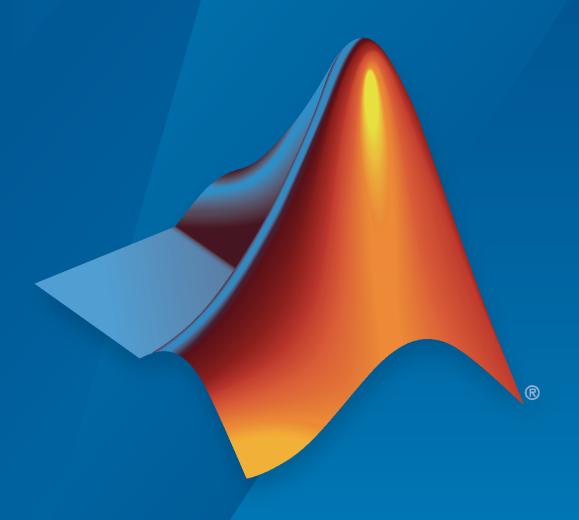
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7

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Contents

	Matrices and Arr
Creating, Concatenating, and Expanding Matric	ces
Removing Rows or Columns from a Matrix	
Reshaping and Rearranging Arrays	
Multidimensional Arrays	
Array Indexing	
	Linear Alge
Matrices in the MATLAB Environment	
Adding and Subtracting Matrices Vector Products and Transpose	
Multiplying Matrices	
Matrix Inverse	
Vector and Matrix Norms Using Multithreaded Computation with Linear	
Systems of Linear Equations	
Computational Considerations	
General Solution	
Overdetermined Systems	
Underdetermined Systems	
Solving for Several Right-Hand Sides	
Iterative Methods	
Multithreaded Computation	
Factorizations	
Introduction	
Cholesky Factorization	
QR Factorization	
Using Multithreaded Computation for Factorize	

Powers and Exponentials	2-26
Eigenvalues	2-30
Eigenvalue Decomposition	2-30
Multiple Eigenvalues	2-30
Schur Decomposition	2-31
Schul Decomposition	2-31
ingular Values	2-33
Batched SVD Calculation	2-35
Low-Rank SVD Approximations	2-35
ADACK : MATI AD	2.25
APACK in MATLAB	2-37
A Brief History	2-37
atrix Exponentials	2-38
raphical Comparison of Exponential Functions	2-42
rupineur computison of Exponential Panetions	2-12
Basic Matrix Operations	2-46
Determine Whether Matrix Is Symmetric Positive Definite	2-54
mage Compression with Low-Rank SVD	2-56
Random Num	bers
Random Num	bers
Why Do Random Numbers Repeat After Startup?	3-2
Why Do Random Numbers Repeat After Startup?	3-2
Why Do Random Numbers Repeat After Startup?	3-2 3-3 3-3
Why Do Random Numbers Repeat After Startup? Create Arrays of Random Numbers Random Number Functions Random Number Generators	3-2 3-3 3-3 3-4
Why Do Random Numbers Repeat After Startup?	3-2 3-3 3-3 3-4
Why Do Random Numbers Repeat After Startup? Create Arrays of Random Numbers Random Number Functions Random Number Generators Random Number Data Types	3-2 3-3 3-3 3-4 3-4
Why Do Random Numbers Repeat After Startup? Create Arrays of Random Numbers Random Number Functions Random Number Generators Random Number Data Types Random Numbers Within a Specific Range	3-2 3-3 3-3 3-4 3-4
Why Do Random Numbers Repeat After Startup? Create Arrays of Random Numbers Random Number Functions Random Number Generators Random Number Data Types Random Numbers Within a Specific Range	3-2 3-3 3-3 3-4 3-4
Why Do Random Numbers Repeat After Startup? Create Arrays of Random Numbers Random Number Functions Random Number Generators Random Number Data Types Random Numbers Within a Specific Range Random Integers	3-2 3-3 3-3 3-4 3-4
Why Do Random Numbers Repeat After Startup? Create Arrays of Random Numbers Random Number Functions Random Number Generators Random Number Data Types Random Numbers Within a Specific Range Random Integers	3-2 3-3 3-3 3-4 3-6 3-7
Why Do Random Numbers Repeat After Startup? Create Arrays of Random Numbers Random Number Functions Random Number Generators Random Number Data Types Random Numbers Within a Specific Range Random Integers Random Numbers from Normal Distribution with Specific Mean and Variance	3-2 3-3 3-3 3-4 3-6 3-7
Why Do Random Numbers Repeat After Startup? Create Arrays of Random Numbers Random Number Functions Random Number Generators Random Number Data Types Candom Numbers Within a Specific Range Candom Integers Candom Numbers from Normal Distribution with Specific Mean and Variance	3-2 3-3 3-3 3-4 3-6 3-7
Treate Arrays of Random Numbers Random Number Functions Random Number Generators Random Number Data Types andom Numbers Within a Specific Range andom Integers andom Numbers from Normal Distribution with Specific Mean and Variance andom Numbers Within a Sphere enerate Random Numbers That Are Repeatable	3-2 3-3 3-3 3-4 3-4 3-6 3-7 3-8 3-9 3-11
Why Do Random Numbers Repeat After Startup? Create Arrays of Random Numbers Random Number Functions Random Number Generators Random Number Data Types Random Numbers Within a Specific Range Random Integers Random Numbers from Normal Distribution with Specific Mean and Variance Random Numbers Within a Sphere Generate Random Numbers That Are Repeatable Specify the Seed	3-2 3-3 3-3 3-4 3-6 3-7 3-8 3-9 3-11 3-11
Why Do Random Numbers Repeat After Startup? Create Arrays of Random Numbers Random Number Functions Random Number Generators Random Number Data Types Random Numbers Within a Specific Range Random Integers Random Numbers from Normal Distribution with Specific Mean and Variance Random Numbers Within a Sphere Generate Random Numbers That Are Repeatable	3-2 3-3 3-3 3-4 3-6 3-7 3-8 3-9 3-11 3-11
Why Do Random Numbers Repeat After Startup? Create Arrays of Random Numbers Random Number Functions Random Number Generators Random Number Data Types Random Numbers Within a Specific Range Random Integers Random Numbers from Normal Distribution with Specific Mean and Variance Random Numbers Within a Sphere Generate Random Numbers That Are Repeatable Specify the Seed Save and Restore the Generator Settings	3-2 3-3 3-3 3-4 3-6 3-7 3-8 3-9 3-11 3-11 3-12
Why Do Random Numbers Repeat After Startup? Create Arrays of Random Numbers Random Number Functions Random Number Generators Random Number Data Types Random Numbers Within a Specific Range Random Integers Random Numbers from Normal Distribution with Specific Mean and Variance Random Numbers Within a Sphere Senerate Random Numbers That Are Repeatable Specify the Seed Save and Restore the Generator Settings	3-2 3-3 3-3 3-4 3-6 3-7 3-8 3-9 3-11 3-11
Why Do Random Numbers Repeat After Startup? Create Arrays of Random Numbers Random Number Functions Random Number Generators Random Number Data Types Random Numbers Within a Specific Range Random Integers Random Numbers from Normal Distribution with Specific Mean and Variance Random Numbers Within a Sphere Generate Random Numbers That Are Repeatable Specify the Seed	3-2 3-3 3-3 3-4 3-6 3-7 3-8 3-9 3-11 3-11 3-12

Creating and Controlling a Random Number Stream	
Choosing a Random Number Generator	
Configuring a Stream	
Restore State of Random Number Generator to Reproduce Output	
Multiple Streams	
Replace Discouraged Syntaxes of rand and randn	
Description of the Discouraged Syntaxes	
Description of Replacement Syntaxes	
Replacement Syntaxes for Initializing the Generator with a State Vector	
If You Are Unable to Upgrade from Discouraged Syntax	
Controlling Random Number Generation	
Sparse Mat	t:
Memory Management	
Computational Efficiency	
Computational Efficiency	•
Computational Efficiency Constructing Sparse Matrices Creating Sparse Matrices Importing Sparse Matrices Accessing Sparse Matrices	
Computational Efficiency Constructing Sparse Matrices Creating Sparse Matrices Importing Sparse Matrices Accessing Sparse Matrices Nonzero Elements	
Computational Efficiency Constructing Sparse Matrices Creating Sparse Matrices Importing Sparse Matrices Accessing Sparse Matrices Nonzero Elements Indices and Values	•
Computational Efficiency Constructing Sparse Matrices Creating Sparse Matrices Importing Sparse Matrices Accessing Sparse Matrices Nonzero Elements	•
Constructing Sparse Matrices Creating Sparse Matrices Importing Sparse Matrices Importing Sparse Matrices Accessing Sparse Matrices Nonzero Elements Indices and Values Indexing in Sparse Matrix Operations Visualizing Sparse Matrices Sparse Matrix Operations	•
Constructing Sparse Matrices Creating Sparse Matrices Importing Sparse Matrices Importing Sparse Matrices Accessing Sparse Matrices Nonzero Elements Indices and Values Indexing in Sparse Matrix Operations Visualizing Sparse Matrices Sparse Matrix Operations Efficiency of Operations	•
Constructing Sparse Matrices Creating Sparse Matrices Importing Sparse Matrices Importing Sparse Matrices Accessing Sparse Matrices Nonzero Elements Indices and Values Indexing in Sparse Matrix Operations Visualizing Sparse Matrices Sparse Matrix Operations Efficiency of Operations Permutations and Reordering	•
Constructing Sparse Matrices Creating Sparse Matrices Importing Sparse Matrices Importing Sparse Matrices Accessing Sparse Matrices Nonzero Elements Indices and Values Indexing in Sparse Matrix Operations Visualizing Sparse Matrices Sparse Matrix Operations Efficiency of Operations Permutations and Reordering Factoring Sparse Matrices	•
Constructing Sparse Matrices Creating Sparse Matrices Importing Sparse Matrices Importing Sparse Matrices Accessing Sparse Matrices Nonzero Elements Indices and Values Indexing in Sparse Matrix Operations Visualizing Sparse Matrices Sparse Matrix Operations Efficiency of Operations Permutations and Reordering Factoring Sparse Matrices Eigenvalues and Singular Values	
Constructing Sparse Matrices Creating Sparse Matrices Importing Sparse Matrices Importing Sparse Matrices Accessing Sparse Matrices Nonzero Elements Indices and Values Indexing in Sparse Matrix Operations Visualizing Sparse Matrices Sparse Matrix Operations Efficiency of Operations Permutations and Reordering Factoring Sparse Matrices	
Constructing Sparse Matrices Creating Sparse Matrices Importing Sparse Matrices Importing Sparse Matrices Accessing Sparse Matrices Nonzero Elements Indices and Values Indexing in Sparse Matrix Operations Visualizing Sparse Matrices Sparse Matrix Operations Efficiency of Operations Permutations and Reordering Factoring Sparse Matrices Eigenvalues and Singular Values	
Constructing Sparse Matrices Creating Sparse Matrices Importing Sparse Matrices Accessing Sparse Matrices Nonzero Elements Indices and Values Indexing in Sparse Matrix Operations Visualizing Sparse Matrices Sparse Matrix Operations Efficiency of Operations Permutations and Reordering Factoring Sparse Matrices Eigenvalues and Singular Values References	•
Constructing Sparse Matrices Creating Sparse Matrices Importing Sparse Matrices Importing Sparse Matrices Accessing Sparse Matrices Nonzero Elements Indices and Values Indexing in Sparse Matrix Operations Visualizing Sparse Matrices Sparse Matrix Operations Efficiency of Operations Permutations and Reordering Factoring Sparse Matrices Eigenvalues and Singular Values References Finite Difference Laplacian	•

	Iterative Methods for Linear Systems	4-56
	Direct vs. Iterative Methods	4-56
	Generic Iterative Algorithm	4-5 7
	Summary of Iterative Methods	4-57
	Choosing an Iterative Solver	4-59
	Preconditioners	4-60
	Equilibration and Reordering	4-62
	Using Linear Operators Instead of Matrices	4-64 4-64
	References	4-04
	Graph and Network Algorit	hmo
	Oraph and Network Algorit	,111115
5		
	Directed and Undirected Graphs	5-2
	What Is a Graph?	5-2
	Creating Graphs	5-5
	Graph Node IDs	5-8 5-8
	Modify or Query Existing Graph	3-8
	Modify Nodes and Edges of Existing Graph	5-10
	Product and Edges of Emisting Graph	5 10
	Add Graph Node Names, Edge Weights, and Other Attributes	5-13
	Graph Plotting and Customization	5-1 7
	Visualize Breadth-First and Depth-First Search	5-28
	Partition Graph with Laplacian Matrix	5-33
	Fartition Graph with Laplacian Matrix	J - JJ
	Add Node Properties to Graph Plot Data Tips	5-36
	· · · · · · · · · · · · · · · · · · ·	
	Build Watts-Strogatz Small World Graph Model	5-41
	Use PageRank Algorithm to Rank Websites	5-48
	Libilo and National Elem	
	Label Graph Nodes and Edges	5-55
	Functions of One Vari	ahla
C [Tunctions of one vari	anie
D		
	Create and Evaluate Polynomials	6-2
	Roots of Polynomials	6-4
	Numeric Roots	6-4
	Roots Using Substitution	6-4
	Roots in a Specific Interval	6-5
	Symbolic Roots	6-7
		- •
	Integrate and Differentiate Polynomials	6-9

	Computational Geom
Twi	angulation Representations
111	2-D and 3-D Domains
	Triangulation Matrix Format
	Querying Triangulations Using the triangulation Class
Wo	orking with Delaunay Triangulations
	Definition of Delaunay Triangulation
	Creating Delaunay Triangulations
Cr	eating and Editing Delaunay Triangulations
Sp	atial Searching
Vo	ronoi Diagrams
	Plot 2-D Voronoi Diagram and Delaunay Triangulation
Туј	pes of Region Boundaries
	Convex Hulls vs. Nonconvex Polygons
	Alpha Shapes
Co	mputing the Convex Hull
	Computing the Convex Hull Using convhull and convhulln
	Convex Hull Computation Using the delaunayTriangulation Class Convex Hull Computation Using alphaShape
	Interpola
Gr	idded and Scattered Sample Data
	Interpolation versus Curve Fitting

Inte	rpolation of 2-D Selections in 3-D Grids
Inte	rpolating Scattered Data
	Scattered Data
	scatteredInterpolant Class
	Interpolating Scattered Data Using the scatteredInterpolant Class
	Interpolation of Complex Scattered Data
	Addressing Problems in Scattered Data Interpolation
Inte	rpolation Using a Specific Delaunay Triangulation
	Nearest-Neighbor Interpolation Using a delaunayTriangulation Query
	Linear Interpolation Using a delaunayTriangulation Query
Extr	apolating Scattered Data
	Factors That Affect the Accuracy of Extrapolation
	Danie Danie De Courseil una i mery Cumptou Soutiereu Duta
	Extrapolation of 3-D Data
No	nalize Data with Differing Magnitudes
TIUP	nalize Data with Differing Magnitudes
Resa	mple Image with Gridded Interpolation
	Optimiz
	Optimiz
Onti	
Opti	mizing Nonlinear Functions
Opti	mizing Nonlinear Functions Minimizing Functions of One Variable
Opti	mizing Nonlinear Functions Minimizing Functions of One Variable Minimizing Functions of Several Variables
Opti	mizing Nonlinear Functions Minimizing Functions of One Variable Minimizing Functions of Several Variables Maximizing Functions
Opti	mizing Nonlinear Functions Minimizing Functions of One Variable Minimizing Functions of Several Variables Maximizing Functions fminsearch Algorithm
-	mizing Nonlinear Functions Minimizing Functions of One Variable Minimizing Functions of Several Variables Maximizing Functions fminsearch Algorithm Reference
Curv	mizing Nonlinear Functions Minimizing Functions of One Variable Minimizing Functions of Several Variables Maximizing Functions fminsearch Algorithm Reference The Fitting via Optimization
Curv	mizing Nonlinear Functions Minimizing Functions of One Variable Minimizing Functions of Several Variables Maximizing Functions fminsearch Algorithm Reference The Fitting via Optimization Optimization Options
Curv	mizing Nonlinear Functions Minimizing Functions of One Variable Minimizing Functions of Several Variables Maximizing Functions fminsearch Algorithm Reference re Fitting via Optimization Optimization Options How to Set Options
Curv	mizing Nonlinear Functions Minimizing Functions of One Variable Minimizing Functions of Several Variables Maximizing Functions fminsearch Algorithm Reference The Fitting via Optimization Optimization Options
Curv	mizing Nonlinear Functions Minimizing Functions of One Variable Minimizing Functions of Several Variables Maximizing Functions fminsearch Algorithm Reference re Fitting via Optimization Optimization Options How to Set Options Options Table
- Curv Set (mizing Nonlinear Functions Minimizing Functions of One Variable Minimizing Functions of Several Variables Maximizing Functions fminsearch Algorithm Reference Fitting via Optimization Optimization Options How to Set Options Options Table Tolerances and Stopping Criteria
Curv Set (Opti	mizing Nonlinear Functions Minimizing Functions of One Variable Minimizing Functions of Several Variables Maximizing Functions fminsearch Algorithm Reference Fitting via Optimization Optimization Options How to Set Options Options Table Tolerances and Stopping Criteria Output Structure mization Solver Iterative Display
Curv Set (Opti Opti	mizing Nonlinear Functions Minimizing Functions of One Variable Minimizing Functions of Several Variables Maximizing Functions fminsearch Algorithm Reference Pe Fitting via Optimization Optimization Options How to Set Options Options Table Tolerances and Stopping Criteria Output Structure mization Solver Iterative Display mization Solver Output Functions
Curv Set (Opti Opti	mizing Nonlinear Functions Minimizing Functions of One Variable Minimizing Functions of Several Variables Maximizing Functions fminsearch Algorithm Reference Fitting via Optimization Optimization Options How to Set Options Options Table Tolerances and Stopping Criteria Output Structure mization Solver Iterative Display
Curv Set (Opti Opti	How to Set Options Options Table Tolerances and Stopping Criteria Output Structure mization Solver Iterative Display mization Solver Output Functions What Is an Output Function? Creating and Using an Output Function Structure of the Output Function
Curv Set (Opti	mizing Nonlinear Functions Minimizing Functions of One Variable Minimizing Functions of Several Variables Maximizing Functions fminsearch Algorithm Reference re Fitting via Optimization Optimization Options How to Set Options Options Table Tolerances and Stopping Criteria Output Structure mization Solver Iterative Display mization Solver Output Functions What Is an Output Function? Creating and Using an Output Function

. 0	
Optimization Solver Plot Functions	
What Is a Plot Function?	
Example: Plot Function	
Optimize Live Editor Task	
What Is the Optimize Live Editor Task?	
Minimize a Nonlinear Function of Seve	
Solve a Scalar Equation	
Optimization Troubleshooting and Tips	
	Function Ha
Parameterizing Functions	
Overview	
Parameterizing Using Nested Function Parameterizing Using Anonymous Fun	
Ondinama	DAGG -4 1 - 4
Orumary	Differential Equations (C
Choose an ODE Solver	
Choose an ODE Solver Ordinary Differential Equations	
Choose an ODE Solver	
Choose an ODE Solver	
Choose an ODE Solver Ordinary Differential Equations Types of ODEs	
Choose an ODE Solver Ordinary Differential Equations Types of ODEs Systems of ODEs Higher-Order ODEs Complex ODEs	
Choose an ODE Solver Ordinary Differential Equations Types of ODEs	
Choose an ODE Solver Ordinary Differential Equations Types of ODEs Systems of ODEs Higher-Order ODEs Complex ODEs Basic Solver Selection Summary of ODE Examples and Files	
Choose an ODE Solver Ordinary Differential Equations Types of ODEs Systems of ODEs Higher-Order ODEs Complex ODEs Basic Solver Selection Summary of ODE Examples and Files Summary of ODE Options	
Choose an ODE Solver Ordinary Differential Equations Types of ODEs Systems of ODEs Higher-Order ODEs Complex ODEs Basic Solver Selection Summary of ODE Examples and Files Summary of ODE Options Options Syntax	
Choose an ODE Solver Ordinary Differential Equations Types of ODEs Systems of ODEs Higher-Order ODEs Complex ODEs Basic Solver Selection Summary of ODE Examples and Files Summary of ODE Options	
Choose an ODE Solver Ordinary Differential Equations Types of ODEs Systems of ODEs Higher-Order ODEs Complex ODEs Basic Solver Selection Summary of ODE Examples and Files Summary of ODE Options Options Syntax Compatibility of Options with Each Sol Usage Examples	ver
Choose an ODE Solver Ordinary Differential Equations Types of ODEs Systems of ODEs Higher-Order ODEs Complex ODEs Basic Solver Selection Summary of ODE Examples and Files Summary of ODE Options Options Syntax Compatibility of Options with Each Sol Usage Examples	ver
Choose an ODE Solver Ordinary Differential Equations Types of ODEs Systems of ODEs Higher-Order ODEs Complex ODEs Basic Solver Selection Summary of ODE Examples and Files Summary of ODE Options Options Syntax Compatibility of Options with Each Sol Usage Examples ODE Event Location What is Event Location?	ver
Choose an ODE Solver Ordinary Differential Equations Types of ODEs Systems of ODEs Higher-Order ODEs Complex ODEs Basic Solver Selection Summary of ODE Examples and Files Summary of ODE Options Options Syntax Compatibility of Options with Each Sol Usage Examples What is Event Location? Writing an Event Function	ver
Choose an ODE Solver Ordinary Differential Equations Types of ODEs Systems of ODEs Higher-Order ODEs Complex ODEs Basic Solver Selection Summary of ODE Examples and Files Summary of ODE Options Options Syntax Compatibility of Options with Each Sol Usage Examples ODE Event Location What is Event Location? Writing an Event Function Event Information	ver
Choose an ODE Solver Ordinary Differential Equations Types of ODEs Systems of ODEs Higher-Order ODEs Complex ODEs Basic Solver Selection Summary of ODE Examples and Files Summary of ODE Options Options Syntax Compatibility of Options with Each Sol Usage Examples ODE Event Location What is Event Location? Writing an Event Function Event Information Limitations	ver
Choose an ODE Solver Ordinary Differential Equations Types of ODEs Systems of ODEs Higher-Order ODEs Complex ODEs Basic Solver Selection Summary of ODE Examples and Files Summary of ODE Options Options Syntax Compatibility of Options with Each Sol Usage Examples ODE Event Location What is Event Location? Writing an Event Function Event Information	ver
Choose an ODE Solver Ordinary Differential Equations Types of ODEs Systems of ODEs Higher-Order ODEs Complex ODEs Basic Solver Selection Summary of ODE Examples and Files Summary of ODE Options Options Syntax Compatibility of Options with Each Sol Usage Examples ODE Event Location What is Event Location? Writing an Event Function Event Information Limitations Simple Event Location: A Bouncing Ba	ver

	Solve Stiff ODEs	11-23
	Solve Differential Algebraic Equations (DAEs)	11-30 11-30
	Consistent Initial Conditions	11-31 11-31
	Imposing Nonnegativity	11-31
	Solve Robertson Problem as Semi-Explicit Differential Algebraic Equations	
	(DAEs)	11-32
	Nonnegative ODE Solution	11-35
	Troubleshoot Common ODE Problems	11-38
	Error Tolerances	11-38
	Problem Scale	11-39
	Solution Components	11-40
	Problem Type	11-42
	Differential Equations	11-43
	Solve Predator-Prey Equations	11-52
	Solve Equations of Motion for Baton Thrown into Air	11-56
	Solve ODE with Strongly State-Dependent Mass Matrix	11-62
	Solve Stiff Transistor Differential Algebraic Equation	11-75
	Solve System of ODEs with Multiple Initial Conditions	11-80
	Solve Celestial Mechanics Problem with High-Order Solvers	11-88
12 [Boundary Value Problems (E	BVPs)
	Solving Boundary Value Problems	12-2
	Boundary Conditions	12-2
	Initial Guess of Solution	12-3
	Finding Unknown Parameters	12-3
	Singular BVPs	12-4
	BVP Solver Selection	12-4
	Evaluating the Solution	12-5 12-6
	DVI Examples and thes	12-0
	Solve BVP with Two Solutions	12-8
	Solve BVP with Unknown Parameter	12-11
	Solve BVP Using Continuation	12-15
	Verify BVP Consistency Using Continuation	12-20

	Solve BVP with Singular Term	12-25
	Solve BVP with Multiple Boundary Conditions	12-29
13 [Partial Differential Equations (I	PDEs)
'	Solving Partial Differential Equations What Types of PDEs Can You Solve with MATLAB? Solving 1-D PDEs Example: The Heat Equation PDE Examples and Files	13-2 13-2 13-2 13-5 13-8
	Solve Single PDE	13-9
	Solve PDE with Discontinuity	13-16
	Solve PDE and Compute Partial Derivatives	13-23
	Solve System of PDEs	13-32
	Solve System of PDEs with Initial Condition Step Functions	13-39
1 <i>1</i> [Delay Differential Equations (I	DEs)
14	Solving Delay Differential Equations Constant Delay DDEs Time-Dependent and State-Dependent DDEs	14-2 14-2 14-2
	DDEs of Neutral Type	14-2 14-3 14-3 14-3 14-4
	DDE with Constant Delays	14-6
	DDE with State-Dependent Delays	14-10
	Cardiovascular Model DDE with Discontinuities	14-14
	DDE of Neutral Type	14-19

Numerical Integr	rati
Integration to Find Arc Length	1
Complex Line Integrals	1
Singularity on Interior of Integration Domain	
Analytic Solution to Integral of Polynomial	
Integration of Numeric Data	
Calculate Tangent Plane to Surface	1
	_
Fourier Trans	foi
Fourier Transforms	
Basic Spectral Analysis	1
Spectral Analysis Quantities	1
Noisy Signal	1
Audio Signal	1
Polynomial Interpolation Using FFT	1
FFT in Mathematics	1
Interpolate Asteroid Data	1
2-D Fourier Transforms	1
Two-Dimensional Fourier Transform	1
2-D Diffraction Pattern	1
Square Wave from Sine Waves	1
Analyzing Cyclical Data with FFT	1
Gate-Based Quantum Algor	it k
Gute-Duseu Quantum Aigor	101
Introduction to Quantum Computing	
Qubit	
Quantum Gate	1
Helper Functions	1
· F	-
Types of Quantum Gates	1
Creation Functions for SimpleGate Objects	1

Creation Functions for CompositeGate Objects	17-22
Local Quantum State Simulation	17-25
Create Circuit	17-25
Simulate Circuit	17-25
Display State Formula	17-26
Plot Possible States	17-27
Query Possible States	17 -2 7
Query Qubit State Probabilities	17-27
Simulate Quantum State Measurement	17-28
Run Quantum Circuit on Hardware Using AWS	17-29
Requirements	
Set Up Access to AWS	
Device Availability	
Connect to Quantum Device	
Create Task to Run Circuit	
Fetch Measurement Output	
Graph Coloring with Grover's Algorithm	17-34
Create State Oracle for Graph Coloring Problem	
Create Diffuser Circuit	
Apply Grover's Algorithm to Graph Coloring Oracle	
Run Circuit on AWS	
Truit Off Out of Tive Control	1, 12
Ground-State Protein Folding Using Variational Quantum Eigenso	
(VQE)	
Model Protein Fold with Qubits	
Write Function to Calculate Energy of Folds	
Compute Minimum Energy for All Folds	17-48
Write CVaR-VQE Objective Function	
Create Circuit Ansatz	
Simulate Iterations of CVaR-VQE	
Run Final Iteration on OPII	17-54

Matrices and Arrays

- "Creating, Concatenating, and Expanding Matrices" on page 1-2
- "Removing Rows or Columns from a Matrix" on page 1-8
- "Reshaping and Rearranging Arrays" on page 1-9
- "Multidimensional Arrays" on page 1-14
- "Array Indexing" on page 1-21

Creating, Concatenating, and Expanding Matrices

The most basic MATLAB® data structure is the matrix. A matrix is a two-dimensional, rectangular array of data elements arranged in rows and columns. The elements can be numbers, logical values (true or false), dates and times, strings, categorical values, or some other MATLAB data type.

Even a single number is stored as a matrix. For example, a variable containing the value 100 is stored as a 1-by-1 matrix of type double.

```
A = 100:
whos A
 Name
           Size
                           Bytes Class
                                           Attributes
 Α
                                8 double
            1x1
```

Constructing a Matrix of Data

If you have a specific set of data, you can arrange the elements in a matrix using square brackets. A single row of data has spaces or commas in between the elements, and a semicolon separates the rows. For example, create a single row of four numeric elements. The size of the resulting matrix is 1by-4 because it has one row and four columns. A matrix of this shape is often referred to as a row vector.

```
A = [12 62 93 -8]
A = 1 \times 4
    12
            62
                93
                           - 8
sz = size(A)
sz = 1 \times 2
      1
             4
```

Now create a matrix with the same numbers, but arrange them in two rows. This matrix has two rows and two columns.

```
A = [12 62; 93 -8]
A = 2 \times 2
     12
            62
     93
            -8
sz = size(A)
sz = 1 \times 2
      2
             2
```

Specialized Matrix Functions

MATLAB has many functions that help create matrices with certain values or a particular structure. For example, the zeros and ones functions create matrices of all zeros or all ones. The first and second arguments of these functions are the number of rows and number of columns of the matrix, respectively.

```
A = zeros(3,2)
A = 3 \times 2
      (-)
               (-)
      0
               0
      0
               (-)
B = ones(2,4)
B = 2 \times 4
              1
                       1
      1
               1
                       1
                               1
```

The diag function places the input elements on the diagonal of a matrix. For example, create a row vector A containing four elements. Then, create a 4-by-4 matrix whose diagonal elements are the elements of A.

```
A = [12 62 93 -8];
B = diag(A)
B = 4 \times 4
     12
              (-)
                      0
                              (-)
      0
             62
                      0
                              0
      0
              0
                    93
                              0
      (-)
              0
                      0
                            -8
```

Concatenating Matrices

You can also use square brackets to append existing matrices. This way of creating a matrix is called *concatenation*. For example, concatenate two row vectors to make an even longer row vector.

```
A = ones(1,4);

B = zeros(1,4);

C = [A B]

C = 1 \times 8

1 1 1 1 0 0 0 0
```

To arrange A and B as two rows of a matrix, use the semicolon.

```
D = [A; B]
D = 2 \times 4
```

1	1	1	1
0	0	0	0

To concatenate several matrices, they must have compatible sizes. In other words, when you concatenate matrices horizontally, they must have the same number of rows. When you concatenate them vertically, they must have the same number of columns.

For example, create two matrices that both have two rows. Horizontally append the second matrix to the first by using square brackets.

```
A = ones(2,3)
A = 2 \times 3
          1 1
    1
           1
     1
B = zeros(2,2)
B = 2 \times 2
     0
           0
     0
            (-)
C = [A B]
C = 2 \times 5
           1
                  1
                         0
                  1
```

An alternative way to concatenate compatible matrices is to use concatenation functions, such as horzcat, vertcat, and cat. Horizontally append the second matrix to the first by using horzcat.

```
D = horzcat(A,B)
D = 2 \times 5
    1 1 1 0
1 1 1 0
```

Generating a Numeric Sequence

The colon is a handy way to create matrices whose elements are sequential and evenly spaced. For example, create a row vector whose elements are the integers from 1 to 10.

```
A = 1:10
A = 1 \times 10
   1 2 3 4 5 6 7 8 9 10
```

You can use the colon operator to create a sequence of numbers within any range, incremented by one.

```
A = -2.5:2.5
A = 1 \times 6
-2.5000 -1.5000 -0.5000 0.5000 1.5000 2.5000
```

To change the value of the sequence increment, specify the increment value in between the starting and ending range values, separated by colons.

```
A = 0:2:10
A = 1 \times 6
0 \quad 2 \quad 4 \quad 6 \quad 8 \quad 10
```

To decrement, use a negative number.

```
A = 6:-1:0
A = 1 \times 7
6 	 5 	 4 	 3 	 2 	 1 	 0
```

You can also increment by noninteger values. If an increment value does not evenly partition the specified range, MATLAB automatically ends the sequence at the last value it can reach before exceeding the range.

```
A = 1:0.2:2.1
A = 1 \times 6
1.0000 \quad 1.2000 \quad 1.4000 \quad 1.6000 \quad 1.8000 \quad 2.0000
```

Expanding a Matrix

You can add one or more elements to a matrix by placing them outside of the existing row and column index boundaries. MATLAB automatically pads the matrix with zeros to keep it rectangular. For example, create a 2-by-3 matrix and add an additional row and column to it by inserting an element in the (3,4) position.

```
A = [10 20 30; 60 70 80]

A = 2 \times 3

10 20 30
60 70 80

A(3,4) = 1

A = 3 \times 4
```

10	20	30	0
60	70	80	0
0	0	0	1

You can also expand the size by inserting a new matrix outside of the existing index ranges.

```
A(4:5.5:6) = [2 3: 4 5]
A = 5 \times 6
    10
          20
    60
         70
                80
                      0
                             0
                                   0
          0
             0
                      1
                             0
     0
          0
             0
                      0
                             2
                                   3
     (-)
           0
                 (-)
                       (-)
                                   5
```

To expand the size of a matrix repeatedly, such as within a for loop, it is a best practice to preallocate space for the largest matrix you anticipate creating. Without preallocation, MATLAB has to allocate memory every time the size increases, slowing down operations. For example, preallocate a matrix that holds up to 10,000 rows and 10,000 columns by initializing its elements to zero.

```
A = zeros(10000, 10000);
```

If you need to preallocate additional elements later, you can expand it by assigning outside of the matrix index ranges or concatenate another preallocated matrix to A.

Empty Arrays

An empty array in MATLAB is an array with at least one dimension length equal to zero. Empty arrays are useful for representing the concept of "nothing" programmatically. For example, suppose you want to find all elements of a vector that are less than 0, but there are none. The find function returns an empty vector of indices, indicating that it did not find any elements less than 0.

```
A = [1 2 3 4];
ind = find(A<0)
ind =
   1x0 empty double row vector</pre>
```

Many algorithms contain function calls that can return empty arrays. It is often useful to allow empty arrays to flow through these algorithms as function arguments instead of handling them as a special case. If you do need to customize empty array handling, you can check for them using the <code>isempty</code> function.

```
TF = isempty(ind)
```

See Also

Related Examples

- "Array Indexing" on page 1-21
- "Reshaping and Rearranging Arrays" on page 1-9
- "Multidimensional Arrays" on page 1-14
- "Create String Arrays"
- "Represent Dates and Times in MATLAB"

Removing Rows or Columns from a Matrix

The easiest way to remove a row or column from a matrix is to set that row or column equal to a pair of empty square brackets []. For example, create a 4-by-4 matrix and remove the second row.

```
A = magic(4)
A = 4 \times 4
    16
          2
                3
                   13
             10
     5
          11
                     8
     9
          7
               6
                      12
          14
                15
                      1
A(2,:) = []
A = 3 \times 4
    16
           2
                 3
                      13
     9
          7
                6
                      12
     4
          14
                15
                       1
```

Now remove the third column.

A(:,3) = []
$$A = 3 \times 3$$

$$16 2 13$$

$$9 7 12$$

$$4 14 1$$

You can extend this approach to any array. For example, create a random 3-by-3-by-3 array and remove all of the elements in the first matrix of the third dimension.

```
B = rand(3,3,3);
B(:,:,1) = [];
```

See Also

Related Examples

- "Reshaping and Rearranging Arrays" on page 1-9
- "Array Indexing" on page 1-21

Reshaping and Rearranging Arrays

Many functions in MATLAB® can take the elements of an existing array and put them in a different shape or sequence. This can be helpful for preprocessing your data for subsequent computations or analyzing the data.

Reshaping

The reshape function changes the size and shape of an array. For example, reshape a 3-by-4 matrix to a 2-by-6 matrix.

```
A = [1 \ 4 \ 7 \ 10; \ 2 \ 5 \ 8 \ 11; \ 3 \ 6 \ 9 \ 12]
A = 3 \times 4
      1
                      7
              4
                             10
      2
              5
                      8
                             11
      3
              6
                             12
B = reshape(A, 2, 6)
B = 2 \times 6
      1
              3
                     5
                             7
                                     9
                                             11
                      6
      2
              4
                              8
                                     10
                                             12
```

As long as the number of elements in each shape are the same, you can reshape them into an array with any number of dimensions. Using the elements from A, create a 2-by-2-by-3 multidimensional array.

Transposing and Flipping

A common task in linear algebra is to work with the transpose of a matrix, which turns the rows into columns and the columns into rows. To do this, use the transpose function or the .' operator.

Create a 3-by-3 matrix and compute its transpose.

```
A = magic(3)
A = 3 \times 3
             1 6
5 7
      8
      3
              9
                     2
      4
B = A.'
B = 3 \times 3
      8
              5
                     9
      1
              7
      6
```

A similar operator ' computes the conjugate transpose for complex matrices. This operation computes the complex conjugate of each element and transposes it. Create a 2-by-2 complex matrix and compute its conjugate transpose.

```
A = [1+i \ 1-i; -i \ i]
A = 2 \times 2 \ complex
   1.0000 + 1.0000i 1.0000 - 1.0000i
   0.0000 - 1.0000i 0.0000 + 1.0000i
B = A'
B = 2 \times 2 \ complex
   1.0000 - 1.0000i 0.0000 + 1.0000i
   1.0000 + 1.0000i 0.0000 - 1.0000i
```

flipud flips the rows of a matrix in an up-to-down direction, and fliplr flips the columns in a leftto-right direction.

```
A = [1 2; 3 4]
A = 2 \times 2
      1
              2
      3
              4
B = flipud(A)
B = 2 \times 2
      3
              4
              2
      1
C = fliplr(A)
```

$$C = 2 \times 2$$

2

4

3

Shifting and Rotating

You can shift elements of an array by a certain number of positions using the circshift function. For example, create a 3-by-4 matrix and shift its columns to the right by 2. The second argument [0 2] tells circshift to shift the rows 0 places and shift the columns 2 places to the right.

To shift the rows of A up by 1 and keep the columns in place, specify the second argument as [-1 0].

C = circshift(A, [-1 0])

The rot90 function can rotate a matrix counterclockwise by 90 degrees.

```
A = [1 2; 3 4]

A = 2 \times 2

1 2
3 4

B = rot90(A)

B = 2 \times 2

2 4
1 3
```

If you rotate 3 more times by using the second argument to specify the number of rotations, you end up with the original matrix A.

