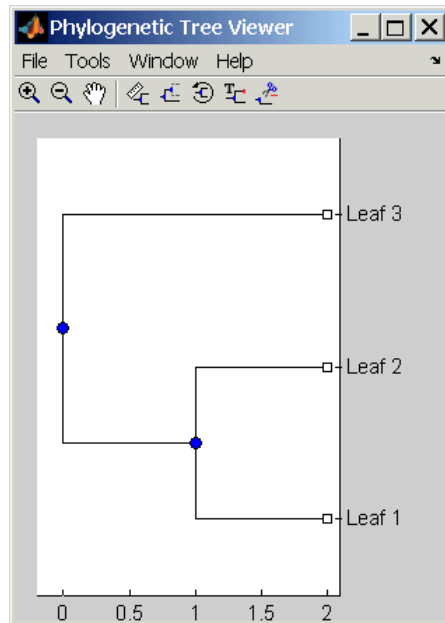
Given a tree with 3 leafs and 2 branches as an example.



In the MATLAB Command window, type

```

B = [1 2 ; 3 4]
tree = phytree(B)
view(tree)
  
```



`Tree = phytree(B, D)` creates an additive 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  $\text{NUMNODES} = \text{NUMLEAVES} + \text{NUMBRANCHES}$ . The last distance in  $D$  is the distance of the root node and is meaningless.

```
b = [1 2 ; 3 4 ]; d = [1 2 1.5 1 0]
view(phytree(b,d))
```

$\text{Tree} = \text{phytree}(B, C)$  creates an ultrametric phylogenetic tree object with branch distances defined by  $C$ .  $C$  is a numeric array of size  $[\text{NUMBRANCHES} \times 1]$  with the coordinates of every branch node. In ultrametric trees, all of the leaves are at the same location (same distance to the root).

```
b = [1 2 ; 3 4]; c = [1 4]'
view(phytree(b,c))
```

$\text{Tree} = \text{phytree}(BC)$  creates an ultrametric phylogenetic binary tree object with branch pointers in  $BC(:, [1 \ 2])$  and branch coordinates in  $BC(:, 3)$ . Same as  $\text{phytree}(B, C)$ .

$\text{Tree} = \text{phytree}(\dots, N)$  specifies the names for the leaves and/or the branches.  $N$  is a cell of strings. If  $\text{NUMEL}(N) == \text{NUMLEAVES}$ , then the names are assigned chronologically to the leaves. If  $\text{NUMEL}(N) == \text{NUMBRANCHES}$ , the names are assigned to the branch nodes. If  $\text{NUMEL}(N) == \text{NUMLEAVES} + \text{NUMBRANCHES}$ , all the nodes are named. Unassigned names default to 'Leaf #' and/or 'Branch #' as required.

$\text{Tree} = \text{phytree}$  creates an empty phylogenetic tree object.

## Method Summary

<code>get (phytree)</code>	Information about phylogenetic tree object
<code>getbyname (phytree)</code>	Branches and leaves from phytree object
<code>getcanonical (phytree)</code>	Calculate canonical form of phylogenetic tree
<code>getnewickstr (phytree)</code>	Create Newick-formatted string



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

## Property Summary

Property	Description
<code>NumLeaves</code>	Number of leaves
<code>NumBranches</code>	Number of branches
<code>NumNodes</code>	Number of nodes ( <code>NumLeaves + NumBranches</code> )
<code>Pointers</code>	Branch to leaf/branch connectivity list
<code>Distances</code>	Edge length for every leaf/branch
<code>LeafNames</code>	Names of the leaves
<code>BranchNames</code>	Names of the branches
<code>NodeNames</code>	Names of all the nodes

## Examples

Create phylogenetic tree for a set of multiply aligned sequences.

```
Sequences = multialignread('aagag.aln')
distances = seqpdist(Sequences)
```

# phytree

---

```
tree = seqlinkage(distances)
phytreetool(tree)
```

## See Also

Bioinformatics Toolbox

- functions — phytree (object constructor), phytreeread, phytreetool, phytreewrite, seqlinkage, seqneighjoin, seqpdist
- phytree object methods — get, getbyname, getcanonical, getnewickstr, pdist, plot, prune, reroot, select, subtree, view, weights

**Purpose** Read phylogenetic tree file

**Syntax** `Tree = phytread(File)`

**Arguments**

*File* Newick formatted tree files (ASCII text file). Enter a filename, a path and filename, 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 phytread.

**Description**

`Tree = phytread(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 only allows binary trees. Non-binary trees are translated into a binary tree with extra branches of length 0.

---

**Examples**

```
tr = phytread('pf00002.tree')
```

**See Also**

Bioinformatics Toolbox functions `phytree` (object constructor), `gethmmtree`, `phytreetool`, `phytreewrite`

# phytreetool

---

**Purpose** View, edit, and explore phylogenetic tree data

**Syntax** `phytreetool(Tree)`  
`phytreetool(File)`

## Arguments

<i>Tree</i>	Phytree object created with the functions <code>phytree</code> or <code>phytreeread</code> .
<i>File</i>	Newick or ClustalW tree formatted file (ASCII text file) with phylogenetic tree data. Enter a filename, a path and filename, or a URL pointing to a file. <i>File</i> 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`
- `phytree` object methods — `plot`, `view`

**Purpose** Write phylogenetic tree object to Newick-formatted file

**Syntax** `phytreewrite('File', Tree)`  
`phytreewrite(Tree)`

## Arguments

*File* Newick formatted file. Enter either a filename or a path and filename supported by your operating system (ASCII text file).

*Tree* Phylogenetic tree object. Tree must be an object created with either the function `phytree` or imported using the function `dnds`.

## 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 filename.

## Examples

Read tree data from a Newick formatted file.

```
tr = phytreeread('pf00002.tree')
```

Remove all the 'mouse' proteins

```
ind = getbyname(tr,'mouse');  
tr = prune(tr,ind);  
view(tr)
```

Write pruned tree data to a file.

# phytreewrite

---

```
phytreewrite('newtree.tree', tr)
```

## See Also

Bioinformatics Toolbox

- functions — `phytree`, `phytreeread`, `phytreetool`, `seqlinkage`
- `phytree` object methods — `getnewickstr`

## Purpose

Draw phylogenetic tree

## Syntax

```
plot(Tree)
plot(Tree, ActiveBranches)
plot(..., 'Type', TypeValue)
plot(..., 'Orientation', OrientationValue)
plot(..., 'BranchLabels', BranchLabelsValue)
plot(..., 'LeafLabels', LeafLabelsValue)
plot(..., 'TerminalLabels', TerminalLabelsValue)
```

## Arguments

Tree	phytree object created with the function <code>phytree</code>
ActiveBranches	Branches veivable in the figure window.
<i>TypeValue</i>	Property to select a method for drawing a phylogenetic tree. Enter 'square', 'angular', or 'radial'. The default value is 'square'.
<i>OrientationValue</i>	Property to orient a phylogram or cladogram tree. Enter 'top', 'bottom', 'left', or 'right'. The default value is 'left'.
<i>BranchLabelsValue</i>	Property to control displaying branch labels. Enter either true or false. The default value is false.
<i>LeafLabelsValue</i>	Property to control displaying leaf labels. Enter either true or false. The default value is false.
<i>TerminalLabels</i>	Property to control displaying terminal labels. Enter either true or false. The default value is false.

## Description

`plot(Tree)` draws a phylogenetic tree object into a MATLAB figure as a phylogram. The significant distances between branches and nodes

## plot (phytree)

---

are in the horizontal direction. Vertical distances have no significance and are selected only for display purposes. Handles to graph elements are stored in the figure field `UserData` so that you can easily modify graphic properties.

`plot(Tree, ActiveBranches)` hides the nonactive branches and all of their descendants. `ActiveBranches` is a logical array of size `numBranches x 1` indicating the active branches.

`plot(..., 'Type', TypeValue)` selects a method for drawing a phylogenetic tree.

`plot(..., 'Orientation', OrientationValue)` orients a phylogenetic tree within a figure window. The `Orientation` property is valid only for phylogram and cladogram trees.

`plot(..., 'BranchLabels', BranchLabelsValue)` hides or displays branch labels placed next to the branch node.

`plot(..., 'LeafLabels', LeafLabelsValue)` hides or displays leaf labels placed next to the leaf nodes.

`plot(..., 'TerminalLabels', TerminalLabelsValue)` hides or displays terminal labels. Terminal labels are placed over the axis tick labels and ignored when `Type= 'radial'`.

`H = plot(...)` returns a structure with handles to the graph elements.

### Examples

```
tr = phytreeread('pf00002.tree')
plot(tr, 'Type', 'radial')
```

Graph element properties can be modified as follows:

```
h=get(gcf, 'UserData')
set(h.branchNodeLabels, 'FontSize', 6, 'Color', [.5 .5 .5])
```

### See Also

Bioinformatics Toolbox

- functions — `phytree` (object constructor), `phytreeread`, `phytreetool`, `seqlinkage`



- `phytree` object method — view

# probelibraryinfo

---

**Purpose** Probe set library information for probe results

**Syntax** ProbeInfo = probelibraryinfo(CELStruct, CDFStruct)

**Description** ProbeInfo = probelibraryinfo(CELStruct, CDFStruct) creates a table of information linking the probe data in a CEL file structure with probe set information from a CDF file structure.

ProbeInfo is a matrix with three columns and the same number of rows as the probes field of the CELStruct. The first column is the probe set ID number to which the corresponding probe belongs. The second column contains the probe pair number and the third column indicates if the probe is a perfect match (1) or mismatch (-1) probe. Probes that do not correspond to a probe set in the CDF library file have probe set ID equal to 0.

Note: Affymetrix probe pair indexing is 0 based while MATLAB indexing is 1 based. The output from probelibraryinfo is 1 based.

## Examples

**1** Get the file Drosophila-121502.cel from

```
http://www.affymetrix.com/support/technical/sample\_data/demo\_data.aff
```

**2** Read the data into MATLAB.

```
celStruct = affyread('Drosophila-121502.cel');  
cdfStruct = affyread('D:\Affymetrix\LibFiles\...  
DrosGenome1\DrosGenome1.CDF');
```

**3** Extract probe set library information.

```
probeinfo = probelibraryinfo(celStruct, cdfStruct);
```

**4** Find out which probeset the 1104th probe belongs to

```
cdfStruct.ProbeSets(probeinfo(1104,1)).Name
```

## See Also

Bioinformatics Toolbox functions affyread, celintensityread, probesetlink, probesetlookup, probesetvalues

**Purpose** Link to NetAffx Web site

**Syntax**

```
probesetlink(AFFYStruct, ID)
URL = probesetlink(AFFYStruct, ID)
probesetlink(..., 'PropertyName', PropertyValue,...)
probesetlink(..., 'Source', SourceValue),
probesetlink(..., 'Browser', BrowserValue)
probesetlink(..., 'NoDisplay', NoDisplayValue)
```

**Description** `probesetlink(AFFYStruct, ID)` displays information from the NetAffx Web site about a probe set (*ID*) from the CHP or CDF structure (*AFFYStruct*). *ID* can be the index of the probe set or the probe set name.

`URL = probesetlink(AFFYStruct, ID)` returns the URL for the information.

`probesetlink(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`probesetlink(..., 'Source', SourceValue)`, when *SourceValue* is true, links to the data source (e.g. GenBank, Flybase) for the probe set.

`probesetlink(..., 'Browser', BrowserValue)`, when *BrowserValue* is true, displays the information in the system Web browser.

`probesetlink(..., 'NoDisplay', NoDisplayValue)`, when *NoDisplayValue* is true, returns the URL but does not open a browser.

Note: NetAffx Web site requires you to register and provide a user name and password.

**Examples** **1** Get the file `Drosophila-121502.chp` from

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

**2** Read the data into MATLAB.

```
chpStruct = affyread('Drosophila-121502.chp',...
                    'D:\Affymetrix\LibFiles\DrosGenome1')
```

# probesetlink

---

**3** Display information from the NetAffx Web site.

```
probesetlink(chpStruct, 'AFFX-YEL018w/_at');
```

## **See Also**

Bioinformatics Toolbox functions `affyread`, `celintensityread`, `probesetlookup`, `probesetplot`, `probelibraryinfo`, `probesetvalues`

<b>Purpose</b>	Gene name for probe set
<b>Syntax</b>	<pre>probesetlookup(AFFYStruct, ID) probesetlookup(AFFYStruct, Name) [Name, NDX, Description, Source, SourceURL] = probesetlookup(...)</pre>
<b>Description</b>	<p><code>probesetlookup(AFFYStruct, ID)</code> returns the gene name for a probe set ID from a CHP or CDF structure (AFFYStruct).</p> <p><code>probesetlookup(AFFYStruct, Name)</code> returns the probe set ID for a gene name (Name) from a CHP or CDF structure (AFFYStruct).</p> <p><code>[Name, NDX, Description, Source, SourceURL] = probesetlookup(...)</code> returns the name, index into the CHP or CDF struct, , description, source, and source URL and for the probe set.</p>
<b>Examples</b>	<ol style="list-style-type: none"><li>1 Get the file <code>Drosophila-121502.chp</code> from <a href="http://www.affymetrix.com/support/technical/sample_data/demo_data.affx">http://www.affymetrix.com/support/technical/sample_data/demo_data.affx</a></li><li>2 Read the data into MATLAB. <pre>chpStruct = affyread('Drosophila-121502.chp',...                     'D:\Affymetrix\LibFiles\DrosGenome1')</pre></li><li>3 Get the gene name. <pre>probesetlookup(chpStruct, 'AFFX-YEL018w/_at')</pre></li></ol>
<b>See Also</b>	Bioinformatics Toolbox functions <code>affyread</code> , <code>celintensityread</code> , <code>probelibraryinfo</code> , <code>probesetlink</code> , <code>probesetplot</code> , <code>probesetvalues</code> , <code>rmabackadj</code>

# probesetplot

---

**Purpose** Plot values for Affymetrix CHP file probe set

**Syntax**

```
probesetplot(CHPStruct, ID, 'PropertyName', PropertyValue)
probesetplot(..., 'GeneName', GeneNameValue)
probesetplot(..., 'Field', FieldValue)
probesetplot(..., 'ShowStats', ShowStatsValue)
```

**Description** `probesetplot(CHPStruct, ID, 'PropertyName', PropertyValue)` plots the PM and MM intensity values for probe set ID. `CHPStruct` is a structure created from an Affymetrix CHP file. ID can be the index of the probe set or the probe set name. Note: the probe set numbers for a CHP file use 0 based indexing while MATLAB uses 1 based indexing. `CHPStruct.ProbeSets(1)` has `ProbeSetNumber 0`.

`probesetplot(..., 'GeneName', GeneNameValue)` when `GeneName` is true, uses the gene name, rather than the probeset name for the title.

`probesetplot(..., 'Field', FieldValue)` shows the data for a field (`FieldValue`). Valid fieldnames are: `Background`, `Intensity`, `StdDev`, `Pixels`, and `Outlier`.

`probesetplot(..., 'ShowStats', ShowStatsValue)` when `ShowStats` is true, adds mean and standard deviation lines to the plot.