Sorting

Sorting the data in an array is also a valuable tool, and MATLAB offers a number of approaches. For example, the sort function sorts the elements of each row or column of a matrix separately in ascending or descending order. Create a matrix A and sort each column of A in ascending order.

```
A = magic(4)
A = 4 \times 4
     16
             2
                          13
                    3
                   10
     5
            11
                           8
      9
            7
                   6
                          12
      4
            14
                   15
                           1
B = sort(A)
B = 4 \times 4
      4
             2
                    3
                           1
      5
            7
                   6
                           8
     9
            11
                   10
                          12
     16
            14
                   15
                          13
```

Sort each row in descending order. The second argument value 2 specifies that you want to sort row-wise.

```
C = sort(A,2,'descend')
C = 4 \times 4
    16
                    3
           13
                    8
                           5
    11
           10
                    7
    12
            9
                           6
    15
           14
                    4
                           1
```

To sort entire rows or columns relative to each other, use the sort rows function. For example, sort the rows of A in ascending order according to the elements in the first column. The positions of the rows change, but the order of the elements in each row are preserved.

```
D = sortrows(A)
D = 4 \times 4
4 \quad 14 \quad 15 \quad 1
```

See Also

Related Examples

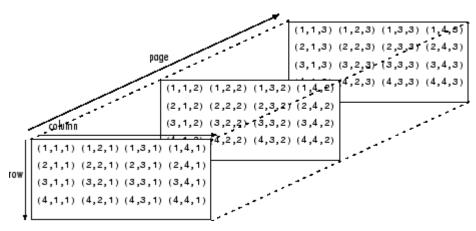
- "Removing Rows or Columns from a Matrix" on page 1-8
- "Array Indexing" on page 1-21

Multidimensional Arrays

A multidimensional array in MATLAB \circledR is an array with more than two dimensions. In a matrix, the two dimensions are represented by rows and columns.

	column			
	(1,1)	(1,2)	(1,3)	(1,4)
row	(2,1)	(2,2)	(2,3)	(2,4)
	(3,1)	(3,2)	(3,3)	(3,4)
	(4,1)	(4,2)	(4,3)	(4,4)

Each element is defined by two subscripts, the row index and the column index. Multidimensional arrays are an extension of 2-D matrices and use additional subscripts for indexing. A 3-D array, for example, uses three subscripts. The first two are just like a matrix, but the third dimension represents *pages* or *sheets* of elements.



Creating Multidimensional Arrays

You can create a multidimensional array by creating a 2-D matrix first, and then extending it. For example, first define a 3-by-3 matrix as the first page in a 3-D array.

Now add a second page. To do this, assign another 3-by-3 matrix to the index value 2 in the third dimension. The syntax A(:,:,2) uses a colon in the first and second dimensions to include all rows and all columns from the right-hand side of the assignment.

$$A(:,:,2) = [10 \ 11 \ 12; \ 13 \ 14 \ 15; \ 16 \ 17 \ 18]$$

$$A = A(:,:,1) =$$

The cat function can be a useful tool for building multidimensional arrays. For example, create a new 3-D array B by concatenating A with a third page. The first argument indicates which dimension to concatenate along.

```
B = cat(3,A,[3 2 1; 0 9 8; 5 3 7])
B =
B(:,:,1) =
    1 2 3
4 5 6
7 8 9
B(:,:,2) =
    10
          11
                12
    13
          14
                15
    16
          17
                18
B(:,:,3) =
     3
          2
                 1
       2
9
     0
                 8
           3
     5
                 7
```

Another way to quickly expand a multidimensional array is by assigning a single element to an entire page. For example, add a fourth page to B that contains all zeros.

Accessing Elements

To access elements in a multidimensional array, use integer subscripts just as you would for vectors and matrices. For example, find the 1,2,2 element of A, which is in the first row, second column, and second page of A.

Α

Use the index vector [1 3] in the second dimension to access only the first and last columns of each page of A.

```
C = A(:,[1 3],:)
C =
C(:,:,1) =
    1
    4
C(:,:,2) =
```

elA = 11

```
10 12
13 15
16 18
```

To find the second and third rows of each page, use the colon operator to create your index vector.

```
D = A(2:3,:,:)

D = D(:,:,1) = 

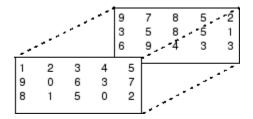
4     5     6     7     8     9

D(:,:,2) = 

13     14     15     16     17     18
```

Manipulating Arrays

Elements of multidimensional arrays can be moved around in many ways, similar to vectors and matrices. reshape, permute, and squeeze are useful functions for rearranging elements. Consider a 3-D array with two pages.



Reshaping a multidimensional array can be useful for performing certain operations or visualizing the data. Use the reshape function to rearrange the elements of the 3-D array into a 6-by-5 matrix.

```
A = [1 \ 2 \ 3 \ 4 \ 5; \ 9 \ 0 \ 6 \ 3 \ 7; \ 8 \ 1 \ 5 \ 0 \ 2];
A(:,:,2) = [9 7 8 5 2; 3 5 8 5 1; 6 9 4 3 3];
B = reshape(A, [6 5])
B = 6 \times 5
      1
              3
      9
              6
                      7
                              5
                                      5
      8
              5
                      2
                              9
                                      3
      2
                      9
                              8
                                      2
              4
      (-)
              3
                      3
                              8
                                      1
                                      3
```

reshape operates columnwise, creating the new matrix by taking consecutive elements down each column of A, starting with the first page then moving to the second page.

Permutations are used to rearrange the order of the dimensions of an array. Consider a 3-D array M.

```
M(:,:,1) = [1 2 3; 4 5 6; 7 8 9];
M(:,:,2) = [0 5 4; 2 7 6; 9 3 1]
M(:,:,1) =
    1 2 3
4 5 6
7 8 9
M(:,:,2) =
    0
        5 4
    2
         7
                6
    9
          3
                1
```

Use the permute function to interchange row and column subscripts on each page by specifying the order of dimensions in the second argument. The original rows of M are now columns, and the columns are now rows.

```
P1 = permute(M,[2 1 3])
P1 =
P1(:,:,1) =
       4 7
5 8
6 9
    1
    2
    3
P1(:,:,2) =
        2
    0
         7
    5
               3
```

Similarly, interchange row and page subscripts of ${\tt M}.$

```
P2 = permute(M,[3 2 1])
P2 =
P2(:,:,1) =
   1 2 3
0 5 4
P2(:,:,2) =
P2(:,:,3) =
   7 8 9
```

9 3 1

When working with multidimensional arrays, you might encounter one that has an unnecessary dimension of length 1. The squeeze function performs another type of manipulation that eliminates dimensions of length 1. For example, use the repmat function to create a 2-by-3-by-1-by-4 array whose elements are each 5, and whose third dimension has length 1.

A = repmat(5,[2 3 1 4])

$$A(:,:,1,4) = 5 5 5 5 5$$

$$szA = size(A)$$

 $szA = 1 \times 4$
2 3 1 4

numdimsA = ndims(A)

numdimsA = 4

Use the squeeze function to remove the third dimension, resulting in a 3-D array.

B = squeeze(A)

$$B(:,:,2) =$$

See Also

Related Examples

- "Creating, Concatenating, and Expanding Matrices" on page 1-2
- "Array Indexing" on page 1-21
- "Reshaping and Rearranging Arrays" on page 1-9

Array Indexing

In MATLAB®, there are three primary approaches to accessing array elements based on their location (index) in the array. These approaches are indexing by position, linear indexing, and logical indexing.

Indexing with Element Positions

The most common way is to explicitly specify the indices of the elements. For example, to access a single element of a matrix, specify the row number followed by the column number of the element.

```
A = [1 \ 2 \ 3 \ 4; \ 5 \ 6 \ 7 \ 8; \ 9 \ 10 \ 11 \ 12; \ 13 \ 14 \ 15 \ 16]
A = 4 \times 4
      1
             2
                     3
                             4
      5
            6
                    7
                            8
      9
            10
                    11
                           12
     13
            14
                 15
e = A(3,2)
e = 10
```

e is the element in the 3,2 position (third row, second column) of A.

You can also reference multiple elements at a time by specifying their indices in a vector. For example, access the first and third elements of the second row of A.

```
r = A(2,[1 \ 3])

r = 1 \times 2

5 7
```

To access elements in a range of rows or columns, use the colon. For example, access the elements in the first through third row and the second through fourth column of A.

An alternative way to compute r is to use the keyword end to specify the second column through the last column. This approach lets you specify the last column without knowing exactly how many columns are in A.

```
r = A(1:3,2:end)
r = 3 \times 3
```

```
2 3 4
6 7 8
10 11 12
```

If you want to access all of the rows or columns, use the colon operator by itself. For example, return the entire third column of A.

```
r = A(:,3)
r = 4×1
3
7
11
15
```

In general, you can use indexing to access elements of any array in MATLAB regardless of its data type or dimensions. For example, directly access a column of a datetime array.

For higher-dimensional arrays, expand the syntax to match the array dimensions. Consider a random 3-by-3-by-3 numeric array. Access the element in the second row, third column, and first sheet of the array.

```
A = rand(3,3,3);

e = A(2,3,1)

e = 0.5469
```

For more information on working with multidimensional arrays, see "Multidimensional Arrays" on page 1-14.

Indexing with a Single Index

Another method for accessing elements of an array is to use only a single index, regardless of the size or dimensions of the array. This method is known as *linear indexing*. While MATLAB displays arrays according to their defined sizes and shapes, they are actually stored in memory as a single column of elements. A good way to visualize this concept is with a matrix. While the following array is displayed as a 3-by-3 matrix, MATLAB stores it as a single column made up of the columns of A appended one after the other. The stored vector contains the sequence of elements 12, 45, 33, 36, 29, 25, 91, 48, 11, and can be displayed using a single colon.

```
A = [12 \ 36 \ 91; \ 45 \ 29 \ 48; \ 33 \ 25 \ 11]
```

```
A = 3 \times 3
    12
            36
                    91
    45
            29
                    48
            25
    33
                    11
Alinear = A(:)
Alinear = 9 \times 1
     12
     45
     33
     36
     29
     25
    91
    48
     11
```

For example, the 3,2 element of A is 25, and you can access it using the syntax A(3,2). You can also access this element using the syntax A(6), since 25 is sixth element of the stored vector sequence.

```
e = A(3,2)
e = 25
elinear = A(6)
elinear = 25
```

While linear indexing can be less intuitive visually, it can be powerful for performing certain computations that are not dependent on the size or shape of the array. For example, you can easily sum all of the elements of A without having to provide a second argument to the sum function.

```
s = sum(A(:))
s = 330
```

The sub2ind and ind2sub functions help to convert between original array indices and their linear version. For example, compute the linear index of the 3,2 element of A.

```
linearidx = sub2ind(size(A),3,2)
linearidx = 6
```

Convert from the linear index back to its row and column form.

```
[row,col] = ind2sub(size(A),6)
row = 3
col = 2
```

Indexing with Logical Values

Using true and false logical indicators is another useful way to index into arrays, particularly when working with conditional statements. For example, say you want to know if the elements of a matrix A

are less than the corresponding elements of another matrix B. The less-than operator returns a logical array whose elements are 1 when an element in A is smaller than the corresponding element in B.

```
A = [1 \ 2 \ 6; \ 4 \ 3 \ 6]
A = 2 \times 3
      1
              3
      4
B = [0 \ 3 \ 7; \ 3 \ 7 \ 5]
B = 2 \times 3
             3
7
      0
      3
ind = A < B
ind = 2x3 logical array
      1 1
        1
              0
```

Now that you know the locations of the elements meeting the condition, you can inspect the individual values using ind as the index array. MATLAB matches the locations of the value 1 in ind to the corresponding elements of A and B, and lists their values in a column vector.

```
Avals = A(ind)
Avals = 3 \times 1
      2
      3
Bvals = B(ind)
Byals = 3 \times 1
      3
      7
      7
```

MATLAB "is" functions also return logical arrays that indicate which elements of the input meet a certain condition. For example, check which elements of a string vector are missing using the ismissing function.

```
str = ["A" "B" missing "D" "E" missing];
ind = ismissing(str)
ind = 1x6 logical array
```

```
0 0 1 0 0 1
```

Suppose you want to find the values of the elements that are not missing. Use the \sim operator with the index vector ind to do this.

```
strvals = str(~ind)
strvals = 1x4 string
   "A" "B" "D" "E"
```

For more examples using logical indexing, see "Find Array Elements That Meet a Condition".

See Also

Related Examples

- "Access Data Using Categorical Arrays"
- "Access Data in Tables"
- "Structure Arrays"
- "Access Data in Cell Array"

External Websites

• Programming: Organizing Data (MathWorks Teaching Resources)

Linear Algebra

- "Matrices in the MATLAB Environment" on page 2-2
- "Systems of Linear Equations" on page 2-10
- "Factorizations" on page 2-20
- "Powers and Exponentials" on page 2-26
- "Eigenvalues" on page 2-30
- "Singular Values" on page 2-33
- "LAPACK in MATLAB" on page 2-37
- "Matrix Exponentials" on page 2-38
- "Graphical Comparison of Exponential Functions" on page 2-42
- "Basic Matrix Operations" on page 2-46
- "Determine Whether Matrix Is Symmetric Positive Definite" on page 2-54
- "Image Compression with Low-Rank SVD" on page 2-56

Matrices in the MATLAB Environment

This topic contains an introduction to creating matrices and performing basic matrix calculations in MATLAB.

The MATLAB environment uses the term *matrix* to indicate a variable containing real or complex numbers arranged in a two-dimensional grid. An *array* is, more generally, a vector, matrix, or higher dimensional grid of numbers. All arrays in MATLAB are rectangular, in the sense that the component vectors along any dimension are all the same length. The mathematical operations defined on matrices are the subject of linear algebra.

Creating Matrices

MATLAB has many functions that create different kinds of matrices. For example, you can create a symmetric matrix with entries based on Pascal's triangle:

Or, you can create an unsymmetric *magic square matrix*, which has equal row and column sums:

```
B = magic(3)
B = \begin{bmatrix} 8 & 1 & 6 \\ 3 & 5 & 7 \\ 4 & 9 & 2 \end{bmatrix}
```

Another example is a 3-by-2 rectangular matrix of random integers. In this case the first input to randi describes the range of possible values for the integers, and the second two inputs describe the number of rows and columns.

A column vector is an *m*-by-1 matrix, a row vector is a 1-by-*n* matrix, and a scalar is a 1-by-1 matrix. To define a matrix manually, use square brackets [] to denote the beginning and end of the array. Within the brackets, use a semicolon; to denote the end of a row. In the case of a scalar (1-by-1 matrix), the brackets are not required. For example, these statements produce a column vector, a row vector, and a scalar:

```
u = [3; 1; 4]
v = [2 0 -1]
s = 7
```

```
u = 3
1
4

v = 2
0
-1

s = 7
```

For more information about creating and working with matrices, see "Creating, Concatenating, and Expanding Matrices" on page 1-2.

Adding and Subtracting Matrices

Addition and subtraction of matrices and arrays is performed element-by-element, or *element-wise*. For example, adding A to B and then subtracting A from the result recovers B:

```
X = A + B
X =
        9
              2
       4
             7
                    10
       5
             12
Y = X - A
       8
              1
                     6
       3
              5
                     7
```

Addition and subtraction require both matrices to have compatible dimensions. If the dimensions are incompatible, an error results:

```
X = A + C
Error using +
Matrix dimensions must agree.
```

For more information, see "Array vs. Matrix Operations".

Vector Products and Transpose

A row vector and a column vector of the same length can be multiplied in either order. The result is either a scalar, called the *inner product*, or a matrix, called the *outer product*:

```
u = [3; 1; 4];
v = [2 0 -1];
x = v*u
x =
2
X = u*v
```

For real matrices, the transpose operation interchanges a_{ij} and a_{ji} . For complex matrices, another consideration is whether to take the complex conjugate of complex entries in the array to form the complex conjugate transpose. MATLAB uses the apostrophe operator (') to perform a complex conjugate transpose, and the dot-apostrophe operator (.') to transpose without conjugation. For matrices containing all real elements, the two operators return the same result.

The example matrix A = pascal(3) is symmetric, so A' is equal to A. However, B = magic(3) is not symmetric, so B' has the elements reflected along the main diagonal:

```
B = magic(3)
B =
      8
             1
                    6
      3
             5
                    7
      4
                    2
X = B'
X =
      8
             3
                    4
      1
             5
                    9
```

For vectors, transposition turns a row vector into a column vector (and vice-versa):

```
x = v'
x = 2
0
-1
```

If x and y are both real column vectors, then the product x*y is not defined, but the two products

```
x'*y
and
v'*x
```

produce the same scalar result. This quantity is used so frequently, it has three different names: *inner* product, *scalar* product, or *dot* product. There is even a dedicated function for dot products named dot.

For a complex vector or matrix, z, the quantity z' not only transposes the vector or matrix, but also converts each complex element to its complex conjugate. That is, the sign of the imaginary part of each complex element changes. For example, consider the complex matrix

```
z = [1+2i \ 7-3i \ 3+4i; \ 6-2i \ 9i \ 4+7i]
```

The complex conjugate transpose of z is:

The unconjugated complex transpose, where the complex part of each element retains its sign, is denoted by z.':

For complex vectors, the two scalar products x'*y and y'*x are complex conjugates of each other, and the scalar product x'*x of a complex vector with itself is real.

Multiplying Matrices

Multiplication of matrices is defined in a way that reflects composition of the underlying linear transformations and allows compact representation of systems of simultaneous linear equations. The matrix product C = AB is defined when the column dimension of A is equal to the row dimension of B, or when one of them is a scalar. If A is m-by-p and B is p-by-n, their product C is m-by-n. The product can actually be defined using MATLAB for loops, colon notation, and vector dot products:

MATLAB uses an asterisk to denote matrix multiplication, as in C = A*B. Matrix multiplication is not commutative; that is, A*B is typically not equal to B*A:

```
Y =

15 28 47
15 34 60
15 28 43
```

A matrix can be multiplied on the right by a column vector and on the left by a row vector:

```
u = [3; 1; 4];

x = A*u

x =

8
17
30

v = [2 0 -1];
y = v*B

y =

12 -7 10
```

Rectangular matrix multiplications must satisfy the dimension compatibility conditions. Since A is 3-by-3 and C is 3-by-2, you can multiply them to get a 3-by-2 result (the common inner dimension cancels):

```
X = A*C

X = 24 17

47 42

79 77
```

However, the multiplication does not work in the reverse order:

```
Y = C*A

Error using *
Incorrect dimensions for matrix multiplication. Check that the number of columns in the first matrix matches the number of rows in the second matrix. To perform elementwise multiplication, use '.*'.
```

You can multiply anything with a scalar:

```
s = 10;

w = s*y

w = 120 -70 100
```

When you multiply an array by a scalar, the scalar implicitly expands to be the same size as the other input. This is often referred to as *scalar expansion*.

Identity Matrix

Generally accepted mathematical notation uses the capital letter I to denote identity matrices, matrices of various sizes with ones on the main diagonal and zeros elsewhere. These matrices have the property that AI = A and IA = A whenever the dimensions are compatible.

The original version of MATLAB could not use I for this purpose because it did not distinguish between uppercase and lowercase letters and i already served as a subscript and as the complex unit. So an English language pun was introduced. The function

```
eye(m,n)
```

returns an m-by-n rectangular identity matrix and eye(n) returns an n-by-n square identity matrix.

Matrix Inverse

If a matrix A is square and nonsingular (nonzero determinant), then the equations AX = I and XA = I have the same solution X. This solution is called the *inverse* of A and is denoted A^{-1} . The inv function and the expression A^{-1} both compute the matrix inverse.

```
A = pascal(3)
A =
       1
              1
                    1
       1
              2
                    3
       1
              3
                    6
X = inv(A)
X =
    3.0000
             -3.0000
                         1.0000
                        -2.0000
   -3.0000
              5.0000
                         1.0000
    1.0000
              -2.0000
A*X
ans =
    1.0000
                    0
    0.0000
               1.0000
                        -0.0000
   -0.0000
               0.0000
                         1.0000
```

The *determinant* calculated by det is a measure of the scaling factor of the linear transformation described by the matrix. When the determinant is exactly zero, the matrix is *singular* and no inverse exists.

```
d = det(A)
d = 1
```

Some matrices are *nearly singular*, and despite the fact that an inverse matrix exists, the calculation is susceptible to numerical errors. The cond function computes the *condition number for inversion*, which gives an indication of the accuracy of the results from matrix inversion. The condition number ranges from 1 for a numerically stable matrix to Inf for a singular matrix.

```
c = cond(A)
c =
61.9839
```

It is seldom necessary to form the explicit inverse of a matrix. A frequent misuse of inv arises when solving the system of linear equations Ax = b. The best way to solve this equation, from the standpoint of both execution time and numerical accuracy, is to use the matrix backslash operator x = Ab. See mldivide for more information.

Kronecker Tensor Product

The Kronecker product, kron(X,Y), of two matrices is the larger matrix formed from all possible products of the elements of X with those of Y. If X is m-by-n and Y is p-by-q, then kron(X,Y) is mp-by-nq. The elements are arranged such that each element of X is multiplied by the entire matrix Y:

```
[X(1,1)*Y \quad X(1,2)*Y \quad . \quad . \quad X(1,n)*Y \\ . \quad . \quad . \quad . \quad . \\ X(m,1)*Y \quad X(m,2)*Y \quad . \quad . \quad X(m,n)*Y]
```

The Kronecker product is often used with matrices of zeros and ones to build up repeated copies of small matrices. For example, if X is the 2-by-2 matrix

$$X = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$$

and I = eye(2,2) is the 2-by-2 identity matrix, then:

```
kron(X,I)
```

and

kron(I,X)

Aside from kron, some other functions that are useful to replicate arrays are repmat, repelem, and blkdiag.

Vector and Matrix Norms

The p-norm of a vector x,

$$\|x\|_p = \left(\sum |x_i|^p\right)^{1/p},$$

is computed by norm(x,p). This operation is defined for any value of p > 1, but the most common values of p are 1, 2, and ∞ . The default value is p = 2, which corresponds to *Euclidean length* or *vector magnitude*:

```
v = [2 0 -1];
[norm(v,1) norm(v) norm(v,inf)]
ans =
     3.0000     2.2361     2.0000
```

The p-norm of a matrix A,

$$||A||_p = \max_{x} \frac{||Ax||_p}{||x||_p},$$

can be computed for p = 1, 2, and ∞ by norm(A, p). Again, the default value is p = 2:

```
A = pascal(3);
[norm(A,1) norm(A) norm(A,inf)]
ans =
    10.0000    7.8730    10.0000
```

In cases where you want to calculate the norm of each row or column of a matrix, you can use vecnorm:

```
vecnorm(A)
ans =
    1.7321    3.7417    6.7823
```

Using Multithreaded Computation with Linear Algebra Functions

MATLAB supports multithreaded computation for a number of linear algebra and element-wise numerical functions. These functions automatically execute on multiple threads. For a function or expression to execute faster on multiple CPUs, a number of conditions must be true:

- 1 The function performs operations that easily partition into sections that execute concurrently. These sections must be able to execute with little communication between processes. They should require few sequential operations.
- 2 The data size is large enough so that any advantages of concurrent execution outweigh the time required to partition the data and manage separate execution threads. For example, most functions speed up only when the array contains several thousand elements or more.
- **3** The operation is not memory-bound; processing time is not dominated by memory access time. As a general rule, complicated functions speed up more than simple functions.

The matrix multiply (X*Y) and matrix power (X^p) operators show significant increase in speed on large double-precision arrays (on order of 10,000 elements). The matrix analysis functions det, rcond, hess, and expm also show significant increase in speed on large double-precision arrays.

Systems of Linear Equations

In this section...

"Computational Considerations" on page 2-10

"General Solution" on page 2-11

"Square Systems" on page 2-11

"Overdetermined Systems" on page 2-13

"Underdetermined Systems" on page 2-15

"Solving for Several Right-Hand Sides" on page 2-17

"Iterative Methods" on page 2-18

"Multithreaded Computation" on page 2-18

Computational Considerations

One of the most important problems in technical computing is the solution of systems of simultaneous linear equations.

In matrix notation, the general problem takes the following form: Given two matrices A and b, does there exist a unique matrix x, so that Ax = b or xA = b?

It is instructive to consider a 1-by-1 example. For example, does the equation

$$7x = 21$$

have a unique solution?

The answer, of course, is yes. The equation has the unique solution x = 3. The solution is easily obtained by division:

$$x = 21/7 = 3$$
.

The solution is *not* ordinarily obtained by computing the inverse of 7, that is 7^{-1} = 0.142857..., and then multiplying 7^{-1} by 21. This would be more work and, if 7^{-1} is represented to a finite number of digits, less accurate. Similar considerations apply to sets of linear equations with more than one unknown; MATLAB solves such equations without computing the inverse of the matrix.

Although it is not standard mathematical notation, MATLAB uses the division terminology familiar in the scalar case to describe the solution of a general system of simultaneous equations. The two division symbols, <code>slash</code>, <code>/</code>, and <code>backslash</code>, <code>\</code>, correspond to the two MATLAB functions <code>mrdivide</code> and <code>mldivide</code>. These operators are used for the two situations where the unknown matrix appears on the left or right of the coefficient matrix:

x = b/A Denotes the solution to the matrix equation xA = b, obtained using mrdivide.

x = A b Denotes the solution to the matrix equation Ax = b, obtained using mldivide.

Think of "dividing" both sides of the equation Ax = b or xA = b by A. The coefficient matrix A is always in the "denominator."

The dimension compatibility conditions for x = A b require the two matrices A and b to have the same number of rows. The solution x then has the same number of columns as b and its row dimension is equal to the column dimension of A. For x = b/A, the roles of rows and columns are interchanged.

In practice, linear equations of the form Ax = b occur more frequently than those of the form xA = b. Consequently, the backslash is used far more frequently than the slash. The remainder of this section concentrates on the backslash operator; the corresponding properties of the slash operator can be inferred from the identity:

```
(b/A)' = (A' \setminus b').
```

The coefficient matrix A need not be square. If A has size m-by-n, then there are three cases:

m = n Square system. Seek an exact solution.

m > n Overdetermined system, with more equations than unknowns. Find a

least-squares solution.

m < n Underdetermined system, with fewer equations than unknowns. Find

a basic solution with at most m nonzero components.

The mldivide Algorithm

The mldivide operator employs different solvers to handle different kinds of coefficient matrices. The various cases are diagnosed automatically by examining the coefficient matrix. For more information, see the "Algorithms" section of the mldivide reference page.

General Solution

The general solution to a system of linear equations Ax = b describes all possible solutions. You can find the general solution by:

- Solving the corresponding homogeneous system Ax = 0. Do this using the null command, by typing null(A). This returns a basis for the solution space to Ax = 0. Any solution is a linear combination of basis vectors.
- **2** Finding a particular solution to the nonhomogeneous system Ax = b.

You can then write any solution to Ax = b as the sum of the particular solution to Ax = b, from step 2, plus a linear combination of the basis vectors from step 1.

The rest of this section describes how to use MATLAB to find a particular solution to Ax = b, as in step 2.

Square Systems

The most common situation involves a square coefficient matrix ${\bf A}$ and a single right-hand side column vector ${\bf b}$.

Nonsingular Coefficient Matrix

If the matrix A is nonsingular, then the solution, $x = A \setminus b$, is the same size as b. For example:

```
A = pascal(3);
u = [3; 1; 4];
```

It can be confirmed that A*x is exactly equal to u.

If A and b are square and the same size, $x = A \setminus b$ is also that size:

It can be confirmed that A*x is exactly equal to b.

Both of these examples have exact, integer solutions. This is because the coefficient matrix was chosen to be pascal(3), which is a full rank matrix (nonsingular).

Singular Coefficient Matrix

A square matrix A is singular if it does not have linearly independent columns. If A is singular, the solution to Ax = b either does not exist, or is not unique. The backslash operator, $A \setminus b$, issues a warning if A is nearly singular or if it detects exact singularity.

If A is singular and Ax = b has a solution, you can find a particular solution that is not unique, by typing

$$P = pinv(A)*b$$

pinv(A) is a pseudoinverse of A. If Ax = b does not have an exact solution, then pinv(A) returns a least-squares solution.

For example:

$$A = [1 & 3 & 7 \\ -1 & 4 & 4 \\ 1 & 10 & 18]$$

is singular, as you can verify by typing

```
rank(A)
ans =
2
```

Since *A* is not full rank, it has some singular values equal to zero.

Exact Solutions. For b = [5;2;12], the equation Ax = b has an exact solution, given by pinv(A)*b

```
ans =
    0.3850
    -0.1103
    0.7066

Verify that pinv(A)*b is an exact solution by typing
A*pinv(A)*b
```

ans = 5.0000 2.0000 12.0000

Least-Squares Solutions. However, if b = [3;6;0], Ax = b does not have an exact solution. In this case, pinv(A)*b returns a least-squares solution. If you type

```
A*pinv(A)*b

ans =
    -1.0000
    4.0000
    2.0000
```

you do not get back the original vector b.

You can determine whether Ax = b has an exact solution by finding the row reduced echelon form of the augmented matrix [A b]. To do so for this example, enter

Since the bottom row contains all zeros except for the last entry, the equation does not have a solution. In this case, pinv(A) returns a least-squares solution.

Overdetermined Systems

This example shows how overdetermined systems are often encountered in various kinds of curve fitting to experimental data.

A quantity y is measured at several different values of time t to produce the following observations. You can enter the data and view it in a table with the following statements.

```
0.8 0.63
1.1 0.6
1.6 0.55
2.3 0.5
```

Try modeling the data with a decaying exponential function

```
y(t) = c_1 + c_2 e^{-t}.
```

The preceding equation says that the vector y should be approximated by a linear combination of two other vectors. One is a constant vector containing all ones and the other is the vector with components $\exp(-t)$. The unknown coefficients, c_1 and c_2 , can be computed by doing a least-squares fit, which minimizes the sum of the squares of the deviations of the data from the model. There are six equations in two unknowns, represented by a 6-by-2 matrix.

```
E = [ones(size(t)) exp(-t)]

E = 6×2

1.0000 1.0000

1.0000 0.7408

1.0000 0.4493

1.0000 0.3329

1.0000 0.2019

1.0000 0.1003
```

Use the backslash operator to get the least-squares solution.

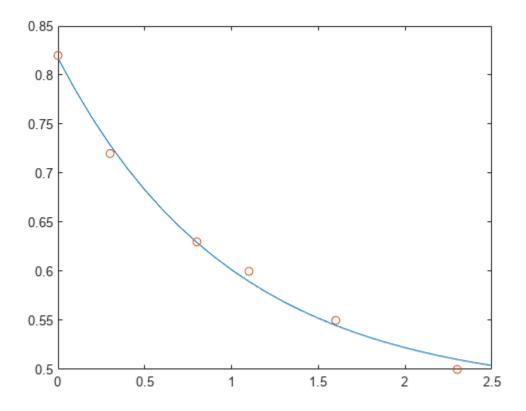
```
c = E\y
c = 2×1
0.4760
0.3413
```

In other words, the least-squares fit to the data is

```
y(t) = 0.4760 + 0.3413e^{-t}.
```

The following statements evaluate the model at regularly spaced increments in t, and then plot the result together with the original data:

```
T = (0:0.1:2.5)';
Y = [ones(size(T)) exp(-T)]*c;
plot(T,Y,'-',t,y,'o')
```



 E^*c is not exactly equal to y, but the difference might well be less than measurement errors in the original data.

A rectangular matrix A is rank deficient if it does not have linearly independent columns. If A is rank deficient, then the least-squares solution to AX = B is not unique. A\B issues a warning if A is rank deficient and produces a least-squares solution. You can use lsqminnorm to find the solution X that has the minimum norm among all solutions.

Underdetermined Systems

This example shows how the solution to underdetermined systems is not unique. Underdetermined linear systems involve more unknowns than equations. The matrix left division operation in MATLAB finds a basic least-squares solution, which has at most m nonzero components for an m-by-n coefficient matrix.

Here is a small, random example:

```
R = [6 8 7 3; 3 5 4 1]

rng(0);

b = randi(8,2,1)

R =

6 8 7 3

3 5 4 1
```

```
b = 7
```

The linear system Rp = b involves two equations in four unknowns. Since the coefficient matrix contains small integers, it is appropriate to use the format command to display the solution in rational format. The particular solution is obtained with

```
format rat
p = R\b
p =

0
17/7
0
-29/7
```

One of the nonzero components is p(2) because R(:,2) is the column of R with largest norm. The other nonzero component is p(4) because R(:,4) dominates after R(:,2) is eliminated.

The complete general solution to the underdetermined system can be characterized by adding p to an arbitrary linear combination of the null space vectors, which can be found using the null function with an option requesting a rational basis.

```
Z = null(R,'r')

Z =

-1/2 -7/6
-1/2 1/2
1 0
1
```

It can be confirmed that R*Z is zero and that the residual R*x - b is small for any vector x, where

$$x = p + Z*q$$

Since the columns of Z are the null space vectors, the product Z^*q is a linear combination of those vectors:

$$Zq = (\overrightarrow{x}_1 \ \overrightarrow{x}_2) \binom{u}{w} = u \overrightarrow{x}_1 + w \overrightarrow{x}_2 \ .$$

To illustrate, choose an arbitrary q and construct x.

```
q = [-2; 1];
 x = p + Z*q;
```

Calculate the norm of the residual.

```
format short
norm(R*x - b)
```

```
ans = 2.6645e-15
```

When infinitely many solutions are available, the solution with minimum norm is of particular interest. You can use lsqminnorm to compute the minimum-norm least-squares solution. This solution has the smallest possible value for norm(p).

```
p = lsqminnorm(R,b)
p =

    -207/137
    365/137
    79/137
    -424/137
```

Solving for Several Right-Hand Sides

Some problems are concerned with solving linear systems that have the same coefficient matrix A, but different right-hand sides b. When the different values of b are available at the same time, you can construct b as a matrix with several columns and solve all of the systems of equations at the same time using a single backslash command: $X = A \setminus [b1 \ b2 \ b3 \ ...]$.

However, sometimes the different values of b are not all available at the same time, which means you need to solve several systems of equations consecutively. When you solve one of these systems of equations using slash (/) or backslash (\), the operator factorizes the coefficient matrix A and uses this matrix decomposition to compute the solution. However, each subsequent time you solve a similar system of equations with a different b, the operator computes the same decomposition of A, which is a redundant computation.

The solution to this problem is to precompute the decomposition of A, and then reuse the factors to solve for the different values of b. In practice, however, precomputing the decomposition in this manner can be difficult since you need to know which decomposition to compute (LU, LDL, Cholesky, and so on) as well as how to multiply the factors to solve the problem. For example, with LU decomposition you need to solve two linear systems to solve the original system Ax = b:

```
[L,U] = lu(A);
x = U \ (L \ b);
```

Instead, the recommended method for solving linear systems with several consecutive right-hand sides is to use decomposition objects. These objects enable you to leverage the performance benefits of precomputing the matrix decomposition, but they *do not* require knowledge of how to use the matrix factors. You can replace the previous LU decomposition with:

```
dA = decomposition(A,'lu');
x = dA\b;
```

If you are unsure which decomposition to use, decomposition(A) chooses the correct type based on the properties of A, similar to what backslash does.

Here is a simple test of the possible performance benefits of this approach. The test solves the same sparse linear system 100 times using both backslash (\) and decomposition.

```
n = 1e3;
A = sprand(n,n,0.2) + speye(n);
```

```
b = ones(n,1);
% Backslash solution
tic
for k = 1:100
    x = A \ b;
end
toc
Elapsed time is 9.006156 seconds.
% decomposition solution
tic
dA = decomposition(A);
for k = 1:100
    x = dA \ b;
end
toc
Elapsed time is 0.374347 seconds.
```

For this problem, the decomposition solution is much faster than using backslash alone, yet the syntax remains simple.

Iterative Methods

If the coefficient matrix A is large and sparse, factorization methods are generally not efficient. Iterative methods generate a series of approximate solutions. MATLAB provides several iterative methods to handle large, sparse input matrices.

Function	Description	
pcg	Preconditioned conjugate gradients method. This method is appropriate for Hermitian positive definite coefficient matrix A.	
bicg	BiConjugate Gradients Method	
bicgstab	BiConjugate Gradients Stabilized Method	
bicgstabl	BiCGStab(l) Method	
cgs	Conjugate Gradients Squared Method	
gmres	Generalized Minimum Residual Method	
lsqr	LSQR Method	
minres	Minimum Residual Method. This method is appropriate for Hermitian coefficient matrix A.	
qmr	Quasi-Minimal Residual Method	
symmlq	Symmetric LQ Method	
tfqmr	Transpose-Free QMR Method	

Multithreaded Computation

MATLAB supports multithreaded computation for a number of linear algebra and element-wise numerical functions. These functions automatically execute on multiple threads. For a function or expression to execute faster on multiple CPUs, a number of conditions must be true:

- 1 The function performs operations that easily partition into sections that execute concurrently. These sections must be able to execute with little communication between processes. They should require few sequential operations.
- The data size is large enough so that any advantages of concurrent execution outweigh the time required to partition the data and manage separate execution threads. For example, most functions speed up only when the array contains several thousand elements or more.
- 3 The operation is not memory-bound; processing time is not dominated by memory access time. As a general rule, complicated functions speed up more than simple functions.

inv, lscov, linsolve, and mldivide show significant increase in speed on large double-precision arrays (on order of 10,000 elements or more) when multithreading is enabled.

Factorizations

In this section...

"Introduction" on page 2-20

"Cholesky Factorization" on page 2-20

"LU Factorization" on page 2-21

"QR Factorization" on page 2-22

"Using Multithreaded Computation for Factorization" on page 2-25

Introduction

All three of the matrix factorizations discussed in this section make use of *triangular* matrices, where all the elements either above or below the diagonal are zero. Systems of linear equations involving triangular matrices are easily and quickly solved using either *forward* or *back substitution*.

Cholesky Factorization

The Cholesky factorization expresses a symmetric matrix as the product of a triangular matrix and its transpose

A = R'R

where R is an upper triangular matrix.

Not all symmetric matrices can be factored in this way; the matrices that have such a factorization are said to be positive definite. This implies that all the diagonal elements of A are positive and that the off-diagonal elements are "not too big." The Pascal matrices provide an interesting example. Throughout this chapter, the example matrix A has been the 3-by-3 Pascal matrix. Temporarily switch to the 6-by-6:

A = pascal(6)

The elements of A are binomial coefficients. Each element is the sum of its north and west neighbors. The Cholesky factorization is

R = chol(A)R =

The elements are again binomial coefficients. The fact that R'R' is equal to A demonstrates an identity involving sums of products of binomial coefficients.

Note The Cholesky factorization also applies to complex matrices. Any complex matrix that has a Cholesky factorization satisfies

$$A' = A$$

and is said to be Hermitian positive definite.