**Examples** **1** Get the file `Drosophila-121502.chp` from

[http://www.affymetrix.com/support/technical/sample\\_data/demo\\_data.affx](http://www.affymetrix.com/support/technical/sample_data/demo_data.affx)

**2** Read the data into MATLAB.

```
chpStruct = affyread('Drosophila-121502.chp',...
                    'D:\Affymetrix\LibFiles\DrosGenome1')
```

**3** Plots PM and MM intensity values.

```
probesetplot(chpStruct, 'AFFX-YEL018w/_at', 'showstats', true);
```

**See Also** Bioinformatics Toolbox functions `affyread`, `celintensityread`, `probesetlink`, `probesetlookup`

**Purpose** Probe set values from probe results

**Syntax** `PSValues = probesetvalues(CELStruct,CDFStruct,PS)`

**Description** `PSValues = probesetvalues(CELStruct,CDFStruct,PS)` creates a table of values for a probe set (*PS*) from the probe data in a CEL file structure (*CELStruct*). *PS* is a probe set index or probe set name from the CDF library file structure (*CDFStruct*). *PSValues* is a matrix with 18 columns and one row for each probe pair in the probe set. The columns correspond to the fields in a CHP probe set data structure:

```
'ProbeSetNumber'
  'ProbePairNumber'
  'UseProbePair'
  'Background'
  'PMPosX'
  'PMPosY'
  'PMIntensity'
  'PMStdDev'
  'PMPixels'
  'PMOutlier'
  'PMMasked'
  'MMPosX'
  'MMPosY'
  'MMIntensity'
  'MMStdDev'
  'MMPixels'
  'MMOutlier'
  'MMMMasked'
```

There are some minor differences between the output of this function and the data in a CHP file. The PM and MM Intensity values in the CHP file are normalized by the Affymetrix software. This function returns the raw intensity values. The 'UseProbePair' and 'Background' fields are only returned by this function for compatibility with the CHP probe set data structure and are always set to zero.

# probesetvalues

---

## Examples

**1** Get the file Drosophila-121502.cel from

[http://www.affymetrix.com/support/technical/sample\\_data/demo\\_data.affx](http://www.affymetrix.com/support/technical/sample_data/demo_data.affx)

**2** Read the data into MATLAB.

```
celStruct = affyread('Drosophila-121502.cel');  
cdfStruct = affyread('D:\Affymetrix\LibFiles\DrosGenome1\...  
DrosGenome1.CDF');
```

**3** Get the values for probe set 147439\_at.

```
psvals = probesetvalues(celStruct,cdfStruct,'147439_at')
```

## See Also

Bioinformatics Toolbox functions `affyread`, `celintensityread`, `probelibraryinfo`, `probesetlink`, `probesetlookup`, `rmabackadj`,



**Purpose** Align two profiles using Needleman-Wunsch global alignment

**Syntax**

```

Prof = proalign(Prof1, Prof2)
[Prof, H1, H2] = proalign(Prof1, Prof2)
proalign(..., 'PropertyName', PropertyValue,...)
proalign(..., 'ScoringMatrix', ScoringMatrixValue)
proalign(..., 'GapOpen', {G1Value, G2Value})
proalign(..., 'ExtendGap', {E1Value, E2Value})
proalign(..., 'ExistingGapAdjust', ExistingGapAdjustValue)
proalign(..., 'TerminalGapAdjust', TerminalGapAdjustValue)
proalign(..., 'ShowScore', ShowScoreValue)

```

**Description** *Prof* = proalign(*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*] = proalign(*Prof1*, *Prof2*) returns pointers that indicate how to rearrange the columns of the original profiles into the new profile.

proalign(..., 'PropertyName', PropertyValue,...) defines optional properties using property name/value pairs.

proalign(..., '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.

proalign(..., '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, 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`

# proteinplot

---

**Purpose** Characteristics for amino acid sequences

**Syntax** `proteinplot (SeqAA)`

**Arguments**

SeqAA	Amino acid sequence or a structure with a field Sequence containing an amino acid sequence.
-------	---

**Description** `proteinplot (SeqAA)` loads an amino acid sequence into the protein plot GUI. `proteinplot` is a tool for analyzing a single amino acid sequence. You can use the results from `proteinplot` to compare the properties of several amino acid sequences. It displays smoothed line plots of various properties such as the hydrophobicity of the amino acids in the sequence.

## Importing sequences into proteinplot

**1** In the **MATLAB Command Window**, type

```
proteinplot(Seq_AA)
```

The `proteinplot` interface opens and the sequence `Seq_AA` is shown in the **Sequence** text box.

**2** Alternatively, type or paste an amino acid sequence into the **Sequence** text box.

You can can import a sequence with the Import dialog box.

**1** Click the **Import Sequence** button. The Import dialog box opens.

**2** From the **Import From** list, select, a variable in the MATLAB workspace, ASCII text file, FASTA formatted file, GenPept formatted file, or accession number in the GenPept database.

## Information about the properties

You can also access information about the properties from the **Help** menu.

- 1 From the **Help** menu, click **References**. The Help Browser opens with a list of properties and references.
- 2 Scroll down to locate the property you are interested in studying.

### Working with Properties

When you click on a property a smoothed plot of the property values along the sequence will be displayed. Multiple properties can be selected from the list by holding down Shift or Ctrl while selecting properties. When two properties are selected, 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 three or more properties are displayed, the values are normalized to the range 0-1.

You can add your own property values by clicking on the Add button next to the property list. This will open up a dialog that allows you to specify the values for each of the amino acids. The Display Text box allows you to specify the text that will be displayed in the selection box on the main proteinplot window. You can also save the property values to an m-file for future use by typing a file name into the Filename box.

The Terminal Selection boxes allow you to choose to plot only part of the sequence. By default all of the sequence is plotted. The default smoothing method is an unweighted linear moving average with a window length of five residues. You can change this using the "Configuration Values" dialog from the Edit menu. The dialog allows you to select the window length from 5 to 29 residues. You can modify the shape of the smoothing window by changing the edge weighting 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 allows you to Import a sequence, save the plot that you have created to a FIG file, you can export the data values in the figure

to a workspace variable or to a MAT file, you can export the figure to a normal figure window for customizing, and you can print the figure.

The Edit menu allows you to 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 allows you to turn the toolbar on and off, and to add a legend to the plot.

The Tools menu allows you to 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 allows you to view this document and to see the references for the sequence properties built into proteinplot

## See Also

Bioinformatics Toolbox functions `aaccount`, `atomiccomp`, `molweight`, `pdbdistplot`, `pdbplot`, `seqtool`

MATLAB function `plotyy`

**Purpose** Remove branch nodes from phylogenetic tree

**Syntax**  
T2 = prune(T1, Nodes)  
T2 = prune(T1, Nodes, 'Mode', 'Exclusive')

## Arguments

T1	Phylogenetic tree object. See phytree.
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 node 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 property (Mode) 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)
```

```
% To :
```

Remove all the 'mouse' proteins use

## prune (phytree)

---

```
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`
- `phytree` object methods — `select`, `get`



**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 that if DATA contains NaN values, then NORMDATA will also contain NaNs 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** malowess, manorm, rmabackadj, rmasummary

# ramachandran

---

**Purpose** Draw Ramachandran plot for Protein Data Bank (PDB) data

**Syntax**

```
ramachandran('PDBid')
ramachandran('File')
ramachandran(PDBData)
Angles = ramachandran(...)
[Angles, Handle] = ramachandran(...)
```

## Arguments

<i>PDBid</i>	Unique identifier for a protein structure record. Each structure in the PDB is represented by a 4-character alphanumeric identifier. For example, 4hbb is the identification code for hemoglobin.
<i>File</i>	Protein Data Bank (PDB) formatted file (ASCII text file). Enter a filename, a path and filename, or a URL pointing to a file. <i>File</i> can also be a MATLAB character array that contains the text for a PDB file.
PDBData	MATLAB structure with PDB formatted data.

## Description

ramachandran generates a plot of the torsion angle PHI (torsion angle between the 'C-N-CA-C' atoms) and the torsion angle PSI (torsion angle between the 'N-CA-C-N' atoms) of the protein sequence.

ramachandran('PDBid') generates the Ramachandran plot for the protein with PDB code ID.

ramachandran('File') generates the Ramachandran plot for protein stored in the PDB file *File*.

ramachandran(PDBData) generates the Ramachandran plot for the protein stored in the structure PDBData, where PDBData is a MATLAB structure obtained by using pdbread or getpdb.

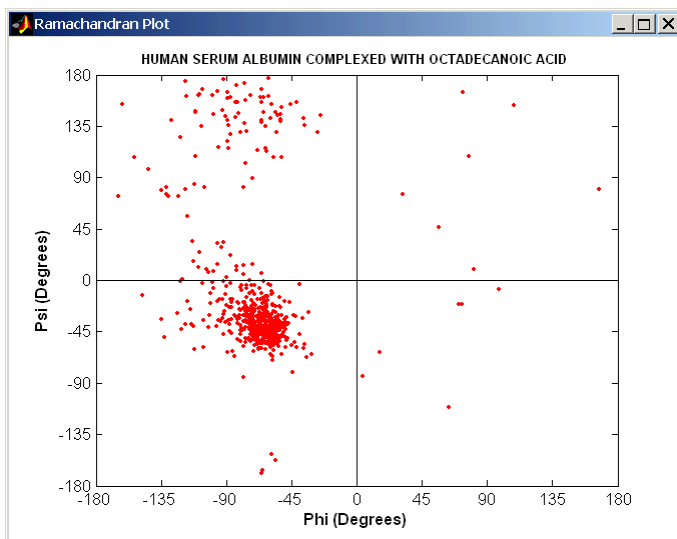
Angles = ramachandran(...) returns an array of the torsion angles PHI, PSI, and OMEGA for the residue sequence.

[Angles, Handle] = ramachandran(...) returns a handle to the plot.

**Examples**

Generate the Ramachandran plot for the human serum albumin complexed with octadecanoic acid.

```
ramachandran('1E7I')
```

**See Also**

Bioinformatics Toolbox functions `getpdb`, `pdbdistplot`, `pdbread`, `pdbplot`

# randfeatures

---

**Purpose** Generate randomized subset of features

**Syntax**

```
[IDX, Z] = randfeatures(X, Group, 'PropertyName',  
PropertyValu...)  
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', PropertyValu...) 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  $0.95.^{(\text{number of classes})}$ .

`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'	$x_{\text{new}} = (x - \text{mean}(x)) / \text{std}(x)$
'softmax'	$x_{\text{new}} = (1 + \exp((\text{mean}(x) - x) / \text{std}(x)))^{-1}$
'minmax'	$x_{\text{new}} = (x - \min(x)) / (\max(x) - \min(x))$

`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.

# randfeatures

---

```
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`,  
`rankfeatures`, `svmclassify`

Statistics Toolbox function `classify`

**Purpose** Generate random sequence from finite alphabet

**Syntax**

```
Seq = randseq(SeqLength)
randseq(..., 'PropertyName', PropertyValue, ...)
randseq(..., 'Alphabet', AlphabetValue)
randseq(..., 'Weights', WeightsValue)
randseq(..., 'FromStructure', FromStructureValue)
randseq(..., 'Case', CaseValue)
randseq(..., 'DataType', DataTypeValue)
```

## Arguments

<i>Length</i>	Number of nucleotide bases or amino acids.
<i>AlphabetValue</i>	Property to select the alphabet for the sequence. Enter 'dna' (default), 'rna', or 'amino'.
<i>WeightsValue</i>	Property to specify a weighted random sequence.
<i>FromStructureValue</i>	Property to specify a weighted random sequence using output structures from the functions from basccount, dimercount, codoncount, or aaccount.
<i>CaseValue</i>	Property to select the case of letters in a sequence when Alphabet is 'char'. Values are 'upper' (default) or 'lower'.
<i>DataTypeValue</i>	Property to select the data type for a sequence. Values are 'char' (default) for letter sequences, and 'uint8' or 'double' for numeric sequences.
	Creates a sequence as an array of <i>DataType</i> .

**Description** `Seq = randseq(SeqLength)` creates a random sequence with a specified length (*SeqLength*)

# randseq

---

`randseq(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`randseq(..., 'Alphabet', AlphabetValue)` generates a sequence from a specific alphabet.

`randseq(..., 'Weights', WeightsValue)` creates a weighted random sequence where the *i*th 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 *i*th element of the nucleotide alphabet is given by `int2nt(i)`, and the *i*th element of the amino acid alphabet is given by `int2aa(i)`.

`randseq(..., 'FromStructure', FromStructureValue)` creates a weighted random sequence with weights given by the output structure from `basecount`, `dimercount`, `codoncount`, or `aaccount`.

`randseq(..., 'Case', CaseValue)` specifies the case for a letter sequence.

`randseq(..., '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)
rankfeatures(..., 'PropertyName', PropertyValue,...)
rankfeatures(..., 'Criterion', CriterionValue)
rankfeatures(..., 'CCWeighting', ALPHA)
rankfeatures(..., 'NWeighting', BETA)
rankfeatures(..., 'NumberOfIndices', N)
rankfeatures(..., '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.

`rankfeatures(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`rankfeatures(..., 'Criterion', CriterionValue)` sets the criterion used to assess the significance of every feature for separating two labeled groups. Options are

'ttest' (default)	Absolute value two-sample T-test with pooled variance estimate
'entropy'	Relative entropy, also known as Kullback-Liebert distance or divergence
'brattacharyya'	Minimum attainable classification error or Chernoff bound

'roc'	Area under the empirical receiver operating characteristic (ROC) curve
'wilcoxon'	Absolute value of the u-statistic of a two-sample unpaired Wilcoxon test, also known as Mann-Whitney

Notes: 1) 'ttest', 'entropy', and 'brattacharyya' assume normal distributed classes while 'roc' and 'wilcoxon' are nonparametric tests. 2) All tests are feature independent.

`rankfeatures(..., '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.

`rankfeatures(..., '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.

# rankfeatures

---

`rankfeatures(..., '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.

`rankfeatures(..., '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. Options are

'none' (default)	Intensities are not cross-normalized.
'meanvar'	$x_{\text{new}} = (x - \text{mean}(x)) / \text{std}(x)$
'softmax'	$x_{\text{new}} = (1 + \exp((\text{mean}(x) - x) / \text{std}(x)))^{-1}$
'minmax'	$x_{\text{new}} = (x - \min(x)) / (\max(x) - \min(x))$

## 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
```

- 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
```

- 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',10);  
plot(t,y(grp==1,:), 'b',t,y(grp==2,:), 'g',t(f),1.35,'vr')
```

## See Also

Statistics Toolbox functions `classify`, `classperf`, `crossvalind`, `randfeatures`, `svmclassify`

# rebasecuts

---

**Purpose** Find restriction enzymes that cut protein sequence

**Syntax**

```
[Enzymes, Sites] = rebasecuts(SeqNT)
rebasecuts(SeqNT, Group)
rebasecuts(SeqNT, [Q, R])
rebasecuts(SeqNT, S)
```

## Arguments

<i>SeqNT</i>	Nucleotide sequence.
<i>Enzymes</i>	Cell array with the names of restriction enzymes from REBASE Version 412.
<i>Sites</i>	Vector of cut sites with the base number before every cut relative to the sequence.
<i>Group</i>	Cell array with the names of valid restriction enzymes.
Q, R, S	Base positions.

## Description

[*Enzymes*, *Sites*] = rebasecuts(*SeqNT*) finds all the restriction enzymes that cut a nucleotide sequence (*SeqNT*).

rebasecuts(*SeqNT*, *Group*) limits the search to a specified list of enzymes (*Group*).

rebasecuts(*SeqNT*, [*Q*, *R*]) limits the search to those enzymes that cut after a specified base position (*Q*) and before a specified base position (*R*) relative to the sequence.

rebasecuts(*SeqNT*, *S*) limits the search to those enzymes that cut just after a specified base position (*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>

## Example

- 1 Enter a nucleotide sequence.

```
seq = 'AGAGGGGTACGCGCTCTGAAAAGCGGGAACCTCGTGGCGCTTTATTAA'
```

- 2 Look for all possible cleavage sites in the sequence seq.