The Cholesky factorization allows the linear system

$$Ax = b$$

to be replaced by

$$R'Rx = b$$
.

Because the backslash operator recognizes triangular systems, this can be solved in the MATLAB environment quickly with

$$x = R \setminus (R' \setminus b)$$

If A is n-by-n, the computational complexity of chol(A) is $O(n^3)$, but the complexity of the subsequent backslash solutions is only $O(n^2)$.

LU Factorization

LU factorization, or Gaussian elimination, expresses any square matrix A as the product of a permutation of a lower triangular matrix and an upper triangular matrix

$$A = LU$$

where L is a permutation of a lower triangular matrix with ones on its diagonal and U is an upper triangular matrix.

The permutations are necessary for both theoretical and computational reasons. The matrix

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

cannot be expressed as the product of triangular matrices without interchanging its two rows. Although the matrix

$$\begin{bmatrix} \varepsilon & 1 \\ 1 & 0 \end{bmatrix}$$

can be expressed as the product of triangular matrices, when ε is small, the elements in the factors are large and magnify errors, so even though the permutations are not strictly necessary, they are desirable. Partial pivoting ensures that the elements of L are bounded by one in magnitude and that the elements of U are not much larger than those of A.

For example:

```
[L,U] = lu(B)
    1.0000
                               0
                          1.0000
    0.3750
               0.5441
    0.5000
               1.0000
U =
    8.0000
               1.0000
                          6.0000
         0
               8.5000
                         -1.0000
         0
                          5.2941
```

The LU factorization of A allows the linear system

```
A*x = b
```

to be solved quickly with

$$x = U \setminus (L \setminus b)$$

Determinants and inverses are computed from the LU factorization using

```
det(A) = det(L)*det(U)
and
inv(A) = inv(U)*inv(L)
```

You can also compute the determinants using det(A) = prod(diag(U)), though the signs of the determinants might be reversed.

QR Factorization

An *orthogonal* matrix, or a matrix with orthonormal columns, is a real matrix whose columns all have unit length and are perpendicular to each other. If *Q* is orthogonal, then

$$Q^{\mathrm{T}}Q = I$$
,

where I is the identity matrix.

The simplest orthogonal matrices are two-dimensional coordinate rotations:

```
\begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix}.
```

For complex matrices, the corresponding term is *unitary*. Orthogonal and unitary matrices are desirable for numerical computation because they preserve length, preserve angles, and do not magnify errors.

The orthogonal, or QR, factorization expresses any rectangular matrix as the product of an orthogonal or unitary matrix and an upper triangular matrix. A column permutation might also be involved:

$$A = QR$$

or

$$AP = QR$$
,

where Q is orthogonal or unitary, R is upper triangular, and P is a permutation.

There are four variants of the QR factorization—full or economy size, and with or without column permutation.

Overdetermined linear systems involve a rectangular matrix with more rows than columns, that is m-by-n with m > n. The full-size QR factorization produces a square, m-by-m orthogonal Q and a rectangular m-by-n upper triangular R:

```
C=gallery('uniformdata',[5 4], 0);
[Q,R] = qr(C)
0 =
              0.1406
    0.6191
                        -0.1899
                                   -0.5058
                                              0.5522
    0.1506
              0.4084
                         0.5034
                                    0.5974
                                              0.4475
    0.3954
             -0.5564
                         0.6869
                                   -0.1478
                                             -0.2008
    0.3167
              0.6676
                         0.1351
                                   -0.1729
                                             -0.6370
    0.5808
              -0.2410
                        -0.4695
                                    0.5792
                                             -0.2207
R =
    1.5346
              1.0663
                         1.2010
                                    1.4036
              0.7245
                         0.3474
                                   -0.0126
         0
                         0.9320
         0
                    0
                                    0.6596
         0
                    0
                                    0.6648
                              0
                    0
                              0
```

In many cases, the last m-n columns of Q are not needed because they are multiplied by the zeros in the bottom portion of R. So the economy-size QR factorization produces a rectangular, m-by-n Q with orthonormal columns and a square n-by-n upper triangular R. For the 5-by-4 example, this is not much of a saving, but for larger, highly rectangular matrices, the savings in both time and memory can be quite important:

In contrast to the LU factorization, the QR factorization does not require any pivoting or permutations. But an optional column permutation, triggered by the presence of a third output argument, is useful for detecting singularity or rank deficiency. At each step of the factorization, the

column of the remaining unfactored matrix with largest norm is used as the basis for that step. This ensures that the diagonal elements of R occur in decreasing order and that any linear dependence among the columns is almost certainly be revealed by examining these elements. For the small example given here, the second column of C has a larger norm than the first, so the two columns are exchanged:

```
[Q,R,P] = qr(C)
   -0.3522
               0.8398
                         -0.4131
                         -0.4739
   -0.7044
              -0.5285
   -0.6163
               0.1241
                          0.7777
R =
  -11.3578
              -8.2762
              7.2460
         0
         0
                    0
P =
     0
           1
           0
     1
```

When the economy-size and column permutations are combined, the third output argument is a permutation vector, rather than a permutation matrix:

```
[Q,R,p] = qr(C,0)
Q =
               0.8398
   -0.3522
              -0.5285
   -0.7044
   -0.6163
               0.1241
R =
  -11.3578
              -8.2762
         0
               7.2460
p =
     2
           1
```

The QR factorization transforms an overdetermined linear system into an equivalent triangular system. The expression $\frac{1}{2}$

```
norm(A*x - b)
equals
norm(Q*R*x - b)
```

 $\label{eq:multiplication} \mbox{ Multiplication by orthogonal matrices preserves the Euclidean norm, so this expression is also equal to \end{to}$

```
norm(R*x - y)
where y = Q'*b. Since the last m-n rows of R are zero, this expression breaks into two pieces:
norm(R(1:n,1:n)*x - y(1:n))
```

and

norm(y(n+1:m))

When A has full rank, it is possible to solve for x so that the first of these expressions is zero. Then the second expression gives the norm of the residual. When A does not have full rank, the triangular structure of R makes it possible to find a basic solution to the least-squares problem.

Using Multithreaded Computation for Factorization

MATLAB software supports multithreaded computation for a number of linear algebra and elementwise numerical functions. These functions automatically execute on multiple threads. For a function or expression to execute faster on multiple CPUs, a number of conditions must be true:

- 1 The function performs operations that easily partition into sections that execute concurrently. These sections must be able to execute with little communication between processes. They should require few sequential operations.
- The data size is large enough so that any advantages of concurrent execution outweigh the time required to partition the data and manage separate execution threads. For example, most functions speed up only when the array contains several thousand elements or more.
- 3 The operation is not memory-bound; processing time is not dominated by memory access time. As a general rule, complicated functions speed up more than simple functions.

lu and qr show significant increase in speed on large double-precision arrays (on order of 10,000 elements).

Powers and Exponentials

This topic shows how to compute matrix powers and exponentials using a variety of methods.

Positive Integer Powers

If A is a square matrix and p is a positive integer, then A^p effectively multiplies A by itself p-1 times. For example:

Inverse and Fractional Powers

If A is square and nonsingular, then $A^{(-p)}$ effectively multiplies inv(A) by itself p-1 times.

```
A^(-3)

ans = 3×3

145.0000 -207.0000 81.0000

-207.0000 298.0000 -117.0000

81.0000 -117.0000 46.0000
```

MATLAB® calculates inv(A) and $A^{(-1)}$ with the same algorithm, so the results are exactly the same. Both inv(A) and $A^{(-1)}$ produce warnings if the matrix is close to being singular.

```
isequal(inv(A),A^(-1))
ans = logical
1
```

Fractional powers, such as $A^{(2/3)}$, are also permitted. The results using fractional powers depend on the distribution of the eigenvalues of the matrix.

```
A^(2/3)

ans = 3×3

0.8901 0.5882 0.3684

0.5882 1.2035 1.3799

0.3684 1.3799 3.1167
```

Element-by-Element Powers

The .^ operator calculates element-by-element powers. For example, to square each element in a matrix you can use A.^2.

A.^2 ans = 3×3 1 1 1 1 1 1 4 9 1 9 36

Square Roots

The sqrt function is a convenient way to calculate the square root of each element in a matrix. An alternate way to do this is $A.^(1/2)$.

```
sqrt(A)
ans = 3×3

1.0000    1.0000    1.0000
1.0000    1.4142    1.7321
1.0000    1.7321    2.4495
```

For other roots, you can use nthroot. For example, calculate A.^(1/3).

```
nthroot(A,3)
```

```
ans = 3×3

1.0000    1.0000    1.0000

1.0000    1.2599    1.4422

1.0000    1.4422    1.8171
```

These element-wise roots differ from the matrix square root, which calculates a second matrix B such that A = BB. The function sqrtm(A) computes $A^(1/2)$ by a more accurate algorithm. The m in sqrtm distinguishes this function from sqrt(A), which, like $A.^(1/2)$, does its job element-by-element.

```
B = sqrtm(A)
B = 3 \times 3
                           0.1937
    0.8775
               0.4387
    0.4387
               1.0099
                           0.8874
    0.1937
               0.8874
                           2.2749
B^2
ans = 3 \times 3
    1.0000
               1.0000
                           1.0000
    1.0000
               2.0000
                           3.0000
```

```
1,0000 3,0000 6,0000
```

Scalar Bases

In addition to raising a matrix to a power, you also can raise a scalar to the power of a matrix.

2^A

```
ans = 3×3

10.4630 21.6602 38.5862

21.6602 53.2807 94.6010

38.5862 94.6010 173.7734
```

When you raise a scalar to the power of a matrix, MATLAB uses the eigenvalues and eigenvectors of the matrix to calculate the matrix power. If [V,D] = eig(A), then $2^A = V 2^D V^{-1}$.

```
[V,D] = eig(A);

V*2^D*V^(-1)

ans = 3×3

10.4630 21.6602 38.5862

21.6602 53.2807 94.6010

38.5862 94.6010 173.7734
```

Matrix Exponentials

The matrix exponential is a special case of raising a scalar to a matrix power. The base for a matrix exponential is Euler's number $e = \exp(1)$.

```
e = \exp(1);

e^A

ans = 3 \times 3

10^3 \times

0.1008 0.2407 0.4368

0.2407 0.5867 1.0654

0.4368 1.0654 1.9418
```

The expm function is a more convenient way to calculate matrix exponentials.

expm(A)

```
ans = 3×3

10<sup>3</sup> ×

0.1008  0.2407  0.4368

0.2407  0.5867  1.0654

0.4368  1.0654  1.9418
```

The matrix exponential can be calculated in a number of ways. See "Matrix Exponentials" on page 2-38 for more information.

Dealing with Small Numbers

The MATLAB functions log1p and expm1 calculate log(1 + x) and $e^x - 1$ accurately for very small values of x. For example, if you try to add a number smaller than machine precision to 1, then the result gets rounded to 1.

```
log(1+eps/2)
ans = 0

However, log1p is able to return a more accurate answer.
log1p(eps/2)
ans = 1.1102e-16

Likewise for e^x - 1, if x is very small then it is rounded to zero.
exp(eps/2)-1
ans = 0

Again, expm1 is able to return a more accurate answer.
expm1(eps/2)
ans = 1.1102e-16
```

Eigenvalues

In this section... "Eigenvalue Decomposition" on page 2-30 "Multiple Eigenvalues" on page 2-31 "Schur Decomposition" on page 2-31

Eigenvalue Decomposition

An eigenvalue and eigenvector of a square matrix A are, respectively, a scalar λ and a nonzero vector v that satisfy

```
Av = \lambda v.
```

With the eigenvalues on the diagonal of a diagonal matrix Λ and the corresponding eigenvectors forming the columns of a matrix V, you have

```
AV = V\Lambda.
```

If V is nonsingular, this becomes the eigenvalue decomposition

```
A = V\Lambda V^{-1}.
```

A good example is the coefficient matrix of the differential equation dx/dt = Ax:

The solution to this equation is expressed in terms of the matrix exponential $x(t) = e^{tA}x(0)$. The statement

```
lambda = eig(A)
```

produces a column vector containing the eigenvalues of A. For this matrix, the eigenvalues are complex:

The real part of each of the eigenvalues is negative, so $e^{\lambda t}$ approaches zero as t increases. The nonzero imaginary part of two of the eigenvalues, $\pm \omega$, contributes the oscillatory component, $\sin(\omega t)$, to the solution of the differential equation.

With two output arguments, eig computes the eigenvectors and stores the eigenvalues in a diagonal matrix:

```
[V,D] = eig(A)
```

```
-0.8326
                 0.2003 - 0.1394i 0.2003 + 0.1394i
  -0.3553
                -0.2110 - 0.6447i - 0.2110 + 0.6447i
  -0.4248
                -0.6930
                                   -0.6930
D =
  -3.0710
                        (-)
                                           0
                                     0
                   -2.4645+17.6008i
       0
                                     -2.4645-17.6008i
       0
                        0
```

The first eigenvector is real and the other two vectors are complex conjugates of each other. All three vectors are normalized to have Euclidean length, norm(v,2), equal to one.

The matrix V*D*inv(V), which can be written more succinctly as V*D/V, is within round-off error of A. And, inv(V)*A*V, or $V\setminus A*V$, is within round-off error of D.

Multiple Eigenvalues

Some matrices do not have an eigenvector decomposition. These matrices are not diagonalizable. For example:

$$A = [\begin{array}{cccc} 1 & -2 & 1 \\ 0 & 1 & 4 \\ 0 & 0 & 3 \end{array}]$$

For this matrix

$$[V,D] = eig(A)$$

produces

V =

There is a double eigenvalue at $\lambda = 1$. The first and second columns of V are the same. For this matrix, a full set of linearly independent eigenvectors does not exist.

Schur Decomposition

Many advanced matrix computations do not require eigenvalue decompositions. They are based, instead, on the Schur decomposition

$$A = USU'$$

where U is an orthogonal matrix and S is a block upper-triangular matrix with 1-by-1 and 2-by-2 blocks on the diagonal. The eigenvalues are revealed by the diagonal elements and blocks of S, while

the columns of U provide an orthogonal basis, which has much better numerical properties than a set of eigenvectors.

For example, compare the eigenvalue and Schur decompositions of this defective matrix:

```
A = [6]
          12
    - 9
         -20
               -33
     4
           9
               15 1;
[V,D] = eig(A)
V =
  -0.4741 + 0.0000i -0.4082 - 0.0000i -0.4082 + 0.0000i
                                     0.8165 + 0.0000i
  -0.3386 + 0.0000i -0.4082 + 0.0000i -0.4082 - 0.0000i
D =
 -1.0000 + 0.0000i
                    0.0000 + 0.0000i
                                      0.0000 + 0.0000i
  0.0000 + 0.0000i 1.0000 + 0.0000i
                                      0.0000 + 0.0000i
  0.0000 + 0.0000i
                    0.0000 + 0.0000i
                                      1.0000 - 0.0000i
[U,S] = schur(A)
U =
  -0.4741
             0.6648
                      0.5774
   0.8127
            0.0782
                      0.5774
           -0.7430
  -0.3386
                      0.5774
S =
  -1.0000
            20.7846
                    -44.6948
            1.0000
        0
                    -0.6096
        0
             0.0000
                      1.0000
```

The matrix A is defective since it does not have a full set of linearly independent eigenvectors (the second and third columns of V are the same). Since not all columns of V are linearly independent, it has a large condition number of about $\sim 1e8$. However, schur is able to calculate three different basis vectors in U. Since U is orthogonal, cond(U) = 1.

The matrix S has the real eigenvalue as the first entry on the diagonal and the repeated eigenvalue represented by the lower right 2-by-2 block. The eigenvalues of the 2-by-2 block are also eigenvalues of A:

```
eig(S(2:3,2:3))
ans =

1.0000 + 0.0000i
1.0000 - 0.0000i
```

Singular Values

A singular value and corresponding singular vectors of a rectangular matrix A are, respectively, a scalar σ and a pair of vectors u and v that satisfy

$$Av = \sigma u$$
$$A^H u = \sigma v.$$

where A^H is the Hermitian transpose of A. The singular vectors u and v are typically scaled to have a norm of 1. Also, if u and v are singular vectors of A, then u and v are singular vectors of A as well.

The singular values σ are always real and nonnegative, even if A is complex. With the singular values in a diagonal matrix Σ and the corresponding singular vectors forming the columns of two orthogonal matrices U and V, you obtain the equations

$$AV = U\Sigma$$
$$A^H U = V\Sigma.$$

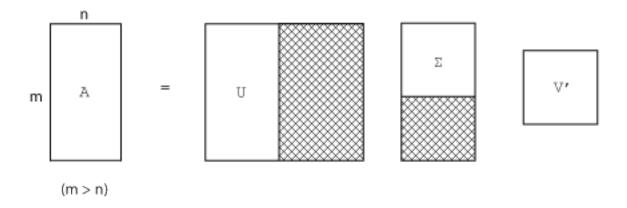
Since U and V are unitary matrices, multiplying the first equation by V^H on the right yields the singular value decomposition equation

$$A = U\Sigma V^H$$
.

The full singular value decomposition of an *m*-by-*n* matrix involves:

- m-by-m matrix U
- m-by-n matrix Σ
- n-by-n matrix V

In other words, U and V are both square, and Σ is the same size as A. If A has many more rows than columns (m > n), then the resulting m-by-m matrix U is large. However, most of the columns in U are multiplied by zeros in Σ . In this situation, the *economy-sized* decomposition saves both time and storage by producing an m-by-n U, an n-by-n Σ and the same V:



The eigenvalue decomposition is the appropriate tool for analyzing a matrix when it represents a mapping from a vector space into itself, as it does for an ordinary differential equation. However, the singular value decomposition is the appropriate tool for analyzing a mapping from one vector space

into another vector space, possibly with a different dimension. Most systems of simultaneous linear equations fall into this second category.

If A is square, symmetric, and positive definite, then its eigenvalue and singular value decompositions are the same. But, as A departs from symmetry and positive definiteness, the difference between the two decompositions increases. In particular, the singular value decomposition of a real matrix is always real, but the eigenvalue decomposition of a real, nonsymmetric matrix might be complex.

For the example matrix

```
A = [9 	 4 	 8 	 7];
```

the full singular value decomposition is

```
[U,S,V] = svd(A)
U =
   -0.6105
              0.7174
                         0.3355
   -0.6646
             -0.2336
                        -0.7098
   -0.4308
             -0.6563
                         0.6194
S =
   14.9359
              5.1883
         0
         0
V =
   -0.6925
              0.7214
```

-0.6925

You can verify that U*S*V' is equal to A to within round-off error. For this small problem, the economy size decomposition is only slightly smaller.

```
[U,S,V] = svd(A,"econ")

U =

-0.6105     0.7174
-0.6646     -0.2336
-0.4308     -0.6563

S =

14.9359     0
0     5.1883
```

-0.7214

```
-0.6925 0.7214
-0.7214 -0.6925
```

Again, U*S*V' is equal to A to within round-off error.

Batched SVD Calculation

If you need to decompose a large collection of matrices that have the same size, it is inefficient to perform all of the decompositions in a loop with svd. Instead, you can concatenate all of the matrices into a multidimensional array and use pagesvd to perform singular value decompositions on all of the array pages with a single function call.

Function	Usage
	Use pagesvd to perform singular value decompositions on the pages of a multidimensional array. This is an efficient way to perform SVD on a large collection of matrices that all have the same size.

For example, consider a collection of three 2-by-2 matrices. Concatenate the matrices into a 2-by-2-by-3 array with the cat function.

```
A = [0 -1; 1 0];

B = [-1 0; 0 -1];

C = [0 1; -1 0];

X = cat(3,A,B,C);
```

Now, use pagesvd to simultaneously perform the three decompositions.

```
[U,S,V] = pagesvd(X);
```

For each page of X, there are corresponding pages in the outputs U, S, and V. For example, the matrix A is on the first page of X, and its decomposition is given by U(:,:,1)*S(:,:,1)*V(:,:,1).

Low-Rank SVD Approximations

For large sparse matrices, using svd to calculate *all* of the singular values and singular vectors is not always practical. For example, if you need to know just a few of the largest singular values, then calculating all of the singular values of a 5000-by-5000 sparse matrix is extra work.

In cases where only a subset of the singular values and singular vectors are required, the svds and svdsketch functions are preferred over svd.

Function	Usage
svds	Use svds to calculate a rank-k approximation of the SVD. You can specify whether the subset of singular values should be the largest, the smallest, or the closest to a specific number. svds generally calculates the best possible rank-k approximation.

Function	Usage
svdsketch	Use svdsketch to calculate a partial SVD of the input matrix satisfying a specified tolerance. While svds requires that you specify the rank, svdsketch adaptively determines the rank of the matrix sketch based on the specified tolerance. The rank-k approximation that svdsketch ultimately uses satisfies the tolerance, but unlike svds, it is not guaranteed to be the best one possible.

For example, consider a 1000-by-1000 random sparse matrix with a density of about 30%.

```
n = 1000;
A = sprand(n,n,0.3);
```

The six largest singular values are

S = svds(A)

S =

130.2184

16.4358

16.4119

16.3688

16.3242

16.2838

Also, the six smallest singular values are

```
S = svds(A,6,"smallest")
```

S =

0.0740

0.0574

0.0388

0.0282 0.0131

0.0066

For smaller matrices that can fit in memory as a full matrix, full(A), using svd(full(A)) might still be quicker than svds or svdsketch. However, for truly large and sparse matrices, using svds or svdsketch becomes necessary.

LAPACK in MATLAB

LAPACK (Linear Algebra Package) is a library of routines that provides fast, robust algorithms for numerical linear algebra and matrix computations. Linear algebra functions and matrix operations in MATLAB are built on LAPACK, and they continue to benefit from the performance and accuracy of its routines.

A Brief History

MATLAB started its life in the late 1970s as an interactive calculator built on top of LINPACK and EISPACK, which were the state-of-the-art Fortran subroutine libraries for matrix computation of the time. For many years MATLAB used translations to C of about a dozen Fortran subroutines from LINPACK and EISPACK.

In the year 2000, MATLAB migrated to using LAPACK, which is the modern replacement for LINPACK and EISPACK. It is a large, multi-author, Fortran library for numerical linear algebra. LAPACK was originally intended for use on supercomputers because of its ability to operate on several columns of a matrix at a time. The speed of LAPACK routines is closely connected to the speed of the Basic Linear Algebra Subroutines (BLAS). The BLAS version is typically hardware-specific and highly optimized.

See Also

More About

"Call LAPACK and BLAS Functions"

External Websites

MATLAB Incorporates LAPACK

Matrix Exponentials

This example shows three of the 19 ways to compute the exponential of a matrix.

For background on the computation of matrix exponentials, see:

Moler, Cleve, and Charles Van Loan. "Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later." *SIAM Review* 45, no. 1 (January 2003): 3–49. https://doi.org/10.1137/S00361445024180.

Start by creating a matrix A.

```
A = \begin{bmatrix} 0 & 1 & 2; & 0.5 & 0 & 1; & 2 & 1 & 0 \end{bmatrix}
A = 3 \times 3
0 & 1.0000 & 2.0000
0.5000 & 0 & 1.0000
2.0000 & 1.0000 & 0
```

Asave = A;

Method 1: Scaling and Squaring

expmdemo1 is an implementation of algorithm 11.3.1 in the book:

Golub, Gene H. and Charles Van Loan. *Matrix Computations, 3rd edition*. Baltimore, MD: Johns Hopkins University Press, 1996.

```
% Scale A by power of 2 so that its norm is < 1/2 .
[f,e] = log2(norm(A, 'inf'));
s = max(0,e+1);
A = A/2^s;
% Pade approximation for exp(A)
X = A;
c = 1/2;
E = eye(size(A)) + c*A;
D = eye(size(A)) - c*A;
q = 6;
p = 1;
for k = 2:q
   c = c * (q-k+1) / (k*(2*q-k+1));
   X = A*X;
   cX = c*X;
   E = E + cX;
     D = D + cX;
   else
     D = D - cX;
   end
   p = \sim p;
end
E = D \setminus E;
```

```
% Undo scaling by repeated squaring
for k = 1:s
    E = E*E;
end

E1 = E

E1 = 3×3

    5.3091    4.0012    5.5778
    2.8088    2.8845    3.1930
    5.1737    4.0012    5.7132
```

Method 2: Taylor Series

expmdemo2 uses the classic definition for the matrix exponential given by the power series

$$e^A = \sum_{k=0}^{\infty} \frac{1}{k!} A^k.$$

 A^0 is the identity matrix with the same dimensions as A. As a practical numerical method, this approach is slow and inaccurate if norm(A) is too large.

```
A = Asave;
% Taylor series for exp(A)
E = zeros(size(A));
F = eye(size(A));
k = 1;
while norm(E+F-E,1) > 0
   E = E + F;
   F = A*F/k;
   k = k+1;
end
E2 = E
E2 = 3 \times 3
    5.3091
               4.0012
                         5.5778
    2.8088
               2.8845
                         3.1930
    5.1737
               4.0012
                         5.7132
```

Method 3: Eigenvalues and Eigenvectors

expmdemo3 assumes that the matrix has a full set of eigenvectors V such that $A = VDV^{-1}$. The matrix exponential can be calculated by exponentiating the diagonal matrix of eigenvalues:

$$e^A = Ve^DV^{-1}$$
.

As a practical numerical method, the accuracy is determined by the condition of the eigenvector matrix.

```
A = Asave;
```

Compare Results

For the matrix in this example, all three methods work equally well.

```
E = expm(Asave);
err1 = E - E1
err1 = 3 \times 3
10^{-14} \times
                       0.0888
    0.3553
             0.1776
            0.1332
                        -0.0444
    0.0888
                0 -0.2665
err2 = E - E2
err2 = 3 \times 3
10^{-14} \times
         0
                    0
                       -0.1776
   -0.0444
                   0 -0.0888
    0.1776
                   0
                        0.0888
err3 = E - E3
err3 = 3 \times 3
10^{-13} \times
   -0.0711
             -0.0444 -0.0799
             -0.0488 -0.0933
   -0.0622
   -0.0711
             -0.0533
                        -0.1066
```

Taylor Series Failure

For some matrices the terms in the Taylor series become very large before they go to zero. Consequently, expmdemo2 fails.

```
A = [-147 72; -192 93];
E1 = expmdemo1(A)
E1 = 2×2
-0.0996 0.0747
-0.1991 0.1494
```

```
E2 = expmdemo2(A)

E2 = 2×2
10<sup>6</sup> ×

-1.1985 -0.5908
-2.7438 -2.0442

E3 = expmdemo3(A)

E3 = 2×2
-0.0996 0.0747
-0.1991 0.1494
```

Eigenvalues and Eigenvectors Failure

Here is a matrix that does not have a full set of eigenvectors. Consequently, expmdemo3 fails.

See Also

expm

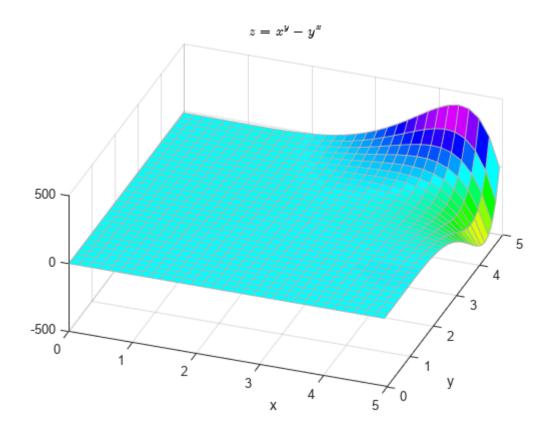
Graphical Comparison of Exponential Functions

This example shows an interesting graphical approach for discovering whether e^{π} is greater than π^e .

The question is: which is greater, e^{π} or π^e ? The easy way to find out is to type it directly at the MATLAB® command prompt. But another way to analyze the situation is to ask a more general question: what is the shape of the function $z(x, y) = x^y - y^x$?

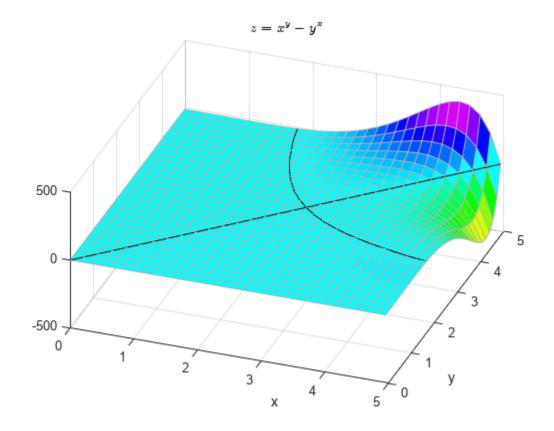
Here is a plot of z.

```
% Define the mesh
x = 0:0.16:5;
y = 0:0.16:5;
[xx,yy] = meshgrid(x,y);
% The plot
zz = xx.^yy-yy.^xx;
h = surf(x,y,zz);
h.EdgeColor = [0.7 0.7 0.7];
view(20,50);
colormap(hsv);
title('$z = x^y-y^x$','Interpreter','latex')
xlabel('x')
ylabel('y')
hold on
```



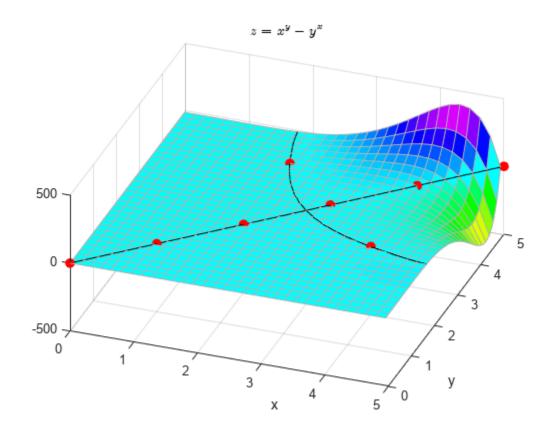
The solution of the equation $x^y - y^x = 0$ has a very interesting shape, and our original question is not easily solved by inspection. Here is a plot of the xy values that yield z = 0.

```
c = contourc(x,y,zz,[0 0]);
list1Len = c(2,1);
xContour = [c(1,2:1+list1Len) NaN c(1,3+list1Len:size(c,2))];
yContour = [c(2,2:1+list1Len) NaN c(2,3+list1Len:size(c,2))];
% Note that the NAN above prevents the end of the first contour line from being
% connected to the beginning of the second line
line(xContour,yContour,'Color','k');
```



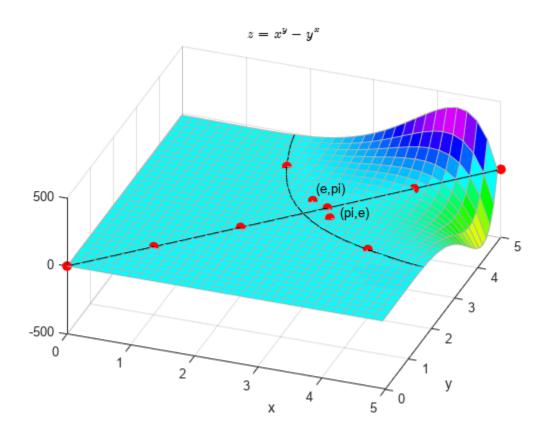
Some combinations of x and y along the black curve are integers. This next plot is of the integer solutions to the equation $x^y - y^x = 0$. Notice that $2^4 = 4^2$ is the *only* integer solution where $x \neq y$.

```
plot([0:5 2 4],[0:5 4 2],'r.','MarkerSize',25);
```



Finally, plot the points (π, e) and (e, π) on the surface. The result shows that e^{π} is indeed larger than π^e (though not by much).

```
e = exp(1);
plot([e pi],[pi e],'r.','MarkerSize',25);
plot([e pi],[pi e],'y.','MarkerSize',10);
text(e,3.3,'(e,pi)','Color','k', ...
    'HorizontalAlignment','left','VerticalAlignment','bottom');
text(3.3,e,'(pi,e)','Color','k','HorizontalAlignment','left',...
    'VerticalAlignment','bottom');
hold off;
```



Verify the results.

e = exp(1);
e^pi
ans = 23.1407
pi^e
ans = 22.4592

See Also

exp|pi

Basic Matrix Operations

This example shows basic techniques and functions for working with matrices in the MATLAB® language.

First, let's create a simple vector with 9 elements called a.

```
a = [1  2  3  4  6  4  3  4  5]
a = 1 \times 9
1  2  3  4  6  4  3  4  5
```

Now let's add 2 to each element of our vector, a, and store the result in a new vector.

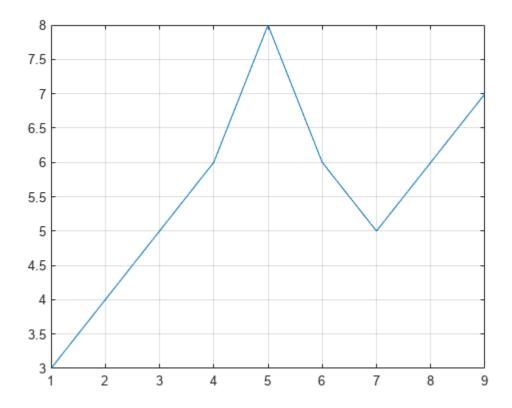
Notice how MATLAB requires no special handling of vector or matrix math.

```
b = a + 2
b = 1 \times 9

3 4 5 6 8 6 5 6 7
```

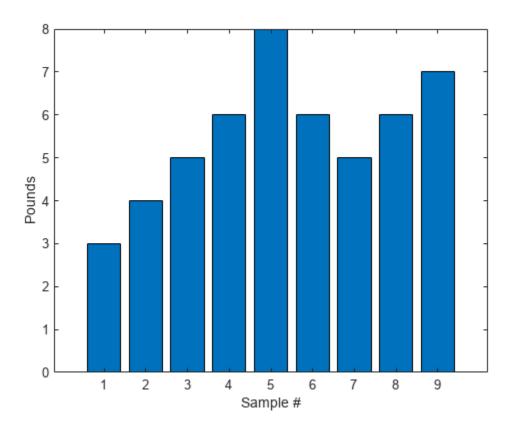
Creating graphs in MATLAB is as easy as one command. Let's plot the result of our vector addition with grid lines.

```
plot(b) grid on
```



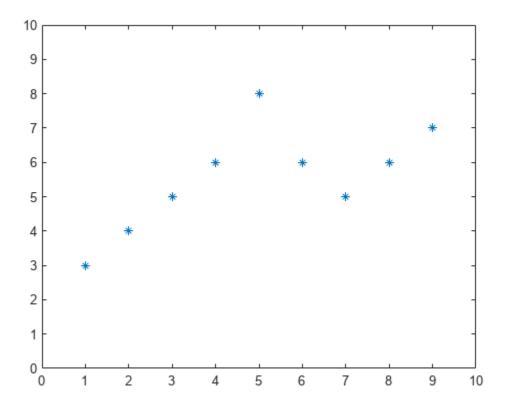
MATLAB can make other graph types as well, with axis labels.

```
bar(b)
xlabel('Sample #')
ylabel('Pounds')
```



MATLAB can use symbols in plots as well. Here is an example using stars to mark the points. MATLAB offers a variety of other symbols and line types.

```
plot(b,'*')
axis([0 10 0 10])
```



One area in which MATLAB excels is matrix computation.

Creating a matrix is as easy as making a vector, using semicolons (;) to separate the rows of a matrix.

$$A = [1 \ 2 \ 0; \ 2 \ 5 \ -1; \ 4 \ 10 \ -1]$$

 $A = 3 \times 3$

We can easily find the transpose of the matrix A.

$$B = A'$$

 $B = 3 \times 3$

Now let's multiply these two matrices together.

Note again that MATLAB doesn't require you to deal with matrices as a collection of numbers. MATLAB knows when you are dealing with matrices and adjusts your calculations accordingly.

$$C = A * B$$
 $C = 3 \times 3$
5 12 24

Instead of doing a matrix multiply, we can multiply the corresponding elements of two matrices or vectors using the .* operator.

$$C = A \cdot * B$$

$$C = 3 \times 3$$

Let's use the matrix A to solve the equation, A*x = b. We do this by using the \ (backslash) operator.

$$b = [1;3;5]$$

$$b = 3 \times 1$$

1 3 5

$$x = A b$$

$$x = 3 \times 1$$

1 0 -1

Now we can show that A*x is equal to b.

$$r = A*x - b$$

$$r = 3 \times 1$$

0

0

0

MATLAB has functions for nearly every type of common matrix calculation.

There are functions to obtain eigenvalues ...

eig(A)

ans =
$$3 \times 1$$

```
3.7321
0.2679
1.0000
```

... as well as the singular values.

```
svd(A)
ans = 3 \times 1
12.3171
0.5149
0.1577
```

The "poly" function generates a vector containing the coefficients of the characteristic polynomial.

The characteristic polynomial of a matrix A is

```
det(\lambda I - A)
p = round(poly(A))
p = 1 \times 4
1 -5 5 -1
```

We can easily find the roots of a polynomial using the roots function.

These are actually the eigenvalues of the original matrix.

```
roots(p) ans = 3 \times 1
```

3.7321 1.0000 0.2679

MATLAB has many applications beyond just matrix computation.

To convolve two vectors ...

```
q = conv(p,p)

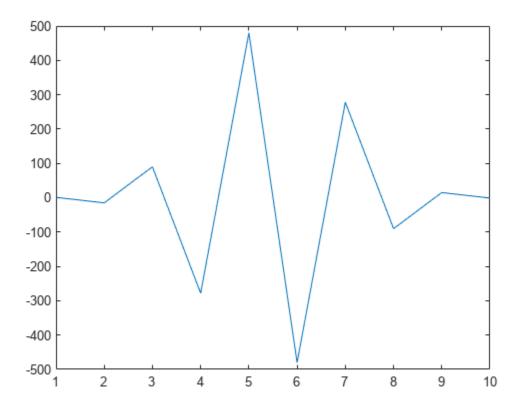
q = 1 \times 7

1 -10 35 -52 35 -10 1
```

... or convolve again and plot the result.

```
r = conv(p,q)
r = 1 \times 10
```

plot(r);



At any time, we can get a listing of the variables we have stored in memory using the who or whos command.

whos

Name	Size	Bytes	Class	Attributes
A B	3x3 3x3	72 72	double double	
a ans	3x3 1x9 3x1	72 72 24	double double double	
b	3x1 1x4	24	double double	
p q	1x7	56	double	
r X	1x10 3x1	80 24	double double	

You can get the value of a particular variable by typing its name.

Α

 $A = 3 \times 3$

You can have more than one statement on a single line by separating each statement with commas or semicolons.