```
[enzymes sites] = rebasecuts(seq)
```

- 3 Find where restriction enzymes CfoI and Tru9I cut the sequence.

```
[enzymes sites] = rebasecuts(seq, {'CfoI','Tru9I'})
```

- 4 Search for any possible enzymes that cut after base 7.

```
enzymes = rebasecuts(seq, 7)
```

- 5 Get the subset of enzymes that cut between base 11 and 37.

```
enzymes = rebasecuts(seq, [11 37])
```

## See Also

Bioinformatics Toolbox functions `cleave`, `seq2regexp`, `seqshowwords`, `restrict`

MATLAB function `regexp`

# redgreencmap

---

**Purpose** Red and green colormap

**Syntax** `redgreencmap(Length)`

**Arguments**

Length Length of the colormap. Enter either 256 or 64. The default value is the length of the colormap of the current figure.

**Description**

`redgreencmap(Length)` returns an M-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.

`redgreencmap`, by itself, is the same length as the current colormap.

**Examples**

Reset the color map of the current figure.

```
pd =gprread('mouse_a1pd.gpr')
mimage(pd,'F635 Median')
colormap(redgreencmap)
```

**See Also**

Bioinformatics Toolbox function `clustergram`  
MATLAB functions `colormap`, `colormapeditor`



**Purpose** Change root of phylogenetic tree

**Syntax**

```
Tree2 = reroot(Tree1)
Tree2 = reroot(Tree1, Node)
Tree2 = reroot(Tree1, Node, Distance)
```

## Arguments

<i>Tree1</i>	Phylogenetic tree (phytree object) created with the function <code>phytree</code> .
<i>Node</i>	Node index returned by the phytree object method <code>getbyname</code> .
<i>Distance</i>	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'.

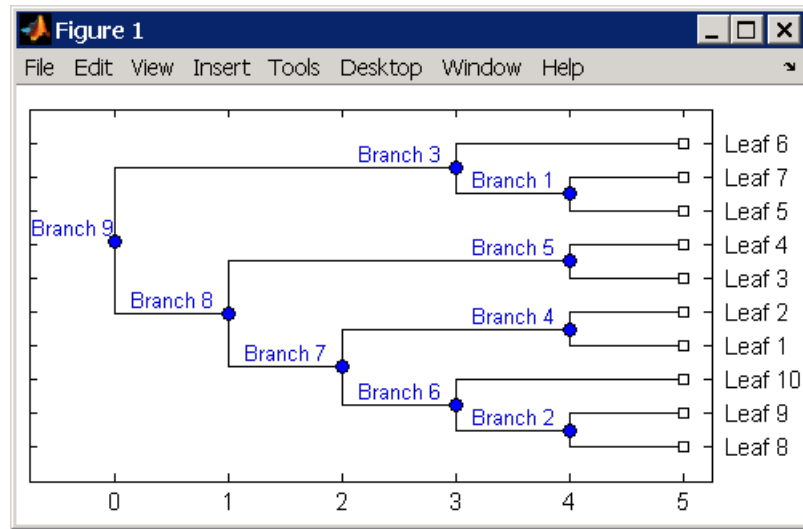
## Examples

**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)
```

MATLAB draws a figure with the phylogenetic tree.

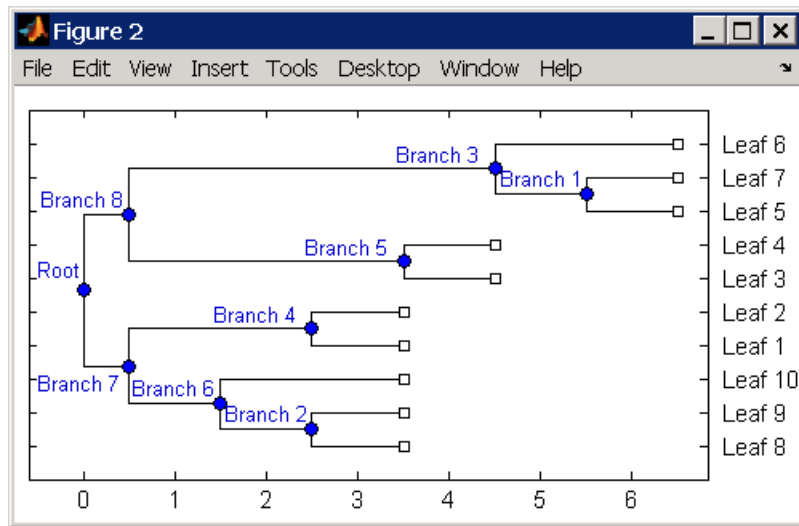
# reroot (phytree)



**2** Place the root at 'Branch 7'.

```
sel = getbyname(tr_1,'Branch 7');  
tr_2 = reroot(tr_1,sel)  
plot(tr_2,'branchlabels',true)
```

MATLAB draws a tree with the root moved to the center of branch 7.

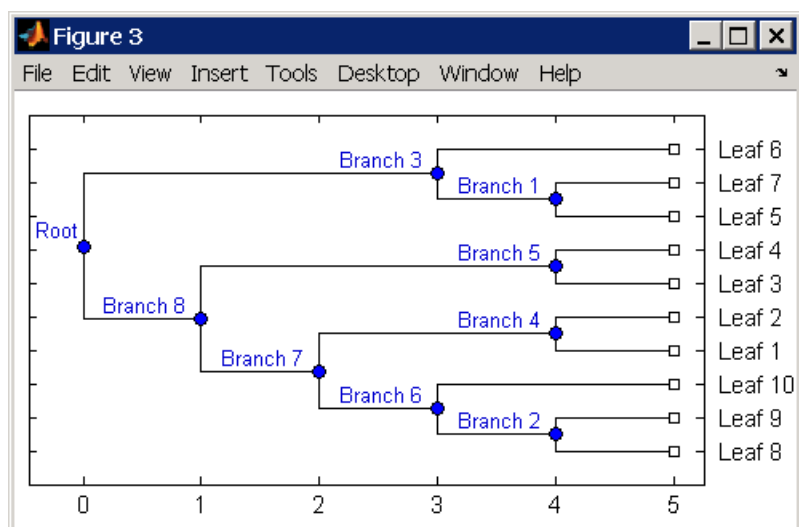


- 3** Move the root to a branch that makes the tree as ultrametric as possible.

```
tr_3 = reroot(tr_2)
plot(tr_3, 'branchlabels', true)
```

MATLAB draws the new tree with the root moved from the center of branch 7 to branch 8.

## reroot (phytree)



### See Also

Bioinformatics Toolbox

- functions — `phytree` (object constructor), `seqneighjoin`
- `phytree` object methods — `get`, `getbyname`, `prune`, `select`

**Purpose** Split nucleotide sequence at restriction site

**Syntax**

```
Fragments = restrict(SeqNT, Enzyme)
Fragments = restrict(SeqNT, Pattern, Position)
[Fragments, CuttingSites] = restrict(...)
[Fragments, CuttingSites, Lengths] = restrict(...)
restrict(..., 'PropertyName', PropertyValue,...)
restrict(..., 'PartialDigest', PartialDigestValue)
```

## Arguments

<i>SeqNT</i>	Nucleotide sequence. Enter either a character string with the characters A, T, 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.
<i>Enzyme</i>	Enter the name of a restriction enzyme from REBASE Version 412.
<i>Pattern</i>	Enter a short nucleotide pattern. Pattern can be a regular expression.
<i>Position</i>	Defines the position on Pattern where the sequence is cut. Position=0 corresponds to the 5' end of the Pattern.
<i>PartialDigestValue</i>	Property to specify a probability for partial digestion. Enter a value from 0 to 1.

## Description

*Fragments* = restrict(*SeqNT*, *Enzyme*) cuts a sequence (*SeqNT*) into fragments at the restriction sites of a restriction enzyme (*Enzyme*). The returned values are stored in a cell array of sequences (*Fragments*).

# restrict

---

`Fragments = restrict(SeqNT, Pattern, Position)` cuts a sequence (*SeqNT*) into fragments at restriction sites specified by a nucleotide pattern (*Pattern*).

`[Fragments, CuttingSites] = restrict(...)` returns a numeric vector with the indices representing the cutting sites. A 0 (zero) is added to the list so `numel(Fragments)==numel(CuttingSites)`. 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(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`restrict(..., 'PartialDigest', PartialDigestValue)` simulates a partial digest where each restriction site in the sequence has a probability (*PartialDigestValue*) 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, go to the REBASE Web site at

<http://rebase.neb.com/rebase/rebase.html>

## Example

**1** Enter a nucleotide sequence.

```
Seq = 'AGAGGGGTACGCGCTCTGAAAAGCGGGAACCTCGTGGCGCTTTATTAA';
```

**2** Use the recognition pattern (sequence) GCGC with the point of cleavage at position 3 to cleave a nucleotide sequence.

```
fragmentsPattern = restrict(Seq, 'GCGC', 3)
```

```
fragmentsPattern =  
    'AGAGGGGTACGCG'  
    'CTCTGAAAAGCGGGAACCTCGTGGCG'  
    'CTTTATTAA'
```

- 3** Use the restriction enzyme HspAI (recognition sequence GCGC with the point of cleavage at position 1) to cleave a nucleotide sequence.

```
fragmentsEnzyme = restrict(Seq, 'HspAI')

fragmentsEnzyme =
  'AGAGGGGTACG'
  'CGCTCTGAAAAGCGGGAACCTCGTGG'
  'CGCTTTATTAA'
```

- 4** Use a regular expression for the enzyme pattern.

```
fragmentsRegExp = restrict(Seq, 'GCG[ ^C]', 3)

fragmentsRegExp =

  'AGAGGGGTACGCGCTCTGAAAAGCG'
  'GGAACCTCGTGGCGCTTTATTAA'
```

- 5** Capture the cutting sites and fragment lengths with the fragments.

```
[fragments, cut_sites, lengths] = restrict(Seq, 'HspAI')

fragments =
  'AGAGGGGTACG'
  'CGCTCTGAAAAGCGGGAACCTCGTGG'
  'CGCTTTATTAA'

cut_sites =
  0
  11
  37

lengths =
  11
  26
  11
```

## restrict

---

### **See Also**

Bioinformatics Toolbox function `cleave`, `seq2regexp`, `seqshowwords`, `rebasecuts`

MATLAB function `regexp`



**Purpose** Reverse mapping for genetic code

**Syntax**

```
map = revgeneticcode
revgeneticcode(GeneticCode)
revgeneticcode(..., 'PropertyName', PropertyValue,...)
revgeneticcode(..., 'Alphabet' AlphabetValue)
revgeneticcode(..., 'ThreeLetterCodes', CodesValue)
```

## Arguments

<i>GeneticCode</i>	Genetic code for translating nucleotide codons to amino acids. Enter a code number or code name from the table Genetic Code on page 2-407 below. If you use a code name, you can truncate the name to the first two characters of the name.
<i>AlphabetValue</i>	Property to select the nucleotide alphabet. Enter either 'dna' or 'rna'. The default value is 'dna'.
<i>CodesValue</i>	Property to select one- or three-letter amino acid codes. Enter true for three-letter codes or false for one-letter codes.

## Genetic Code

Code Number	Code Name	Code Number	Code Name
1	Standard	12	Alternative Yeast Nuclear
2	Vertebrate Mitochondrial	13	Ascidian Mitochondrial
3	Yeast Mitochondrial	14	Flatworm Mitochondrial

# revgeneticcode

Code Number	Code Name	Code Number	Code Name
4	Mold, Protozoan, Coelenterate Mitochondrial, and Mycoplasma /Spiroplasma	15	Blepharisma Nuclear
5	Invertebrate Mitochondrial	16	Chlorophycean Mitochondrial
6	Ciliate, Dasycladacean, and Hexamita Nuclear	21	Trematode Mitochondrial
9	Echinoderm Mitochondrial	22	Scenedesmus Obliquus Mitochondrial
10	Euplotid Nuclear	23	Thraustochytrium Mitochondrial
11	Bacterial and Plant Plastid		

## Description

`map = revgeneticcode` returns a structure containing the reverse mapping for the standard genetic code.

`revgeneticcode(GeneticCode)` returns a structure containing the reverse mapping for an alternate genetic code.

`revgeneticcode(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`revgeneticcode(..., 'Alphabet' AlphabetValue)` defines the nucleotide alphabet to use in the map.

revgeneticcode(..., 'ThreeLetterCodes', CodesValue) returns the mapping structure with three-letter amino acid codes as field names instead of the default single-letter codes if ThreeLetterCodes is true.

## References

[1] NCBI Web page describing genetic codes,  
<http://www.ncbi.nlm.nih.gov/Taxonomy/Utils/wprintgc.cgi?mode=c>

## Examples

```

moldcode = revgeneticcode(4, 'Alphabet', 'rna');
wormcode = revgeneticcode('Flatworm Mitochondrial',...
                          'ThreeLetterCode', true);

```

```
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' }

```

# revgeneticcode

---

Starts: {'TTG' 'CTG' 'ATG'}

## 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**

```
BackgroundAdjustedMatrix = rmabackadj(PMData)
BackgroundAdjustedMatrix = rmabackadj(..., 'Method',
MethodValue, ...)
BackgroundAdjustedMatrix = rmabackadj(..., 'Truncate',
TruncateValue, ...)
BackgroundAdjustedMatrix = rmabackadj(..., 'Showplot',
ShowplotValue, ...)
```

## Arguments

<i>PMData</i>	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.)
<i>MethodValue</i>	Property to control 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'.
<i>TruncateValue</i>	Property to control the background noise model. Enter either true (use a truncated Gaussian distribution) or false (use a nontruncated Gaussian distribution). Default is true.
<i>ShowplotValue</i>	Property to control the plotting of a histogram showing the distribution of PM probe intensity values (blue) and the convoluted probability distribution function (red), with estimated parameters. 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.

## Description

*BackgroundAdjustedMatrix* = `rmabackadj(PMData)` returns the background adjusted values of probe intensities 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.

*BackgroundAdjustedMatrix* = `rmabackadj(..., 'PropertyName', PropertyValue, ...)` defines optional properties that use property name/value pairs in any order. These property name/value pairs are as follows:

*BackgroundAdjustedMatrix* = `rmabackadj(..., 'Method', MethodValue, ...)` controls 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'.

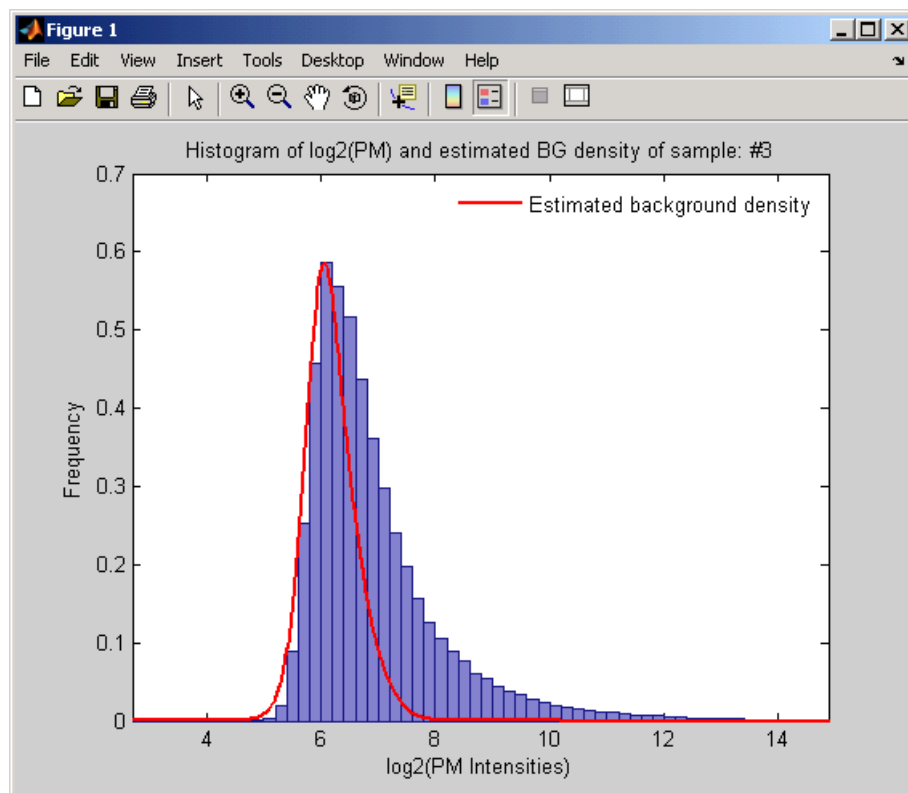
*BackgroundAdjustedMatrix* = `rmabackadj(..., 'Truncate', TruncateValue, ...)` controls the background noise model used. When *TruncateValue* is false, `rmabackadj` uses nontruncated Gaussian as the background noise model. Default is true.