If you don't assign a variable to store the result of an operation, the result is stored in a temporary variable called ans.

```
sqrt(-1)
ans = 0.0000 + 1.0000i
```

As you can see, MATLAB easily deals with complex numbers in its calculations.

See Also

More About

• "Array vs. Matrix Operations"

Determine Whether Matrix Is Symmetric Positive Definite

This topic explains how to use the chol and eig functions to determine whether a matrix is symmetric positive definite (a symmetric matrix with all positive eigenvalues).

Method 1: Attempt Cholesky Factorization

The most efficient method to check whether a matrix is symmetric positive definite is to attempt to use chol on the matrix. If the factorization fails, then the matrix is not symmetric positive definite.

Create a square symmetric matrix and use a try/catch block to test whether chol(A) succeeds.

```
A = [1 -1 0; -1 5 0; 0 0 7]
A = .3 \times .3
        -1 0
5 0
    1
    - 1
     (-)
try chol(A)
    disp('Matrix is symmetric positive definite.')
    disp('Matrix is not symmetric positive definite')
end
ans = 3 \times 3
                             0
    1.0000 -1.0000
         0 2.0000
                             0
                 0
                        2.6458
```

Matrix is symmetric positive definite.

The drawback of this method is that it cannot be extended to also check whether the matrix is symmetric positive semi-definite (where the eigenvalues can be positive or zero).

Method 2: Check Eigenvalues

While it is less efficient to use eig to calculate all of the eigenvalues and check their values, this method is more flexible since you can also use it to check whether a matrix is symmetric positive semi-definite. Still, for small matrices the difference in computation time between the methods is negligible to check whether a matrix is symmetric positive definite.

This method requires that you use issymmetric to check whether the matrix is symmetric before performing the test (if the matrix is not symmetric, then there is no need to calculate the eigenvalues).

```
tf = issymmetric(A)
tf = logical
    1

d = eig(A)
```

```
d = 3×1
     0.7639
     5.2361
     7.0000

isposdef = all(d > 0)
isposdef = logical
     1
```

You can extend this method to check whether a matrix is symmetric positive semi-definite with the command all($d \ge 0$).

Numerical Considerations

The methods outlined here might give different results for the same matrix. Since both calculations involve round-off errors, each algorithm checks the definiteness of a matrix that is slightly different from A. In practice, the use of a tolerance is a more robust comparison method, since eigenvalues can be numerically zero within machine precision and be slightly positive or slightly negative.

For example, if a matrix has an eigenvalue on the order of eps, then using the comparison isposdef = all(d > 0) returns true, even though the eigenvalue is numerically zero and the matrix is better classified as symmetric positive *semi*-definite.

To perform the comparison using a tolerance, you can use the modified commands

```
tf = issymmetric(A)
d = eig(A)
isposdef = all(d > tol)
issemidef = all(d > -tol)
```

The tolerance defines a radius around zero, and any eigenvalues within that radius are treated as zeros. A good choice for the tolerance in most cases is length(d)*eps(max(d)), which takes into account the magnitude of the largest eigenvalue.

See Also

chol|eig

More About

• "Factorizations" on page 2-20

Image Compression with Low-Rank SVD

This example shows how to use svdsketch to compress an image. svdsketch uses a low-rank matrix approximation to preserve important features of the image, while filtering out less important features. As the tolerance used with svdsketch increases in magnitude, more features are filtered out, changing the level of detail in the image.

Load Image

Load the image street1.jpg, which is a picture of a city street. The 3-D matrix that forms this image is uint8, so convert the image to a grayscale matrix. View the image with an annotation of the original matrix rank.

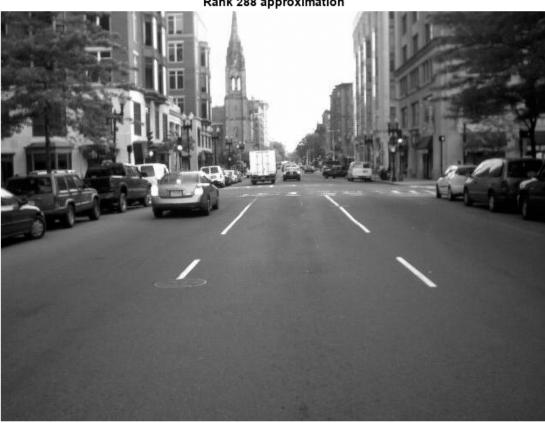
```
A = imread('street1.jpg');
A = rgb2gray(A);
imshow(A)
title(['Original (',sprintf('Rank %d)',rank(double(A)))])
```



Compress Image

Use svdsketch to calculate a low-rank matrix that approximates A within a tolerance of 1e-2. Form the low-rank matrix by multiplying the SVD factors returned by svdsketch, convert the result to uint8, and view the resulting image.

```
[U1,S1,V1] = svdsketch(double(A),1e-2);
Anew1 = uint8(U1*S1*V1');
imshow(uint8(Anew1))
title(sprintf('Rank %d approximation', size(S1,1)))
```



Rank 288 approximation

svdsketch produces a rank 288 approximation, which results in some minor graininess in some of the boundary lines of the image.

Now, compress the image a second time using a tolerance of 1e-1. As the magnitude of the tolerance increases, the rank of the approximation produced by svdsketch generally decreases.

```
[U2,S2,V2] = svdsketch(double(A),1e-1);
Anew2 = uint8(U2*S2*V2');
imshow(Anew2)
title(sprintf('Rank %d approximation', size(S2,1)))
```



Rank 48 approximation

This time, svdsketch produces a rank 48 approximation. Most of the major aspects of the image are still visible, but the additional compression increases the blurriness.

Limit Subspace Size

svdsketch adaptively determines what rank to use for the matrix sketch based on the specified
tolerance. However, you can use the MaxSubspaceDimension name-value pair to specify the
maximum subspace size that should be used to form the matrix sketch. This option can produce
matrices that do not satisfy the tolerance, since the subspace you specify might be too small. In these
cases, svdsketch returns a matrix sketch with the maximum allowed subspace size.

Use svdsketch with a tolerance of 1e-1 and a maximum subspace size of 15. Specify a fourth output to return the relative approximation error.

```
[U3,S3,V3,apxErr] = svdsketch(double(A),le-1,'MaxSubspaceDimension',15);
```

Compare the relative approximation error of the result with the specified tolerance. apxErr contains one element since svdsketch only needs one iteration to compute the answer.

```
apxErr <= 1e-1
```

```
ans = logical
```

The result indicates that the matrix sketch does not satisfy the specified tolerance.

View the heavily compressed rank 15 image.

```
Anew3 = uint8(U3*S3*V3');
imshow(Anew3)
title(sprintf('Rank %d approximation', size(S3,1)))
```



Rank 15 approximation

Compare Results

Finally, view all of the images side-by-side for comparison.

```
tiledlayout(2,2,'TileSpacing','Compact')
nexttile
imshow(A)
title('Original')
nexttile
imshow(Anew1)
title(sprintf('Rank %d approximation',size(S1,1)))
nexttile
```

```
imshow(Anew2)
title(sprintf('Rank %d approximation', size(S2,1)))
nexttile
imshow(Anew3)
title(sprintf('Rank %d approximation', size(S3,1)))
```

Original



Rank 288 approximation



Rank 48 approximation



Rank 15 approximation



See Also

svd | svds | svdsketch

More About

- "Singular Values" on page 2-33
- "Resample Image with Gridded Interpolation" on page 8-53

Random Numbers

- "Why Do Random Numbers Repeat After Startup?" on page 3-2
- "Create Arrays of Random Numbers" on page 3-3
- "Random Numbers Within a Specific Range" on page 3-6
- "Random Integers" on page 3-7
- "Random Numbers from Normal Distribution with Specific Mean and Variance" on page 3-8
- "Random Numbers Within a Sphere" on page 3-9
- "Generate Random Numbers That Are Repeatable" on page 3-11
- "Generate Random Numbers That Are Different" on page 3-14
- "Managing the Global Stream Using RandStream" on page 3-16
- "Creating and Controlling a Random Number Stream" on page 3-19
- "Multiple Streams" on page 3-28
- "Replace Discouraged Syntaxes of rand and randn" on page 3-32
- "Controlling Random Number Generation" on page 3-36

Why Do Random Numbers Repeat After Startup?

All the random number functions, rand, randn, randi, and randperm, draw values from a shared random number generator. Every time you start MATLAB, the generator resets itself to the same state. Therefore, a command such as rand(2,2) returns the same result any time you execute it immediately following startup. Also, any script or function that calls the random number functions returns the same result whenever you restart.

If you want to avoid repeating the same random number arrays when MATLAB restarts, then execute the command,

```
rng('shuffle');
```

before calling rand, randi, or randperm. This command ensures that you do not repeat a result from a previous MATLAB session.

If you want to repeat a result that you got at the start of a MATLAB session without restarting, you can reset the generator to the startup state at any time using

```
rng('default');
```

When you execute rng('default'), the ensuing random number commands return results that match the output of a new MATLAB session. For example,

```
rng('default');
A = rand(2,2)
A =
    0.8147    0.1270
    0.9058    0.9134
```

The values in A match the output of rand(2,2) whenever you restart MATLAB.

See Also

rng

Create Arrays of Random Numbers

In this section... "Random Number Functions" on page 3-3 "Random Number Generators" on page 3-4 "Random Number Data Types" on page 3-4

MATLAB uses algorithms to generate pseudorandom and pseudoindependent numbers. These numbers are not strictly random and independent in the mathematical sense, but they pass various statistical tests of randomness and independence, and their calculation can be repeated for testing or diagnostic purposes.

The rand, randi, randn, and randperm functions are the primary functions for creating arrays of random numbers. The rng function allows you to control the seed and algorithm that generates random numbers.

Random Number Functions

There are four fundamental random number functions: rand, randi, randn, and randperm. The rand function returns floating-point numbers between 0 and 1 that are drawn from a uniform distribution. For example:

```
rng('default')
r1 = rand(1000,1);
```

r1 is a 1000-by-1 column vector containing real floating-point numbers drawn from a uniform distribution. All the values in r1 are in the open interval (0, 1). A histogram of these values is roughly flat, which indicates a fairly uniform sampling of numbers.

The randi function returns double integer values drawn from a discrete uniform distribution. For example,

```
r2 = randi(10, 1000, 1);
```

r2 is a 1000-by-1 column vector containing integer values drawn from a discrete uniform distribution whose range is in the close interval [1, 10]. A histogram of these values is roughly flat, which indicates a fairly uniform sampling of integers between 1 and 10.

The randn function returns arrays of real floating-point numbers that are drawn from a standard normal distribution. For example:

```
r3 = randn(1000,1);
```

r3 is a 1000-by-1 column vector containing numbers drawn from a standard normal distribution. A histogram of r3 looks like a roughly normal distribution whose mean is 0 and standard deviation is 1.

You can use the randperm function to create a double array of random integer values that have no repeated values. For example,

```
r4 = randperm(15,5);
```

r4 is a 1-by-5 array containing integers randomly selected from the range [1, 15]. Unlike randi, which can return an array containing repeated values, the array returned by randperm has no repeated values.

Successive calls to any of these functions return different results. This behavior is useful for creating several different arrays of random values.

Random Number Generators

MATLAB offers several generator algorithm options, which are summarized in the table.

Value	Generator Name	Generator Keyword
'twister'	Mersenne Twister (used by default stream at MATLAB startup)	mt19937ar
'simdTwister'	SIMD-oriented Fast Mersenne Twister	dsfmt19937
'combRecursive'	Combined multiple recursive	mrg32k3a
'multFibonacci'	Multiplicative Lagged Fibonacci	mlfg6331_64
'philox'	Philox 4x32 generator with 10 rounds	philox4x32_10
'threefry'	Threefry 4x64 generator with 20 rounds	threefry4x64_20
'v4'	Legacy MATLAB version 4.0 generator	mcg16807
'v5uniform'	Legacy MATLAB version 5.0 uniform generator	swb2712
'v5normal'	Legacy MATLAB version 5.0 normal generator	shr3cong

Use the rng function to set the seed and generator used by the rand, randi, randn, and randperm functions. For example, rng(0, 'twister') reset the generator to its default state. To avoid repetition of random number arrays when MATLAB restarts, see "Why Do Random Numbers Repeat After Startup?" on page 3-2

For more information about controlling the random number generator's state to repeat calculations using the same random numbers, or to guarantee that different random numbers are used in repeated calculations, see "Controlling Random Number Generation" on page 3-36.

Random Number Data Types

rand and randn functions generate values in double precision by default.

```
rng('default')
A = rand(1,5);
class(A)
ans = 'double'
To specify the class as double explicitly:
rng('default')
B = rand(1,5,'double');
class(B)
```

```
ans = 'double'
isequal(A,B)
ans =
1
```

rand and randn can also generate values in single precision.

```
rng('default')
A = rand(1,5,'single');
class(A)
ans = 'single'
```

The values are the same as if you had cast the double precision values from the previous example. The random stream that the functions draw from advances the same way regardless of what class of values is returned.

A,B

```
A = 0.8147 0.9058 0.1270 0.9134 0.6324
B = 0.8147 0.9058 0.1270 0.9134 0.6324
```

randi supports both integer types and single or double precision.

```
A = randi([1 10],1,5,'double');
class(A)
ans = 'double'
B = randi([1 10],1,5,'uint8');
class(B)
ans = 'uint8'
```

See Also

rng | rand | randi | randn | randperm

Related Examples

- "Controlling Random Number Generation" on page 3-36
- "Generate Random Numbers That Are Repeatable" on page 3-11
- "Generate Random Numbers That Are Different" on page 3-14
- "Random Numbers Within a Specific Range" on page 3-6
- "Random Integers" on page 3-7
- "Random Numbers from Normal Distribution with Specific Mean and Variance" on page 3-8

Random Numbers Within a Specific Range

This example shows how to create an array of random floating-point numbers that are drawn from a uniform distribution in the open interval (50, 100).

By default, rand returns normalized values (between 0 and 1) that are drawn from a uniform distribution. To change the range of the distribution to a new range, (a, b), multiply each value by the width of the new range, (b - a) and then shift every value by a.

First, initialize the random number generator to make the results in this example repeatable.

```
rng(0,'twister');
```

Create a vector of 1000 random values. Use the rand function to draw the values from a uniform distribution in the open interval, (50,100).

```
a = 50;

b = 100;

r = (b-a).*rand(1000,1) + a;
```

Verify the values in r are within the specified range.

```
r_range = [min(r) max(r)]
r_range =
    50.0261    99.9746
```

The result is in the open interval, (50,100).

Note Some combinations of a and b make it theoretically possible for your results to include a or b. In practice, this is extremely unlikely to happen.

See Also

rng

Related Examples

- "Random Numbers from Normal Distribution with Specific Mean and Variance" on page 3-8
- "Random Numbers Within a Sphere" on page 3-9
- "Create Arrays of Random Numbers" on page 3-3

Random Integers

This example shows how to create an array of random integer values that are drawn from a discrete uniform distribution on the set of numbers -10, -9,...,9, 10.

The simplest randi syntax returns double-precision integer values between 1 and a specified value, imax. To specify a different range, use the imin and imax arguments together.

First, initialize the random number generator to make the results in this example repeatable.

```
rng(0,'twister');
```

Create a 1-by-1000 array of random integer values drawn from a discrete uniform distribution on the set of numbers -10, -9,...,9, 10. Use the syntax, randi([imin imax],m,n).

```
r = randi([-10 \ 10], 1, 1000);
```

Verify that the values in r are within the specified range.

```
[rmin,rmax] = bounds(r)
rmin = -10
rmax = 10
```

See Also

rng | randi

Related Examples

• "Create Arrays of Random Numbers" on page 3-3

Random Numbers from Normal Distribution with Specific Mean and Variance

This example shows how to create an array of random floating-point numbers that are drawn from a normal distribution having a mean of 500 and variance of 25.

The randn function returns a sample of random numbers from a normal distribution with mean 0 and variance 1. The general theory of random variables states that if x is a random variable whose mean is μ_x and variance is σ_x^2 , then the random variable, y, defined by y = ax + b, where a and b are constants, has mean $\mu_y = a\mu_x + b$ and variance $\sigma_y^2 = a^2\sigma_x^2$. You can apply this concept to get a sample of normally distributed random numbers with mean 500 and variance 25.

First, initialize the random number generator to make the results in this example repeatable.

```
rng(0,'twister');
```

Create a vector of 1000 random values drawn from a normal distribution with a mean of 500 and a standard deviation of 5.

```
a = 5;
b = 500;
y = a.*randn(1000,1) + b;
```

Calculate the sample mean, standard deviation, and variance.

```
stats = [\text{mean}(y) \text{ std}(y) \text{ var}(y)]

stats = 1 \times 3

499.8368 4.9948 24.9483
```

The mean and variance are not 500 and 25 exactly because they are calculated from a sampling of the distribution.

See Also

rng | randn

- "Random Numbers Within a Specific Range" on page 3-6
- "Random Numbers Within a Sphere" on page 3-9
- "Create Arrays of Random Numbers" on page 3-3

Random Numbers Within a Sphere

This example shows how to create random points within the volume of a sphere, as described by Knuth [1]. The sphere in this example is centered at the origin and has a radius of 3.

One way to create points inside a sphere is to specify them in spherical coordinates. Then you can convert them to Cartesian coordinates to plot them.

First, initialize the random number generator to make the results in this example repeatable.

```
rng(0, 'twister')
```

Calculate an elevation angle for each point in the sphere. These values are in the open interval, $(-\pi/2, \pi/2)$, but are not uniformly distributed.

```
rvals = 2*rand(1000,1)-1;
elevation = asin(rvals);
```

Create an azimuth angle for each point in the sphere. These values are uniformly distributed in the open interval, $(0, 2\pi)$.

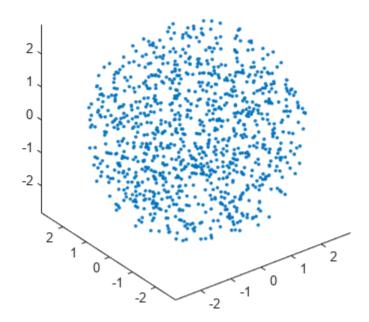
```
azimuth = 2*pi*rand(1000,1);
```

Create a radius value for each point in the sphere. These values are in the open interval, (0, 3), but are not uniformly distributed.

```
radii = 3*(rand(1000,1).^(1/3));
```

Convert to Cartesian coordinates and plot the result.

```
[x,y,z] = sph2cart(azimuth,elevation,radii);
figure
plot3(x,y,z,'.')
axis equal
```



If you want to place random numbers on the surface of the sphere, then specify a constant radius value to be the last input argument to sph2cart. In this case, the value is 3.

[x,y,z] = sph2cart(azimuth,elevation,3);

References

[1] Knuth, D. *The Art of Computer Programming*. Vol. 2, 3rd ed. Reading, MA: Addison-Wesley Longman, 1998, pp. 134–136.

See Also

rng | rand | sph2cart

- "Random Numbers Within a Specific Range" on page 3-6
- "Random Numbers from Normal Distribution with Specific Mean and Variance" on page 3-8
- "Create Arrays of Random Numbers" on page 3-3

Generate Random Numbers That Are Repeatable

Specify the Seed

This example shows how to repeat arrays of random numbers by specifying the seed first. Every time you initialize the generator using the same seed, you always get the same result.

First, initialize the random number generator to make the results in this example repeatable.

```
rng('default');
```

Now, initialize the generator using a seed of 1.

```
rng(1);
```

Then, create an array of random numbers.

```
A = rand(3,3)

A = 

0.4170    0.3023    0.1863    0.7203    0.1468    0.3456    0.0001    0.0923    0.3968
```

Repeat the same command.

```
A = rand(3,3)

A =

0.5388    0.2045    0.6705
0.4192    0.8781    0.4173
0.6852    0.0274    0.5587
```

The first call to rand changed the state of the generator, so the second result is different.

Now, reinitialize the generator using the same seed as before. Then reproduce the first matrix, A.

```
rng(1);
A = rand(3,3)

A =

0.4170  0.3023  0.1863
0.7203  0.1468  0.3456
0.0001  0.0923  0.3968
```

In some situations, setting the seed alone will not guarantee the same results. This is because the generator that the random number functions draw from might be different than you expect when your code executes. For long-term repeatability, specify the seed and the generator type together.

For example, the following code sets the seed to 1 and the generator to Mersenne Twister.

```
rng(1,'twister');
```

Set the seed and generator type together when you want to:

- Ensure that the behavior of code you write today returns the same results when you run that code in a future MATLAB release.
- Ensure that the behavior of code you wrote in a previous MATLAB release returns the same results using the current release.
- Repeat random numbers in your code after running someone else's random number code.

See the rng reference page for a list of available generators.

Save and Restore the Generator Settings

This example shows how to create repeatable arrays of random numbers by saving and restoring the generator settings. The most common reason to save and restore generator settings is to reproduce the random numbers generated at a specific point in an algorithm or iteration. For example, you can use the generator settings as an aid in debugging. Unlike reseeding, which reinitializes the generator, this approach allows you to save and restore the generator settings at any point.

First, initialize the random number generator to make the results in this example repeatable.

```
rng(1, 'twister');
```

Create an array of random integer values between 1 and 10.

```
A = randi(10,3,3)

A = 3 \times 3

5 4 2

8 2 4

1 1 4
```

The first call to randi changed the state of the generator. Save the generator settings after the first call to randi in a structure s.

```
s = rng;
```

Create another array of random integer values between 1 and 10.

```
A = randi(10,3,3)

A = 3 \times 3

6 3 7

5 9 5

7 1 6
```

Now, return the generator to the previous state stored in s and reproduce the second array A.

```
rng(s);

A = randi(10,3,3)

A = 3 \times 3

6 3 7

5 9 5
```

7 1 6

See Also

rng

- "Generate Random Numbers That Are Different" on page 3-14
- "Controlling Random Number Generation" on page 3-36

Generate Random Numbers That Are Different

This example shows how to avoid repeating the same random number arrays when MATLAB restarts. This technique is useful when you want to combine results from the same random number commands executed at different MATLAB sessions.

All the random number functions, rand, randn, randi, and randperm, draw values from a shared random number generator. Every time you start MATLAB, the generator resets itself to the same state. Therefore, a command such as rand(2,2) returns the same result any time you execute it immediately following startup. Also, any script or function that calls the random number functions returns the same result whenever you restart.

One way to get different random numbers is to initialize the generator using a different seed every time. Doing so ensures that you don't repeat results from a previous session.

Execute the rng('shuffle') command once in your MATLAB session before calling any of the random number functions.

```
rng('shuffle')
```

You can execute this command in a MATLAB Command Window, or you can add it to your startup file, which is a special script that MATLAB executes every time you restart.

Now, execute a random number command.

```
A = rand(2,2);
```

Each time you call rng('shuffle'), it reseeds the generator using a different seed based on the current time.

Note Frequent reseeding of the generator does not improve the statistical properties of the output and does not make the output more random in any real sense. Reseeding can be useful when you restart MATLAB or before you run a large calculation involving random numbers. However, reseeding the generator too frequently within a session is not a good idea because the statistical properties of your random numbers can be adversely affected.

Alternatively, specify different seeds explicitly in different MATLAB sessions. For example, generate random numbers in one MATLAB session.

```
rng(1);
A = rand(2,2);
```

Use different seeds to generate random numbers in another MATLAB session.

```
rng(2);
B = rand(2,2);
```

Arrays A and B are different because the generator is initialized with a different seed before each call to the rand function.

To generate multiple independent streams that are guaranteed to not overlap, and for which tests that demonstrate independence of the values between streams have been carried out, you can use

RandStream.create. For more information about generating multiple streams, see "Multiple Streams" on page 3-28.

See Also

rng

- "Generate Random Numbers That Are Repeatable" on page 3-11
- "Controlling Random Number Generation" on page 3-36
- "Startup Options in MATLAB Startup File"

Managing the Global Stream Using RandStream

The rand, randi, and randperm functions draw random numbers from an underlying random number stream, called the *global stream*. The global stream is a RandStream object. A simple way to control the global stream is to use the rng function. For more comprehensive control, the RandStream class enables you to create a separate stream from the global stream, get a handle to the global stream, and control random number generation.

Use rng to set the random number generator to the default seed (0) and algorithm (Mersenne Twister). Save the generator settings.

```
rng('default')
s = rng

s = struct with fields:
    Type: 'twister'
    Seed: 0
    State: [625x1 uint32]
```

Create a 1-by-6 row vector of uniformly distributed random values between 0 and 1.

```
x = rand(1,6)

x = 1 \times 6

0.8147 0.9058 0.1270 0.9134 0.6324 0.0975
```

Use RandStream.getGlobalStream to return a handle to the global stream, that is, the current global stream that rand generates random numbers from. If you use RandStream.getGlobalStream to get a handle to the global stream, you can see the changes you made to the global stream using rng.

Change the generator seed and algorithm, and create a new random row vector. Show the current global stream that rand generates random numbers from.

```
 \begin{array}{l} \operatorname{rng}(1, \operatorname{'philox'}) \\ \operatorname{xnew} = \operatorname{rand}(1, 6) \\ \\ \operatorname{xnew} = 1 \times 6 \\ \\ \operatorname{0.5361} \quad \operatorname{0.2319} \quad \operatorname{0.7753} \quad \operatorname{0.2390} \quad \operatorname{0.0036} \quad \operatorname{0.5262} \\ \\ \operatorname{globalStream} = \operatorname{RandStream.getGlobalStream} \\ \\ \operatorname{globalStream} = \\ \operatorname{philox} 4 \times 32 \ 10 \quad \operatorname{random stream} \quad (\operatorname{current global stream}) \\ \end{array}
```

```
Seed: 1
NormalTransform: Inversion
```

Next, restore the original generator settings and create a random vector. The result matches the original row vector x created with the default generator.

```
rng(s)

xold = rand(1,6)

xold = 1 \times 6

0.8147 0.9058 0.1270 0.9134 0.6324 0.0975
```

By default, random number generation functions, such as rand, use the global random number stream. To specify a different stream, create another RandStream object. Pass it as the first input argument to rand. For example, create a 1-by-6 vector of random numbers using the SIMD-oriented Fast Mersenne Twister.

When you call the rand function with myStream as the first input argument, it draws numbers from myStream and does not affect the results of the global stream.

If you want to set myStream as a global stream, you can use the RandStream.setGlobalStream object function.

In many cases, the rng function is all you need to control the global stream, but the RandStream class allows control over some advanced features, such as the choice of algorithm used for normal random values.

For example, create a RandStream object and specify the transformation algorithm to generate normally distributed pseudorandom values when using randn. Generate normally distributed pseudorandom values using the Polar transformation algorithm, instead of the default Ziggurat transformation algorithm.

Set myStream as the global stream. Create 6 random numbers with normal distribution from the global stream.

```
RandStream.setGlobalStream(myStream) randn(1,6) ans = 1 \times 6 0.2543 -0.7733 -1.7416 0.3686 0.5965 -0.0191
```

See Also

rng | RandStream

- "Multiple Streams" on page 3-28
- "Creating and Controlling a Random Number Stream" on page 3-19
- "Controlling Random Number Generation" on page 3-36
- "Create Arrays of Random Numbers" on page 3-3

Creating and Controlling a Random Number Stream

```
"Substreams" on page 3-19

"Choosing a Random Number Generator" on page 3-21

"Configuring a Stream" on page 3-24

"Restore State of Random Number Generator to Reproduce Output" on page 3-25
```

The RandStream class allows you to create a random number stream. This is useful for several reasons:

- You can generate random values without affecting the state of the global stream.
- You can separate sources of randomness in a simulation.
- You can use a generator that is configured differently than the one MATLAB software uses at startup.

With a RandStream object, you can create your own stream, set the writable properties, and use the stream to generate random numbers. You can control the stream you create the same way you control the global stream. You can even replace the global stream with the stream you create.

To create a stream, use the RandStream function.

```
myStream = RandStream('mlfg6331_64');
rand(myStream,1,5)

ans =
    0.6986    0.7413    0.4239    0.6914    0.7255
```

The random stream myStream acts separately from the global stream. If you call the rand, randn, randi, and randperm functions with myStream as the first argument, they draw from the stream you created. If you call rand, randn, randi, and randperm without myStream, they draw from the global stream.

You can make myStream the global stream using the RandStream.setGlobalStream method.

Substreams

You can use substreams to get different results that are statistically independent from a stream. Unlike seeds, where the locations along the sequence of random numbers are not exactly known, the

spacing between substreams is known, so any chance of overlap can be eliminated. In short, substreams are a more-controlled way to do many of the same things that seeds have traditionally been used for. Substreams are also a more lightweight solution than parallel streams.

Substreams provide a quick and easy way to ensure that you get different results from the same code at different times. To use the Substream property of a RandStream object, create a stream using a generator that supports substreams. For a list of generator algorithms that support substreams and their properties, see the table in the next section. For example, generate several random numbers in a loop.

```
mvStream = RandStream('mlfq6331 64');
RandStream.setGlobalStream(myStream)
for i = 1:5
    myStream.Substream = i;
    z = rand(1,i)
end
    0.6986
z =
    0.9230
              0.2489
    0.0261
              0.2530
                         0.0737
z =
    0.3220
              0.7405
                         0.1983
                                   0.1052
    0.2067
              0.2417
                         0.9777
                                   0.5970
                                              0.4187
```

In another loop, you can generate random values that are independent from the first set of 5 iterations.

```
for i = 6:10
    myStream.Substream = i;
    z = rand(1,11-i)
end
z =
    0.2650
               0.8229
                         0.2479
                                    0.0247
                                               0.4581
z =
    0.3963
               0.7445
                         0.7734
                                    0.9113
    0.2758
               0.3662
                         0.7979
    0.6814
               0.5150
z =
    0.5247
```

Substreams are useful in serial computation. Substreams can recreate all or part of a simulation by returning to a particular checkpoint in stream. For example, you can return to the 6th substream in the loop. The result contains the same values as the 6th output above.

```
myStream.Substream = 6;
z = rand(1,5)
z =
    0.2650    0.8229    0.2479    0.0247    0.4581
```

Choosing a Random Number Generator

MATLAB offers several generator algorithm options. The table summarizes the key properties of the available generator algorithms and the keywords used to create them. To return a list of all the available generator algorithms, use the RandStream.list method.

Keyword	Generator	Multiple Stream and Substream Support	Approximate Period In Full Precision
mt19937ar	Mersenne twister (used by default stream at MATLAB startup)	No	2 ¹⁹⁹³⁷ -1
dsfmt19937	SIMD-oriented fast Mersenne twister	No	2 ¹⁹⁹³⁷ -1
mcg16807	Multiplicative congruential generator	No	2 ³¹ -2
mlfg6331_64	Multiplicative lagged Fibonacci generator	Yes	2^{124} (2^{51} streams of length 2^{72})
mrg32k3a	Combined multiple recursive generator	Yes	2^{191} (2^{63} streams of length 2^{127})
philox4x32_10	Philox 4x32 generator with 10 rounds	Yes	2 ¹⁹³ (2 ⁶⁴ streams of length 2 ¹²⁹)
threefry4x64_20	Threefry 4x64 generator with 20 rounds	Yes	2 ⁵¹⁴ (2 ²⁵⁶ streams of length 2 ²⁵⁸)
shr3cong	Shift-register generator summed with linear congruential generator	No	264
swb2712	Modified subtract with borrow generator	No	21492

The generators mcg16807, shr3cong, and swb2712 provide for backwards compatibility with earlier versions of MATLAB. mt19937ar and dsfmt19937 are designed primarily for sequential applications. The remaining generators provide explicit support for parallel random number generation.

Depending on the application, some generators might be faster or return values with more precision. All pseudorandom number generators are based on deterministic algorithms, and all generators pass a sufficiently specific statistical test for randomness. One way to check the results of a Monte Carlo simulation is to rerun the simulation with two or more different generator algorithms, and the choice of generators in MATLAB provides you with the means to do that. Although it is unlikely that your results will differ by more than the Monte Carlo sampling error when using different generators, there are examples in the literature where this kind of validation has turned up flaws in a particular generator algorithm. (See [13] for an example.)

Generator Algorithms

mt19937ar

The Mersenne Twister, as described in [11], has period $2^{19937} - 1$ and each U(0,1) value is created using two 32-bit integers. The possible values are multiples of 2^{-53} in the interval (0, 1). This generator does not support multiple streams or substreams. The randn algorithm used by default for mt19937ar streams is the ziggurat algorithm [7], but with the mt19937ar generator underneath.

Note This generator is identical to the one used by the rand function beginning in MATLAB Version 7, activated by rand('twister',s).

dsfmt19937

The double precision SIMD-oriented Fast Mersenne Twister, as described in [12], is a faster implementation of the Mersenne Twister algorithm. The period is $2^{19937} - 1$ and the possible values are multiples of 2^{-52} in the interval (0, 1). The generator produces double precision values in [1, 2) natively, which are transformed to create U(0,1) values. This generator does not support multiple streams or substreams.

mcg16807

A 32-bit multiplicative congruential generator, as described in [14], with multiplier $a=7^5$, modulo $m=2^{31}-1$. This generator has a period of $2^{31}-2$ and does not support multiple streams or substreams. Each U(0,1) value is created using a single 32-bit integer from the generator; the possible values are all multiples of $(2^{31}-1)^{-1}$ strictly within the interval (0, 1). For mcg16807 streams, the default algorithm used by randn is the polar algorithm (described in [1]).

Note This generator is identical to the one used beginning in MATLAB Version 4 by both the rand and randn functions, activated using rand('seed',s) or randn('seed',s).

mlfq6331 64

A 64-bit multiplicative lagged Fibonacci generator, as described in [10], with lags l=63, k=31. This generator is similar to the MLFG implemented in the SPRNG package. It has a period of approximately 2^{124} . It supports up to 2^{61} parallel streams, via parameterization, and 2^{51} substreams each of length 2^{72} . Each U(0,1) value is created using one 64-bit integer from the generator; the possible values are all multiples of 2^{-64} strictly within the interval (0, 1). The randn algorithm used by default for mlfg6331_64 streams is the ziggurat algorithm [7], but with the mlfg6331_64 generator underneath.

mrg32k3a

A 32-bit combined multiple recursive generator, as described in [2]. This generator is similar to the CMRG implemented in the RngStreams package in C. It has a period of 2^{191} and supports up to 2^{63} parallel streams through sequence splitting, each of length 2^{127} . It also supports 2^{51} substreams, each of length 2^{76} . Each U(0,1) value is created using two 32-bit integers from the generator; the possible values are multiples of 2^{-53} strictly within the interval (0, 1). The randn

algorithm used by default for mrg32k3a streams is the ziggurat algorithm [7], but with the mrg32k3a generator underneath.

philox4x32 10

A 4x32 generator with 10 rounds as described in [15]. This generator uses a Feistel network and integer multiplication. The generator is specifically designed for high performance in highly parallel systems such as GPUs. It has a period of 2^{193} (2^{64} streams of length 2^{129}).

threefry4x64 20

A 4x64 generator with 20 rounds as described in [15]. This generator is a non-cryptographic adaptation of the Threefish block cipher from the Skein Hash Function. It has a period of 2^{514} (2^{256} streams of length 2^{258}).

shr3cong

Marsaglia's SHR3 shift-register generator summed with a linear congruential generator with multiplier a=69069, addend b=1234567, and modulus 2^{-32} . SHR3 is a 3-shift-register generator defined as $u=u(\mathbf{I}+\mathbf{L}^{13})(\mathbf{I}+\mathbf{R}^{17})(\mathbf{I}+\mathbf{L}^5)$, where \mathbf{I} is the identity operator, \mathbf{L} is the left shift operator, and \mathbf{R} is the right shift operator. The combined generator (the SHR3 part is described in [7]) has a period of approximately 2^{64} . This generator does not support multiple streams or substreams. Each U(0,1) value is created using one 32-bit integer from the generator; the possible values are all multiples of 2^{-32} strictly within the interval (0,1). The randn algorithm used by default for shr3cong streams is the earlier form of the ziggurat algorithm [9], but with the shr3cong generator underneath. This generator is identical to the one used by the randn function beginning in MATLAB Version 5, activated using randn ('state',s).

Note The SHR3 generator used in [6] (1999) differs from the one used in [7] (2000). MATLAB uses the most recent version of the generator, presented in [7].

swb2712

A modified Subtract-with-Borrow generator, as described in [8]. This generator is similar to an additive lagged Fibonacci generator with lags 27 and 12, but it is modified to have a much longer period of approximately 2^{1492} . The generator works natively in double precision to create U(0,1) values, and all values in the open interval (0,1) are possible. The randn algorithm used by default for swb2712 streams is the ziggurat algorithm [7], but with the swb2712 generator underneath.

Note This generator is identical to the one used by the rand function beginning in MATLAB Version 5, activated using rand('state',s).

Transformation Algorithms

Inversion

Computes a normal random variate by applying the standard normal inverse cumulative distribution function to a uniform random variate. Exactly one uniform value is consumed per normal value.

Polar

The polar rejection algorithm, as described in [1]. Approximately 1.27 uniform values are consumed per normal value, on average.

Ziggurat

The ziggurat algorithm, as described in [7]. Approximately 2.02 uniform values are consumed per normal value, on average.

Configuring a Stream

A random number stream s has properties that control its behavior. To access or change a property, use the syntax p = s.Property and s.Property = p.

For example, you can configure the transformation algorithm to generate normally distributed pseudorandom values when using randn. Generate normally distributed pseudorandom values using the default Ziggurat transformation algorithm.

```
s1 = RandStream('mt19937ar');
s1.NormalTransform
ans = 'Ziggurat'
r1 = randn(s1,1,10);
```

Configure the stream to use the Polar transformation algorithm to generate normally distributed pseudorandom values.

When generating random numbers with uniform distribution using rand, you can also configure the stream to generate antithetic pseudorandom values, that is, the usual values subtracted from 1 for uniform values.

Create 6 random numbers with uniform distribution from the stream s.

```
s2 = RandStream('mt19937ar');
r1 = rand(s2,1,6)

r1 =
    0.8147    0.9058    0.1270    0.9134    0.6324    0.0975
```

Restore the initial state of the stream. Create another 6 random numbers with the Antithetic property set to true. Check that these 6 random numbers are equal to the previously generated random numbers subtracted from 1.

```
reset(s2)
s2.Antithetic = true;
r2 = rand(s2,1,6)
r2 =
    0.1853    0.0942    0.8730    0.0866    0.3676    0.9025
isequal(r1,1 - r2)
```

```
ans =
```

Instead of setting the properties of a stream one-by-one, you can save and restore all properties of a stream s by using A = get(s) and set(s,A), respectively. For example, configure all properties of the stream s2 to be the same as the stream s1.

```
A = qet(s1)
A =
               Type: 'mt19937ar'
         NumStreams: 1
        StreamIndex: 1
          Substream: 1
               Seed: 0
              State: [625x1 uint32]
    NormalTransform: 'Polar'
         Antithetic: 0
      FullPrecision: 1
set(s2,A)
               Type: 'mt19937ar'
         NumStreams: 1
        StreamIndex: 1
          Substream: 1
               Seed: 0
              State: [625x1 uint32]
    NormalTransform: 'Polar'
         Antithetic: 0
      FullPrecision: 1
```

The get and set functions enable you to save and restore a stream's entire configuration so that results are exactly reproducible later on.