*BackgroundAdjustedMatrix* = `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. 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 *Data*.
- `..., 'Showplot', [3,5,7], ...)` plots the intensity values in columns 3, 5, and 7 of *Data*.
- `..., '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, which contains Affymetrix probe-level data, including `pmMatrix`, a matrix of PM probe intensity values from multiple CEL files.

```
load prostatecancerpdata
```

- 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 prostatecancerpdata.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/repository/devel/vignette/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

affyinvarsetnorm, affyread, celintensityread, probelibraryinfo, probesetlink, probesetlookup, probesetvalues, quantilenorm, rmasummary

# rmasummary

---

**Purpose** Calculate gene (probe set) expression values from Affymetrix microarray probe-level data using Robust Multi-array Average (RMA) procedure

**Syntax**  
*ExpressionMatrix* = rmasummary(*ProbeIndices*, *Data*)  
*ExpressionMatrix* = rmasummary(..., 'Output', *OutputValue*)

## Arguments

<i>ProbeIndices</i>	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.
<i>Data</i>	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.)
<i>OutputValue</i>	Property to control the scale of the returned gene expression values. <i>OutputValue</i> can be: <ul style="list-style-type: none"><li>• 'log'</li><li>• 'log2'</li><li>• 'log10'</li><li>• 'natural'</li><li>• @<i>functionname</i></li></ul> In the last instance, the data is transformed as defined by the function <i>functionname</i> . 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  $Y_{ijn}$  denote the background adjusted, base 2 log transformed and quantile-normalized PM probe intensity value of chip  $i$  and probe  $j$ .  $Y_{ijn}$  follows a linear additive model:

$$Y_{ijn} = U_{in} + A_{jn} + E_{ijn}; i = 1, \dots, I; j = 1, \dots, J; n = 1, \dots, N$$

where:

$U_{in}$  = gene expression of the probe set  $n$  on chip  $i$

$A_{jn}$  = probe affinity effect for the  $j$ th probe in the probe set

$E_{ijn}$  = residual for the  $j$ th probe on the  $i$ th chip

The RMA methods assumes  $A_1 + A_2 + \dots + A_J = 0$  for all probe sets. A robust procedure, median polish, is used to estimate  $U_i$  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, ...)` defines optional properties that use property

name/value pairs in any order. These property name/value pairs are as follows:

*ExpressionMatrix* = rmasummary(..., 'Output', *OutputValue*) controls 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, which contains Affymetrix data variables, including *pmMatrix*, a matrix of PM probe intensity values from multiple CEL files.

```
load prostatecancerpmdata
```

- 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*. (You will

use the probeIndices column vector provided to supply information on the probe indices.)

```
ExpressionMatrix = rmasummary(probeIndices, NormMatrix);
```

The prostatecancerpdata.mat file used in the above previous 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

affyinvarsetnorm, celintensityread, mainvarsetnorm, malowess, manorm, quantilenorm, rmabackadj

# rna2dna

---

**Purpose** Convert RNA sequence of nucleotides to DNA sequence

**Syntax** `SeqDNA = rna2dna(SeqRNA)`

**Arguments**

<code>SeqRNA</code>	Nucleotide sequence for RNA. Enter a character string with the characters A, C, U, G, and the ambiguous nucleotide bases N, R, Y, K, M, S, W, B, D, H, and V.
---------------------	---

**Description** `SeqDNA = rna2dna(SeqRNA)` converts any uracil nucleotides in an RNA sequence into thymine (U→T), and returns in the same format as DNA. For example, if the RNA sequence is an integer sequence then so is `SeqRNA`.

**Example**

```
rna2dna('ACGAUGAGUCAUGCUU')  
  
ans =  
ACGATGAGTCATGCTT
```

**See Also** Bioinformatics Toolbox

- `function` — `dna2rna`

MATLAB

- `functions` — `strrep`, `regexp`

**Purpose** Read trace data from SCF file

**Syntax** `[Sample, Probability, Comments] = scfread('File')`  
`[A, C, T, G, ProbA, ProbC, ProbG, ProbT, Comments]`  
`= scfread ('File')`

## Arguments

*File* SCF formatted file. Enter a filename or a path and filename.

## Description

scfread reads data from a SCF formatted file into a MATLAB structure.

`[Sample, Probability, Comments] = scfread('File')` reads an SCF formatted file and returns the sample data in the structure `Sample`, with fields `A`, `C`, `T`, `G`, probability data in the structure `Probability`, and comment information from the file in `Comments`.

`[A, C, T, G, ProbA, ProbC, ProbG, ProbT, Comments] = scfread ('File')` reads an SCF formatted file and returns the sample data and probabilities for nucleotides 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](http://www.mrc-lmb.cam.ac.uk/pubseq/manual/formats_unix_2.html)

## Examples

Examples of SCF files can be found at

`ftp://ftp.ncbi.nih.gov/pub/TraceDB/example/`

Unzip the file `bcm-example.tgz` with SCF files to your MATLAB working directory.

```
[Sample, Probability, Comments] = scfread('HCIUP1D61207.scf')
```

```
Sample =
```

# scfread

---

```
A: [10827x1 double]
C: [10827x1 double]
G: [10827x1 double]
T: [10827x1 double]
```

```
Probability =
  prob_A: [742x1 double]
  prob_C: [742x1 double]
  prob_G: [742x1 double]
  prob_T: [742x1 double]
```

```
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(..., 'PropertyName', PropertyValue,...)
select(..., 'Reference', ReferenceValue)
select(..., 'Criteria', CriteriaValue)
select(..., 'Threshold', ThresholdValue)
select(..., 'Exclude', ExcludeValue),
select(..., 'Propagate', PropagateValue)
```

## Arguments

<i>Tree</i>	Phylogenetic tree (phytree object) created with the function phytree.
<i>N</i>	Number of closest nodes to the root node.
<i>ReferenceValue</i>	Property to select a reference point for measuring distance.
<i>CriteriaValue</i>	Property to select a criteria for measuring distance.
<i>ThresholdValue</i>	Property to select a distance value. Nodes with distances below this value are selected.
<i>ExcludeValue</i>	Property to remove (exclude) branch or leaf nodes from the output. Enter 'none', 'branches', or 'leaves'. The default value is 'none'.
<i>PropagateValue</i>	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

## select (phytree)

---

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, ...)` defines optional properties using property name/value pairs.

`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 = inf`; 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. vips_human):
ind = getbyname(tr,'vips_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
- phytree object methods — get, pdist, prune

# seq2regexp

**Purpose** Convert sequence with ambiguous characters to regular expression

**Syntax**

```
seq2regexp(Seq)
seq2regexp(..., 'PropertyName', PropertyValue, ...)
seq2regexp(..., 'Alphabet', AlphabetValue)
seq2regexp(..., 'Ambiguous', AmbiguousValue)
```

## Arguments

*Seq* Amino acid or nucleotide sequence as a string of characters. You can also enter a structure with the field *Sequence*.

*AlphabetValue* Property to select the sequence alphabet. Enter either 'AA' amino acids or 'NT' for nucleotides. The default value is 'NT'.

*AmbiguousValue* Property to control returning ambiguous characters in the regular expression. Enter either true (include ambiguous characters) or false (return only unambiguous characters). The default value is true.

## Nucleotide Conversions

Nucleotide Letter	Nucleotide	Nucleotide Letter	Nucleotide
A—A	Adenosine	S—[GC]	(Strong)
C—C	Cytosine	W—[AT]	(Weak)
G—G	Guanine	B—[GTC]	
T—T	Thymidine	D—[GAT]	
U—U	Uridine	H—[ACT]	
R—[GA]	(Purine)	V—[GCA]	
Y—[TC]	(Pyrimidine)	N—[AGCT]	Any nucleotide

Nucleotide Letter	Nucleotide	Nucleotide Letter	Nucleotide
K—[GT]	(Keto)	- — -	Gap of indeterminate length
M—[AC]	(Amino)	?—?	Unknown

### Amino Acid Conversion

Amino Acid Letter	Description
B—[DN]	Aspartic acid or asparagine
Z—[EQ]	Glutamic acid or glutamine
X—[ARNDCQEGHILKMFSTWYV]	Any amino acid

## Description

`seq2regexp(Seq)` converts ambiguous nucleotide or amino acid symbols in a sequence into a regular expression format using IUB/IUPAC codes.

`seq2regexp(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`seq2regexp(..., 'Alphabet', AlphabetValue)` selects the sequence alphabet for nucleotide sequences or amino acid sequences.

`seq2regexp(..., 'Ambiguous', AmbiguousValue)`, when *AmbiguousValue* is false, removes the ambiguous characters from the output regular expressions. For example,

- If *Seq* = 'ACGTK', and *AmbiguousValue* is true (default), MATLAB returns ACGT[GTK] with the unambiguous characters G, T, and the ambiguous character K.
- If *Seq* = 'ACGTK', and *AmbiguousValue* is false, MATLAB returns ACGT[GT] with only the unambiguous characters.

# seq2regexp

---

## Example

- 1 Convert a nucleotide sequence into a regular expression.

```
seq2regexp( 'ACWTMAN' )  
  
ans =  
AC[ATW]T[ACM]A[ACGTRYKMSWBDHVN]
```

- 2 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`, `regexp`

**Purpose** Calculate complementary strand of nucleotide sequence

**Syntax** `SeqC = seqcomplement(SeqNT)`

**Arguments**

*SeqNT* 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*.

**Description**

`SeqC = seqcomplement(SeqNT)` calculates the complementary strand (A→T, C→G, G→C, T→A) of a DNA sequence and returns a sequence in the same format as *SeqNT*. For example, if *SeqNT* is an integer sequence then so is *SeqC*.

**Example**

Return the complement of a DNA nucleotide sequence.

```
s = 'ATCG';  
seqcomplement(s)  
  
ans =  
TAGC
```

**See Also**

Bioinformatics Toolbox functions `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

<i>Seqs</i>	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 <i>Sequence</i> .
<i>Profile</i>	Sequence profile. Enter a profile from the function <i>seqprofile</i> . 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.
<i>ScoringMatrixValue</i>	Scoring matrix. The default value is BLOSUM50 for amino acid sequences or NUC44 for nucleotide sequences. <i>ScoringMatrix</i> can also be a 21x21, 5x5, 20x20, or 4x4 numeric array. For the gap-included cases, gap scores (last row/column) are set to <code>mean(diag(ScoringMatrix))</code> for a gap matching with another gap, and set to <code>mean(nodiag(ScoringMatrix))</code> 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`, `proalign`, `seqdisp`, `seqprofile`

# seqdisp

---

**Purpose** Format long sequence output for easy viewing

**Syntax**

```
seqdisp(Seq)
seqdisp(..., 'PropertyName', PropertyValue,...)
seqdisp(..., 'Row', RowValue)
seqdisp(..., 'Column', ColumnValue)
seqdisp(..., 'ShowNumbers', ShowNumbersValue)
```

## Arguments

<i>Seq</i>	Nucleotide or amino acid sequence. Enter a character array, a FASTA filename, or a MATLAB structure with the field <i>Sequence</i> . Multiply aligned sequences are allowed.  FASTA files can have the file extension <i>fa</i> , <i>fasta</i> , <i>fas</i> , <i>fsa</i> , or <i>fst</i> .
<i>Row</i>	Property to select the length of each row. Enter an integer. The default length is 60.
<i>Column</i>	Property to select the column width or number of symbols before displaying a space. Enter an integer. The default column width is 10.
<i>ShowNumbers</i>	Property to control displaying numbers at the start of each row. Enter either <i>true</i> (default) to show numbers or <i>false</i> to hide numbers.

**Description** `seqdisp(Seq)` displays a sequence (*Seq*) in rows with a default row length of 60 and a default column width of 10.

`seqdisp(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`seqdisp(..., 'Row', RowValue)` specifies the length of each row for the displayed sequence.

`seqdisp(..., 'Column', ColumnValue)` specifies the number of letters to display before adding a space. Row must be larger than and evenly divisible by Column.

`seqdisp(..., 'ShowNumbers', ShowNumbersValue)` when `ShowNumbers` is false, turns off the position numbers at the start of each row off.

## 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'; 'ATCGACYGGTTCGGTTCGCTCGAAN']
fastawrite('local.fa', hdr, seq);
seqdisp('local.fa', 'ShowNumbers', false')
```

```
ans =
>Sequence A
  1 TAGCTGRCCA AGGCCAAGCG AGCTTN
>Sequence B
  1 ATCGACYGGT TCGGTTCGC TCGAAN
```

## See Also

Bioinformatics Toolbox function `multialignread`, `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

<i>Seq1, Seq2</i>	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 <i>Sequence</i> .
<i>Window</i>	Enter an integer for the size of a window.
<i>Number</i>	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.

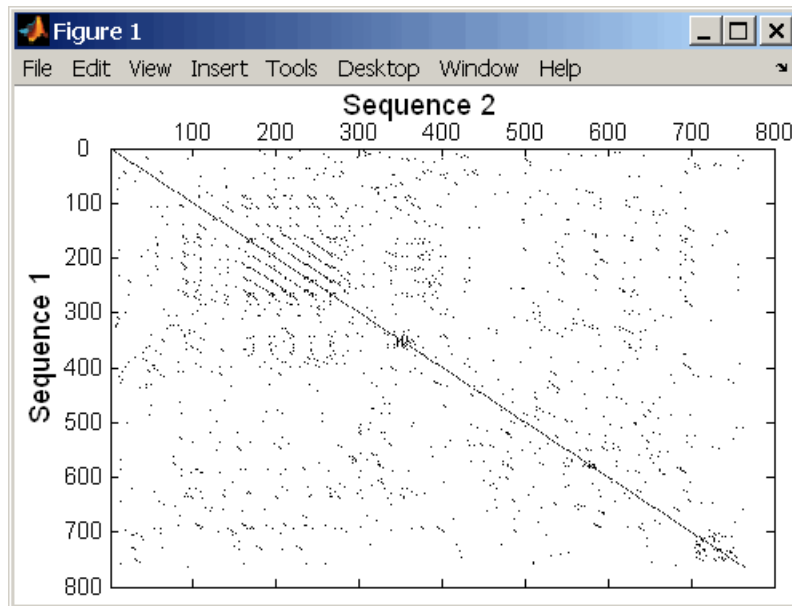
`[Matches, Matrix] = seqdotplot(...)` returns the dotplot as a sparse matrix.

## 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)
```



```
Matches = seqdotplot(moufflon,takin,11,7)  
Matches =  
    5552
```

```
[Matches, Matrix] = seqdotplot(moufflon,takin,11,7)
```

## See Also

Bioinformatics Toolbox functions `nwalign`, `swalign`

# seqlinkage

---

**Purpose** Construct phylogenetic tree from pairwise distances

**Syntax**

```
Tree = seqlinkage(Dist)
Tree = seqlinkage(Dist, Method)
Tree = seqlinkage(Dist, Method, Names)
```

## Arguments

<i>Dist</i>	Pairwise distances generated from the function <code>seqpdist</code> .
<i>Method</i>	Property to select a distance method. Enter a method from the table below.
<i>Names</i>	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 <i>Dist</i> .