Restore State of Random Number Generator to Reproduce Output

The State property is the internal state of the random number generator. You can save the state of the global stream at a certain point in your simulation when generating random numbers to reproduce the results later on.

Use RandStream.getGlobalStream to return a handle to the global stream, that is, the current global stream that rand generates random numbers from. Save the state of the global stream.

```
globalStream = RandStream.getGlobalStream;
myState = globalStream.State;
```

Using myState, you can restore the state of globalStream and reproduce previous results.

```
A = rand(1,100);
globalStream.State = myState;
B = rand(1,100);
isequal(A,B)
ans = logical
1
```

rand, randi, randn, and randperm access the global stream. Since all of these functions access the same underlying stream, a call to one affects the values produced by the others at subsequent calls.

```
globalStream.State = myState;
A = rand(1,100);
globalStream.State = myState;
C = randi(100);
B = rand(1,100);
isequal(A,B)
ans = logical
0
```

You can also reset a stream to its initial settings using the reset function.

```
reset(globalStream)
A = rand(1,100);
reset(globalStream)
B = rand(1,100);
isequal(A,B)
ans = logical
1
```

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See Also

rng | RandStream

- "Managing the Global Stream Using RandStream" on page 3-16
- "Multiple Streams" on page 3-28
- "Controlling Random Number Generation" on page 3-36
- "Create Arrays of Random Numbers" on page 3-3

Multiple Streams

Using Multiple Independent Streams

MATLAB® software includes generator algorithms that enable you to create multiple independent random number streams. For example, the four generator types that support multiple independent streams are the Combined Multiple Recursive ('mrg32k3a'), the Multiplicative Lagged Fibonacci ('mlfg6331_64'), the Philox 4x32 ('philox4x32_10'), and the Threefry 4x64 ('threefry4x64_20') generators. You can create multiple independent streams that are guaranteed to not overlap, and for which tests that demonstrate (pseudo)independence of the values between streams have been carried out. For more information about generator algorithms that support multiple streams, see the table of generator algorithms in "Creating and Controlling a Random Number Stream" on page 3-19.

The RandStream.create function enables you to create streams that have the same generator algorithm and seed value, but are statistically independent.

```
[s1,s2,s3] = RandStream.create('mlfg6331 64','NumStreams',3)
s1 =
mlfg6331 64 random stream
      StreamIndex: 1
      NumStreams: 3
             Seed: 0
 NormalTransform: Ziggurat
s2 =
mlfg6331 64 random stream
      StreamIndex: 2
      NumStreams: 3
             Seed: 0
 NormalTransform: Ziggurat
s3 =
mlfg6331 64 random stream
      StreamIndex: 3
      NumStreams: 3
             Seed: 0
 NormalTransform: Ziggurat
```

As evidence of independence, you can see that these streams are largely uncorrelated.

```
r1 = rand(s1,100000,1);

r2 = rand(s2,100000,1);

r3 = rand(s3,100000,1);

corrcoef([r1,r2,r3])

ans = 3×3

1.0000 0.0007 0.0052

0.0007 1.0000 0.0000

0.0052 0.0000 1.0000
```

Depending on the application, creating only some of the streams in a set of independent streams can be useful if you need to simulate some events. Specify the StreamIndices parameter to create only some of the streams from a set of multiple streams. The StreamIndex property returns the index of each stream you create.

Multiple streams, since they are statistically independent, can be used to verify the precision of a simulation. For example, a set of independent streams can be used to repeat a Monte Carlo simulation several times in different MATLAB sessions or on different processors and determine the variance in the results. This makes multiple streams useful in large-scale parallel simulations.

Using Seeds to Get Different Results

For generator types that do not explicitly support independent streams, different seeds provide a method to create multiple streams. By using different seeds, you can create streams that return different values and act separately from one another. However, using a generator specifically designed for multiple independent streams is a better option, as the statistical properties across streams have been carefully verified.

Create two streams with different seeds by using the Mersenne twister generator.

Use the first stream in one MATLAB session to generate random numbers.

```
r1 = rand(s1, 100000, 1);
```

Use the second stream in another MATLAB session to generate random numbers.

```
r2 = rand(s2, 100000, 1);
```

With different seeds, streams typically return values that are uncorrelated.

```
corrcoef([r1,r2])
```

```
ans = 2×2
1.0000 0.0030
0.0030 1.0000
```

The two streams with different seeds may appear uncorrelated since the state space of the Mersenne Twister is so much larger (2^{19937} elements) than the number of possible seeds (2^{32}). The chances of overlap in different simulation runs are pretty remote unless you use a large number of different seeds. Using widely spaced seeds does not increase the level of randomness. In fact, taking this strategy to the extreme and reseeding a generator before each call can result in the sequence of values that are not statistically independent and identically distributed.

Seeding a stream is most useful if you use it as an initialization step, perhaps at MATLAB startup, or before running a simulation.

Using Substreams to Get Different Results

Another method to get different results from a stream is to use substreams. Unlike seeds, where the locations along the sequence of random numbers are not exactly known, the spacing between substreams is known, so any chance of overlap can be eliminated. Like independent parallel streams, research has been done to demonstrate statistical independence across substreams. In short, substreams are a more controlled way to do many of the same things that seeds have traditionally been used for, and a more lightweight solution than parallel streams.

Substreams provide a quick and easy way to ensure that you get different results from the same code at different times. For example, generate several random numbers in a loop.

```
defaultStream = RandStream('mlfg6331 64');
RandStream.setGlobalStream(defaultStream)
for i = 1:5
    defaultStream.Substream = i;
    z = rand(1,i)
end
z = 0.6986
z = 1 \times 2
    0.9230
               0.2489
z = 1 \times 3
    0.0261
               0.2530
                           0.0737
z = 1 \times 4
    0.3220
               0.7405
                           0.1983
                                      0.1052
z = 1 \times 5
    0.2067
               0.2417
                           0.9777
                                      0.5970
                                                  0.4187
```

In another loop, you can generate random values that are independent from the first set of 5 iterations.

```
for i = 6:10
    defaultStream.Substream = i;
    z = rand(1,11-i)
end
z = 1 \times 5
    0.2650
                0.8229
                            0.2479
                                        0.0247
                                                    0.4581
z = 1 \times 4
                0.7445
                            0.7734
                                        0.9113
    0.3963
z = 1 \times 3
    0.2758
                0.3662
                            0.7979
z = 1 \times 2
    0.6814
                0.5150
z = 0.5247
```

Each of these substreams can reproduce its loop iteration. For example, you can return to the 6th substream in the loop.

```
defaultStream.Substream = 6;

z = rand(1,5)

z = 1 \times 5

0.2650 0.8229 0.2479 0.0247 0.4581
```

See Also

rng | RandStream

- "Managing the Global Stream Using RandStream" on page 3-16
- "Controlling Random Number Generation" on page 3-36
- "Creating and Controlling a Random Number Stream" on page 3-19
- "Create Arrays of Random Numbers" on page 3-3

Replace Discouraged Syntaxes of rand and randn

```
In this section...

"Description of the Discouraged Syntaxes" on page 3-32

"Description of Replacement Syntaxes" on page 3-32

"Replacement Syntaxes for Initializing the Generator with an Integer Seed" on page 3-33

"Replacement Syntaxes for Initializing the Generator with a State Vector" on page 3-34

"If You Are Unable to Upgrade from Discouraged Syntax" on page 3-34
```

Description of the Discouraged Syntaxes

In earlier versions of MATLAB, you controlled the random number generator used by the rand and randn functions with the 'seed', 'state' or 'twister' inputs. For example:

```
rand('seed',sd)
randn('seed',sd)
rand('state',s)
randn('state',s)
rand('twister',5489)
```

These syntaxes referred to different types of generators, and they are no longer recommended for the following reasons:

- The terms 'seed' and 'state' are misleading names for the generators.
- All of the generators except 'twister' are flawed.
- They unnecessarily use different generators for rand and randn.

To assess the impact of replacing discouraged syntaxes in your existing code, execute the following commands at the start of your MATLAB session:

```
warning('on','MATLAB:RandStream:ActivatingLegacyGenerators')
warning('on','MATLAB:RandStream:ReadingInactiveLegacyGeneratorState')
```

Description of Replacement Syntaxes

Use the rng function to control the shared generator used by rand, randn, randi and all other random number generation functions like randperm, sprand, and so on. To learn how to use the rng function when replacing discouraged syntaxes, take a few moments to understand their function. This should help you to see which new rng syntax best suits your needs.

The first input to rand(Generator,s) or randn(Generator,s) specified the type of the generator, as described here.

```
Generator = 'seed' referred to the MATLAB v4 generator, not to the seed initialization value.

Generator = 'state' referred to the MATLAB v5 generators, not to the internal state of the generator.

Generator = 'twister' referred to the Mersenne Twister generator, now the MATLAB startup generator.
```

The v4 and v5 generators are no longer recommended unless you are trying to exactly reproduce the random numbers generated in earlier versions of MATLAB. The simplest way to update your code is to use rng. The rng function replaces the names for the rand and randn generators as follows.

rand/randn Generator Name	rng Generator Name	
'seed'	'v4'	
'state'	'v5uniform' (for rand)	
	'v5normal' (for randn)	
'twister'	'twister' (recommended)	

Replacement Syntaxes for Initializing the Generator with an Integer Seed

The most common uses of the integer seed sd in the rand(Generator,sd) syntax were to:

- Reproduce exactly the same random numbers each time (e.g., by using a seed such as 0, 1, or 3141879)
- Try to ensure that MATLAB always gives different random numbers in separate runs (for example, by using a seed such as sum(100*clock))

The following table shows replacements for syntaxes with an integer seed sd.

- The first column shows the discouraged syntax with rand and randn.
- The second column shows how to exactly reproduce the discouraged behavior with the new rng function. In most cases, this is done by specifying a legacy generator type such as the v4 or v5 generators, which is no longer recommended.
- The third column shows the recommended alternative, which does not specify the optional generator type input to rng. Therefore, if you *always* omit the Generator input, rand, randn, and randi just use the default Mersenne Twister generator that is used at MATLAB startup. In future releases when new generators supersede the Mersenne Twister, this code will use the new default.

Discouraged rand/randn Syntax	Not Recommended: Reproduce Discouraged Behavior Exactly By Specifying Generator Type	Recommended Alternative: Does Not Override Generator Type
rand('twister',5489)	rng(5489,'twister')	rng('default')
rand('seed',sd)	rng(sd,'v4')	rng(sd)
randn('seed',sd)		
rand('state',sd)	<pre>rng(sd,'v5uniform')</pre>	
randn('state',sd)	rng(sd,'v5normal')	
rand('seed',sum(100*clock))	rng(sum(100*clock),'v4')	rng('shuffle')

Replacement Syntaxes for Initializing the Generator with a State Vector

The most common use of the state vector (shown here as st) in the rand(Generator, st) syntax was to reproduce exactly the random numbers generated at a specific point in an algorithm or iteration. For example, you could use this vector as an aid in debugging.

The rng function changes the pattern of saving and restoring the state of the random number generator as shown in the next table. The example in the left column assumes that you are using the v5 uniform generator. The example in the right column uses the new syntax, and works for any generator you use.

Discouraged Syntax Using rand/randn	New Syntax Using rng	
<pre>% Save v5 generator state. st = rand('state');</pre>	% Get generator settings. s = rng;	
% Call rand. x = rand;	% Call rand. x = rand;	
<pre>% Restore v5 generator state. rand('state',st);</pre>	<pre>% Restore previous generator % settings. rng(s);</pre>	
% Call rand again and hope		
<pre>% for the same results. y = rand</pre>	% Call rand again and % get the same results. y = rand	

For a demonstration, see this instructional video.

If You Are Unable to Upgrade from Discouraged Syntax

If there is code that you are not able or not permitted to modify and you know that it uses the discouraged random number generator control syntaxes, it is important to remember that when you use that code MATLAB will switch into legacy mode. In legacy mode, rand and randn are controlled by separate generators, each with their own settings.

Calls to rand in legacy mode use one of the following:

- The 'v4' generator, controlled by rand('seed', ...)
- The 'v5uniform' generator, controlled by rand('state', ...)
- The 'twister' generator, controlled by rand('twister', ...)

Calls to randn in legacy mode use one of the following:

- The 'v4' generator, controlled by randn('seed', ...)
- The 'v5normal' generator, controlled by randn('state', ...)

If code that you rely on puts MATLAB into legacy mode, use the following command to escape legacy mode and get back to the default startup generator:

rng default

Alternatively, to guard around code that puts MATLAB into legacy mode, use:

See Also

rng | rand | randn

Related Examples

• "Create Arrays of Random Numbers" on page 3-3

Controlling Random Number Generation

This example shows how to use the rng function, which provides control over random number generation.

(Pseudo)Random numbers in MATLAB® come from the rand, randi, and randn functions. Many other functions call those three, but those are the fundamental building blocks. All three depend on a single shared random number generator that you can control using rng.

It's important to realize that "random" numbers in MATLAB are not unpredictable at all, but are generated by a deterministic algorithm. The algorithm is designed to be sufficiently complicated so that its output *appears* to be an independent random sequence to someone who does not know the algorithm, and can pass various statistical tests of randomness. The function that is introduced here provides ways to take advantage of the determinism to

- repeat calculations that involve random numbers, and get the same results, or
- guarantee that different random numbers are used in repeated calculations

and to take advantage of the apparent randomness to justify combining results from separate calculations.

"Starting Over"

If you look at the output from rand, randi, or randn in a new MATLAB session, you'll notice that they return the same sequences of numbers each time you restart MATLAB. It's often useful to be able to reset the random number generator to that startup state, without actually restarting MATLAB. For example, you might want to repeat a calculation that involves random numbers, and get the same result.

rng provides a very simple way to put the random number generator back to its default settings.

```
rng default
rand % returns the same value as at startup
ans = 0.8147
```

What are the "default" random number settings that MATLAB starts up with, or that rng default gives you? If you call rng with no inputs, you can see that it is the Mersenne Twister generator algorithm, seeded with 0.

```
rng
```

```
ans = struct with fields:
    Type: 'twister'
    Seed: 0
State: [625x1 uint32]
```

You'll see in more detail below how to use the above output, including the State field, to control and change how MATLAB generates random numbers. For now, it serves as a way to see what generator rand, randi, and randn are currently using.

Non-Repeatability

Each time you call rand, randi, or randn, they draw a new value from their shared random number generator, and successive values can be treated as statistically independent. But as mentioned above,

each time you restart MATLAB those functions are reset and return the same sequences of numbers. Obviously, calculations that use the *same* "random" numbers cannot be thought of as statistically independent. So when it's necessary to combine calculations done in two or more MATLAB sessions as if they *were* statistically independent, you cannot use the default generator settings.

One simple way to avoid repeating the same random numbers in a new MATLAB session is to choose a different seed for the random number generator. rng gives you an easy way to do that, by creating a seed based on the current time.

```
rng shuffle
rand
ans = 0.1481
```

Each time you use 'shuffle', it reseeds the generator with a different seed. You can call rng with no inputs to see what seed it actually used.

```
rng
ans = struct with fields:
    Type: 'twister'
    Seed: 48366163
    State: [625x1 uint32]

rng shuffle % creates a different seed each time rng
ans = struct with fields:
    Type: 'twister'
    Seed: 48366170
    State: [625x1 uint32]

rand
ans = 0.5435
```

'shuffle' is a very easy way to reseed the random number generator. You might think that it's a good idea, or even necessary, to use it to get "true" randomness in MATLAB. For most purposes, though, it is not necessary to use 'shuffle' at all. Choosing a seed based on the current time does not improve the statistical properties of the values you'll get from rand, randi, and randn, and does not make them "more random" in any real sense. While it is perfectly fine to reseed the generator each time you start up MATLAB, or before you run some kind of large calculation involving random numbers, it is actually not a good idea to reseed the generator too frequently within a session, because this can affect the statistical properties of your random numbers.

What 'shuffle' does provide is a way to avoid repeating the same sequences of values. Sometimes that is critical, sometimes it's just "nice", but often it is not important at all. Bear in mind that if you use 'shuffle', you may want to save the seed that rng created so that you can repeat your calculations later on. You'll see how to do that below.

More Control over Repeatability and Non-Repeatability

So far, you've seen how to reset the random number generator to its default settings, and reseed it using a seed that is created using the current time. rng also provides a way to reseed it using a specific seed.

You can use the same seed several times, to repeat the same calculations. For example, if you run this code twice ...

```
rng(1) % the seed is any non-negative integer < 2^32
x = randn(1,5)

x = 1×5
    -0.6490    1.1812   -0.7585   -1.1096   -0.8456

rng(1)
x = randn(1,5)
x = 1×5
    -0.6490    1.1812   -0.7585   -1.1096   -0.8456</pre>
```

 \dots you get exactly the same results. You might do this to recreate x after having cleared it, so that you can repeat what happens in subsequent calculations that depend on x, using those specific values.

On the other hand, you might want to choose *different* seeds to ensure that you don't repeat the same calculations. For example, if you run this code in one MATLAB session ...

```
rng(2)
x2 = sum(randn(50,1000),1); % 1000 trials of a random walk
and this code in another ...
rng(3)
x3 = sum(randn(50,1000),1);
```

... you could combine the two results and be confident that they are not simply the same results repeated twice.

```
x = [x2 x3];
```

As with 'shuffle' there is a caveat when reseeding MATLAB's random number generator, because it affects all subsequent output from rand, randi, and randn. Unless you need repeatability or uniqueness, it is usually advisable to simply generate random values without reseeding the generator. If you do need to reseed the generator, that is usually best done at the command line, or in a spot in your code that is not easily overlooked.

Choosing a Generator Type

Not only can you reseed the random number generator as shown above, you can also choose the type of random number generator that you want to use. Different generator types produce different sequences of random numbers, and you might, for example, choose a specific type because of its statistical properties. Or you might need to recreate results from an older version of MATLAB that used a different default generator type.

One other common reason for choosing the generator type is that you are writing a validation test that generates "random" input data, and you need to guarantee that your test can always expect exactly the same predictable result. If you call rng with a seed before creating the input data, it reseeds the random number generator. But if the generator type has been changed for some reason, then the output from rand, randi, and randn will not be what you expect from that seed. Therefore, to be 100% certain of repeatability, you can also specify a generator type.

For example,

```
rng(0,'twister')
```

causes rand, randi, and randn to use the Mersenne Twister generator algorithm, after seeding it with 0.

```
Using 'combRecursive'
rng(0,'combRecursive')
```

selects the Combined Multiple Recursive generator algorithm, which supports some parallel features that the Mersenne Twister does not.

This command

```
rng(0,'v4')
```

selects the generator algorithm that was the default in MATLAB 4.0.

And of course, this command returns the random number generator to its default settings.

```
rng default
```

However, because the default random number generator settings may change between MATLAB releases, using 'default' does not guarantee predictable results over the long-term. 'default' is a convenient way to reset the random number generator, but for even more predictability, specify a generator type and a seed.

On the other hand, when you are working interactively and need repeatability, it is simpler, and usually sufficient, to call rng with just a seed.

Saving and Restoring Random Number Generator Settings

Calling rng with no inputs returns a scalar structure with fields that contain two pieces of information described already: the generator type, and the integer with which the generator was last reseeded.

```
s = rng
s = struct with fields:
    Type: 'twister'
    Seed: 0
    State: [625x1 uint32]
```

The third field, State, contains a copy of the generator's current state vector. This state vector is the information that the generator maintains internally in order to generate the next value in its sequence of random numbers. Each time you call rand, randi, or randn, the generator that they share updates its internal state. Thus, the state vector in the settings structure returned by rng contains the information necessary to repeat the sequence, beginning from the point at which the state was captured.

While just being able to see this output is informative, rng also accepts a settings structure as an *input*, so that you can save the settings, including the state vector, and restore them later to repeat calculations. Because the settings contain the generator type, you'll know exactly what you're getting, and so "later" might mean anything from moments later in the same MATLAB session, to years (and

multiple MATLAB releases) later. You can repeat results from any point in the random number sequence at which you saved the generator settings. For example

```
x1 = randn(10,10); % move ahead in the random number sequence
                   % save the settings at this point
x2 = randn(1,5)
x2 = 1 \times 5
   0.8404
           -0.8880
                        0.1001
                                -0.5445
                                             0.3035
                   % move ahead in the random number sequence
x3 = randn(5,5);
rng(s);
                   % return the generator back to the saved state
x2 = randn(1,5)
                   % repeat the same numbers
x2 = 1 \times 5
           -0.8880
                        0.1001 -0.5445
   0.8404
                                             0.3035
```

Notice that while reseeding provides only a coarse reinitialization, saving and restoring the generator state using the settings structure allows you to repeat *any* part of the random number sequence.

The most common way to use a settings structure is to restore the generator state. However, because the structure contains not only the state, but also the generator type and seed, it's also a convenient way to temporarily switch generator types. For example, if you need to create values using one of the legacy generators from MATLAB 5.0, you can save the current settings at the same time that you switch to use the old generator ...

```
previousSettings = rng(0,'v5uniform')
previousSettings = struct with fields:
    Type: 'twister'
    Seed: 0
    State: [625x1 uint32]
```

... and then restore the original settings later.

```
rng(previousSettings)
```

You should not modify the contents of any of the fields in a settings structure. In particular, you should not construct your own state vector, or even depend on the format of the generator state.

Writing Simpler, More Flexible, Code

rng allows you to either

- · reseed the random number generator, or
- save and restore random number generator settings

without having to know what type it is. You can also return the random number generator to its default settings without having to know what those settings are. While there are situations when you might *want* to specify a generator type, rng affords you the simplicity of not *having* to specify it.

If you are able to avoid specifying a generator type, your code will automatically adapt to cases where a different generator needs to be used, and will automatically benefit from improved properties in a new default random number generator type.

rng and RandStream

rng provides a convenient way to control random number generation in MATLAB for the most common needs. However, more complicated situations involving multiple random number streams and parallel random number generation require a more complicated tool. The RandStream class is that tool, and it provides the most powerful way to control random number generation. The two tools are complementary, with rng providing a much simpler and concise syntax that is built on top of the flexibility of RandStream.

Sparse Matrices

- "Computational Advantages of Sparse Matrices" on page 4-2
- "Constructing Sparse Matrices" on page 4-4
- "Accessing Sparse Matrices" on page 4-8
- "Sparse Matrix Operations" on page 4-14
- "Finite Difference Laplacian" on page 4-28
- "Graphical Representation of Sparse Matrices" on page 4-32
- "Graphs and Matrices" on page 4-38
- "Sparse Matrix Reordering" on page 4-44
- "Iterative Methods for Linear Systems" on page 4-56

Computational Advantages of Sparse Matrices

```
In this section...

"Memory Management" on page 4-2

"Computational Efficiency" on page 4-2
```

Memory Management

Using sparse matrices to store data that contains a large number of zero-valued elements can both save a significant amount of memory and speed up the processing of that data. sparse is an attribute that you can assign to any two-dimensional MATLAB matrix that is composed of double or logical elements.

The sparse attribute allows MATLAB to:

- Store only the nonzero elements of the matrix, together with their indices.
- Reduce computation time by eliminating operations on zero elements.

For full matrices, MATLAB stores every matrix element internally. Zero-valued elements require the same amount of storage space as any other matrix element. For sparse matrices, however, MATLAB stores only the nonzero elements and their indices. For large matrices with a high percentage of zero-valued elements, this scheme significantly reduces the amount of memory required for data storage.

The whos command provides high-level information about matrix storage, including size and storage class. For example, this whos listing shows information about sparse and full versions of the same matrix.

```
M full = magic(1100);
                                % Create 1100-by-1100 matrix.
M \text{ full}(M \text{ full} > 50) = 0;
                                % Set elements >50 to zero.
M_sparse = sparse(M_full);
                              % Create sparse matrix of same.
whos
  Name
                                                           Attributes
                    Size
                                         Bytes Class
  M full
                 1100×1100
                                       9680000 double
  M sparse
                 1100×1100
                                          9608
                                                double
                                                           sparse
```

Notice that the number of bytes used is fewer in the sparse case, because zero-valued elements are not stored.

Computational Efficiency

Sparse matrices also have significant advantages in terms of computational efficiency. Unlike operations with full matrices, operations with sparse matrices do not perform unnecessary low-level arithmetic, such as zero-adds (x+0) is always (x+0). The resulting efficiencies can lead to dramatic improvements in execution time for programs working with large amounts of sparse data.

See Also

More About

• "Sparse Matrix Operations" on page 4-14

Constructing Sparse Matrices

```
In this section...

"Creating Sparse Matrices" on page 4-4

"Importing Sparse Matrices" on page 4-7
```

Creating Sparse Matrices

MATLAB never creates sparse matrices automatically. Instead, you must determine if a matrix contains a large enough percentage of zeros to benefit from sparse techniques.

The *density* of a matrix is the number of nonzero elements divided by the total number of matrix elements. For matrix M, this would be

```
nnz(M) / prod(size(M));
or
nnz(M) / numel(M);
```

Matrices with very low density are often good candidates for use of the sparse format.

Converting Full to Sparse

You can convert a full matrix to sparse storage using the sparse function with a single argument.

For example:

```
5
A = \begin{bmatrix} 0 \end{bmatrix}
                           0
               2
                     0
        1
               3
                     0
                           0
        0
                           01;
S = sparse(A)
 S =
    (3,1)
                        2
    (2,2)
                        3
    (3,2)
                        4
    (4,3)
                        5
    (1,4)
```

The printed output lists the nonzero elements of S, together with their row and column indices. The elements are sorted by columns, reflecting the internal data structure.

You can convert a sparse matrix to full storage using the full function, provided the matrix order is not too large. For example, A = full(S) reverses the example conversion.

Converting a full matrix to sparse storage is not the most frequent way of generating sparse matrices. If the order of a matrix is small enough that full storage is possible, then conversion to sparse storage rarely offers significant savings.

Creating Sparse Matrices Directly

You can create a sparse matrix from a list of nonzero elements using the sparse function with five arguments.

```
S = sparse(i,j,s,m,n)
```

i and j are vectors of row and column indices, respectively, for the nonzero elements of the matrix. s is a vector of nonzero values whose indices are specified by the corresponding (i, j) pairs. m is the row dimension of the resulting matrix, and n is the column dimension.

The matrix S of the previous example can be generated directly with

The sparse command has a number of alternate forms. The example above uses a form that sets the maximum number of nonzero elements in the matrix to length(s). If desired, you can append a sixth argument that specifies a larger maximum, allowing you to add nonzero elements later without reallocating the sparse matrix.

The matrix representation of the second difference operator is a good example of a sparse matrix. It is a tridiagonal matrix with -2s on the diagonal and 1s on the super- and subdiagonal. There are many ways to generate it—here's one possibility.

```
D = sparse(1:n,1:n,-2*ones(1,n),n,n);
E = sparse(2:n,1:n-1,ones(1,n-1),n,n);
S = E+D+E'
S =
   (1,1)
                - 2
   (2,1)
                 1
   (1,2)
                 1
   (2,2)
                - 2
   (3,2)
                 1
   (2,3)
                 1
   (3,3)
                -2
   (4,3)
                 1
   (3,4)
                 1
   (4,4)
                -2
   (5,4)
                 1
                 1
   (4,5)
                -2
   (5,5)
```

Now F = full(S) displays the corresponding full matrix.

```
F = full(S)
F =
```

- 2	1	0	0	0
1	- 2	1	0	0
0	1	-2	1 -2	0
0	0	1	- 2	1 -2
0	0	0	1	- 2

Creating Sparse Matrices from Their Diagonal Elements

Creating sparse matrices based on their diagonal elements is a common operation, so the function spdiags handles this task. Its syntax is

```
S = spdiags(B,d,m,n)
```

To create an output matrix **S** of size *m*-by-*n* with elements on **p** diagonals:

- B is a matrix of size min(m,n)-by-p. The columns of B are the values to populate the diagonals of S.
- d is a vector of length p whose integer elements specify which diagonals of S to populate.

That is, the elements in column j of B fill the diagonal specified by element j of d.

Note If a column of B is longer than the diagonal it's replacing, super-diagonals are taken from the lower part of the column of B, and sub-diagonals are taken from the upper part of the column of B.

As an example, consider the matrix \boldsymbol{B} and the vector \boldsymbol{d} .

```
B = \begin{bmatrix} 41 & 11 & 0 \\ 52 & 22 & 0 \\ 63 & 33 & 13 \\ 74 & 44 & 24 \end{bmatrix};
d = \begin{bmatrix} -3 & 0 \\ 2 \end{bmatrix};
```

Use these matrices to create a 7-by-4 sparse matrix A:

```
A = spdiags(B,d,7,4)
A =
   (1,1)
                 11
   (4,1)
                 41
   (2,2)
                 22
   (5,2)
                 52
   (1,3)
                 13
   (3,3)
                 33
   (6,3)
                 63
   (2,4)
                 24
   (4,4)
                 44
                 74
   (7,4)
```

In its full form, A looks like this:

```
full(A)
```

```
ans =
    11
            (-)
                   13
                           (-)
     0
           22
                   0
                          24
     (-)
            0
                   33
                          0
    41
            0
                          44
                   0
     0
            52
                   0
                           0
     0
             0
                   63
                           0
                    0
                          74
```

spdiags can also extract diagonal elements from a sparse matrix, or replace matrix diagonal elements with new values. Type help spdiags for details.

Importing Sparse Matrices

You can import sparse matrices from computations outside the MATLAB environment. Use the spconvert function in conjunction with the load command to import text files containing lists of indices and nonzero elements. For example, consider a three-column text file T.dat whose first column is a list of row indices, second column is a list of column indices, and third column is a list of nonzero values. These statements load T.dat into MATLAB and convert it into a sparse matrix S:

```
load T.dat
S = spconvert(T)
```

The save and load commands can also process sparse matrices stored as binary data in MAT-files.

See Also

sparse | spconvert

More About

• "Sparse Matrix Operations" on page 4-14

Accessing Sparse Matrices

```
In this section...

"Nonzero Elements" on page 4-8

"Indices and Values" on page 4-9

"Indexing in Sparse Matrix Operations" on page 4-9

"Visualizing Sparse Matrices" on page 4-12
```

Nonzero Elements

There are several commands that provide high-level information about the nonzero elements of a sparse matrix:

- nnz returns the number of nonzero elements in a sparse matrix.
- nonzeros returns a column vector containing all the nonzero elements of a sparse matrix.
- nzmax returns the amount of storage space allocated for the nonzero entries of a sparse matrix.

To try some of these, load the supplied sparse matrix west0479, one of the Harwell-Boeing collection.

This matrix models an eight-stage chemical distillation column.

Try these commands.

```
nnz(west0479)
ans =
        1887
format short e
west0479
west0479 =
  (25,1)
              1.0000e+00
              -3.7648e-02
  (31,1)
  (87,1)
              -3.4424e-01
  (26, 2)
              1.0000e+00
  (31, 2)
              -2.4523e-02
  (88, 2)
              -3.7371e-01
  (27,3)
              1.0000e+00
  (31,3)
              -3.6613e-02
  (89,3)
              -8.3694e-01
  (28,4)
              1.3000e+02
```

```
:

nonzeros(west0479)

ans =

1.0000e+00

-3.7648e-02

-3.4424e-01

1.0000e+00

-2.4523e-02

-3.7371e-01

1.0000e+00

-3.6613e-02

-8.3694e-01

1.3000e+02
```

Note Use **Ctrl+C** to stop the nonzeros listing at any time.

Note that initially nnz has the same value as nzmax by default. That is, the number of nonzero elements is equivalent to the number of storage locations allocated for nonzeros. However, MATLAB does not dynamically release memory if you zero out additional array elements. Changing the value of some matrix elements to zero changes the value of nnz, but not that of nzmax.

However, you can add as many nonzero elements to the matrix as desired. You are not constrained by the original value of nzmax.

Indices and Values

For any matrix, full or sparse, the find function returns the indices and values of nonzero elements. Its syntax is

```
[i,j,s] = find(S);
```

find returns the row indices of nonzero values in vector i, the column indices in vector j, and the nonzero values themselves in the vector s. The example below uses find to locate the indices and values of the nonzeros in a sparse matrix. The sparse function uses the find output, together with the size of the matrix, to recreate the matrix.

```
S1 = west0479;
[i,j,s] = find(S1);
[m,n] = size(S1);
S2 = sparse(i,j,s,m,n);
```

Indexing in Sparse Matrix Operations

Because sparse matrices are stored in compressed sparse column format, there are different costs associated with indexing into a sparse matrix than there are with indexing into a full matrix. Such costs are negligible when you need to change only a few elements in a sparse matrix, so in those cases it's normal to use regular array indexing to reassign values:

```
B = speye(4);
[i,j,s] = find(B);
[i,j,s]
ans =
     1
           1
                  1
     2
           2
                  1
     3
           3
                  1
     4
           4
                  1
B(3,1) = 42;
[i,j,s] = find(B);
[i,j,s]
ans =
     1
           1
                  1
     3
                 42
           1
     2
           2
                 1
     3
           3
                  1
                  1
```

In order to store the new matrix with 42 at (3,1), MATLAB inserts an additional row into the nonzero values vector and subscript vectors, then shifts all matrix values after (3,1).

Using linear indexing to access or assign an element in a large sparse matrix will fail if the linear index exceeds 2^48-1, which is the current upper bound for the number of elements allowed in a matrix.

```
S = spalloc(2^30, 2^30, 2);

S(end) = 1
```

Maximum variable size allowed by the program is exceeded.

To access an element whose linear index is greater than intmax, use array indexing:

```
S(2^30,2^30) = 1

S = (1073741824,1073741824) 1
```

While the cost of indexing into a sparse matrix to change a single element is negligible, it is compounded in the context of a loop and can become quite slow for large matrices. For that reason, in cases where many sparse matrix elements need to be changed, it is best to vectorize the operation instead of using a loop. For example, consider a sparse identity matrix:

```
n = 10000;
A = 4*speye(n);
```

Changing the elements of A within a loop is slower than a similar vectorized operation:

```
tic
A(1:n-1,n) = -1;
A(n,1:n-1) = -1;
toc
```

Elapsed time is 0.003344 seconds.

```
tic for k = 1:n-1 C(k,n) = -1; C(n,k) = -1; end toc Elapsed time is 0.448069 seconds.
```

Since MATLAB stores sparse matrices in compressed sparse column format, it needs to shift multiple entries in A during each pass through the loop.

Preallocating the memory for a sparse matrix and then filling it in an element-wise manner similarly causes a significant amount of overhead in indexing into the sparse array:

```
S1 = spalloc(1000,1000,100000);
tic;
for n = 1:100000
    i = ceil(1000*rand(1,1));
    j = ceil(1000*rand(1,1));
    S1(i,j) = rand(1,1);
end
toc

Elapsed time is 2.577527 seconds.
```

Constructing the vectors of indices and values eliminates the need to index into the sparse array, and thus is significantly faster:

```
i = ceil(1000*rand(100000,1));
j = ceil(1000*rand(100000,1));
v = zeros(size(i));
for n = 1:100000
    v(n) = rand(1,1);
end

tic;
S2 = sparse(i,j,v,1000,1000);
toc

Elapsed time is 0.017676 seconds.
```

For that reason, it's best to construct sparse matrices all at once using a construction function, like the sparse or spdiags functions.

For example, suppose you wanted the sparse form of the coordinate matrix C:

```
C = \begin{pmatrix} 4 & 0 & 0 & 0 & -1 \\ 0 & 4 & 0 & 0 & -1 \\ 0 & 0 & 4 & 0 & -1 \\ 0 & 0 & 0 & 4 & -1 \\ 1 & 1 & 1 & 1 & 4 \end{pmatrix}
```

Construct the five-column matrix directly with the sparse function using the triplet pairs for the row subscripts, column subscripts, and values:

```
i = [1 5 2 5 3 5 4 5 1 2 3 4 5]';

j = [1 1 2 2 3 3 4 4 5 5 5 5 55]';
```

```
s = [4 1 4 1 4 1 4 1 -1 -1 -1 -1 4]';
C = sparse(i,j,s)
C =
   (1,1)
   (5,1)
                 1
   (2,2)
   (5,2)
                 1
   (3,3)
                 4
   (5,3)
                 1
   (4,4)
                 4
   (5,4)
                 1
   (1,5)
                - 1
   (2,5)
                - 1
   (3,5)
                - 1
   (4,5)
                - 1
   (5,5)
                 4
```

The ordering of the values in the output reflects the underlying storage by columns. For more information on how MATLAB stores sparse matrices, see John R. Gilbert, Cleve Moler, and Robert Schreiber's Sparse Matrices In MATLAB: Design and Implementation, (*SIAM Journal on Matrix Analysis and Applications*, 13:1, 333–356 (1992)).

Visualizing Sparse Matrices

It is often useful to use a graphical format to view the distribution of the nonzero elements within a sparse matrix. The MATLAB spy function produces a template view of the sparsity structure, where each point on the graph represents the location of a nonzero array element.

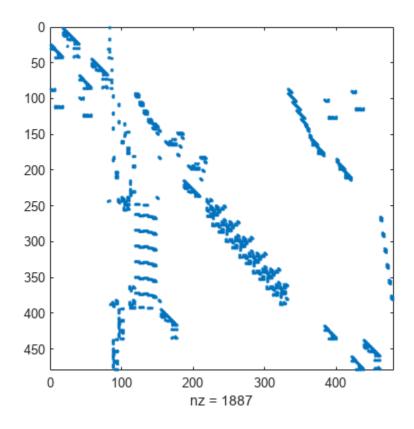
For example:

Load the supplied sparse matrix west0479, one of the Harwell-Boeing collection.

```
load west0479
```

View the sparsity structure.

```
spy(west0479)
```



See Also

sparse

More About

- "Computational Advantages of Sparse Matrices" on page 4-2
- "Constructing Sparse Matrices" on page 4-4
- "Sparse Matrix Operations" on page 4-14

Sparse Matrix Operations

Efficiency of Operations

Computational Complexity

The computational complexity of sparse operations is proportional to nnz, the number of nonzero elements in the matrix. Computational complexity also depends linearly on the row size m and column size n of the matrix, but is independent of the product m*n, the total number of zero and nonzero elements.

The complexity of fairly complicated operations, such as the solution of sparse linear equations, involves factors like ordering and fill-in, which are discussed in the previous section. In general, however, the computer time required for a sparse matrix operation is proportional to the number of arithmetic operations on nonzero quantities.

Algorithmic Details

Sparse matrices propagate through computations according to these rules:

- Functions that accept a matrix and return a scalar or constant-size vector always produce output in full storage format. For example, the size function always returns a full vector, whether its input is full or sparse.
- Functions that accept scalars or vectors and return matrices, such as zeros, ones, rand, and eye, always return full results. This is necessary to avoid introducing sparsity unexpectedly. The sparse analog of zeros(m,n) is simply sparse(m,n). The sparse analogs of rand and eye are sprand and speye, respectively. There is no sparse analog for the function ones.
- Unary functions that accept a matrix and return a matrix or vector preserve the storage class of the operand. If S is a sparse matrix, then chol(S) is also a sparse matrix, and diag(S) is a sparse vector. Columnwise functions such as max and sum also return sparse vectors, even though these vectors can be entirely nonzero. Important exceptions to this rule are the sparse and full functions.
- Binary operators yield sparse results if both operands are sparse, and full results if both are full. For mixed operands, the result is full unless the operation preserves sparsity. If S is sparse and F is full, then S+F, S*F, and F\S are full, while S.*F and S&F are sparse. In some cases, the result might be sparse even though the matrix has few zero elements.
- Matrix concatenation using either the cat function or square brackets produces sparse results for mixed operands.

Permutations and Reordering

A permutation of the rows and columns of a sparse matrix S can be represented in two ways:

- A permutation matrix P acts on the rows of S as P*S or on the columns as S*P'.
- A permutation vector p, which is a full vector containing a permutation of 1:n, acts on the rows of S as S(p,:), or on the columns as S(:,p).

For example:

```
p = [1 3 4 2 5]

I = eye(5,5);
```

```
P = I(p,:)
e = ones(4,1);
S = diag(11:11:55) + diag(e,1) + diag(e,-1)
p =
     1
            3
                   4
                          2
                                 5
P =
     1
            0
                   0
                          0
                                 0
     0
            0
                   1
                          0
                                 0
     0
            0
                   0
                          1
                                 0
     0
            1
                   0
                          0
                                 0
     0
            0
                   0
                          0
                                 1
S =
            1
                   0
                          0
                                 0
    11
           22
                   1
                          0
                                 0
     1
     0
            1
                  33
                          1
                                 0
     0
            0
                         44
                                 1
                   1
     0
            0
                   0
                          1
                                55
```

You can now try some permutations using the permutation vector p and the permutation matrix P. For example, the statements S(p,:) and P*S return the same matrix.

```
S(p,:)
ans =
            1
                   0
                          0
                                  0
    11
                          1
     0
            1
                  33
                                  0
     0
            0
                         44
                   1
                                 1
     1
           22
                   1
                           0
                                  0
     0
            0
                   0
                           1
                                55
P*S
ans =
                          0
    11
            1
                   0
                                  0
            1
                  33
     0
                          1
                                  0
     0
            0
                   1
                         44
                                  1
     1
           22
                   1
                           0
                                  0
            0
                   0
                           1
                                55
```

Similarly, S(:,p) and S*P' both produce

```
S*P'
ans =
    11
            0
                  0
                         1
                                0
     1
           1
                  0
                        22
                                0
     0
          33
                  1
                         1
                                0
```

```
0 1 44 0 1
0 0 1 0 55
```

If P is a sparse matrix, then both representations use storage proportional to n and you can apply either to S in time proportional to nnz(S). The vector representation is slightly more compact and efficient, so the various sparse matrix permutation routines all return full row vectors with the exception of the pivoting permutation in LU (triangular) factorization, which returns a matrix compatible with the full LU factorization.

To convert between the two permutation representations:

```
n = 5;
I = speye(n);
Pr = I(p,:);
Pc = I(:,p);
pc = (1:n)*Pc
pc =
            3
     1
                         2
                                5
                  4
pr = (Pr*(1:n)')'
pr =
     1
            3
                  4
                         2
                                5
```

The inverse of P is simply R = P'. You can compute the inverse of p with r(p) = 1:n.

```
r(p) = 1:5
r =
1 4 2 3 5
```

Reordering for Sparsity

Reordering the columns of a matrix can often make its LU or QR factors sparser. Reordering the rows and columns can often make its Cholesky factors sparser. The simplest such reordering is to sort the columns by nonzero count. This is sometimes a good reordering for matrices with very irregular structures, especially if there is great variation in the nonzero counts of rows or columns.

The colperm computes a permutation that orders the columns of a matrix by the number of nonzeros in each column from smallest to largest.

Reordering to Reduce Bandwidth

The reverse Cuthill-McKee ordering is intended to reduce the profile or bandwidth of the matrix. It is not guaranteed to find the smallest possible bandwidth, but it usually does. The symrcm function actually operates on the nonzero structure of the symmetric matrix A + A', but the result is also useful for nonsymmetric matrices. This ordering is useful for matrices that come from one-dimensional problems or problems that are in some sense *long and thin*.

Approximate Minimum Degree Ordering

The degree of a node in a graph is the number of connections to that node. This is the same as the number of off-diagonal nonzero elements in the corresponding row of the adjacency matrix. The

approximate minimum degree algorithm generates an ordering based on how these degrees are altered during Gaussian elimination or Cholesky factorization. It is a complicated and powerful algorithm that usually leads to sparser factors than most other orderings, including column count and reverse Cuthill-McKee. Because keeping track of the degree of each node is very time-consuming, the approximate minimum degree algorithm uses an approximation to the degree, rather than the exact degree.

These MATLAB functions implement the approximate minimum degree algorithm:

- symamd Use with symmetric matrices.
- colamd Use with nonsymmetric matrices and symmetric matrices of the form A*A' or A'*A.

See "Reordering and Factorization of Sparse Matrices" on page 4-18 for an example using symamd.

You can change various parameters associated with details of the algorithms using the spparms function.

For details on the algorithms used by colamd and symamd, see [5]. The approximate degree the algorithms use is based on [1].

Nested Dissection Ordering

Like the approximate minimum degree ordering, the nested dissection ordering algorithm implemented by the <code>dissect</code> function reorders the matrix rows and columns by considering the matrix to be the adjacency matrix of a graph. The algorithm reduces the problem down to a much smaller scale by collapsing together pairs of vertices in the graph. After reordering the small graph, the algorithm then applies projection and refinement steps to expand the graph back to the original size.

The nested dissection algorithm produces high quality reorderings and performs particularly well with finite element matrices compared to other reordering techniques. For more information about the nested dissection ordering algorithm, see [7].

Factoring Sparse Matrices

LU Factorization

If S is a sparse matrix, the following command returns three sparse matrices L, U, and P such that P*S = L*U.

```
[L,U,P] = lu(S);
```

lu obtains the factors by Gaussian elimination with partial pivoting. The permutation matrix P has only n nonzero elements. As with dense matrices, the statement [L,U] = lu(S) returns a permuted unit lower triangular matrix and an upper triangular matrix whose product is S. By itself, lu(S) returns L and U in a single matrix without the pivot information.

The three-output syntax [L,U,P] = lu(S) selects P via numerical partial pivoting, but does not pivot to improve sparsity in the LU factors. On the other hand, the four-output syntax [L,U,P,Q] = lu(S) selects P via threshold partial pivoting, and selects P and Q to improve sparsity in the LU factors.

You can control pivoting in sparse matrices using

```
lu(S,thresh)
```

where thresh is a pivot threshold in [0,1]. Pivoting occurs when the diagonal entry in a column has magnitude less than thresh times the magnitude of any sub-diagonal entry in that column. thresh = 0 forces diagonal pivoting. thresh = 1 is the default. (The default for thresh is 0.1 for the four-output syntax).

When you call lu with three or less outputs, MATLAB automatically allocates the memory necessary to hold the sparse L and U factors during the factorization. Except for the four-output syntax, MATLAB does not use any symbolic LU prefactorization to determine the memory requirements and set up the data structures in advance.

Reordering and Factorization of Sparse Matrices

This example shows the effects of reordering and factorization on sparse matrices.

If you obtain a good column permutation p that reduces fill-in, perhaps from symrcm or colamd, then computing lu(S(:,p)) takes less time and storage than computing lu(S).

Create a sparse matrix using the Bucky ball example.

```
B = bucky;
```

B has exactly three nonzero elements in each row and column.

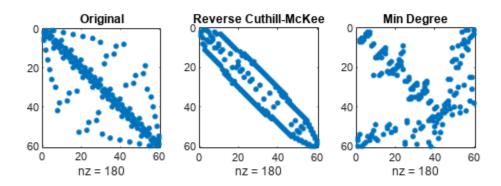
Create two permutations, r and m using symrcm and symamd respectively.

```
r = symrcm(B);
m = symamd(B);
```

The two permutations are the symmetric reverse Cuthill-McKee ordering and the symmetric approximate minimum degree ordering.

Create spy plots to show the three adjacency matrices of the Bucky Ball graph with these three different numberings. The local, pentagon-based structure of the original numbering is not evident in the others.

```
figure
subplot(1,3,1)
spy(B)
title('Original')
subplot(1,3,2)
spy(B(r,r))
title('Reverse Cuthill-McKee')
subplot(1,3,3)
spy(B(m,m))
title('Min Degree')
```



The reverse Cuthill-McKee ordering, r, reduces the bandwidth and concentrates all the nonzero elements near the diagonal. The approximate minimum degree ordering, m, produces a fractal-like structure with large blocks of zeros.

To see the fill-in generated in the LU factorization of the Bucky ball, use speye, the sparse identity matrix, to insert -3s on the diagonal of B.

$$B = B - 3*speye(size(B));$$

Since each row sum is now zero, this new B is actually singular, but it is still instructive to compute its LU factorization. When called with only one output argument, lu returns the two triangular factors, L and U, in a single sparse matrix. The number of nonzeros in that matrix is a measure of the time and storage required to solve linear systems involving B.

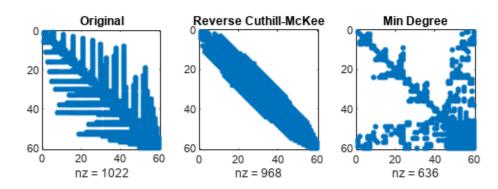
Here are the nonzero counts for the three permutations being considered.

- lu(B) (Original): 1022
- lu(B(r,r)) (Reverse Cuthill-McKee): 968
- lu(B(m,m)) (Approximate minimum degree): 636

Even though this is a small example, the results are typical. The original numbering scheme leads to the most fill-in. The fill-in for the reverse Cuthill-McKee ordering is concentrated within the band, but it is almost as extensive as the first two orderings. For the approximate minimum degree ordering, the relatively large blocks of zeros are preserved during the elimination and the amount of fill-in is significantly less than that generated by the other orderings.

The spy plots below reflect the characteristics of each reordering.

```
figure
subplot(1,3,1)
spy(lu(B))
title('Original')
subplot(1,3,2)
spy(lu(B(r,r)))
title('Reverse Cuthill-McKee')
subplot(1,3,3)
spy(lu(B(m,m)))
title('Min Degree')
```



Cholesky Factorization

If S is a symmetric (or Hermitian), positive definite, sparse matrix, the statement below returns a sparse, upper triangular matrix R so that R'*R = S.

```
R = chol(S)
```

chol does not automatically pivot for sparsity, but you can compute approximate minimum degree and profile limiting permutations for use with chol(S(p,p)).

Since the Cholesky algorithm does not use pivoting for sparsity and does not require pivoting for numerical stability, chol does a quick calculation of the amount of memory required and allocates all

the memory at the start of the factorization. You can use symbfact, which uses the same algorithm as chol, to calculate how much memory is allocated.

QR Factorization

MATLAB computes the complete QR factorization of a sparse matrix S with

```
[Q,R] = qr(S)
or
[Q,R,E] = qr(S)
```

but this is often impractical. The unitary matrix ${\bf Q}$ often fails to have a high proportion of zero elements. A more practical alternative, sometimes known as "the Q-less QR factorization," is available.

With one sparse input argument and one output argument

$$R = qr(S)$$

returns just the upper triangular portion of the QR factorization. The matrix R provides a Cholesky factorization for the matrix associated with the normal equations:

$$R'*R = S'*S$$

However, the loss of numerical information inherent in the computation of S'*S is avoided.

With two input arguments having the same number of rows, and two output arguments, the statement

$$[C,R] = qr(S,B)$$

applies the orthogonal transformations to B, producing C = Q'*B without computing Q.

The O-less OR factorization allows the solution of sparse least squares problems

```
minimize ||Ax - b||_2
```

with two steps:

If A is sparse, but not square, MATLAB uses these steps for the linear equation solving backslash operator:

```
x = A b
```

Or, you can do the factorization yourself and examine R for rank deficiency.

It is also possible to solve a sequence of least squares linear systems with different right-hand sides, b, that are not necessarily known when R = qr(A) is computed. The approach solves the "seminormal equations R'*R*x = A'*b with

```
x = R \setminus (R' \setminus (A'*b))
```

and then employs one step of iterative refinement to reduce round off error:

```
r = b - A*x;

e = R \setminus (R' \setminus (A'*r));

x = x + e
```

Incomplete Factorizations

The ilu and ichol functions provide approximate, *incomplete* factorizations, which are useful as preconditioners for sparse iterative methods.

The ilu function produces three incomplete lower-upper (ILU) factorizations: the zero-fill ILU (ILU(0)), a Crout version of ILU (ILUC(tau)), and ILU with threshold dropping and pivoting (ILUTP(tau)). The ILU(0) never pivots and the resulting factors only have nonzeros in positions where the input matrix had nonzeros. Both ILUC(tau) and ILUTP(tau), however, do threshold-based dropping with the user-defined drop tolerance tau.

For example:

shows that A has 7840 nonzeros, and its complete LU factorization has 126478 nonzeros. On the other hand, the following code shows the different ILU outputs:

```
[L,U] = ilu(A);
nnz(L)+nnz(U)-size(A,1)
ans =
        7840
norm(A-(L*U).*spones(A),'fro')./norm(A,'fro')
ans =
   4.8874e-17
opts.type = 'ilutp';
opts.droptol = 1e-4;
[L,U,P] = ilu(A, opts);
nnz(L)+nnz(U)-size(A,1)
ans =
       31147
norm(P*A - L*U, 'fro')./norm(A, 'fro')
ans =
   9.9224e-05
```

These calculations show that the zero-fill factors have 7840 nonzeros, the ILUTP(1e-4) factors have 31147 nonzeros, and the ILUC(1e-4) factors have 31083 nonzeros. Also, the relative error of the product of the zero-fill factors is essentially zero on the pattern of A. Finally, the relative error in the factorizations produced with threshold dropping is on the same order of the drop tolerance, although this is not guaranteed to occur. See the ilu reference page for more options and details.

The ichol function provides zero-fill incomplete Cholesky factorizations (IC(0)) as well as threshold-based dropping incomplete Cholesky factorizations (ICT(tau)) of symmetric, positive definite sparse matrices. These factorizations are the analogs of the incomplete LU factorizations above and have many of the same characteristics. For example:

shows that A has 195228 nonzeros, and its complete Cholesky factorization without reordering has 7762589 nonzeros. By contrast:

IC(0) has nonzeros only in the pattern of the lower triangle of A, and on the pattern of A, the product of the factors matches. Also, the ICT(1e-4) factors are considerably sparser than the complete Cholesky factor, and the relative error between A and L*L' is on the same order of the drop tolerance. It is important to note that unlike the factors provided by chol, the default factors provided by ichol are lower triangular. See the ichol reference page for more information.

Eigenvalues and Singular Values

Two functions are available that compute a few specified eigenvalues or singular values. svds is based on eigs.

Functions to Compute a Few Eigenvalues or Singular Values

Function	Description	
eigs	Few eigenvalues	
svds	Few singular values	

These functions are most frequently used with sparse matrices, but they can be used with full matrices or even with linear operators defined in MATLAB code.

The statement

```
[V,lambda] = eigs(A,k,sigma)
```

finds the k eigenvalues and corresponding eigenvectors of the matrix A that are nearest the "shift" sigma. If sigma is omitted, the eigenvalues largest in magnitude are found. If sigma is zero, the eigenvalues smallest in magnitude are found. A second matrix, B, can be included for the generalized eigenvalue problem: $A\upsilon=\lambda B\upsilon$.

The statement

```
[U,S,V] = svds(A,k)
```

finds the k largest singular values of A and

```
[U,S,V] = svds(A,k,'smallest')
```

finds the k smallest singular values.

The numerical techniques used in eigs and svds are described in [6].

Smallest Eigenvalue of Sparse Matrix

This example shows how to find the smallest eigenvalue and eigenvector of a sparse matrix.

Set up the five-point Laplacian difference operator on a 65-by-65 grid in an L-shaped, two-dimensional domain.

```
L = numgrid('L',65);
A = delsq(L);
```

Determine the order and number of nonzero elements.

```
size(A)

ans = 1 \times 2

2945 2945

nnz(A)

ans = 14473
```

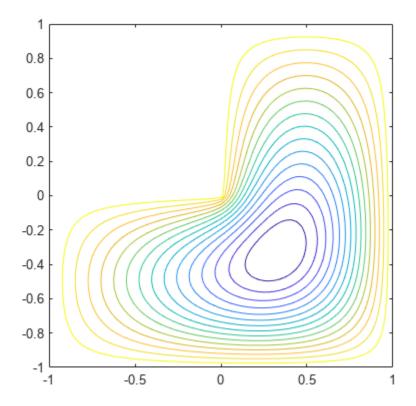
A is a matrix of order 2945 with 14,473 nonzero elements.

Compute the smallest eigenvalue and eigenvector.

```
[v,d] = eigs(A,1,'smallestabs');
```

Distribute the components of the eigenvector over the appropriate grid points and produce a contour plot of the result.

```
L(L>0) = full(v(L(L>0)));
x = -1:1/32:1;
contour(x,x,L,15)
axis square
```



References

- [1] Amestoy, P. R., T. A. Davis, and I. S. Duff, "An Approximate Minimum Degree Ordering Algorithm," *SIAM Journal on Matrix Analysis and Applications*, Vol. 17, No. 4, Oct. 1996, pp. 886-905.
- [2] Barrett, R., M. Berry, T. F. Chan, et al., *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods*, SIAM, Philadelphia, 1994.
- [3] Davis, T.A., Gilbert, J. R., Larimore, S.I., Ng, E., Peyton, B., "A Column Approximate Minimum Degree Ordering Algorithm," *Proc. SIAM Conference on Applied Linear Algebra*, Oct. 1997, p. 29.
- [4] Gilbert, John R., Cleve Moler, and Robert Schreiber, "Sparse Matrices in MATLAB: Design and Implementation," SIAM J. Matrix Anal. Appl., Vol. 13, No. 1, January 1992, pp. 333-356.
- [5] Larimore, S. I., An Approximate Minimum Degree Column Ordering Algorithm, MS Thesis, Dept. of Computer and Information Science and Engineering, University of Florida, Gainesville, FL, 1998.
- [6] Saad, Yousef, Iterative Methods for Sparse Linear Equations. PWS Publishing Company, 1996.
- [7] Karypis, George and Vipin Kumar. "A Fast and High Quality Multilevel Scheme for Partitioning Irregular Graphs." *SIAM Journal on Scientific Computing*. Vol. 20, Number 1, 1999, pp. 359–392.

See Also

More About

- "Computational Advantages of Sparse Matrices" on page 4-2
- "Constructing Sparse Matrices" on page 4-4
- "Accessing Sparse Matrices" on page 4-8

Finite Difference Laplacian

This example shows how to compute and represent the finite difference Laplacian on an L-shaped domain.

Domain

The numgrid function numbers points within an L-shaped domain. The spy function is a useful tool for visualizing the pattern of nonzero elements in a matrix. Use these two functions to generate and display an L-shaped domain.

```
n = 32;
R = 'L';
G = numgrid(R,n);
spy(G)
title('A Finite Difference Grid')
```



Show a smaller version of the matrix as a sample.

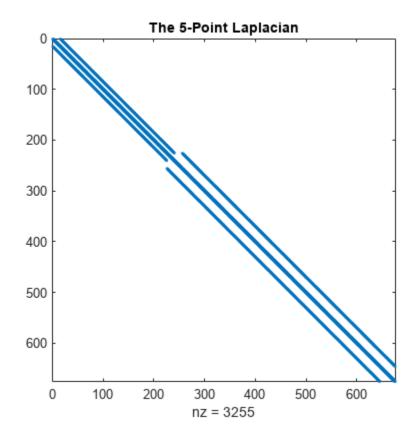
```
g = numgrid(R, 10)
g = 10 \times 10
      0
                    0
                            0
                                   0
                                           0
                                                  0
                                                          0
                                                                 0
                                                                         0
      0
             1
                    5
                            9
                                  13
                                          17
                                                 25
                                                         33
                                                                41
                                                                         0
                                  14
                                          18
                                                                42
                           10
                                                 26
```

0	3	7	11	15	19	27	35	43	0
0	4	8	12	16	20	28	36	44	0
0	0	0			21	29	37	45	0
0	0	0	0	0	22	30	38	46	0
0	0	0	0	0	23	31	39	47	0
0	0	0	0	0	24	32	40	48	0
0	0	0	0	0	0	0	0	0	0

Discrete Laplacian

Use delsq to generate the discrete Laplacian. Use the spy function again to get a graphical feel of the matrix elements.

```
D = delsq(G);
spy(D)
title('The 5-Point Laplacian')
```



Determine the number of interior points.

```
N = sum(G(:)>0)
N = 675
```

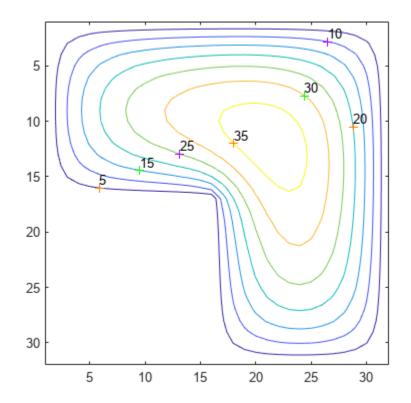
Dirichlet Boundary Value Problem

Solve the Dirichlet boundary value problem for the sparse linear system. The problem setup is: delsq(u) = 1 in the interior, u = 0 on the boundary.

```
rhs = ones(N,1);
if (R == 'N') % For nested dissection, turn off minimum degree ordering.
    spparms('autommd',0)
    u = D\rhs;
    spparms('autommd',1)
else
    u = D\rhs; % This is used for R=='L' as in this example
end
```

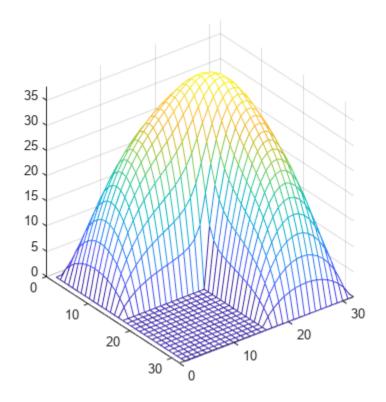
Map the solution onto the L-shaped grid and plot it as a contour map.

```
U = G;
U(G>0) = full(u(G(G>0)));
clabel(contour(U));
prism
axis square ij
```



Now show the solution as a mesh plot.

```
mesh(U)
axis([0 n 0 n 0 max(max(U))])
axis square ij
```



See Also

spy

Graphical Representation of Sparse Matrices

This example shows the finite element mesh for a NASA airfoil, including two trailing flaps. More information about the history of airfoils is available at NACA Airfoils (nasa.gov).

The data is stored in the file airfoil.mat. The data consists of 4253 pairs of (x,y) coordinates of the mesh points. It also contains an array of 12,289 pairs of indices, (i,j), specifying connections between the mesh points.

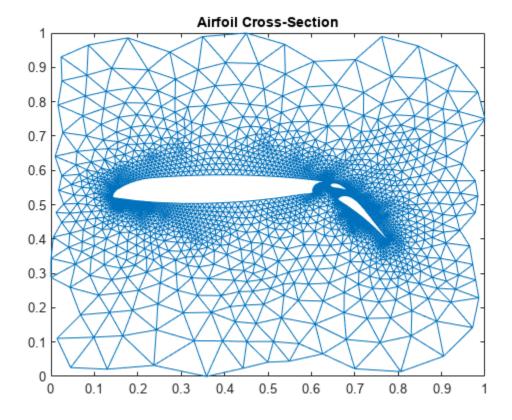
Load the data file into the workspace.

load airfoil

View Finite Element Mesh

First, scale x and y by 2^{-32} to bring them into the range [0, 1]. Then form a sparse adjacency matrix from the (i,j) connections and make it positive definite. Finally, plot the adjacency matrix using (x,y) as the coordinates for the vertices (mesh points).

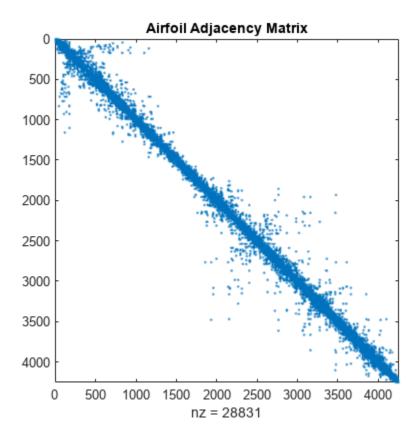
```
% Scaling x and y
x = pow2(x,-32);
y = pow2(y,-32);
% Forming the sparse adjacency matrix and making it positive definite
n = max(max(i),max(j));
A = sparse(i,j,-1,n,n);
A = A + A';
d = abs(sum(A)) + 1;
A = A + diag(sparse(d));
% Plotting the finite element mesh
gplot(A,[x y])
title('Airfoil Cross-Section')
```



Visualize Sparsity Pattern

You can use spy to visualize the nonzero elements in a matrix, so it is a particularly useful function to see the sparsity pattern in sparse matrices. spy(A) plots the sparsity pattern of the matrix A.

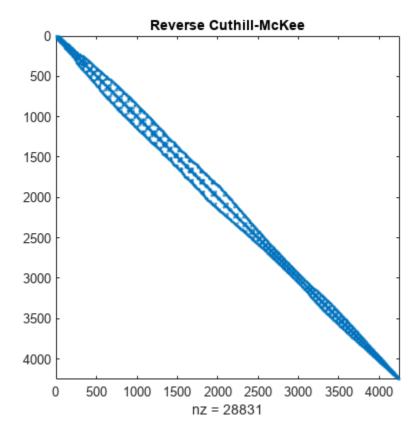
spy(A)
title('Airfoil Adjacency Matrix')



Symmetric Reordering - Reverse Cuthill-McKee

symrcm uses the Reverse Cuthill-McKee technique for reordering the adjacency matrix. r = symrcm(A) returns a permutation vector r such that A(r,r) tends to have its diagonal elements closer to the diagonal than A. This form is a good preordering for LU or Cholesky factorization of matrices that come from "long, skinny" problems. It works for both symmetric and nonsymmetric matrices.

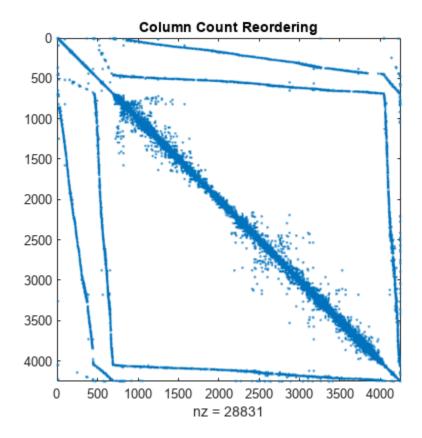
```
r = symrcm(A);
spy(A(r,r))
title('Reverse Cuthill-McKee')
```



Symmetric Reordering - Column Permutations

Use j = COLPERM(A) to return a permutation vector that reorders the columns of the sparse matrix A in nondecreasing order of nonzero count. This form is sometimes useful as a preordering for LU factorization, as in lu(A(:,j)).

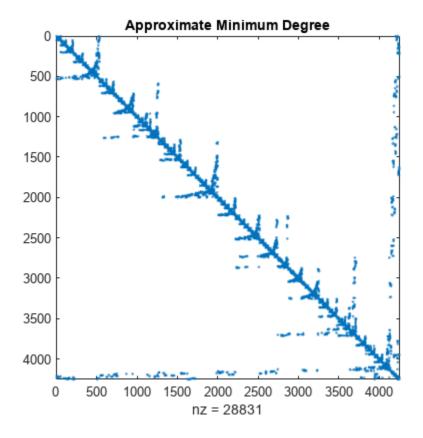
```
j = colperm(A);
spy(A(j,j))
title('Column Count Reordering')
```



Symmetric Reordering - Symmetric Approximate Minimum Degree

symamd gives a symmetric approximate minimum degree permutation. For a symmetric positive definite matrix A, the command p = symamd(S) returns the permutation vector p such that S(p,p) tends to have a sparser Cholesky factor than S. Sometimes symamd works well for symmetric indefinite matrices too.

```
m = symamd(A);
spy(A(m,m))
title('Approximate Minimum Degree')
```



See Also symamd | symrcm | colperm | spy

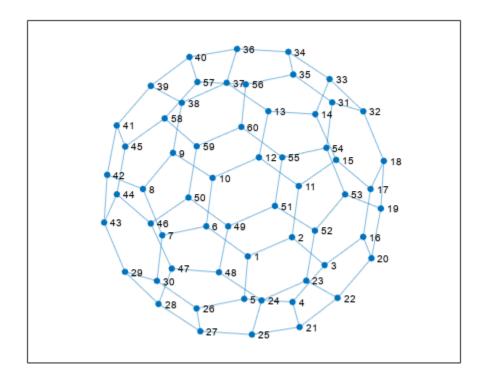
Graphs and Matrices

This example shows an application of sparse matrices and explains the relationship between graphs and matrices.

A graph is a set of nodes with specified connections, or edges, between them. Graphs come in many shapes and sizes. One example is the connectivity graph of the Buckminster Fuller geodesic dome, which is also in the shape of a soccer ball or a carbon-60 molecule.

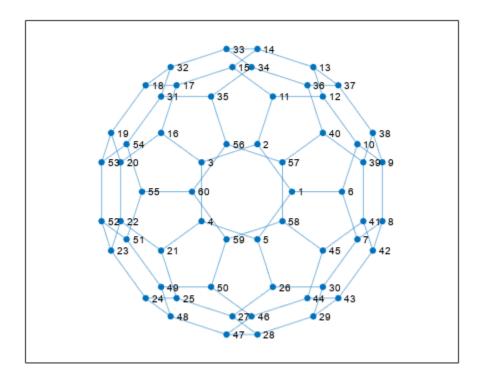
In MATLAB®, you can use the bucky function to generate the graph of the geodesic dome.

```
[B,V] = bucky;
G = graph(B);
p = plot(G);
axis equal
```



You also can specify coordinates for the nodes to change the display of the graph.

```
p.XData = V(:,1);
p.YData = V(:,2);
```

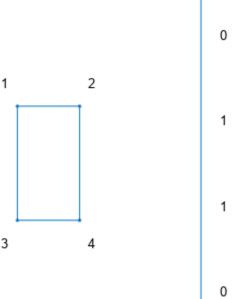


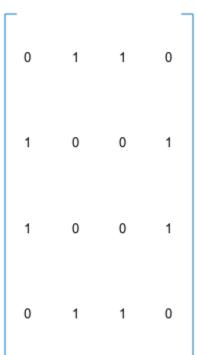
The bucky function can be used to create the graph because it returns an adjacency matrix. An adjacency matrix is one way to represent the nodes and edges in a graph.

To construct the adjacency matrix of a graph, the nodes are numbered 1 to N. Then each element (i,j) of the N-by-N matrix is set to 1 if node i is connected to node j, and 0 otherwise. Thus, for undirected graphs the adjacency matrix is symmetric, but this need not be the case for directed graphs.

For example, here is a simple graph and its associated adjacency matrix.

```
% Define a matrix A.
A = [0 \ 1 \ 1 \ 0 \ ; \ 1 \ 0 \ 0 \ 1 \ ; \ 1 \ 0 \ 0 \ 1 \ ; \ 0 \ 1 \ 1 \ 0];
% Draw a picture showing the connected nodes.
cla
subplot(1,2,1);
gplot(A,[0 1;1 1;0 0;1 0],'.-');
text([-0.2, 1.2 -0.2, 1.2],[1.2, 1.2, -.2, -.2],('1234')', ...
   'HorizontalAlignment','center')
axis([-1 2 -1 2], 'off')
% Draw a picture showing the adjacency matrix.
subplot(1,2,2);
xtemp = repmat(1:4,1,4);
ytemp = reshape(repmat(1:4,4,1),16,1)';
text(xtemp-.5,ytemp-.5,char('0'+A(:)),'HorizontalAlignment','center');
line([.25 0 0 .25 NaN 3.75 4 4 3.75],[0 0 4 4 NaN 0 0 4 4])
axis off tight
```



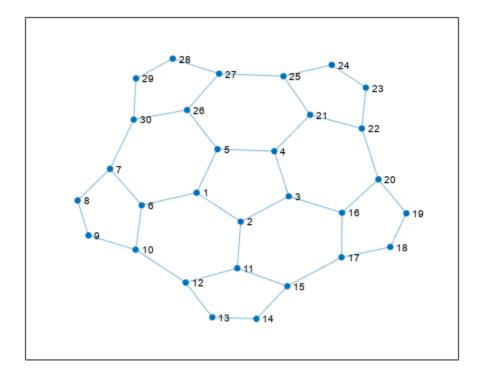


Sparse matrices are particularly helpful for representing very large graphs. This is because each node is usually connected to only a few other nodes. As a result, the density of nonzero entries in the adjacency matrix is often relatively small for large graphs. The bucky ball adjacency matrix is a good example, since it is a 60-by-60 symmetric sparse matrix with only 180 nonzero elements. The density of this matrix is just 5%.

Since the adjacency matrix defines the graph, you can plot a portion of the bucky ball by using a subset of the entries in the adjacency matrix.

Use the adjacency function to create a new adjacency matrix for the graph. Display the nodes in one hemisphere of the bucky ball by indexing into the adjacency matrix to create a new, smaller graph.

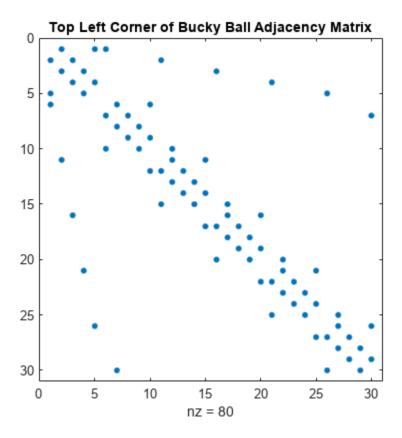
```
figure
A = adjacency(G);
H = graph(A(1:30,1:30));
h = plot(H);
```



To visualize the adjacency matrix of this hemisphere, use the spy function to plot the silhouette of the nonzero elements in the adjacency matrix.

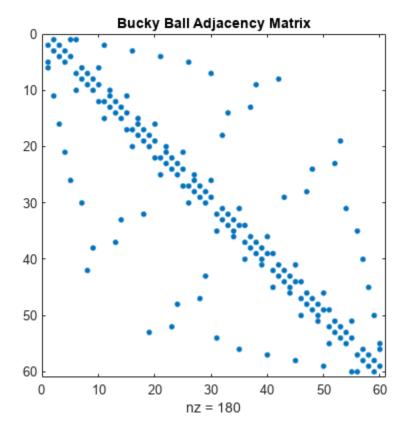
Note that the matrix is symmetric, since if node i is connected to node j, then node j is connected to node i.

```
spy(A(1:30,1:30))
title('Top Left Corner of Bucky Ball Adjacency Matrix')
```



Finally, here is a spy plot of the entire bucky ball adjacency matrix.

spy(A)
title('Bucky Ball Adjacency Matrix')



See Also spy | graph

Sparse Matrix Reordering

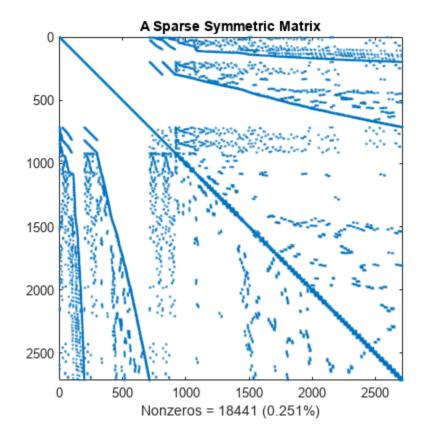
This example shows how reordering the rows and columns of a sparse matrix can influence the speed and storage requirements of a matrix operation.

Visualizing a Sparse Matrix

A spy plot shows the nonzero elements in a matrix.

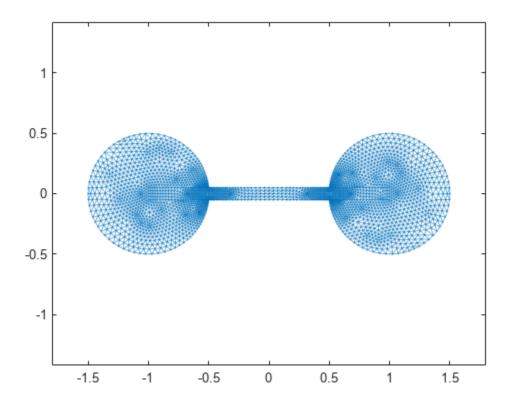
This spy plot shows a sparse symmetric positive definite matrix derived from a portion of the barbell matrix. This matrix describes connections in a graph that resembles a barbell.

```
load barbellgraph.mat
S = A + speye(size(A));
pct = 100 / numel(A);
spy(S)
title('A Sparse Symmetric Matrix')
nz = nnz(S);
xlabel(sprintf('Nonzeros = %d (%.3f%%)',nz,nz*pct));
```



Here is a plot of the barbell graph.