## 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) such as is generated by the function `seqpdist`.

`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

The Bioinformatics Toolbox

- functions — `phytree` (object constructor), `phytreewrite`, `seqpdist`, `seqneighjoin`
- `phytree` object methods — `plot`, `view`

# seqlogo

---

**Purpose** Sequence logo for nucleotide and amino acid sequences

**Syntax**

```
seqlogo(Seqs)
seqlogo(Profile)
DisplayInfo = seqlogo(Seqs)
DisplayInfo = seqlogo(..., 'Displaylogo', DisplaylogoValue).
seqlogo(..., 'Alphabet', AlphabetValue)
seqlogo(..., 'Startat', StartatValue)
seqlogo(..., 'Endat', EndatValue)
seqlogo(..., 'SSCorrection', SSCorrectionValue).
```

**Arguments**

<i>Seqs</i>	Set of pairwise or 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 <i>Sequence</i> .
<i>Displaylogo</i>	Property to control drawing a sequence logo. Enter either true or false.

**Description** `seqlogo(Seqs)` displays a sequence logo for a set of aligned sequences (*Seqs*). 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  $\log_2(4)$  bits for nucleotide sequences and  $\log_2(20)$  bits for amino acid sequences.

`seqlogo(Profile)` displays a sequence logo for a sequence profile (*P*) returned by the function `seqprofile`.

*Profile* For amino acids, frequency distribution matrix of size [20 x sequence length]. For nucleotides, matrix of size [4 x sequence length] using the DNA alphabet. If gaps were included, *Profile* may have 21 (or 5) rows, but `seqlogo` ignores gaps.

The alphabet for nucleic acids is colored as follows



A	Green
C	Blue
G	Yellow
T, U	Red

The alphabet for proteins is colored according to chemical property as follows

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

Ambiguous symbols not in the list above are added to the logo and colored purple.

`DisplayInfo = seqlogo(Seqs)` returns a cell array of unique symbols in a sequence (`Seqs`) and the information weight matrix used for graphically displaying the logo.

`DisplayInfo = seqlogo(..., 'Displaylogo', DisplaylogoValue)`. when `Displaylogo` is false, returns display information, but does not draw the sequence logo.

`seqlogo(..., 'Alphabet', AlphabetValue)` selects the alphabet for nucleotide sequences ('NT') or amino acid sequences ('AA'). The default is 'NT'. If you provide amino acid sequences to `seqlogo`, you must select 'AA' for the Alphabet.

`seqlogo(..., 'Startat', StartatValue)` specifies the starting position for the sequences (`Seqs`). The default starting position is 1.

`seqlogo(..., 'Endat', EndatValue)` specifies the ending position for the sequences (`Seqs`). The default ending position is the maximum length of the sequences (`Seqs`).

`seqlogo(..., 'SSCorrection', SSCorrectionValue)`. when `SSCorrection` is `false`, no estimation is made for the number of bits. A simple calculation of bits tends to overestimate the conservation at a particular location. To compensate for this overestimation, when `SSCorrection` is `true`, a rough estimate is applied as an approximate correction. This correction works better when the number of sequences is greater than 50. The default is `true`.

## Reference

Schneider, T.D., Stephens, R.M., "Sequence Logos: A new way to display consensus sequences," *Nucleic Acids Research*, Vol. 18, pp. 6097-6100, 1990.

## Examples

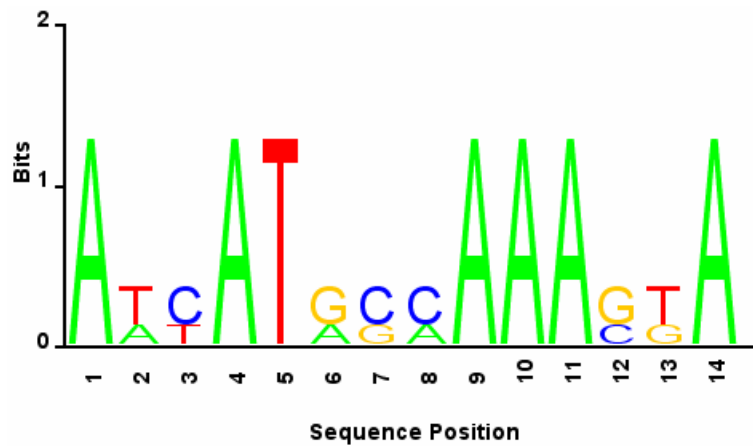
**1** Get a series of aligned sequences.

```
S = {'ATTATAGCAA ACTA', ...  
     'AACATGCCAAAGTA', ...  
     'ATCATGCAAAAGGA' }
```

**2** Display the sequence logo.

```
seqlogo(S)
```

MATLAB draws a figure.



- 3** Notice that correction for small samples prevents you from seeing columns with information equal to  $\log_2(4) = 2$  bits, but you can turn this adjustment off.

```
seqlogo(S, 'sscCorrection', false)
```

## 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 strmatch, regexp

**Purpose** Neighbor-joining method for phylogenetic tree reconstruction

**Syntax**

```
Tree = seqneighjoin(Dist)
Tree = seqneighjoin(Dist, Method)
Tree = seqneighjoin(Dist, Method, Names)
seqneighjoin(..., 'PropertyName', PropertyValue,...)
seqneighjoin(..., 'Reroot', RerootValue)
```

## Arguments

<i>Dist</i>	Matrix or vector returned by the function seqpdist
<i>Method</i>	Method to compute the distances between nodes. Enter 'equivar' (default), 'firstorder', or 'average'.
<i>Names</i>	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 <i>Dist</i> .

## Description

*Tree = seqneighjoin(Dist)* computes a phylogenetic tree object from pairwise distances (*Dist*) between the species or products using the neighbor-joining method.

*Tree = seqneighjoin(Dist, Method)* selects a method (*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).

The following table describes the values for *Method*.

# seqneighjoin

---

'equivar' (default)	Assumes equal variance and independence of evolutionary distance estimates ( $a = 1/2$ ). Such as in Studier and Keppler, JMBE (1988).
'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(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`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.

## References

[1] Saitou N, Nei M (1987), "The neighbor-joining method: A new method for reconstructing phylogenetic trees", *Molecular Biology and Evolution*. 4(4):406-25.

[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 JA, Keppler KJ (1988), “A note on the neighbor-joining algorithm of Saitou and Nei”, *Molecular Biology and Evolution*, 5(6):729-31.

## 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)
```

## See Also

Bioinformatics Toolbox functions `multialign`, `phytree` (object constructor), `seqlinkage` (alternative method to create a phylogenetic tree), `seqpdist`

Methods of `phytree` object `reroot`, `view`

# seqpdist

---

**Purpose** Calculate pairwise distance between sequences

**Syntax**

```
D = seqpdist(Seqs)
seqpdist(..., 'PropertyName', PropertyValue,...)
seqpdist(..., 'Method', MethodValue)
seqpdist(..., 'Indels', IndelsValue)
seqpdist(..., 'Optargs', OptargsValue)
seqpdist(..., 'PairwiseAlignment', PairwiseAlignmentValue)
seqpdist(..., 'JobManager', JobManagerValue)
seqpdist(..., 'WaitInQueue', WaitInQueueValue)
seqpdist(..., 'Squareform', SquareformValue)
seqpdist(..., 'Alphabet', AlphabetValue)
seqpdist(..., 'ScoringMatrix', ScoringMatrixValue)
seqpdist(..., 'Scale', ScaleValue)
seqpdist(..., 'GapOpen', GapOpenValue)
seqpdist(..., 'ExtendGap', ExtendGapValue)
```

## Arguments

<i>Seqs</i>	Cell array with nucleotide or amino acid sequences.
<i>MethodValue</i>	Property to select the method for calculating pairwise distances.
<i>IndelsValue</i>	Property to indicate treatment of gaps.
<i>OptargsValue</i>	Property to pass required arguments by the distance method selected with the property Method.
<i>PairwiseAlignmentValue</i>	Property to force pairwise alignment.
<i>JobManagerValue</i>	JobManager object representing an available distributed MATLAB resource. Enter a jobmanager object returned by the Distributed Computing Toolbox function findResource.



<i>WaitInQueueValue</i>	Property to control waiting for a distributed MATLAB resource to be available. Enter either true or false. The default value is false.
<i>SquareFormValue</i>	Property to control formatting the output as a square or triangular matrix.
<i>AlphabetValue</i>	Property to select an alphabet. Enter either 'NT' for nucleotides or 'AA' for amino acids.
<i>ScoringMatrixValue</i>	Property to select a scoring matrix for pairwise alignment.
<i>ScaleValue</i>	Property to select a scale factor for the scoring matrix.
<i>GapOpenValue</i>	Property to select a gap penalty.
<i>ExtendedGapValue</i>	Property to select a penalty for extending a gap.

## Description

$D = \text{seqpdist}(\text{Seqs})$  returns a vector  $D$  containing biological distances between each pair of sequences stored in the  $M$  elements of the a cell array of sequences ( $\text{Seqs}$ ).

$D$  is an 1-by- $(M*(M-1)/2)$  row vector corresponding to the  $M*(M-1)/2$  pairs of the  $M$  sequences in  $\text{Seqs}$ . The output  $D$  is arranged in the order  $((2,1), (3,1), \dots, (M,1), (3,2), \dots (M,2), \dots (M,M-1))$ . 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  $D((J-1)*(M-J)/2+I-J)$ .  $\text{Seqs}$  can also be a vector of structures with the field `Sequence` or a matrix of chars.

$\text{seqpdist}(\dots, 'PropertyName', PropertyValue, \dots)$  enters optional arguments as property name/value pairs.

$\text{seqpdist}(\dots, 'Method', MethodValue)$  selects a method ( $MethodValue$ ) to compute distances between every pair of sequences.

Distances defined for both nucleotides and amino acids:

# seqpdist

'p-distance'	<p>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.</p> $d = p$
'Jukes-Cantor' (default)	<p>Maximum likelihood estimate of the number of substitutions between two sequences. p is described with the method 'p-distance'. For nucleotides</p> $d = -3/4 \log(1 - p * 4/3)$ <p>For amino acids</p> $d = -19/20 \log(1 - p * 20/19)$
'alignment-score'	<p>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:</p> $d = (1 - \text{score12}/\text{score11}) * (1 - \text{score12}/\text{score22})$ <p>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 <math>d = 0</math>.</p>

Distances defined only for nucleotides and no scoring of gaps:

'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 and transversion nucleotide substitution.
'Tamura'	Considers separately the transitional and transversion 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).
'Hasegawa'	Considers separately the transitional and transversion nucleotide substitution and the background nucleotide frequencies. Background frequencies can be computed from the input sequences or given by setting the Optargs to [gA gC gG gT].
'Nei-Tamura'	Considers separately the transitional substitution between purines, the transitional substitution between pyrimidines and the transversion substitution and the background nucleotide frequencies. Background frequencies can be computed from the input sequences or given by setting the Optargs to [gA gC gG gT].

Distances defined only for amino acids and no scoring of gaps:

'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'. 'a' can be set by 'Optargs'. The default value is 2.

A user defined distance function can also be specified using @, for example, @distfun, the distance function must be of the form:

```
function D = distfun(S1, S2, OptArgsValue)
```

The function `distfun` should take as arguments two same-length sequences (NT or AA) plus zero or more additional problem-dependent arguments in `OptArgsValue`, and returning a scalar that represents the distance between S1 and S2.

`seqpdist(..., 'Indels', IndelsValue)` indicates how to treat sites with gaps. Options 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 at the input *Seqs*.

`seqpdist(..., 'Optargs', OptargsValue)` passes optional arguments required or accepted by some distance methods. Use a cell array to pass more than one input argument (for example, the nucleotide

frequencies in the Tajima-Nei distance function can be specified instead of computing them from the input sequences).

`seqpdist(..., 'PairwiseAlignment', PairwiseAlignmentValue)`, when *PairwiseAlignmentValue* is true, ignores multiple alignment of the input sequences (if any) and forces a pairwise alignment of input sequences. If the input sequences are not prealigned, this flag is set automatically. Pairwise alignment can be slow for a large number of sequences. The default value is false.

`seqpdist(..., 'JobManager', JobManagerValue)` distributes pairwise alignments into a cluster of computers using the Distributed Computing Toolbox. *JobManagerValue* is a jobmanager object such as the one returned by Distributed Computing Toolbox function `findResource`.

`seqpdist(..., 'WaitInQueue', WaitInQueueValue)`, when *WaitInQueueValue* is true, `multialign` waits in the job manager queue for an available worker. When *WaitInQueueValue* is false (default) and there are no workers immediately available, `multialign` stops and displays an error message. Use this property with the Distributed Computing Toolbox and the `multialign` property `WaitInQueue`.

`seqpdist(..., 'Squareform', SquareformValue)`, when *SquareFormValue* is true, converts the output into a square formatted matrix so that  $D(I,J)$  denotes the distance between the  $I$ th and  $J$ th sequences. The output matrix is symmetric and has a zero diagonal. Setting the property `Squareform` to true is the same as using the function `squareform` in the Statistical Toolbox.

`seqpdist(..., 'Alphabet', AlphabetValue)` specifies whether the sequences are amino acids ('AA') or nucleotides ('NT'). The default value is 'AA'.

The remaining input properties are analogous to the function `nwalign` and are used when the property `PairwiseAlignment` = true or the property `Method` = 'alignment-score'. For more information about these properties, see the functions `nwalign`.

# seqpdist

---

`seqpdist(..., 'ScoringMatrix', ScoringMatrixValue)` specifies the scoring matrix to be used for the alignment. The default value is BLOSUM50 for amino acids and NUC44 for nucleotides.

`seqpdist(..., 'Scale', ScaleValue)` indicates the scale factor of the scoring matrix to return the score using arbitrary units. If the scoring matrix info also provides a scale factor, then both are used.

`seqpdist(..., 'GapOpen', GapOpenValue)` specifies the penalty for opening a gap in the alignment. The default gap open penalty is 8.

`seqpdist(..., 'ExtendGap', ExtendGapValue)` specifies the penalty for extending a gap in the alignment. If `ExtendGap` is not specified, then extensions to gaps are scored with the same value as `GapOpen`.

## Examples

- 1 Load a multiple alignment of amino acids.