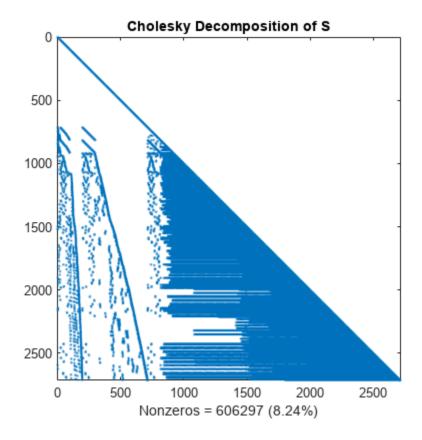
```
G = graph(S,'omitselfloops');
p = plot(G,'XData',xy(:,1),'YData',xy(:,2),'Marker','.');
axis equal
```



Computing the Cholesky Factor

Compute the Cholesky factor L, where S = L*L'. Notice that L contains many more nonzero elements than the unfactored S, because the computation of the Cholesky factorization creates **fill-in** nonzeros. These fill-in values slow down the algorithm and increase storage cost.

```
L = chol(S,'lower');
spy(L)
title('Cholesky Decomposition of S')
nc(1) = nnz(L);
xlabel(sprintf('Nonzeros = %d (%.2f%%)',nc(1),nc(1)*pct));
```



Reordering to Speed Up Calculation

By reordering the rows and columns of a matrix, it is possible to reduce the amount of fill-in that factorization creates, thereby reducing the time and storage cost of subsequent calculations.

Several different reorderings supported by MATLAB® are:

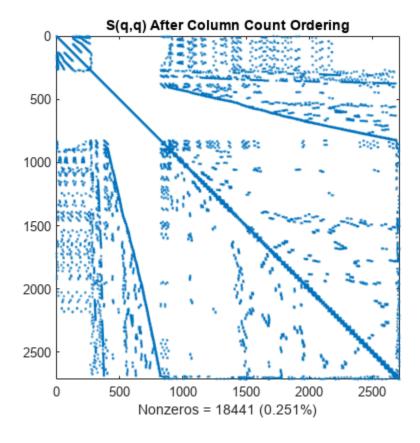
- colperm: Column count
- symrcm: Reverse Cuthill-McKee
- amd: Minimum degree
- dissect: Nested dissection

Test the effects of these sparse matrix reorderings on the barbell matrix.

Column Count Reordering

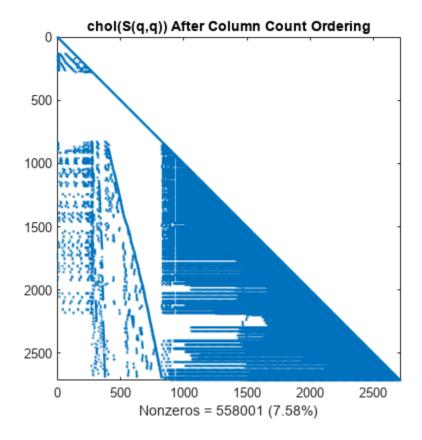
The colperm command uses the column count reordering algorithm to move rows and columns with higher nonzero count towards the end of the matrix.

```
q = colperm(S);
spy(S(q,q))
title('S(q,q) After Column Count Ordering')
nz = nnz(S);
xlabel(sprintf('Nonzeros = %d (%.3f%%)',nz,nz*pct));
```



For this matrix, the column count ordering can barely reduce the time and storage for Cholesky factorization.

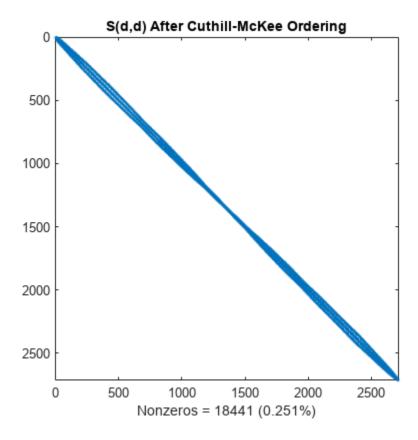
```
L = chol(S(q,q),'lower');
spy(L)
title('chol(S(q,q)) After Column Count Ordering')
nc(2) = nnz(L);
xlabel(sprintf('Nonzeros = %d (%.2f%%)',nc(2),nc(2)*pct));
```



Reverse Cuthill-McKee Reordering

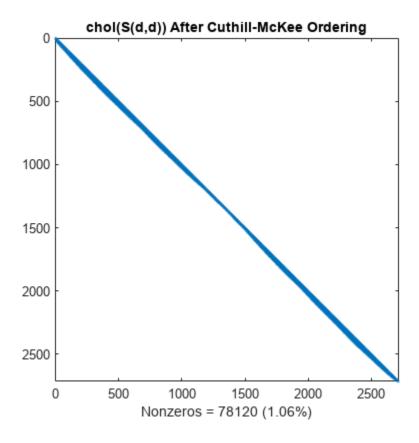
The symrcm command uses the reverse Cuthill-McKee reordering algorithm to move all nonzero elements closer to the diagonal, reducing the bandwidth of the original matrix.

```
d = symrcm(S);
spy(S(d,d))
title('S(d,d) After Cuthill-McKee Ordering')
nz = nnz(S);
xlabel(sprintf('Nonzeros = %d (%.3f%%)',nz,nz*pct));
```



The fill-in produced by Cholesky factorization is confined to the band, so factorizing the reordered matrix takes less time and less storage.

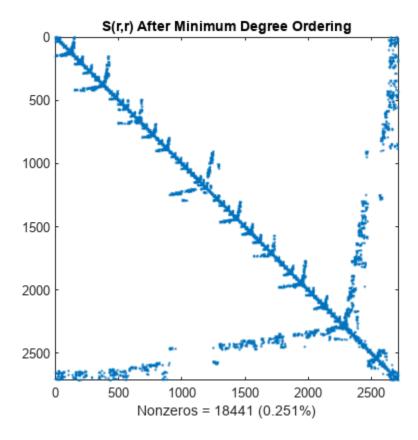
```
L = chol(S(d,d),'lower');
spy(L)
title('chol(S(d,d)) After Cuthill-McKee Ordering')
nc(3) = nnz(L);
xlabel(sprintf('Nonzeros = %d (%.2f%)', nc(3),nc(3)*pct));
```



Minimum Degree Reordering

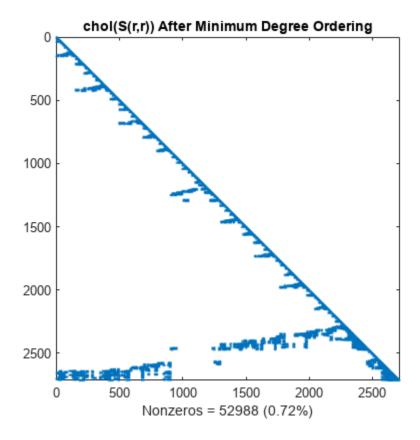
The amd command uses an approximate minimum degree algorithm (a powerful graph-theoretic technique) to produce large blocks of zeros in the matrix.

```
r = amd(S);
spy(S(r,r))
title('S(r,r) After Minimum Degree Ordering')
nz = nnz(S);
xlabel(sprintf('Nonzeros = %d (%.3f%)',nz,nz*pct));
```



The Cholesky factorization preserves the blocks of zeros produced by the minimum degree algorithm. This structure can significantly reduce time and storage costs.

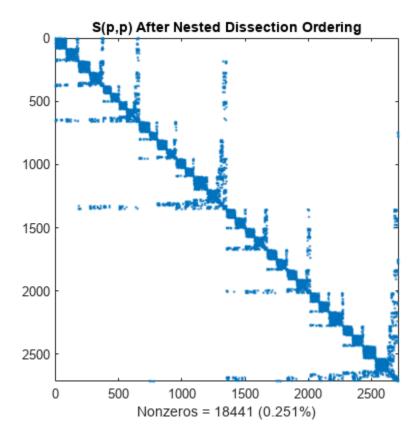
```
L = chol(S(r,r),'lower');
spy(L)
title('chol(S(r,r)) After Minimum Degree Ordering')
nc(4) = nnz(L);
xlabel(sprintf('Nonzeros = %d (%.2f%%)',nc(4),nc(4)*pct));
```



Nested Dissection Permutation

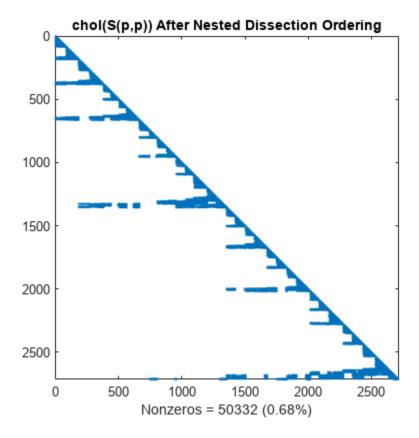
The dissect function uses graph-theoretic techniques to produce fill-reducing orderings. The algorithm treats the matrix as the adjacency matrix of a graph, coarsens the graph by collapsing vertices and edges, reorders the smaller graph, and then uses refinement steps to uncoarsen the small graph and produce a reordering of the original graph. The result is a powerful algorithm that frequently produces the least amount of fill-in compared to the other reordering algorithms.

```
p = dissect(S);
spy(S(p,p))
title('S(p,p) After Nested Dissection Ordering')
nz = nnz(S);
xlabel(sprintf('Nonzeros = %d (%.3f%)',nz,nz*pct));
```



Similar to the minimum degree ordering, the Cholesky factorization of the nested dissection ordering mostly preserves the nonzero structure of S(d,d) below the main diagonal.

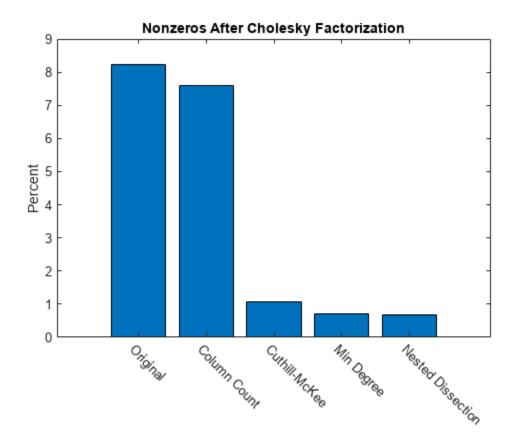
```
L = chol(S(p,p),'lower');
spy(L)
title('chol(S(p,p)) After Nested Dissection Ordering')
nc(5) = nnz(L);
xlabel(sprintf('Nonzeros = %d (%.2f%%)',nc(5),nc(5)*pct));
```



Summarizing Results

This bar chart summarizes the effects of reordering the matrix before performing the Cholesky factorization. While the Cholesky factorization of the original matrix had about 8% of its elements as nonzeros, using dissect or symamd reduces that density to less than 1%.

```
labels = {'Original','Column Count','Cuthill-McKee',...
    'Min Degree','Nested Dissection'};
bar(nc*pct)
title('Nonzeros After Cholesky Factorization')
ylabel('Percent');
ax = gca;
ax.XTickLabel = labels;
ax.XTickLabelRotation = -45;
```



See Also
spy | chol | nnz | symrcm | colperm | symamd

Iterative Methods for Linear Systems

One of the most important and common applications of numerical linear algebra is the solution of linear systems that can be expressed in the form A*x = b. When A is a large sparse matrix, you can solve the linear system using iterative methods, which enable you to trade-off between the run time of the calculation and the precision of the solution. This topic describes the iterative methods available in MATLAB to solve the equation A*x = b.

Direct vs. Iterative Methods

There are two types of methods for solving linear equations A*x = b:

• **Direct methods** are variants of Gaussian elimination. These methods use the individual matrix elements directly, through matrix operations such as LU, QR, or Cholesky factorization. You can use direct methods to solve linear equations with a high level of precision, but these methods can be slow when operating on large sparse matrices. The speed of solving a linear system with a direct method strongly depends on the density and fill pattern of the coefficient matrix.

For example, this code solves a small linear system.

```
A = magic(5);
b = sum(A,2);
x = A\b;
norm(A*x-b)
ans =
1.4211e-14
```

MATLAB implements direct methods through the matrix division operators / and \, as well as functions such as decomposition, lsgminnorm, and linsolve.

• Iterative methods produce an approximate solution to the linear system after a finite number of steps. These methods are useful for large systems of equations where it is reasonable to trade-off precision for a shorter run time. Iterative methods use the coefficient matrix only indirectly, through a matrix-vector product or an abstract linear operator. Iterative methods can be used with any matrix, but they are typically applied to large sparse matrices for which direct solves are slow. The speed of solving a linear system with an indirect method does not depend as strongly on the fill pattern of the coefficient matrix as a direct method. However, using an iterative method typically requires tuning parameters for each specific problem.

For example, this code solves a large sparse linear system that has a symmetric positive definite coefficient matrix.

```
A = delsq(numgrid('L',400));
b = ones(size(A,1),1);
x = pcg(A,b,[],1000);
norm(b-A*x)
pcg converged at iteration 796 to a solution with relative residual 9.9e-07.
ans =
   3.4285e-04
```

MATLAB implements a variety of iterative methods that have different strengths and weaknesses depending on the properties of the coefficient matrix ${\bf A}$.

Direct methods are usually faster and more generally applicable than indirect methods if there is enough storage available to carry them out. Generally, you should attempt to use x = A b first. If the direct solve is too slow, then you can try using iterative methods.

Generic Iterative Algorithm

Most iterative algorithms that solve linear equations follow a similar process:

- Start with an initial guess for the solution vector x0. (This is usually a vector of zeros unless you specify a better guess.)
- 2 Compute the residual norm res = norm(b-A*x0).
- 3 Compare the residual against the specified tolerance. If res \leq tol, end the computation and return the computed answer for x0.
- 4 Apply A*x0 and update the magnitude and direction of the vector x0 based on the value of the residual and other calculated quantities. This is the step where most computation is done.
- **5** Repeat Steps 2 through 4 until the value of x0 is good enough to satisfy the tolerance.

Iterative methods differ in how they update the magnitude and direction of x0 in Step 4, and some have slightly different convergence criteria in Steps 2 and 3, but this captures the basic process that all iterative solvers follow.

Summary of Iterative Methods

MATLAB has several functions that implement iterative methods for systems of linear equations. These methods are designed to solve Ax = b or minimize the norm ||b - Ax||. Several of these methods have similarities and are based on the same underlying algorithms, but each algorithm has benefits in certain situations [1], [2].

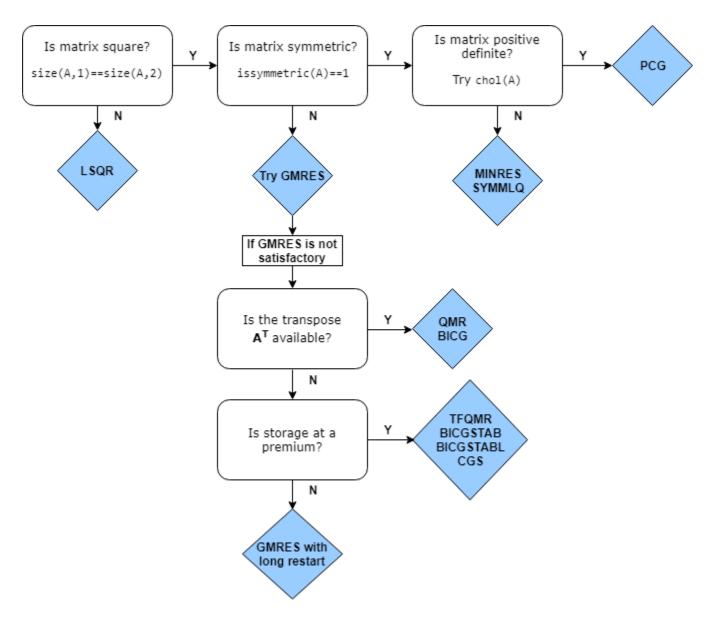
Description	Notes
pcg (preconditioned conjugate gradients)	Coefficient matrix must be symmetric positive definite.
	Most effective solver for symmetric positive definite systems since storage for only a limited number of vectors is required.
lsqr (least squares)	The only solver available for rectangular systems.
	• Analytically equivalent to the method of conjugate gradients (PCG) applied to the normal equations (A'*A)*x = A'*b.

Description	Notes
minres (minimum residual)	Coefficient matrix must be symmetric but does not need to be positive definite.
	Each iteration minimizes the residual error in the 2-norm, so the algorithm is guaranteed to make progress from step to step.
	Does not suffer from breakdowns (when an algorithm becomes unable to make progress toward a solution and halts).
symmlq (symmetric LQ)	Coefficient matrix must be symmetric but does not need to be positive definite.
	Solves a projected system and keeps the residual orthogonal to all previous ones.
	Does not suffer from breakdowns (when an algorithm becomes unable to make progress toward a solution and halts).
bicg (biconjugate gradient)	Coefficient matrix must be square.
	bicg is computationally cheap, but convergence is irregular and unreliable.
	bicg is historically important because many other iterative algorithms were developed as improvements on it.
bicgstab (biconjugate gradient stabilized)	Coefficient matrix must be square.
	Uses BiCG steps alternating with GMRES(1) steps for additional stability.
bicgstabl (biconjugate gradient stabilized (1))	Coefficient matrix must be square.
	Uses BiCG steps alternating with GMRES(2) steps for additional stability.
cgs (conjugate gradient squared)	Coefficient matrix must be square.
	Requires the same number of operations per iteration as bicg, but avoids using the transpose by working with a squared residual.

Description	Notes
gmres (generalized minimum residual)	Coefficient matrix must be square.
	• One of the most dependable algorithms, since the residual norm is minimized in each iteration.
	Work and required storage rise linearly with iteration count.
	 Choosing an appropriate restart value is essential to avoid unnecessary work and storage.
qmr (quasi-minimal residual)	Coefficient matrix must be square.
	 Overhead per iteration is slightly more than bicg, but this provides more stability.
tfqmr (transpose-free quasi-minimal residual)	Coefficient matrix must be square.
	Best solver to try for symmetric indefinite systems when memory is limited.

Choosing an Iterative Solver

This flowchart of iterative solvers in MATLAB gives a rough idea of the situations where each solver is useful. You can generally use gmres for almost all square, nonsymmetric problems. There are some cases where the biconjugate gradients algorithms (bicg, bicgstab, cgs, and so on) are more efficient than gmres, but their unpredictable convergence behavior often makes gmres a better initial choice.



Preconditioners

The convergence rate of iterative methods is dependent on the spectrum (eigenvalues) of the coefficient matrix. Therefore, you can improve the convergence and stability of most iterative methods by transforming the linear system to have a more favorable spectrum (clustered eigenvalues or a condition number near 1). This transformation is performed by applying a second matrix, called a preconditioner, to the system. This process transforms the linear system

$$Ax = b$$

into an equivalent system

$$\widetilde{A}\widetilde{x} = \widetilde{b}$$
.

The ideal preconditioner transforms the coefficient matrix A into an identity matrix, since any iterative method will converge in one iteration with such a preconditioner. In practice, finding a good

preconditioner requires trade-offs. The transformation is performed in one of three ways: left preconditioning, right preconditioning, or split preconditioning.

The first case is called *left preconditioning* since the preconditioner matrix M appears on the left of A:

$$\left(M^{-1}A\right)x = \left(M^{-1}b\right).$$

These iterative solvers use left preconditioning:

- bicg
- gmres
- gmr

In *right preconditioning, M* appears on the right of *A*:

$$(A M^{-1})(M x) = b .$$

These iterative solvers use right preconditioning:

- lsqr
- bicgstab
- bicgstabl
- cqs
- tfgmr

Finally, for symmetric coefficient matrices A, split preconditioning ensures that the transformed system is still symmetric. The preconditioner $M = HH^T$ gets split and the factors appear on different sides of A:

$$(H^{-1}AH^{-T})H^Tx = (H^{-1}b)$$

The solver algorithm for split preconditioned systems is based on the above equation, but in practice there is no need to compute H. The solver algorithm multiplies and solves with M directly.

These iterative solvers use split preconditioning:

- pcg
- minres
- symmlq

In all cases, the preconditioner M is chosen to accelerate convergence of the iterative method. When the residual error of an iterative solution stagnates or makes little progress between iterations, it often means you need to generate a preconditioner matrix to incorporate into the problem.

The iterative solvers in MATLAB allow you to specify a single preconditioner matrix M, or two preconditioner matrix factors such that $M = M_1 M_2$. This makes it easy to specify a preconditioner in its factorized form, such as M = LU. Note that in the split preconditioned case, where $M = HH^T$ also holds, there is not a relation between the M1 and M2 inputs and the H factors.

In some cases, preconditioners occur naturally in the mathematical model of a given problem. In the absence of natural preconditioners, you can use one of the incomplete factorizations in this table to

generate a preconditioner matrix. Incomplete factorizations are essentially incomplete direct solves that are quick to calculate.

Function	Factorization	Description
ilu	A≈LU	Incomplete LU factorization for square or rectangular matrices.
ichol	A ≈ L L*	Incomplete Cholesky factorization for symmetric positive definite matrices.

See "Incomplete Factorizations" on page 4-22 for more information about ilu and ichol.

Preconditioner Example

Consider the five-point finite difference approximation to Laplace's equation on a square, two-dimensional domain. The following commands use the preconditioned conjugate gradient (PCG) method with the preconditioner M = L*L', where L is the zero-fill incomplete Cholesky factor of A. For this system, pcg is unable to find a solution without specifying a preconditioner matrix.

```
A = delsq(numgrid('S',250));
b = ones(size(A,1),1);
tol = 1e-3;
maxit = 100;
L = ichol(A);
x = pcg(A,b,tol,maxit,L,L');
pcg converged at iteration 92 to a solution with relative residual 0.00076.
```

pcg requires 92 iterations to achieve the specified tolerance. However, using a different preconditioner can yield better results. For example, using ichol to construct a modified incomplete Cholesky allows pcg to meet the specified tolerance after only 39 iterations.

```
L = ichol(A,struct('type','nofill','michol','on'));
x = pcg(A,b,tol,maxit,L,L');
pcg converged at iteration 39 to a solution with relative residual 0.00098.
```

Equilibration and Reordering

For computationally tough problems, you might need a better preconditioner than the one generated by ilu or ichol directly. For example, you might want to generate a better quality preconditioner or minimize the amount of computation being done. In these cases, you can use *equilibration* to make the coefficient matrix more diagonally dominant (which can lead to a better quality preconditioner) and *reordering* to minimize the number of nonzeros in matrix factors (which can reduce memory requirements and may improve the efficiency of subsequent calculations).

If you use both equilibration and reordering to generate a preconditioner, the process is:

- 1 Use equilibrate on the coefficient matrix.
- 2 Reorder the equilibrated matrix using a sparse matrix reordering function, such as dissect or symrcm.
- **3** Generate the final preconditioner using ilu or ichol.

Here is an example that uses equilibration and reordering to generate a preconditioner for a sparse coefficient matrix.

1 Create the coefficient matrix A and a vector of ones b for the right-hand side of the linear equation. Calculate an estimation of the condition number for A.

```
load west0479;
A = west0479;
b = ones(size(A,1),1);
condest(A)
ans =
    1.4244e+12
```

Use equilibrate to improve the condition number of the coefficient matrix.

```
[P,R,C] = equilibrate(A);
Anew = R*P*A*C;
bnew = R*P*b;
condest(Anew)
ans =
5.1042e+04
```

2 Reorder the equilibrated matrix using dissect.

```
q = dissect(Anew);
Anew = Anew(q,q);
bnew = bnew(q);
```

3 Generate a preconditioner using an incomplete LU factorization.

```
[L,U] = ilu(Anew);
```

4 Solve the linear system with gmres using the preconditioner matrices, a tolerance of 1e-10, 50 maximum outer iterations, and 30 inner iterations.

```
tol = 1e-10;
maxit = 50;
restart = 30;
[xnew, flag, relres] = gmres(Anew,bnew,restart,tol,maxit,L,U);
x(q) = xnew;
x = C*x(:);
```

Now, compare the relres relative residual returned by gmres (which includes the preconditioners) to the relative residual without the preconditioners resnew and the relative residual without equilibration res. The results show that even though the linear systems are all equivalent, the different methods apply different weights to each element, and this can significantly affect the value of the residual.

```
relres
resnew = norm(Anew*xnew - bnew) / norm(bnew)
res = norm(A*x - b) / norm(b)

relres =
    8.7537e-11
resnew =
    3.6805e-08
res =
    5.1415e-04
```

Using Linear Operators Instead of Matrices

The iterative solvers in MATLAB do not *require* that you provide a numeric matrix for A. Since the calculations performed by the solvers use the result of the matrix-vector multiplication A*x or A'*x, you can instead provide a function that calculates the result of those linear operations. A function that calculates these quantities is often called a linear operator.

In addition to using a linear operator instead of a coefficient matrix A, you can also use a linear operator instead of a matrix for the preconditioner M. In that case, the function needs to calculate $M\x$ or $M'\x$, as indicated on the reference page for the solver.

Using linear operators enables you to exploit patterns in A or M to calculate the value of the linear operations more efficiently than if the solver used the matrix explicitly to carry out the full matrix-vector multiplication. It also means you do not need the memory to store the coefficient or preconditioner matrices, since the linear operator typically calculates the result of the matrix-vector multiplication without forming the matrix at all.

For example, consider the coefficient matrix

When A multiplies a vector, most of the elements in the resulting vector are zeros. The nonzero elements in the result correspond with the nonzero tridiagonal elements of A. So, for a given vector x, the linear operator function simply needs to add together three vectors to calculate the value of A*x:

```
function y = linearOperatorA(x)
y = -1*[0; x(1:end-1)] ...
+ 2*x ...
+ -1*[x(2:end); 0];
end
```

Most iterative solvers require the linear operator function for A to return the value of A*x. Likewise, for the preconditioner matrix M, the function generally must calculate $M\x$. For the solvers lsqr, qmr, and bicg, the linear operator functions must also return the value for A'*x or $M'\x$ when requested. See the iterative solver reference pages for examples and descriptions of linear operator functions.

References

- [1] Barrett, R., M. Berry, T. F. Chan, et al., *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods*, SIAM, Philadelphia, 1994.
- [2] Saad, Yousef, Iterative Methods for Sparse Linear Equations. PWS Publishing Company, 1996.

See Also

More About

• "Systems of Linear Equations" on page 2-10

Graph and Network Algorithms

- "Directed and Undirected Graphs" on page 5-2
- "Modify Nodes and Edges of Existing Graph" on page 5-10
- "Add Graph Node Names, Edge Weights, and Other Attributes" on page 5-13
- "Graph Plotting and Customization" on page 5-17
- "Visualize Breadth-First and Depth-First Search" on page 5-28
- "Partition Graph with Laplacian Matrix" on page 5-33
- "Add Node Properties to Graph Plot Data Tips" on page 5-36
- "Build Watts-Strogatz Small World Graph Model" on page 5-41
- "Use PageRank Algorithm to Rank Websites" on page 5-48
- "Label Graph Nodes and Edges" on page 5-55

Directed and Undirected Graphs

In this section...

"What Is a Graph?" on page 5-2

"Creating Graphs" on page 5-5

"Graph Node IDs" on page 5-8

"Modify or Query Existing Graph" on page 5-8

What Is a Graph?

A graph is a collection of *nodes* and *edges* that represents relationships:

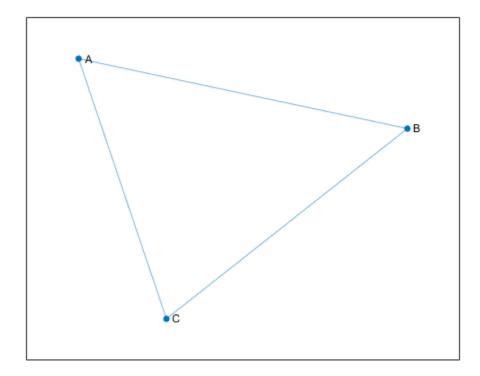
- **Nodes** are vertices that correspond to objects.
- **Edges** are the connections between objects.
- The graph edges sometimes have **Weights**, which indicate the strength (or some other attribute) of each connection between the nodes.

These definitions are general, as the exact meaning of the nodes and edges in a graph depends on the specific application. For instance, you can model the friendships in a social network using a graph. The graph nodes are people, and the edges represent friendships. The natural correspondence of graphs to physical objects and situations means that you can use graphs to model a wide variety of systems. For example:

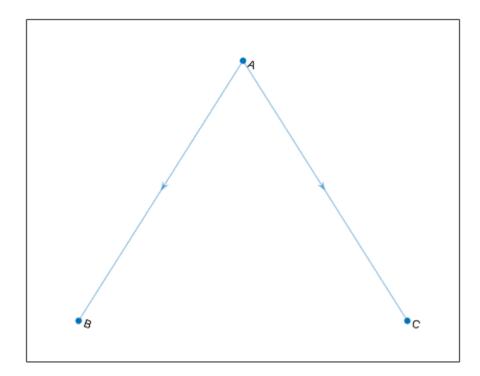
- Web page linking The graph nodes are web pages, and the edges represent hyperlinks between pages.
- Airports The graph nodes are airports, and the edges represent flights between airports.

In MATLAB, the graph and digraph functions construct objects that represent undirected and directed graphs.

• **Undirected graphs** have edges that do not have a direction. The edges indicate a *two-way* relationship, in that each edge can be traversed in both directions. This figure shows a simple undirected graph with three nodes and three edges.



• **Directed graphs** have edges with direction. The edges indicate a *one-way* relationship, in that each edge can only be traversed in a single direction. This figure shows a simple directed graph with three nodes and two edges.



The exact position, length, or orientation of the edges in a graph illustration typically do not have meaning. In other words, the same graph can be visualized in several different ways by rearranging the nodes and/or distorting the edges, as long as the underlying structure does not change.

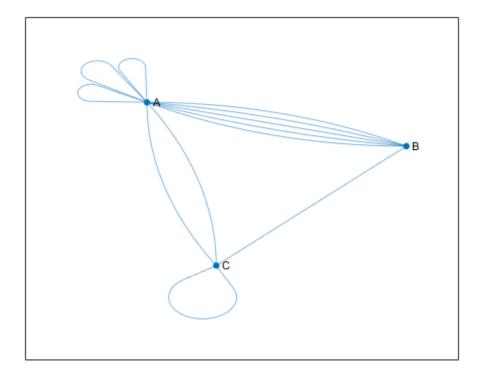
Self-loops and Multigraphs

Graphs created using graph and digraph can have one or more *self-loops*, which are edges connecting a node to itself. Additionally, graphs can have multiple edges with the same source and target nodes, and the graph is then known as a *multigraph*. A multigraph may or may not contain self-loops.

For the purposes of graph algorithm functions in MATLAB, a graph containing a node with a single self-loop is not a multigraph. However, if the graph contains a node with *multiple* self-loops, it is a multigraph.

For example, the following figure shows an undirected multigraph with self-loops. Node A has three self-loops, while node C has one. The graph contains these three conditions, any one of which makes it a multigraph.

- Node A has three self-loops.
- Nodes A and B have five edges between them.
- · Nodes A and C have two edges between them.



To determine whether a given graph is a multigraph, use the ismultigraph function.

Creating Graphs

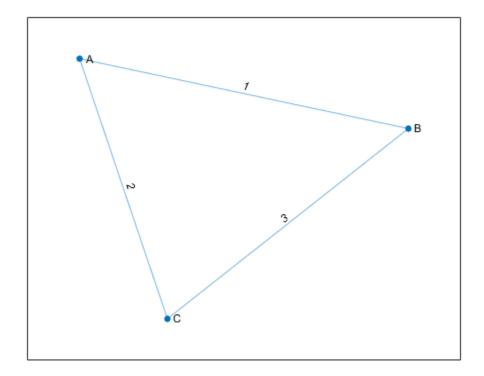
The primary ways to create a graph include using an adjacency matrix or an edge list.

Adjacency Matrix

One way to represent the information in a graph is with a square *adjacency matrix*. The nonzero entries in an adjacency matrix indicate an edge between two nodes, and the value of the entry indicates the weight of the edge. The diagonal elements of an adjacency matrix are typically zero, but a nonzero diagonal element indicates a *self-loop*, or a node that is connected to itself by an edge.

- When you use graph to create an undirected graph, the adjacency matrix must be symmetric. In practice, the matrices are frequently triangular to avoid repetition. To construct an undirected graph using only the upper or lower triangle of the adjacency matrix, use graph(A, 'upper') or graph(A, 'lower').
- When you use digraph to create a directed graph, the adjacency matrix does not need to be symmetric.
- For large graphs, the adjacency matrix contains many zeros and is typically a sparse matrix.
- You cannot create a multigraph from an adjacency matrix.

For example, consider this undirected graph.



You can represent the graph with this adjacency matrix:

$$\begin{pmatrix}
0 & 1 & 2 \\
1 & 0 & 3 \\
2 & 3 & 0
\end{pmatrix}$$

To construct the graph in MATLAB, input:

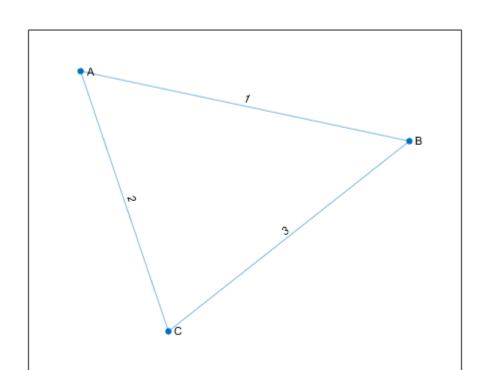
```
A = [0 1 2; 1 0 3; 2 3 0];
node_names = {'A','B','C'};
G = graph(A,node_names)

G =
   graph with properties:
   Edges: [3×2 table]
   Nodes: [3×1 table]
```

You can use the graph or digraph functions to create a graph using an adjacency matrix, or you can use the adjacency function to find the weighted or unweighted sparse adjacency matrix of a preexisting graph.

Edge List

Another way to represent the information in a graph is by listing all of the edges.



For example, consider the same undirected graph.

Now represent the graph by the edge list

Edge Weight

(A,B) 1

(A,C) 2

(B,C) 3

From the edge list it is easy to conclude that the graph has three unique nodes, A, B, and C, which are connected by the three listed edges. If the graph had disconnected nodes, they would not be found in the edge list, and would have to be specified separately.

In MATLAB, the list of edges is separated by column into *source* nodes and *target* nodes. For directed graphs the edge direction (from source to target) is important, but for undirected graphs the source and target node are interchangeable. One way to construct this graph using the edge list is to use separate inputs for the source nodes, target nodes, and edge weights:

```
source_nodes = {'A','A','B'};
target_nodes = {'B','C','C'};
edge_weights = [1 2 3];
G = graph(source nodes, target nodes, edge weights);
```

Both graph and digraph permit construction of a simple graph or multigraph from an edge list. After constructing a graph, G, you can look at the edges (and their properties) with the command G.Edges. The order of the edges in G.Edges is sorted by source node (first column) and secondarily

by target node (second column). For undirected graphs, the node with the smaller index is listed as the source node, and the node with the larger index is listed as the target node.

Since the underlying implementation of graph and digraph depends on sparse matrices, many of the same indexing costs apply. Using one of the previous methods to construct a graph all at once from the triplet pairs (source,target,weight) is quicker than creating an empty graph and iteratively adding more nodes and edges. For best performance, minimize the number of calls to graph, digraph, addedge, addnode, rmedge, and rmnode.

Graph Node IDs

By default, all of the nodes in a graph created using graph or digraph are numbered. Therefore, you always can refer to them by their numeric *node index*.

If the graph has node names (that is, G.Nodes contains a variable Name), then you also can refer to the nodes in a graph using their names. Thus, named nodes in a graph can be referred to by either their node indices or node names. For example, node 1 can be called, 'A'.

The term *node ID* encompasses both aspects of node identification. The node ID refers to both the node index and the node name.

For convenience, MATLAB remembers which type of node ID you use when you call most graph functions. So if you refer to the nodes in a graph by their node indices, most graph functions return a numeric answer that also refers to the nodes by their indices.

```
A = [0 1 1 0; 1 0 1 0; 1 1 0 1; 0 0 1 0];
G = graph(A, { 'a', 'b', 'c', 'd'});
p = shortestpath(G,1,4)
p =
```

However, if you refer to the nodes by their names, then most graph functions return an answer that also refers to the nodes by their names (contained in a cell array of character vectors or string array).

```
p1 = shortestpath(G,'a','d')
p1 =
    1×3 cell array
    {'a'}    {'c'}    {'d'}
```

Use findnode to find the numeric node ID for a given node name. Conversely, for a given numeric node ID, index into G.Nodes.Name to determine the corresponding node name.

Modify or Query Existing Graph

After you construct a graph or digraph object, you can use a variety of functions to modify the graph structure or to determine how many nodes or edges the graph has. This table lists some available functions for modifying or querying graph and digraph objects.

	Add
addedge	Add one or more edges to a graph

rmedge	Remove one or more edges from a graph		
addnode	Add one or more nodes to a graph		
rmnode	Remove one or more nodes from a graph		
findnode	Locate a specific node in a graph		
findedge	Locate a specific edge in a graph		
numnodes	Find the number of nodes in a graph		
numedges	Find the number of edges in a graph		
edgecount	Number of edges between specified nodes		
flipedge	Reverse the direction of directed graph edges		
reordernodes	Permute the order of the nodes in a graph		
subgraph	Extract subgraph		

See "Modify Nodes and Edges of Existing Graph" on page 5-10 for some common graph modification examples.

See Also

graph|digraph

More About

- "Modify Nodes and Edges of Existing Graph" on page 5-10
- "Add Graph Node Names, Edge Weights, and Other Attributes" on page 5-13
- "Graph Plotting and Customization" on page 5-17

Modify Nodes and Edges of Existing Graph

This example shows how to access and modify the nodes and/or edges in a graph or digraph object using the addedge, rmedge, addnode, rmnode, findedge, findnode, and subgraph functions.

Add Nodes

Create a graph with four nodes and four edges. The corresponding elements in s and t specify the end nodes of each graph edge.

```
s = [1 1 1 2];
t = [2 3 4 3];
G = graph(s,t)

G =
   graph with properties:
   Edges: [4x1 table]
   Nodes: [4x0 table]
```

View the edge list of the graph.

G.Edges

```
ans=4×1 table
EndNodes

1 2
1 3
1 4
2 3
```

Use addnode to add five nodes to the graph. This command adds five disconnected nodes with node IDs 5, 6, 7, 8, and 9.

```
G = addnode(G,5)

G =
  graph with properties:
  Edges: [4x1 table]
  Nodes: [9x0 table]
```

Remove Nodes

Use rmnode to remove nodes 3, 5, and 6 from the graph. All edges connected to one of the removed nodes also are removed. The remaining six nodes in the graph are renumbered to reflect the new number of nodes.

```
G = rmnode(G,[3 5 6])
G =
  graph with properties:
```

```
Edges: [2x1 table] Nodes: [6x0 table]
```

Add Edges

Use addedge to add two edges to G. The first edge is between node 1 and node 5, and the second edge is between node 2 and node 5. This command adds two new rows to G.Edges.

```
G = addedge(G,[1 2],[5 5])
G =
  graph with properties:
  Edges: [4x1 table]
  Nodes: [6x0 table]
```

Remove Edges

Use rmedge to remove the edge between node 1 and node 3. This command removes a row from G.Edges.

```
G = rmedge(G,1,3)

G =
  graph with properties:
  Edges: [3x1 table]
  Nodes: [6x0 table]
```

Determine Edge Index

Determine the edge index for the edge between nodes 1 and 5. The edge index, ei, is a row number in G. Edges.

```
ei = findedge(G,1,5)
ei = 2
```

Determine Node Index

Add node names to the graph, and then determine the node index for node 'd'. The numeric node index, ni, is a row number in G.Nodes. You can use both ni and the node name, 'd', to refer to the node when using other graph functions, like shortestpath.

```
G.Nodes.Name = {'a' 'b' 'c' 'd' 'e' 'f'}';
ni = findnode(G,'d')
ni = 4
```

Extract Subgraph

Use subgraph to extract a piece of the graph containing only two nodes.

```
H = subgraph(G,[1 2])
```

```
H =
  graph with properties:
  Edges: [1x1 table]
  Nodes: [2x1 table]
```

View the edge list of the subgraph.