```
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, dndsm1, phytree (object constructor), seqlinkage
- phytree object method — pdist

# seqprofile

---

**Purpose** Calculate sequence profile from set of multiply aligned sequences

**Syntax**

```
Profile = seqprofile(Seqs, 'PropertyName', PropertyValue ...)  
[Profile, Symbols] = seqprofile(Seqs)  
seqprofile(..., 'Alphabet', AlphabetValue)  
seqprofile(..., 'Counts', CountsValue)  
seqprofile(..., 'Gaps', GapsValue)  
seqprofile(..., 'Ambiguous', AmbiguousValue),  
seqprofile(..., 'Limits', LimitsValue)
```

## Arguments

Seqs	Set of multiply aligned sequences. Enter an array of strings, cell array of strings, or an array of structures with the field Sequence.
Alphabet	Sequence alphabet. Enter 'NT' (nucleotides), 'AA' (amino acids), or 'none'. The default alphabet is 'AA'.  When Alphabet is 'none', the symbol list is based on the observed symbols. Every character can be a symbol except for a hyphen (-) and a period (.), which are reserved for gaps.
Count	Property to control returning frequency (ratio of counts/total counts) or counts. Enter either true (counts) or false (frequency). The default value is false.
Gaps	Property to control counting gaps in a sequence. Enter 'all' (counts all gaps), 'noflanks' (counts all gaps except those at the flanks of every sequence), or 'none'. The default value is 'none'.



Ambiguous	Property to control counting ambiguous symbols. Enter 'Count' to add partial counts to the standard symbols.
Limits	Property to specify using part of the sequences. Enter a [1x2] vector with the first position and the last position to include in the profile. The default value is [1, SeqLength].

## Description

`Profile = seqprofile(Seqs, 'PropertyName', PropertyValue ...)` returns a matrix (Profile) 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 a unique symbol list (Symbols) where every symbol in the list corresponds to a row in the profile (Profile).

`seqprofile(..., 'Alphabet', AlphabetValue)` selects a nucleotide alphabet, amino acid alphabet, or no alphabet.

`seqprofile(..., 'Counts', CountsValue)` when Counts is true, returns the counts instead of the frequency.

`seqprofile(..., 'Gaps', GapsValue)` appends a row to the bottom of a profile (Profile) with the count for gaps.

`seqprofile(..., '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(..., 'Limits', LimitsValue)` specifies the start and end positions for the profile relative to the indices of the multiple alignment.

# seqprofile

---

## Examples

```
seqs = fastaread('pf00002.fa');  
[P,S] = seqprofile(seqs,'limits',[50 60],'gaps','all')
```

## See Also

Bioinformatics Toolbox functions `fastaread`, `multialignread`, `seqconsensus`, `seqdisp`, `seqlogo`

**Purpose** Calculate reverse complement of nucleotide sequence

**Syntax** `SeqRC = seqrcomplement(SeqNT)`

## 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`.

## Description

`seqrcomplement` calculates the reverse complementary strand of a DNA sequence.

`SeqRC = seqrcomplement(SeqNT)` calculates the reverse complementary strand 3' → 5' (A→T, C→G, G→C, T→A) for a DNA sequence and returns a sequence in the same format as `SeqNT`. For example, if `SeqNT` is an integer sequence then so is `SeqRC`.

## Examples

Reverse a DNA nucleotide sequence and then return its complement.

```
s = 'ATCG'  
seqrcomplement(s)
```

```
ans =  
CGAT
```

## See Also

Bioinformatics Toolbox functions `codoncount`, `palindromes`, `seqcomplement`, `seqreverse`, `seqtool`

# seqreverse

---

**Purpose** Reverse the letters or numbers in nucleotide sequence

**Syntax** SeqR = seqreverse(SeqNT)

## Arguments

SeqNT	Enter a 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.
SeqR	Returns a sequence in the same format as the nucleotide sequence. For example, if SeqNT is an integer sequence, then so is SeqR.

**Description** seqreverse calculates the reverse strand of a DNA or RNA sequence. SeqR = seqreverse(SeqNT) calculates the reverse strand 3' → 5' of the nucleotide sequence.

**Examples** Reverse a nucleotide sequence.

```
s = 'ATCG'  
seqreverse(s)  
  
ans =  
GCTA
```

**See Also** Bioinformatics Toolbox functions seqcomplement, seqrcomplement, seqtool  
MATLAB function flip1r

**Purpose** Display open reading frames in sequence

**Syntax**

```
seqshoworfs(SeqNT)
seqshoworfs(..., 'PropertyName', PropertyValue,...)
seqshoworfs(..., 'Frames', FramesValue)
seqshoworfs(..., 'GeneticCode', GeneticCodeValue)
seqshoworfs(..., 'MinimumLength', MinimumLengthValue)
seqshoworfs(..., 'AlternativeStartCodons', StartCodonsValue)
seqshoworfs(..., 'Color', ColorValue)
seqshoworfs(..., 'Columns', ColumnsValue)
```

## Arguments

<i>SeqNT</i>	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.
<i>FramesValue</i>	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.
<i>GeneticCodeValue</i>	Genetic code name. Enter a code number or a code name from the table see Genetic Code on page 2-133.
<i>MinimumLengthValue</i>	Property to set the minimum number of codons in an ORF.
<i>StartCodonsValue</i>	Property to control using alternative start codons. Enter either true or false. The default value is false.

<i>ColorValue</i>	Property to select the color for highlighting the reading frame. Enter either a 1-by-3 RGB vector specifying the intensity (0 to 255) of the red, green, and blue components of the color, or a character from the following list: 'b'—blue, 'g'—green, 'r'—red, 'c'—cyan, 'm'—magenta, or 'y'—yellow.  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 COLOR should be a 1-by-6 cell array of color values.
<i>ColumnsValue</i>	Property to specify the number of columns in the output.

## 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(..., '*PropertyName*', *PropertyValue*,...) defines optional properties using property name/value pairs.

seqshoworfs(..., '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(..., 'GeneticCode', *GeneticCodeValue*) specifies the genetic code to use for finding open reading frames.

seqshoworfs(..., 'MinimumLength', *MinimumLengthValue*) sets the minimum number of codons for an ORF to be considered valid. The default value is 10.

`seqshoworfs(..., 'AlternativeStartCodons', StartCodonsValue)` 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 of alternative start codons, see

```
http://www.ncbi.nlm.nih.gov/Taxonomy/Utils/  
wprintgc.cgi?mode=t#SG1
```

`seqshoworfs(..., 'Color', ColorValue)` selects 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 frame.

`seqshoworfs(..., 'Columns', ColumnsValue)` specifies how many columns per line to use in the output. The default value is 64.

## Examples

Look for the open reading frames in a random nucleotide sequence.

```
s = randseq(200, 'alphabet', 'dna');  
seqshoworfs(s);
```

Identify the open reading frames in a GenBank sequence.

```
HLA_DQB1 = getgenbank('NM_002123');  
seqshoworfs(HLA_DQB1.Sequence);
```

## See Also

Bioinformatics Toolbox functions `codoncount`, `geneticcode`, `seqdisp`, `seqshowwords`, `seqwordcount`, `cpgisland`, `seqtool`

MATLAB function `regexp`

# seqshowwords

---

**Purpose** Graphically display words in sequence

**Syntax**

```
seqshowwords(Seq, Word)
seqshowwords(..., 'PropertyName', PropertyValue,...)
seqshowwords(..., 'Color', ColorValue)
seqshowwords(..., 'Columns', ColumnsValue)
seqshowwords(..., 'Alphabet', AlphabetValue)
```

## Arguments

<i>Seq</i>	Enter either a nucleotide or amino acid sequence. You can also enter a structure with the field <i>Sequence</i> .
<i>Word</i>	Enter a short character sequence.
<i>ColorValue</i>	Property to select the color for highlighted characters. Enter a 1-by-3 RGB vector specifying the intensity (0255) of the red, green, and blue components, or enter a character from the following list: 'b'— blue, 'g'— green, 'r'— red, 'c'— cyan, 'm'— magenta, or 'y'— yellow.  The default color is red 'r'.
<i>ColumnsValue</i>	Property to specify the number of characters in a line. Default value is 64.
<i>AlphabetValue</i>	Property to select the alphabet. Enter 'AA' for amino acid sequences or 'NT' for nucleotide sequences. The default is 'NT'.

**Description** `seqshowwords(Seq, Word)` displays the sequence with all occurrences of a word highlighted, and returns a structure with the start and stop positions for all occurrences of the word in the sequence.

`seqshowwords(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`seqshowwords(..., 'Color', ColorValue)` selects the color used to highlight the words in the output display.



`seqshowwords(..., 'Columns', ColumnsValue)` specifies how many columns per line to use in the output.

`seqshowwords(..., 'Alphabet', AlphabetValue)` selects the alphabet for the sequence (*Seq*) and the word (*Word*).

If the search word (*Word*) contains nucleotide or amino acid symbols that represent multiple possible symbols, then `seqshowwords` shows all 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'.

## Examples

This example shows two matches, 'TAGT' and 'TAAT', for the word 'BART'.

```
seqshowwords('GCTAGTAACGTATATATAAT', 'BART')
```

```
ans =  
  Start: [3 17]  
  Stop: [6 20]
```

```
000001 GCTAGTAACGTATATATAAT
```

`seqshowwords` does not highlight overlapping patterns multiple times. This example highlights two places, the first occurrence of 'TATA' and the 'TATATATA' immediately after 'CG'. The final 'TA' is not highlighted because the preceding 'TA' is part of an already matched pattern.

```
seqshowwords('GCTATAACGTATATATATA', 'TATA')
```

```
ans =  
  Start: [3 10 14]  
  Stop: [6 13 17]
```

```
000001 GCTATAACGTATATATATA
```

# seqshowwords

---

To highlight all multiple repeats of TA, use the regular expression 'TA(TA)\*TA'.

```
seqshowwords('GCTATAACGTATATATATA', 'TA(TA)*TA')
```

```
ans =  
    Start: [3 10]  
    Stop: [6 19]
```

```
000001 GCTATAACGTATATATATA
```

## See Also

Bioinformatics Toolbox functions `palindromes`, `cleave`, `restrict`, `seqdisp`, `seqtool`, `seqwordcount`

MATLAB functions `strfind`, `regexp`

**Purpose**

Open interactive tool to explore biological sequences

**Syntax**

```
seqtool(Seq)
seqtool(..., 'PropertyName', PropertyValue, ...)
seqtool(..., 'Alphabet', AlphabetValue)
```

**Arguments**

*Seq* Struct with a field *Sequence*, a character array, or a filename with an extension of *.gbk*, *.gpt*, *.fasta*, *.fa*, or *.ebi*

**Description**

`seqtool(Seq)` loads a sequence (*Seq*) into the seqtool GUI.

`seqtool(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`seqtool(..., 'Alphabet', AlphabetValue)` specifies an alphabet (*AlphabetValue*) for the sequence (*Seq*). The default value is 'AA' except when all of the symbols in the sequence are A, C, G, T, and -, then *AlphabetValue* is set to 'NT'. Use 'AA' when you want to force an amino acid sequence alphabet.

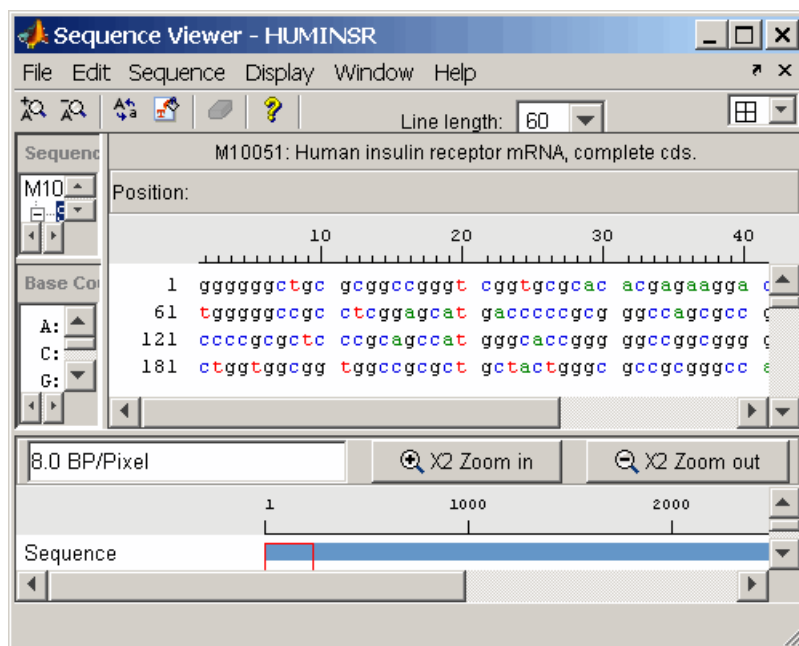
**Example**

**1** Get a sequence from Genbank.

```
S = getgenbank('M10051')
```

**2** Open the sequence tool window with the sequence.

```
seqtool(S)
```



## 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
```

# seqwordcount

---

## See Also

Bioinformatics Toolbox functions `codoncount`, `seqshoworfs`, `seqshowwords`, `seqtool`, `seq2regex`

MATLAB functions `strfind`

**Purpose** Sequence alignment with color

**Syntax**

```
showalignment(Alignment)  
showalignment(..., 'PropertyName', PropertyValue,...)  
showalignment(..., 'MatchColor', MatchColorValue)  
showalignment(..., 'SimilarColor', SimilarColorValue)  
showalignment(..., 'StartPointers', StartPointersValue)  
showalignment(..., 'Columns', ColumnsValue)
```

## Arguments

*Alignment* For pairwise alignments, matches and similar residues are highlighted and *Alignment* is the output from one of the functions `nalign` or `swalign`. For multiple sequence alignment highly conserved columns are highlighted and *Alignment* is the output from the function `multialign`.

*MatchColorValue* Property to select the color to highlight matching characters. Enter a 1-by-N RGB vector specifying the intensity (0 to 255) of the red, green, and blue components, or enter a character from the following list: 'b' – blue, 'g' – green, 'r' – red, 'c' – cyan, 'm' – magenta, or 'y' – yellow.

The default color is red, 'r'.

*SimilarColorValue* Property to select the color to highlight similar characters. Enter a 1-by-3 RGB vector or color character. The default color is magenta.

# showalignment

---

<i>StartersPointersValue</i>	Property to specify the starting indices of the aligned sequences. <i>StartPointers</i> is the two element vector returned as the third output of the function <i>swalign</i> .
<i>ColumnsValue</i>	Property to specify the number of characters in a line. Enter the number of characters to display in one row. The default value is 64.

## Description

`showalignment(Alignment)` displays an alignment in a MATLAB figure window.

`showalignment(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`showalignment(..., 'MatchColor', MatchColorValue)` selects the color to highlight the matches in the output display. The default color is red. For example, to use cyan, enter 'c' or [0 255 255].

`showalignment(..., 'SimilarColor', SimilarColorValue)` selects the color to highlight similar residues that are not exact matches. The default color is magenta.

The following options are only available when showing pairwise alignments:

`showalignment(..., 'StartPointers', StartPointersValue)` specifies the starting indices in the original sequences of a local alignment.

`showalignment(..., 'Columns', ColumnsValue)` specifies how many columns per line to use in the output, and labels the start of each row with the sequence positions.

## Examples

Enter two amino acid sequences and show their alignment.

```
[Score, Alignment] = nwalignment('VSPAGMASGYD', 'IPGKASYD');  
showalignment(Alignment);
```



```
Identities = 6/11 (55%), Positives = 7/11 (64%)
```

```
VSPAGMASGYD  
: | | || ||  
I-P-GKAS-YD
```

Enter a multiplyaligned set of sequences and show their alignment.

```
gag = multialignread('aagag.aln');  
showalignment(gag)
```

### See Also

Bioinformatics Toolbox functions `nwalign`, `swalign`

# showhmmprof

---

**Purpose** Plot Hidden Markov Model (HMM) profile

**Syntax**

```
showhmmprof(Model)  
showhmmprof(..., 'PropertyName', PropertyValue,...)  
showhmmprof(..., 'Scale', ScaleValue)  
showhmmprof(..., 'Order', OrderValue)
```

## Arguments

*Model* Hidden Markov model created with the functions `gethmmprof` and `pfamhmmread` functions.

*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,...)` defines optional properties using property name/value pairs.

`showhmmprof(..., '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(..., '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`

# sptread

---

**Purpose** Read data from SPOT file

**Syntax**

```
SPOTData = sptread('File')
sptread(..., 'PropertyName', PropertyValue,...)
sptread(..., 'CleanColNames', CleanColNamesValue)
```

## Arguments

<i>File</i>	SPOT formatted file (ASCII text file). Enter a filename, a path and filename, or URL pointing to a file. <i>File</i> can also be a MATLAB character array that contains the text for a SPOT file.
<i>CleanColNamesValue</i>	Property to control using valid MATLAB variable names.

## Description

`SPOTData = sptread('File')` reads a SPOT formatted file (*File*) and creates a MATLAB structure (SPOTData) containing the following fields:

- Header
- Data
- Blocks
- Columns
- Rows
- IDs
- ColumnNames
- Indices
- Shape

`sptread(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`sptread(..., 'CleanColNames', CleanColNamesValue)` The column names in the SPOT 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 MATLAB 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.

```
spotStruct = sptread('spotdata.txt')
mimage(spotStruct, 'Rmedian');
```

- 2 Alternatively, 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, geosoftread, gprread, imageneread, maboxplot, magetfield,

# subtree (phytree)

---

**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 = phytread('pf00002.tree')
```

**2** Get the subtree that contains the VIPS and CGRR human proteins.

```
sel = getbyname(tr,{'vips_human','cgr_human'});  
sel = any(sel,2);  
tr = subtree(tr,sel)  
view(tr);
```

**See Also** Bioinformatics Toolbox

- functions — `phytree` (object constructor)
- `phytree` object methods — `get`, `getbyname`, `prune`, `select`

---

<b>Purpose</b>	Classify data using support vector machine
<b>Syntax</b>	<pre>Group = svmclassify(SVMStruct, Sample) svmclassify(..., 'PropertyName', PropertyValue,...) svmclassify(..., 'Showplot', ShowplotValue)</pre>
<b>Description</b>	<p><code>Group = svmclassify(SVMStruct, Sample)</code> classifies each row of the data in <code>Sample</code> using the information in a support vector machine classifier structure <code>SVMStruct</code>, created using the function <code>svmtrain</code>. <code>Sample</code> must have the same number of columns as the data used to train the classifier in <code>svmtrain</code>. <code>Group</code> indicates the group to which each row of <code>Sample</code> has been assigned.</p>

---

**Note** If a data point falls on the boundary line, it is classified as a 1.

---

`svmclassify(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`svmclassify(..., 'Showplot', ShowplotValue)` when `Showplot` is true, plots the sample data on the figure created using the `showplot` option in `svmtrain`.

## Example

**1** Load sample data.

```
load fisheriris

data = [meas(:,1), meas(:,2)];
```

**2** Extract the Setosa class.

```
groups = ismember(species,'setosa');
```

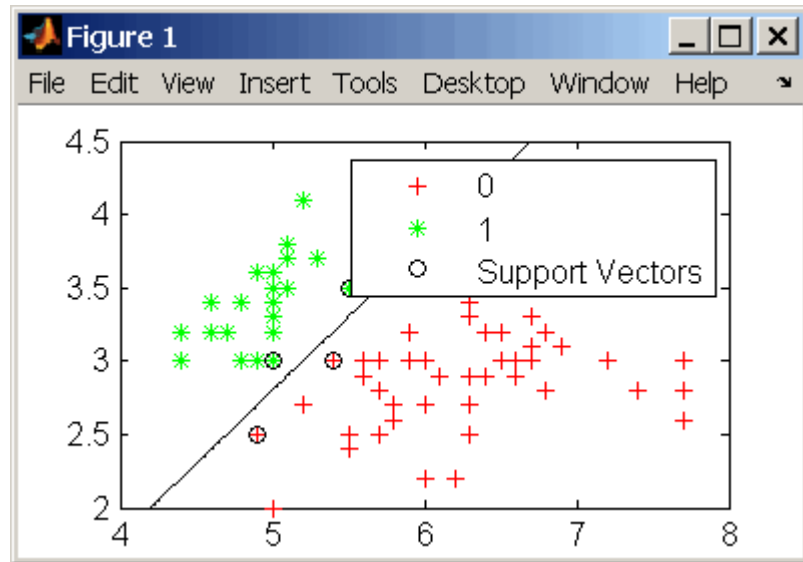
**3** Randomly select training and test sets

```
[train, test] = crossvalind('holdOut',groups);
cp = classperf(groups);
```

# svmclassify

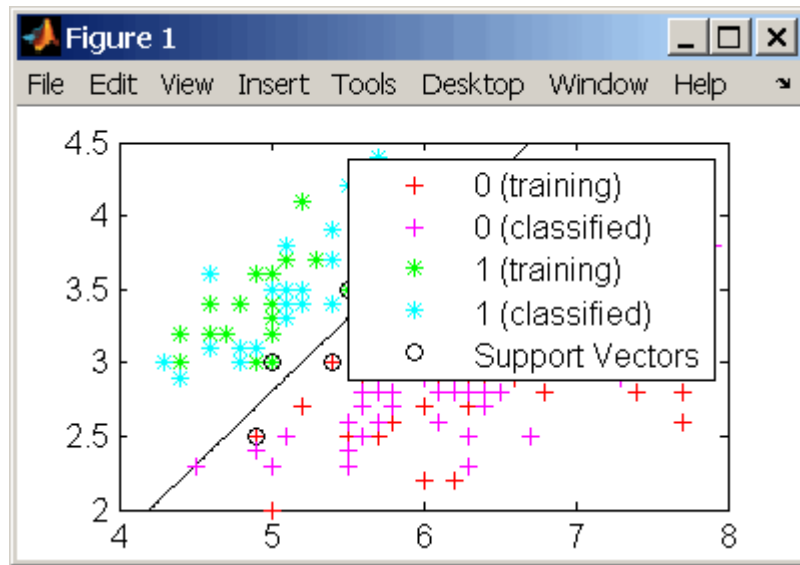
4 Use a linear support vector machine classifier.

```
svmStruct = svmtrain(data(train,:),groups(train),...  
                    'showplot',true);
```



```
classes = svmclassify(svmStruct,data(test,:), 'showplot',true);
```





**5** See how well the classifier performed.

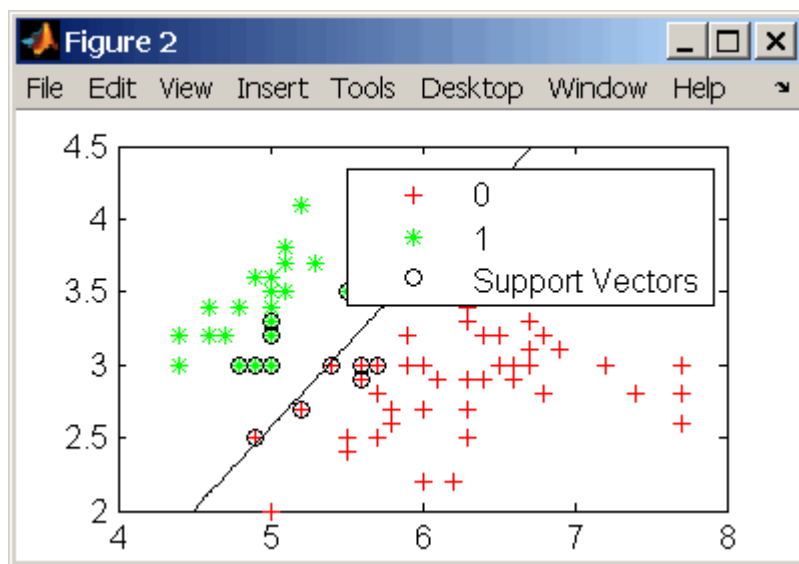
```
classperf(cp,classes,test);
cp.CorrectRate
```

```
ans =
    0.9867
```

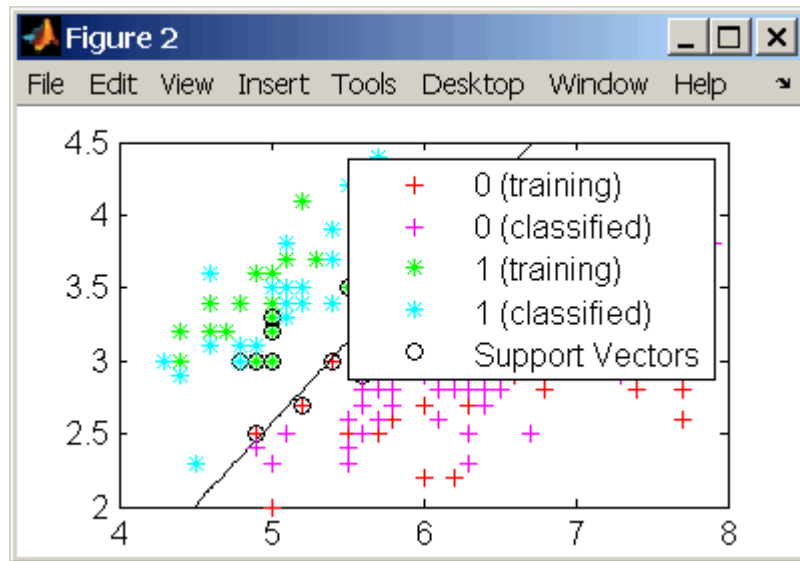
**6** If you have the Optimization Toolbox you can use a 1-norm soft margin support vector machine classifier.

```
figure
svmStruct = svmtrain(data(train,:),groups(train),...
                    'showplot',true,'boxconstraint',1);
```

# svmclassify



```
classes = svmclassify(svmStruct,data(test,:), 'showplot', true);
```



7 See how well the classifier performed.

```
classperf(cp,classes,test);  
cp.CorrectRate
```

```
ans =  
    0.9933
```

## 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., Vandewalle, J., Least Squares Support Vector Machines, World Scientific, Singapore, 2002.
- [3] Scholkopf, B., 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 `knnclassify`, `classperf`, `crossvalind`, `svmtrain`

Statistical Toolbox functions `classify`

Optimization Toolbox function `quadprog`

**Purpose** Train support vector machine classifier

**Syntax**

```
SVMStruct = svmtrain(Training, Group)
svmtrain(..., 'PropertyName', PropertyValue,...)
svmtrain(..., 'Kernel_Function', Kernel_FunctionValue)
svmtrain(..., 'RBF_Sigma', RBFSigmaValue)
svmtrain(..., 'Polyorder', PolyorderValue)
svmtrain(..., 'Mlp_Params', Mlp_ParamsValue)
svmtrain(..., 'Method', MethodValue)
svmtrain(..., 'QuadProg_Opts', QuadProg_OptsValue)
svmtrain(..., 'BoxConstraint', BoxConstraintValue)
svmtrain(..., 'Autoscale', AutoscaleValue)
svmtrain(..., 'ShowPlot', ShowPlotValue)
```

## Arguments

<i>Training</i>	Matrix of training data.
<i>Group</i>	Numeric vector, string array, or cell array of strings for classifying data in <i>Training</i> into two groups. It has the same length as <i>Training</i> and defines two groups by specifying the group to which each corresponding row in <i>Training</i> belongs.
<i>SVMStruct</i>	<i>SVMStruct</i> contains information about the trained classifier that <code>svmclassify</code> uses for classification. It also contains the support vectors in the field <code>SupportVector</code> .

## Description

`SVMStruct = svmtrain(Training, Group)` trains a support vector machine classifier (SVM) using data (*Training*) 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*.

`svmtrain(..., 'PropertyName', PropertyValue,...)` defines optional properties using property name/value pairs.

`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'	Linear kernel or dot product. Default value
'quadratic'	Quadratic kernel
'polynomial'	Polynomial kernel (default order 3)
'rbf'	Gaussian radial basis function kernel
'mlp'	Multilayer perceptron kernel (default scale 1)
Function handle	A handle to a kernel function specified using @, for example @kfun, or an anonymous function

A kernel function must be of the form

```
function K = kfun(U, V)
```

The returned value *K* is a matrix of size *m*-by-*n*, where *U* and *V* have *m* and *n* rows respectively. 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)
```

`svmtrain(..., 'RBF_Sigma', RBFSigmaValue)` specifies the scaling factor, *sigma*, in the radial basis function kernel. The default is 1. *RBFSigmaValue* must be a positive number.

`svmtrain(..., 'Polyorder', PolyorderValue)` specifies the order of a polynomial kernel. The default order is 3.

`svmtrain(..., 'Mlp_Params', Mlp_ParamsValue)` specifies the parameters of the multilayer perceptron (mlp) kernel as a vector with two parameters [ $p_1$ ,  $p_2$ ].  $K = \tanh(p_1 * U * V + p_2)$ ,  $p_1 > 0$ , and  $p_2 < 0$ . Default values are  $p_1 = 1$  and  $p_2 = -1$ .

`svmtrain(..., 'Method', MethodValue)` specifies the method to find the separating hyperplane. The options are

'QP'      Quadratic programming (requires the Optimization Toolbox)

'LS'      Least-squares method

---

**Note** If you installed the Optimization Toolbox, the 'QP' method is the default. If not, the only available method is 'LS'.

---

`svmtrain(..., 'QuadProg_Opts', QuadProg_OptsValue)` allows you to pass an options structure, created using `optimset`, to the Optimization Toolbox function `quadprog` when using the 'QP' method. See the `optimset` reference page for more details.

`svmtrain(..., 'BoxConstraint', BoxConstraintValue)` allows you to set box constraints for the two-norm soft margin. It can be supplied either as a strictly positive numeric scalar or as an array of strictly positive values of the same length as *Training*. If it is supplied as a scalar value, it is automatically rescaled by  $N/(2*N_1)$  for the data points of group one and by  $N/(2*N_2)$  for the data points of group two.  $N_1$  is the number of elements in group one,  $N_2$  is the number of elements in group two, and  $N = N_1 + N_2$ . This rescaling is done to take into account unbalanced groups, that is cases where  $N_1$  and  $N_2$  have very different values. If the box constraints are supplied as an array, then each array element is taken as a box constraint for the data point with the same index. The default value for the box constraint is a

scalar value of  $\frac{1}{\sqrt{\epsilon}}$ , which is appropriate only for separable data. In realistic applications, an optimal value for the box constraint should be determined for each classification problem using cross validation.

`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 false.

`svmtrain(..., 'ShowPlot', ShowPlotValue)`, when using two-dimensional data and *ShowPlotValue* is true, creates a plot of the grouped data and plots the separating line for the classifier.

## Memory Usage and Out of Memory Error

When the function `svmtrain` 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  $8 \times (n+1)^2$  bytes of contiguous memory. Without that size of contiguous memory, MATLAB displays an "out of memory" message.

Training an SVM with a large number of samples leads the function to run slowly, and require a large amount of memory. If you run out of memory or the optimization step is taking a very long time, try using a smaller number of samples and use cross validation to test the performance of the classifier.

## Example

1 Load sample data.

```
load fisheriris  
  
data = [meas(:,1), meas(:,2)];
```

2 Extract the Setosa class.

```
groups = ismember(species, 'setosa');
```

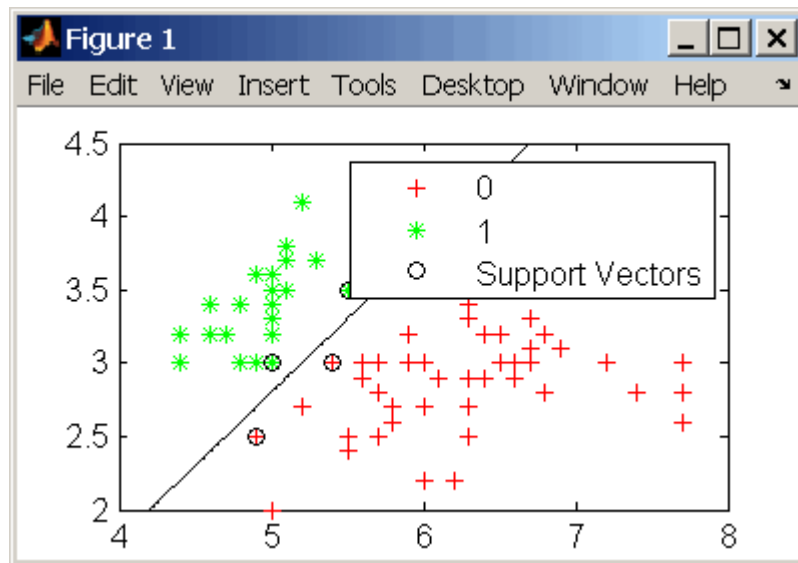
3 Randomly select training and test sets



```
[train, test] = crossvalind('holdOut',groups);  
cp = classperf(groups);
```

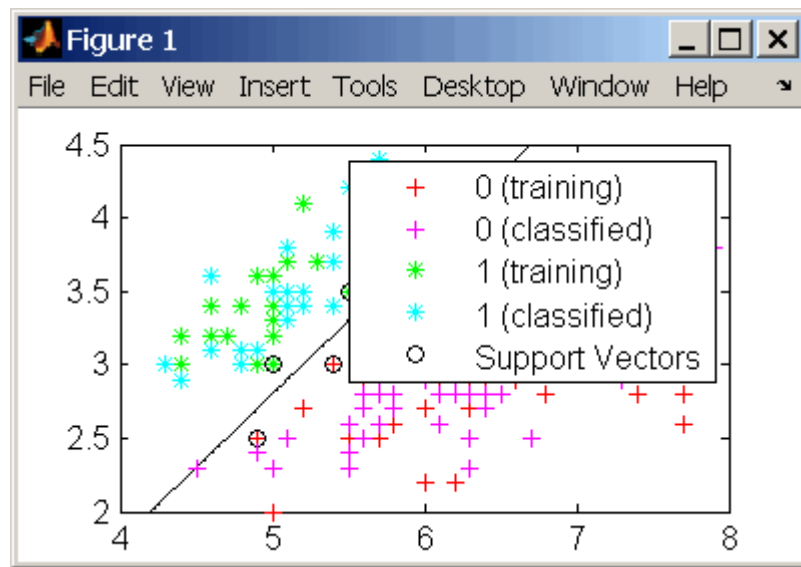
**4** Use a linear support vector machine classifier.

```
svmStruct = svmtrain(data(train,:),groups(train),'showplot',true);
```



```
classes = svmclassify(svmStruct,data(test,:), 'showplot',true);
```

# svmtrain



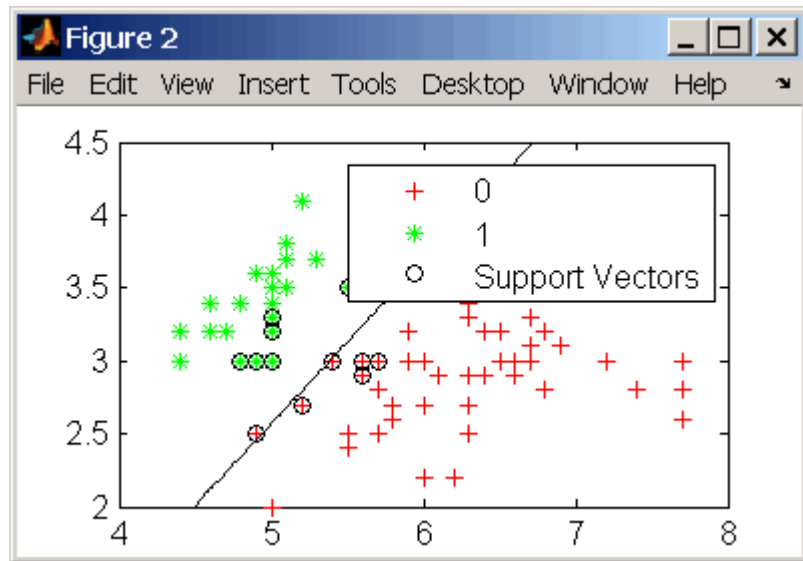
5 See how well the classifier performed.

```
classperf(cp,classes,test);  
cp.CorrectRate
```

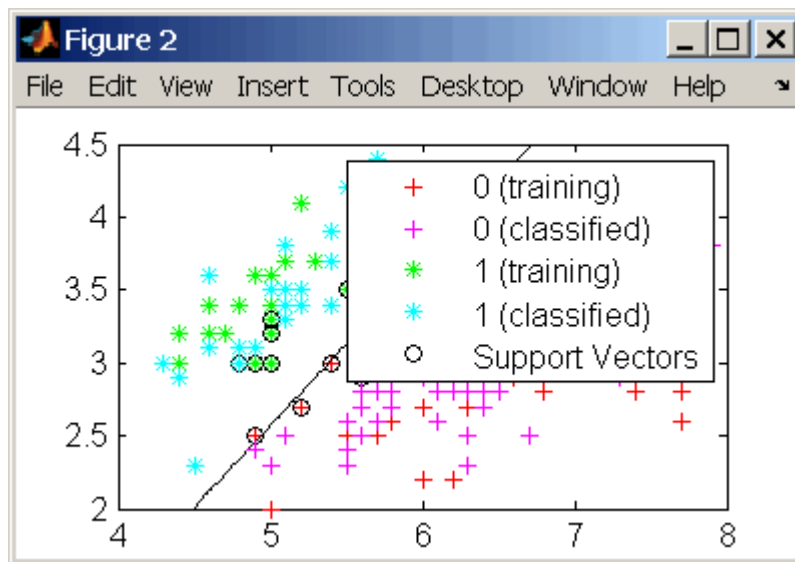
```
ans =  
    0.9867
```

6 If you have the Optimization Toolbox you can use a 1-norm soft margin support vector machine classifier.

```
figure  
svmStruct = svmtrain(data(train,:),groups(train),...  
                    'showplot',true,'boxconstraint',1);
```



```
classes = svmclassify(svmStruct,data(test,:), 'showplot', true);
```



7 See how well the classifier performed.

```
classperf(cp,classes,test);  
cp.CorrectRate
```

```
ans =  
    0.9933
```

## 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., Vandewalle, J., Least Squares Support Vector Machines, World Scientific, Singapore, 2002.
- [3] Scholkopf, B., 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 `knnclassify`, `svmclassify`

Statistics Toolbox functions `classify`

Optimization Toolbox functions `optimset`, `quadprog`

# swalign

---

**Purpose**                      Locally align two sequences using Smith-Waterman algorithm

**Syntax**

```
swalign(Seq1, Seq2)
[Score, Alignment] = swalign(Seq1, Seq2)
[Score, Alignment, Start] = swalign(Seq1, Seq2)
swalign(..., 'PropertyName', PropertyValue,...)
swalign(..., 'Alphabet', AlphabetValue)
swalign(..., 'ScoringMatrix', ScoringMatrixValue)
swalign(..., 'Scale', ScaleValue)
swalign(..., 'GapOpen', GapOpenValue)
swalign(..., 'ExtendGap', ExtendGapValue)
swalign(..., 'Showscore', ShowscoreValue)
```

## Arguments

<i>Seq1, Seq2</i>	Nucleotide or amino acid sequences. Enter a character string or vector of integers. You can also enter a structure with the field <i>Sequence</i> .
<i>AlphabetValue</i>	Property to select an amino acid or nucleotide sequences. Enter either 'AA' or 'NT'. The default value is 'AA'.
<i>ScoringMatrixValue</i>	Property to select the scoring matrix. Enter the name of a scoring matrix. Values are 'PAM40', 'PAM250', DAYHOFF, GONNET, 'BLOSUM30' increasing by 5 to 'BLOSUM90', or 'BLOSUM62', or 'BLOSUM100'.  The default value when <i>AlphabetValue</i> = 'aa' is 'BLOSUM50', while the default value when <i>AlphabetValue</i> = 'nt' is nuc44.
<i>ScaleValue</i>	Property to specify a scaling factor for a scoring matrix.

<i>GapOpenValue</i>	Property to specify the gap open penalty. Enter an integer for the gap penalty. Default value is 8.
<i>ExtendGapValue</i>	Property to specify the extended gap open penalty. Enter an integer for the extended gap penalty. The default value equals the GapOpen value.
<i>ShowscoreValue</i>	Property to control displaying the scoring space and the winning path. Enter either true or false. The default value is false.

## Description

`swalign(Seq1, Seq2)` returns the alignment score in bits for the optimal alignment. The scale factor used to calculate the score is provided by the scoring matrix. If this is not defined, then `swalign` returns the raw score.

`[Score, Alignment] = swalign(Seq1, Seq2)` returns a 3-by-n character array showing the two sequences and the local alignment between them. Amino acids that match are indicated with the symbol |, while related amino acids (nonmatches with a positive scoring matrix value) are indicated with the symbol :.

`[Score, Alignment, Start] = swalign(Seq1, Seq2)` returns a 2-by-1 vector with the starting point indices where the alignment begins for each sequence.

`swalign(..., 'PropertyName', PropertyValue, ...)` defines optional properties using property name/value pairs.

`swalign(..., 'Alphabet', AlphabetValue)` specifies whether the sequences are amino acids ('AA') or nucleotides ('NT'). The default value is 'AA'.

`swalign(..., 'ScoringMatrix', ScoringMatrixValue)` specifies the scoring matrix to use for the alignment. The default is 'blosum50' for Alphabet = 'AA' or 'NUC44' for Alphabet = NT.

`swalign(..., 'Scale', ScaleValue)` indicates the scale factor of the scoring matrix to return the score using arbitrary units. If the scoring matrix also provides a scale factor, then both are used.

`swalign(..., 'GapOpen', GapOpenValue)` specifies the penalty for opening a gap in the alignment. The default gap open penalty is 8.

`swalign(..., 'ExtendGap', ExtendGapValue)` specifies the penalty for extending a gap in the alignment. If `ExtendGap` is not specified, then extensions to gaps are scored with the same value as `GapOpen`.

`swalign(..., 'Showscore', ShowscoreValue)` displays the scoring space and the winning path.

Scores are 'raw' scores which mean the final score is an accumulation of using the scoring matrix values at each position of the alignment. Accumulation means that it is the sum of the amino acid matches (including the gap penalties). If the provided scoring matrix (or the one used by default) has a `Scale` entry, then the score is returned in 'bits'.

## Examples

Return the score in bits and the local alignment using the default `ScoringMatrix('BLOSUM50')` and default values for the `GapOpen` and `ExtendGap` values.

```
[Score, Alignment] = swalign('VSPAGMASGYD', 'IPGKASYD')
```

```
Score =  
      8.6667
```

```
Alignment =  
PAGMASGYD  
| | || ||  
P-GKAS-YD
```

Align two amino sequences using a specified scoring matrix ('pam250') and a gap open penalty of 5.

```
[Score, Alignment] = swalign('HEAGAWGHEE', 'PAWHEAE', ...  
                             'ScoringMatrix', 'pam250', ...
```



```
'GapOpen',5)
```

```
Score =
      8
Alignment =
GAWGHE
: || ||
PAW-HE
```

Align two amino sequences and return the Score in nat units (nats).

```
[Score, Alignment] = swalign('HEAGAWGHEE', 'PAWHEAE', ...
                             'Scale', log(2))
```

```
Score =
      6.4694
Alignment =
AWGHE
|| ||
AW-HE
```

## References

- [1] Durbin R, Eddy S, Krogh A, Mitchison G (1998), *Biological Sequence Analysis*. Cambridge University Press.
- [2] Smith T, Waterman M (1981), "Identification of common molecular subsequences", *Journal Molecular Biology*, 147:195-197.

## See Also

Bioinformatics Toolbox functions `blosum`, `nt2aa`, `nwalign`, `pam`, `seqdotplot`, `showalignment`

# traceplot

---

**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, T.  
`traceplot(A, C, G, T)` creates a trace plot from data in vectors A, C, G, T.  
`h = traceplot()` returns a structure with the handles of the lines corresponding to A, C, G, T.

**Examples**  

```
tstruct = scfread('sample.scf');  
traceplot(tstruct)
```

**See Also** Bioinformatics Toolbox

- `function` — `scfread`

**Purpose** Draw figure from biograph object

**Syntax**  
`view(BGobj)`  
`BGobjHandle = view(BGobj)`

**Arguments**

<code>BGobj</code>	Biograph object created with the function <code>biograph</code> .
--------------------	---

**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])
```

# view (biograph)

---

## See Also

Bioinformatics Toolbox

- function — biograph (object constructor)
- biograph object methods — dolayout, getancestors, getdescendants, getedgesbynodeid, getnodesbyid, getrelatives, view

MATLAB

- functions — get, set

**Purpose** View phylogenetic tree

**Syntax** `view(Tree)`  
`view(Tree, IntNodes)`

## Arguments

<i>Tree</i>	Phylogenetic tree (phytree object) created with the function <code>phytree</code> .
<i>IntNodes</i>	Nodes from the phytree object to initially display in the <i>Tree</i> .

## 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

```
tr = phytreeread('pf00002.tree')
view(tree)
```

## See Also

Bioinformatics Toolbox

- functions — `phytree` (object constructor), `phytreeread`, `phytreetool`, `seqlinkage`, `seqneighjoin`
- phytree object method — `plot`

# weights (phytree)

---

**Purpose** Calculate weights for phylogenetic tree

**Syntax** `W = weights(Tree)`

**Arguments**

<code>Tree</code>	Phylogenetic tree (phytree object) created with the function <code>phytree</code> .
-------------------	---

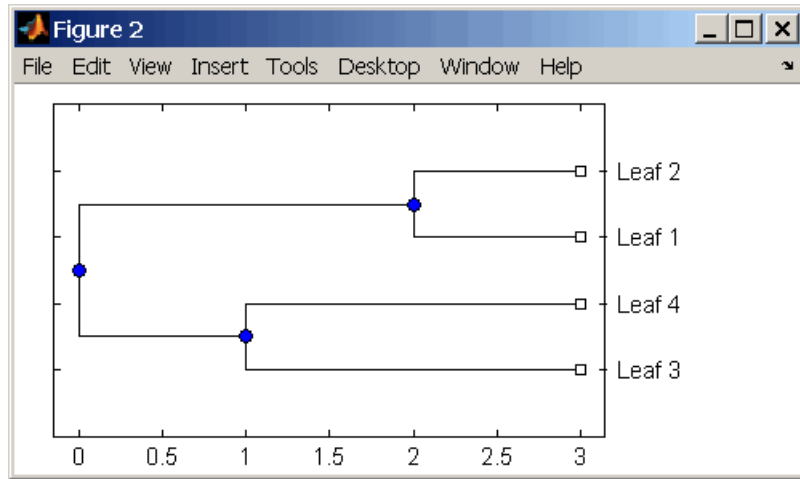
**Description** `W = weights(Tree)` calculates branch proportional weights for every leaf in a tree (`Tree`) using the Thompson-Higgins-Gibson method. The distance of every segment of the tree is adjusted by dividing it by the number of leaves it contains. The sequence weights are the result of normalizing 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.

## weights (phytree)

---

### See Also

Bioinformatics Toolbox

- functions — `multialign`, `phytree` (object constructor), `profalign`, `seqlinkage`



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