H.Edges

Modify Node and Edge Tables with Variables Editor

The node and edge information for a graph object is contained in two properties: Nodes and Edges. Both of these properties are tables containing variables to describe the attributes of the nodes and edges in the graph. Since Nodes and Edges are both tables, you can use the Variables editor to interactively view or edit the tables. You cannot add or remove nodes or edges using the Variables editor, and you also cannot edit the EndNodes property of the Edges table. The Variables editor is useful for managing extra node and edge attributes in the Nodes and Edges tables. For more information, see "Create and Edit Variables".

See Also

graph | digraph | addedge | rmedge | addnode | rmnode | findedge | findnode | subgraph

More About

• "Directed and Undirected Graphs" on page 5-2

Add Graph Node Names, Edge Weights, and Other Attributes

This example shows how to add attributes to the nodes and edges in graphs created using graph and digraph. You can specify node names or edge weights when you originally call graph or digraph to create a graph. However, this example shows how to add attributes to a graph after it has been created.

Create Graph

Create a directed graph. The corresponding elements in s and t define the source and target nodes of each edge in the graph.

```
s = [1 1 2 2 3];
t = [2 4 3 4 4];
G = digraph(s,t)

G =
    digraph with properties:
        Edges: [5x1 table]
        Nodes: [4x0 table]
```

Add Node Names

Add node names to the graph by adding the variable, Name, to the G.Nodes table. The Name variable must be specified as an N-by-1 cell array of character vectors or string array, where N=numnodes(G). It is important to use the Name variable when adding node names, as this variable name is treated specially by some graph functions.

```
G.Nodes.Name = {'First' 'Second' 'Third' 'Fourth'}';
```

View the new **Nodes** table.

G.Nodes

```
ans=4×1 table
Name

{'First' }
{'Second'}
{'Third' }
{'Fourth'}
```

Use table indexing to view the names of nodes 1 and 4.

Add Edge Weights

Add edge weights to the graph by adding the variable, Weight, to the G.Edges table. The Weight variable must be an M-by-1 numeric vector, where M = numedges(G). It is important to use the Weight variable when adding edge weights, as this variable name is treated specially by some graph functions.

```
G.Edges.Weight = [10 20 30 40 50]';
```

View the new Edges table.

G.Edges

ans=5×2 table EndN	lodes	Weight
{'First' } {'First' } {'Second'} {'Second'} {'Third' }	{'Second'} {'Fourth'} {'Third' } {'Fourth'} {'Fourth'}	10 20 30 40 50

Use table indexing to view the first and third rows of G. Edges.

G.Edges([1 3],:)

Add Custom Attributes

In principle you can add any variable to G.Nodes and G.Edges that defines an attribute of the graph nodes or edges. Adding custom attributes can be useful, since functions like subgraph and reordernodes preserve the graph attributes.

For example, add a variable named Power to G.Edges to indicate whether each edge is 'on' or 'off'.

```
G.Edges.Power = {'on' 'on' 'on' 'off' 'off'}';
G.Edges
ans=5×3 table
             EndNodes
                                    Weight
                                                Power
    {'First' }
{'First' }
                    {'Second'}
                                      10
                                               {'on' }
                                               {'on' }
{'on' }
                    {'Fourth'}
                                      20
    {'Second'}
                    {'Third' }
                                      30
    {'Second'}
                    {'Fourth'}
                                      40
                                               {'off'}
    {'Third' }
                    {'Fourth'}
                                      50
                                               {'off'}
```

Add a variable named Size to G. Nodes to indicate the physical size of each node.

Modify Tables with Variables Editor

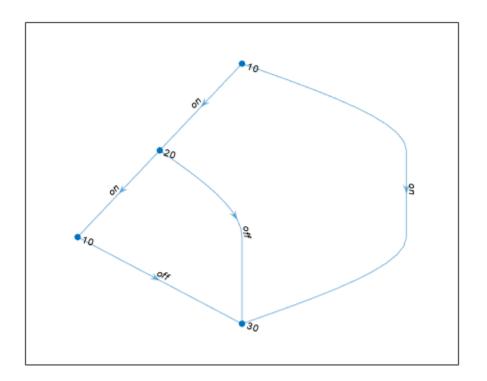
Since Nodes and Edges are both tables, you can use the Variables editor to interactively view or edit the tables. For more information, see "Create and Edit Variables".

Label Nodes and Edges of Graph Plot

When you plot a graph, you can use the variables in G.Nodes and G.Edges to label the graph nodes and edges. This practice is convenient, since these variables are already guaranteed to have the correct number of elements.

Plot the graph and label the edges using the Power variable in G.Edges. Label the nodes using the Size variable in G.Nodes.

```
p = plot(G, 'EdgeLabel', G. Edges. Power, 'NodeLabel', G. Nodes. Size)
```



```
GraphPlot with properties:
   NodeColor: [0 0.4470 0.7410]
  MarkerSize: 4
      Marker: 'o'
   EdgeColor: [0 0.4470 0.7410]
   LineWidth: 0.5000
   LineStyle: '-'
   NodeLabel: {'10' '20' '10' '30'}
EdgeLabel: {'on' 'on' 'on' 'off' 'off'}
        XData: [2 1.5000 1 2]
        YData: [4 3 2 1]
        ZData: [0 0 0 0]
Show all properties
```

See Also

graph | digraph

More About

- "Directed and Undirected Graphs" on page 5-2
- "Modify Nodes and Edges of Existing Graph" on page 5-10

Graph Plotting and Customization

This example shows how to plot graphs, and then customize the display to add labels or highlighting to the graph nodes and edges.

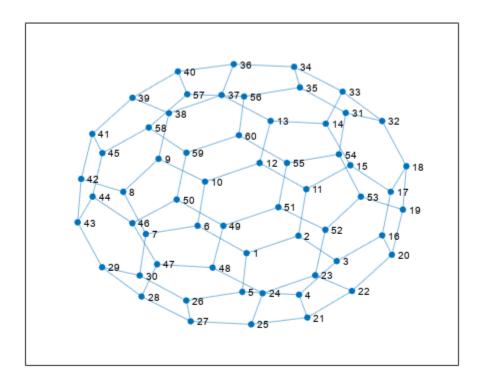
Graph Plotting Objects

Use the plot function to plot graph and digraph objects. By default, plot examines the size and type of graph to determine which layout to use. The resulting figure window contains no axes tick marks. However, if you specify the (x,y) coordinates of the nodes with the XData, YData, or ZData name-value pairs, then the figure includes axes ticks.

Node labels are included automatically in plots of graphs that have 100 or fewer nodes. The node labels use the node names if available; otherwise, the labels are numeric node indices.

For example, create a graph using the buckyball adjacency matrix, and then plot the graph using all of the default options. If you call plot and specify an output argument, then the function returns a handle to a GraphPlot object. Subsequently, you can use this object to adjust properties of the plot. For example, you can change the color or style of the edges, the size and color of the nodes, and so on.

```
G = graph(bucky);
p = plot(G)
```



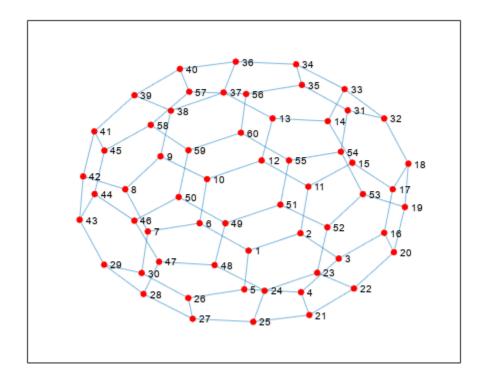
p =
 GraphPlot with properties:

Show all properties

After you have a handle to the GraphPlot object, use dot indexing to access or change the property values. For a complete list of the properties that you can adjust, see GraphPlot Properties.

Change the value of NodeColor to 'red'.

```
p.NodeColor = 'red';
```



Determine the line width of the edges.

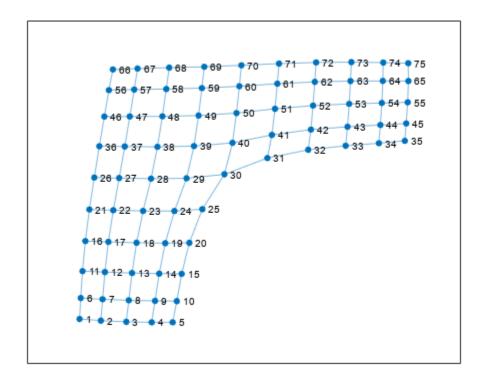
```
p.LineWidth
```

```
ans = 0.5000
```

Create and Plot Graph

Create and plot a graph representing an L-shaped membrane constructed from a square grid with a side of 12 nodes. Specify an output argument with plot to return a handle to the GraphPlot object.

```
n = 12;
A = delsq(numgrid('L',n));
G = graph(A,'omitselfloops')
G =
  graph with properties:
  Edges: [130x2 table]
  Nodes: [75x0 table]
```



```
p =
   GraphPlot with properties:

   NodeColor: [0 0.4470 0.7410]
   MarkerSize: 4
        Marker: 'o'
   EdgeColor: [0 0.4470 0.7410]
   LineWidth: 0.5000
   LineStyle: '-'
   NodeLabel: {1x75 cell}
```

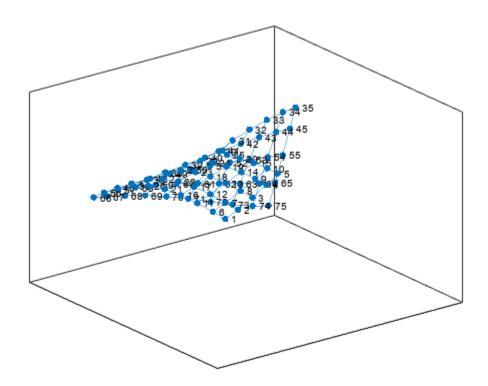
Show all properties

Change Graph Node Layout

Use the layout function to change the layout of the graph nodes in the plot. The different layout options automatically compute node coordinates for the plot. Alternatively, you can specify your own node coordinates with the XData, YData, and ZData properties of the GraphPlot object.

Instead of using the default 2-D layout method, use layout to specify the 'force3' layout, which is a 3-D force directed layout.

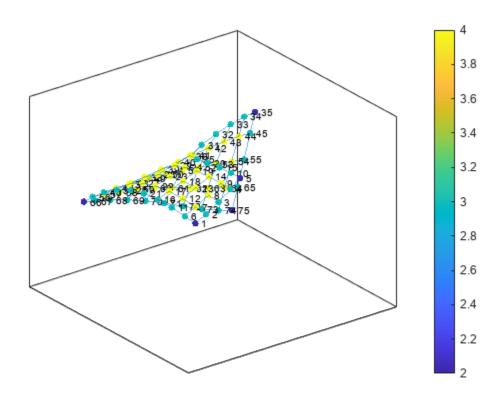
```
layout(p,'force3')
view(3)
```



Proportional Node Coloring

Color the graph nodes based on their degree. In this graph, all of the interior nodes have the same maximum degree of 4, nodes along the boundary of the graph have a degree of 3, and the corner nodes have the smallest degree of 2. Store this node coloring data as the variable NodeColors in G.Nodes.

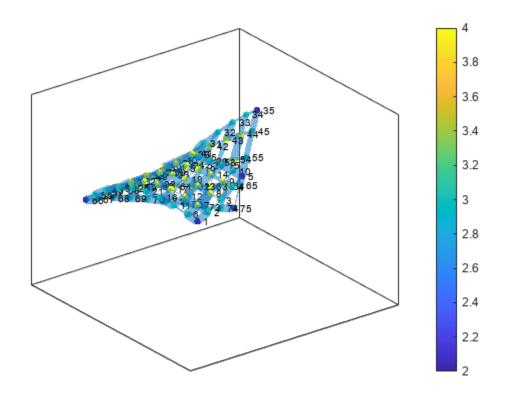
```
G.Nodes.NodeColors = degree(G);
p.NodeCData = G.Nodes.NodeColors;
colorbar
```



Edge Line Width by Weight

Add some random integer weights to the graph edges, and then plot the edges such that their line width is proportional to their weight. Since an edge line width approximately greater than 7 starts to become cumbersome, scale the line widths such that the edge with the greatest weight has a line width of 7. Store this edge width data as the variable LWidths in G.Edges.

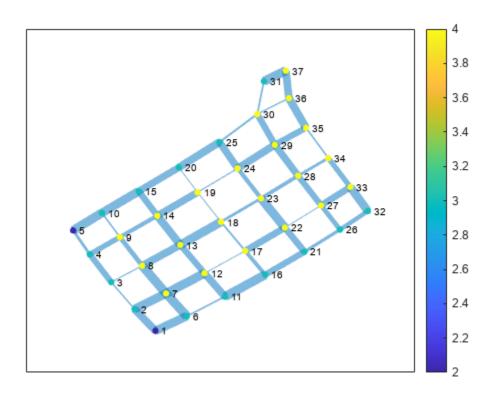
```
G.Edges.Weight = randi([10 250],130,1);
G.Edges.LWidths = 7*G.Edges.Weight/max(G.Edges.Weight);
p.LineWidth = G.Edges.LWidths;
```



Extract Subgraph

Extract and plot the top right corner of G as a subgraph, to make it easier to read the details on the graph. The new graph, H, inherits the NodeColors and LWidths variables from G, so that recreating the previous plot customizations is straightforward. However, the nodes in H are renumbered to account for the new number of nodes in the graph.

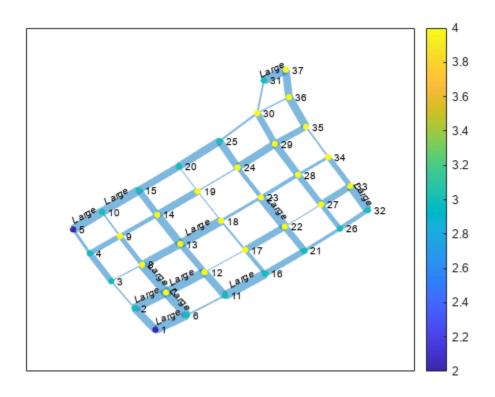
```
H = subgraph(G,[1:31 36:41]);
p1 = plot(H, 'NodeCData', H.Nodes.NodeColors, 'LineWidth', H.Edges.LWidths);
colorbar
```



Label Nodes and Edges

Use labeledge to label the edges whose width is larger than 6 with the label, 'Large'. The labelnode function works in a similar manner for labeling nodes.

labeledge(p1,find(H.Edges.LWidths > 6),'Large')



Highlight Shortest Path

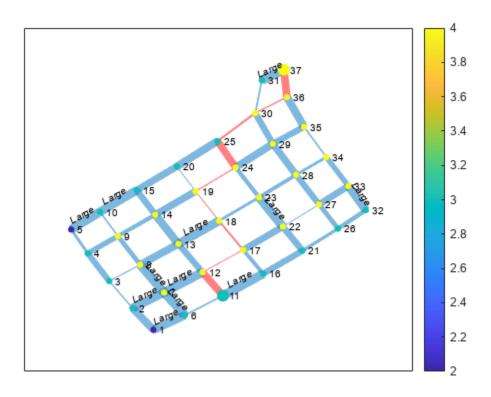
Find the shortest path between node 11 and node 37 in the subgraph, H. Highlight the edges along this path in red, and increase the size of the end nodes on the path.

```
path = shortestpath(H,11,37)

path = 1×10

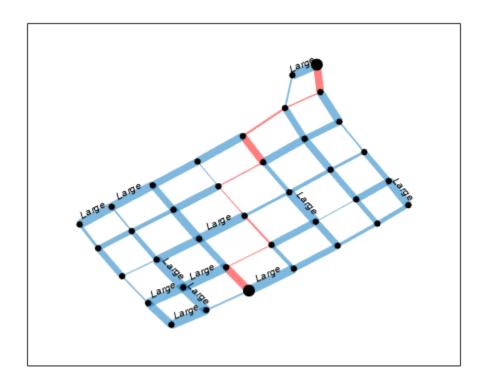
    11    12    17    18    19    24    25    30    36    37

highlight(p1,[11 37])
highlight(p1,path,'EdgeColor','r')
```



Remove the node labels and colorbar, and make all of the nodes black.

```
p1.NodeLabel = {};
colorbar off
p1.NodeColor = 'black';
```

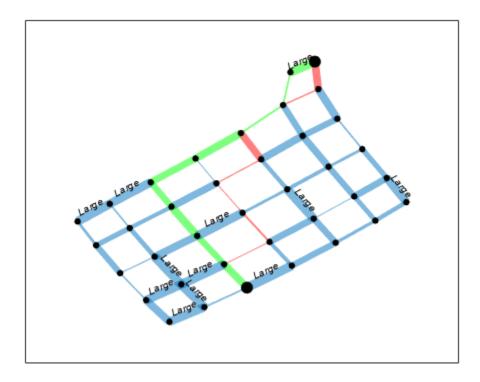


Find a different shortest path that ignores the edge weights. Highlight this path in green.

```
path2 = shortestpath(H,11,37,'Method','unweighted')
path2 = 1 \times 10
    11
          12
                 13
                        14
                              15
                                     20
                                           25
                                                  30
                                                        31
                                                               37
```

highlight(p1,path2,'EdgeColor','g')

5-26



Plotting Large Graphs

It is common to create graphs that have hundreds of thousands, or even millions, of nodes and/or edges. For this reason, plot treats large graphs slightly differently to maintain readability and performance. The plot function makes these adjustments when working with graphs that have more than 100 nodes:

- 1 The default graph layout method is always 'subspace'.
- **2** The nodes are no longer labeled automatically.
- **3** The MarkerSize property is set to 2. (Smaller graphs have a marker size of 4).
- 4 The ArrowSize property of directed graphs is set to 4. (Smaller directed graphs use an arrow size of 7).

See Also

graph | digraph | plot | GraphPlot

More About

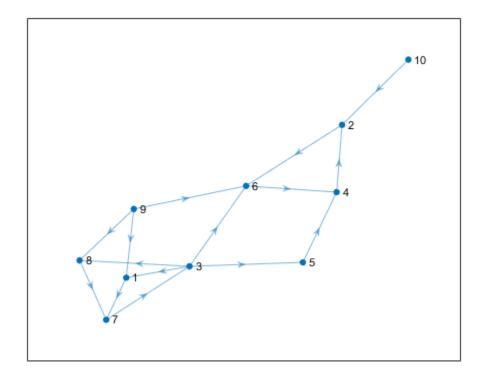
- "Directed and Undirected Graphs" on page 5-2
- GraphPlot
- "Add Node Properties to Graph Plot Data Tips" on page 5-36

Visualize Breadth-First and Depth-First Search

This example shows how to define a function that visualizes the results of bfsearch and dfsearch by highlighting the nodes and edges of a graph.

Create and plot a directed graph.

```
s = [1 2 3 3 3 3 4 5 6 7 8 9 9 9 10];
t = [7 6 1 5 6 8 2 4 4 3 7 1 6 8 2];
G = digraph(s,t);
plot(G)
```



Perform a depth-first search on the graph. Specify 'allevents' to return all events in the algorithm. Also, specify Restart as true to ensure that the search visits every node in the graph.

discovernode	1	NaN	NaN	NaN
edgetonew	NaN	1	7	1
discovernode	7	NaN	NaN	NaN
edgetonew	NaN	7	3	10
discovernode	3	NaN	NaN	NaN
edgetodiscovered	NaN	3	1	3
edgetonew	NaN	3	5	4
discovernode	5	NaN	NaN	NaN
edgetonew	NaN	5	4	8
discovernode	4	NaN	NaN	NaN
edgetonew	NaN	4	2	7
discovernode	2	NaN	NaN	NaN
edgetonew	NaN	2	6	2
discovernode	6	NaN	NaN	NaN
edgetodiscovered	NaN	6	4	9
finishnode	6	NaN	NaN	NaN
finishnode	2	NaN	NaN	NaN
finishnode	4	NaN	NaN	NaN
finishnode	5	NaN	NaN	NaN
edgetofinished	NaN	3	6	5
edgetonew	NaN	3	8	6
discovernode	8	NaN	NaN	NaN
edgetodiscovered	NaN	8	7	11
finishnode	8	NaN	NaN	NaN
finishnode	3	NaN	NaN	NaN
finishnode	7	NaN	NaN	NaN
finishnode	1	NaN	NaN	NaN
startnode	9	NaN	NaN	NaN
discovernode	9	NaN	NaN	NaN
edgetofinished	NaN	9	1	12
edgetofinished	NaN	9	6	13
edgetofinished	NaN	9	8	14
finishnode	9	NaN	NaN	NaN
startnode	10	NaN	NaN	NaN
discovernode	10	NaN	NaN	NaN
edgetofinished	NaN	10	2	15
finishnode	10	NaN	NaN	NaN

The values in the table, T, are useful for visualizing the search. The function visualize_search.m shows one way to use the results of searches performed with bfsearch and dfsearch to highlight the nodes and edges in the graph according to the table of events, T. The function pauses before each step in the algorithm, so you can slowly step through the search by pressing any key.

Save visualize search.m in the current folder.

```
function visualize_search(G,t)
% G is a graph or digraph object, and t is a table resulting from a call to
% BFSEARCH or DFSEARCH on that graph.
%
% Example inputs: G = digraph([1 2 3 3 3 3 4 5 6 7 8 9 9 9 10], ...
%        [7 6 1 5 6 8 2 4 4 3 7 1 6 8 2]);
% t = dfsearch(G, 1, 'allevents', 'Restart', true);
% Copyright 1984-2019 The MathWorks, Inc.
isundirected = isa(G, 'graph');
```

```
if isundirected
    % Replace graph with corresponding digraph, because we need separate
    % edges for both directions
    [src, tgt] = findedge(G);
    G = digraph([src; tgt], [tgt; src], [1:numedges(G), 1:numedges(G)]);
end
h = plot(G,'NodeColor',[0.5 0.5 0.5],'EdgeColor',[0.5 0.5 0.5], ...
    'EdgeLabelMode', 'auto');
for ii=1:size(t,1)
    switch t.Event(ii)
        case 'startnode'
            highlight(h,t.Node(ii),'MarkerSize',min(h.MarkerSize)*2);
        case 'discovernode'
            highlight(h,t.Node(ii),'NodeColor','r');
        case 'finishnode'
            highlight(h,t.Node(ii),'NodeColor','k');
        otherwise
            if isundirected
                a = G.Edges.Weight;
                b = t.EdgeIndex(ii);
                edgeind = intersect(find(a == b),...
                    findedge(G,t.Edge(ii,1),t.Edge(ii,2)));
            else
                edgeind = t.EdgeIndex(ii);
            end
            switch t.Event(ii)
                case 'edgetonew'
                    highlight(h,'Edges',edgeind,'EdgeColor','b');
                case 'edgetodiscovered'
                    highlight(h, 'Edges', edgeind, 'EdgeColor', [0.8 0 0.8]);
                case 'edgetofinished'
                    highlight(h, 'Edges', edgeind, 'EdgeColor', [0 0.8 0]);
            end
    end
    nodeStr = t.Node;
    if isnumeric(nodeStr)
        nodeStr = num2cell(nodeStr);
        nodeStr = cellfun(@num2str, nodeStr, 'UniformOutput', false);
    end
    edgeStr = t.Edge;
    if isnumeric(edgeStr)
        edgeStr = num2cell(edgeStr);
        edgeStr = cellfun(@num2str, edgeStr, 'UniformOutput', false);
    end
    if ~isnan(t.Node(ii))
        title([char(t{ii, 1}) ' on Node ' nodeStr{ii}]);
    else
        title([char(t{ii, 1}) ' on Edge (' edgeStr{ii, 1} ', '...
            edgeStr{ii, 2},') with edge index ' sprintf('%d ', t{ii, 4})]);
    end
    disp('Strike any key to continue...')
    pause
```

```
end
disp('Done.')
close all
```

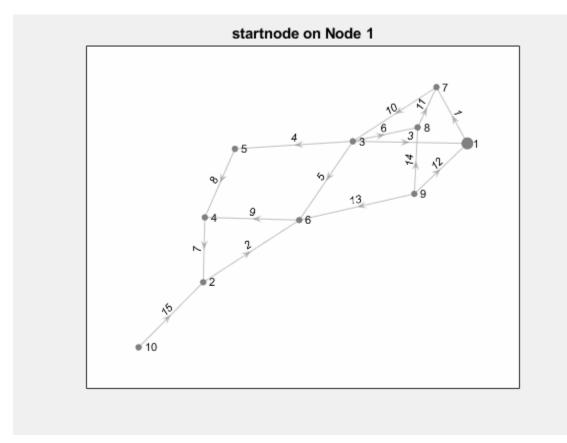
Use this command to run visualize search.m on graph G and search result T:

```
visualize_search(G,T)
```

The graph begins as all gray, and then a new piece of the search result appears each time you press a key. The search results are highlighted according to:

- 'startnode' Starting nodes increase in size.
- 'discovernode' Nodes turn red as they are discovered.
- 'finishnode' Nodes turn black after they are finished.
- 'edgetonew' Edges that lead to undiscovered nodes turn blue.
- 'edgetodiscovered' Edges that lead to discovered nodes turn magenta.
- 'edgetofinished' Edges that lead to finished nodes turn *green*.

This .gif animation shows what you see when you step through the results of visualize_search.m.



See Also

bfsearch | dfsearch | graph | digraph

More About

"Directed and Undirected Graphs" on page 5-2 $\,$

Partition Graph with Laplacian Matrix

This example shows how to use the Laplacian matrix of a graph to compute the Fiedler vector. The Fiedler vector can be used to partition the graph into two subgraphs.

Load Data

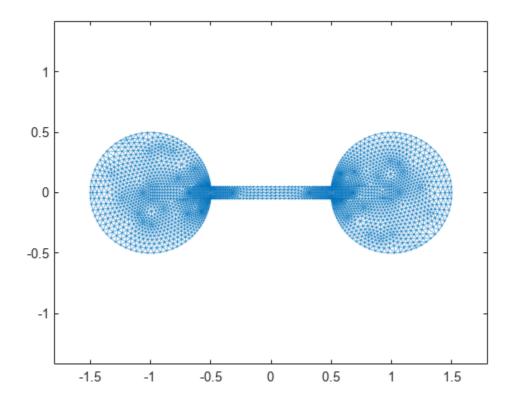
Load the data set barbellgraph.mat, which contains the sparse adjacency matrix and node coordinates of a barbell graph.

load barbellgraph.mat

Plot Graph

Plot the graph using the custom node coordinates xy.

```
G = graph(A,'omitselfloops');
p = plot(G,'XData',xy(:,1),'YData',xy(:,2),'Marker','.');
axis equal
```



Calculate Laplacian Matrix and Fiedler Vector

Calculate the Laplacian matrix of the graph. Then, calculate the two smallest magnitude eigenvalues and corresponding eigenvectors using eigs.

```
L = laplacian(G);
[V,D] = eigs(L,2,'smallestabs');
```

The Fiedler vector is the eigenvector corresponding to the second smallest eigenvalue of the graph. The *smallest* eigenvalue is zero, indicating that the graph has one connected component. In this case, the second column in V corresponds to the second smallest eigenvalue D(2,2).

```
D
D = 2 \times 2
10^{-3} \times 0.0000 \qquad 0
0 \qquad 0.2873
w = V(:,2);
```

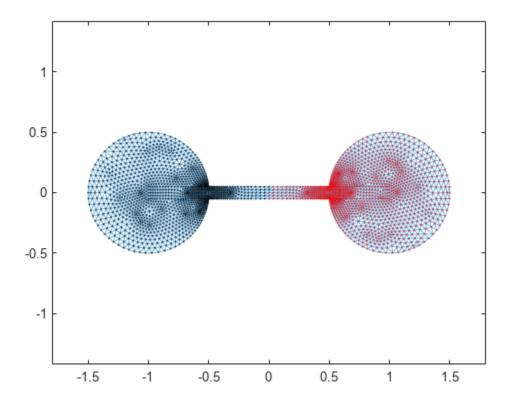
Finding the Fiedler vector using eigs is scalable to larger graphs, since only a subset of the eigenvalues and eigenvectors are computed, but for smaller graphs it is equally feasible to convert the Laplacian matrix to full storage and use eig(full(L)).

Partition Graph

Partition the graph into two subgraphs using the Fiedler vector w. A node is assigned to subgraph A if it has a positive value in w. Otherwise, the node is assigned to subgraph B. This practice is called a *sign cut* or *zero threshold cut*. The sign cut minimizes the weight of the cut, subject to the upper and lower bounds on the weight of any nontrivial cut of the graph.

Partition the graph using the sign cut. Highlight the subgraph of nodes with w>=0 in red, and the nodes with w<0 in black.

```
highlight(p,find(w>=0),'NodeColor','r') % subgraph A
highlight(p,find(w<0),'NodeColor','k') % subgraph B</pre>
```



For the bar bell graph, this partition bisects the graph nicely into two equal sets of nodes. However, the sign cut does not always produce a balanced cut.

It is always possible to bisect a graph by calculating the median of w and using it as a threshold value. This partition is called the *median cut*, and it guarantees an equal number of nodes in each subgraph.

You can use the median cut by first shifting the values in w by the median:

$$w_{med} = w - median(w);$$

Then, partition the graph by sign in w_med . For the bar bell graph, the median of w is close to zero, so the two cuts produce similar bisections.

See Also

graph | digraph | laplacian | subgraph

More About

• "Directed and Undirected Graphs" on page 5-2

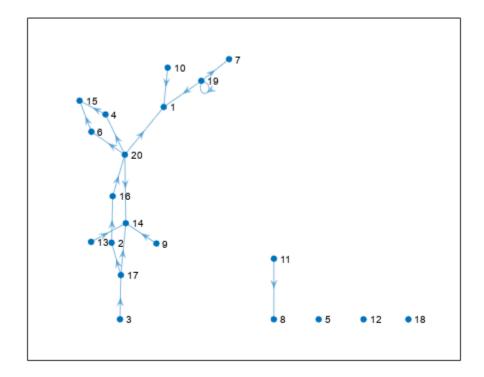
Add Node Properties to Graph Plot Data Tips

This example shows how to customize **GraphPlot** data tips to display extra node properties of a graph.

Plot GraphPlot Object with Data Tip

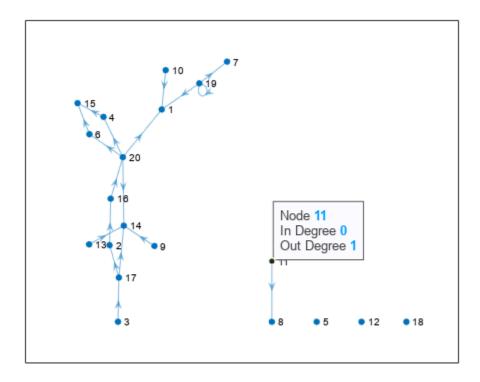
Create a GraphPlot graphics object for a random directed graph. Add an extra node property wifi to the graph.

```
rng default
G = digraph(sprandn(20, 20, 0.05));
G.Nodes.wifi = randi([0 1], 20, 1) == 1;
h = plot(G);
```



Add a data tip to the graph. The data tip enables you to select nodes in the graph plot and view properties of the nodes.

```
dt = datatip(h,4,3);
```



By default, the data tips for an undirected graph display the node number and degree. For directed graphs, the display includes the node number, in-degree, and out-degree.

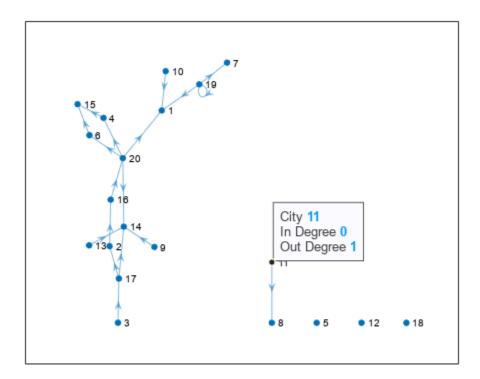
Customize Existing Data in Data Tip

You can customize the display of data tips for graphics objects by adding, editing, or removing rows of data from the appropriate object properties. For this GraphPlot object:

- The GraphPlot object handle is h.
- The h.DataTipTemplate property contains an object that controls the display of the data tips.
- The h.DataTipTemplate.DataTipRows property holds the data for the data tips as DataTipTextRow objects.
- Each DataTipTextRow object has Label and Value properties. You can adjust the label or data that is displayed in the data tip by modifying these properties.

Change the label for the Node row in the data tip so that it displays as "City".

h.DataTipTemplate.DataTipRows(1).Label = "City";

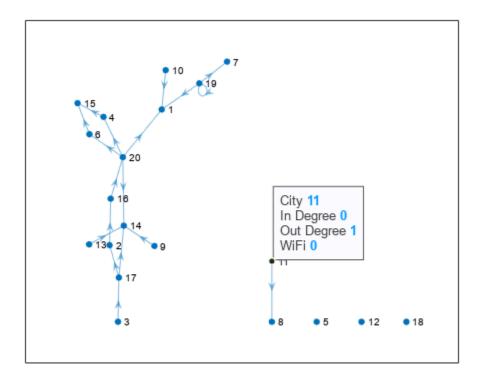


The data tip now displays a city number.

Add Data to Data Tip

The dataTipTextRow function creates a new row of data as an object that can be inserted into the DataTipRows property. Use dataTipTextRow to create a new row of data for the data tip labeled "WiFi" that references the values in the G.Nodes.wifi property of the graph. Add this data tip row to the DataTipRows property as the last row.

```
row = dataTipTextRow('WiFi',G.Nodes.wifi);
h.DataTipTemplate.DataTipRows(end+1) = row;
```



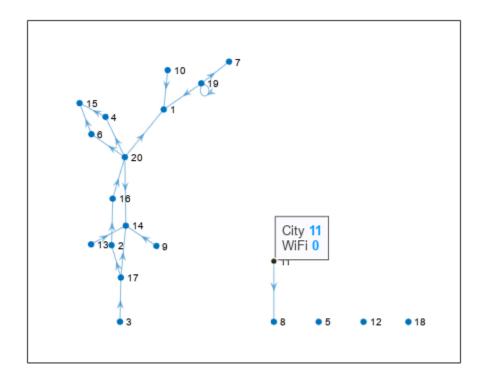
The data tip display now includes a Wi-Fi® value for each node.

Remove Data from Data Tip

To remove rows of data from the data tip, you can index into the <code>DataTipRows</code> property and assign the rows an empty matrix []. This is the same method you might use to delete rows or columns from a matrix.

Delete the in-degree and out-degree rows from the data tip. Since these appear as the second and third rows in the data tip display, they correspond to the second and third rows of the DataTipRows property.

h.DataTipTemplate.DataTipRows(2:3) = [];



The data tip display now only displays the city number and Wi-Fi status.

See Also

datatip | graph | digraph | DataTipTemplate Properties

More About

- "Create Custom Data Tips"
- "Interactively Explore Plotted Data"

Build Watts-Strogatz Small World Graph Model

This example shows how to construct and analyze a Watts-Strogatz small-world graph. The Watts-Strogatz model is a random graph that has small-world network properties, such as clustering and short average path length.

Algorithm Description

Creating a Watts-Strogatz graph has two basic steps:

- 1 Create a ring lattice with N nodes of mean degree 2K. Each node is connected to its K nearest neighbors on either side.
- For each edge in the graph, rewire the target node with probability β . The rewired edge cannot be a duplicate or self-loop.

After the first step the graph is a perfect ring lattice. So when $\beta = 0$, no edges are rewired and the model returns a ring lattice. In contrast, when $\beta = 1$, all of the edges are rewired and the ring lattice is transformed into a random graph.

The file WattsStrogatz.m implements this graph algorithm for undirected graphs. The input parameters are N, K, and beta according to the algorithm description above.

View the file WattsStrogatz.m.

```
% Copyright 2015 The MathWorks, Inc.
function h = WattsStrogatz(N.K.beta)
% H = WattsStrogatz(N,K,beta) returns a Watts-Strogatz model graph with N
% nodes, N*K edges, mean node degree 2*K, and rewiring probability beta.
% beta = 0 is a ring lattice, and beta = 1 is a random graph.
% Connect each node to its K next and previous neighbors. This constructs
% indices for a ring lattice.
s = repelem((1:N)',1,K);
t = s + repmat(1:K,N,1);
t = mod(t-1.N)+1:
% Rewire the target node of each edge with probability beta
for source=1:N
    switchEdge = rand(K, 1) < beta;
    newTargets = rand(N, 1);
    newTargets(source) = 0;
    newTargets(s(t==source)) = 0;
    newTargets(t(source, ~switchEdge)) = 0;
    [~, ind] = sort(newTargets, 'descend');
    t(source, switchEdge) = ind(1:nnz(switchEdge));
end
h = graph(s,t);
```

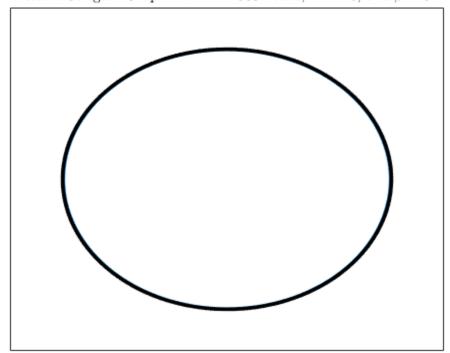
end

Ring Lattice

Construct a ring lattice with 500 nodes using the WattsStrogatz function. When beta is 0, the function returns a ring lattice whose nodes all have degree 2K.

```
h = WattsStrogatz(500,25,0);
plot(h,'NodeColor','k','Layout','circle');
title('Watts-Strogatz Graph with $N = 500$ nodes, $K = 25$, and $\beta = 0$', ...
'Interpreter','latex')
```

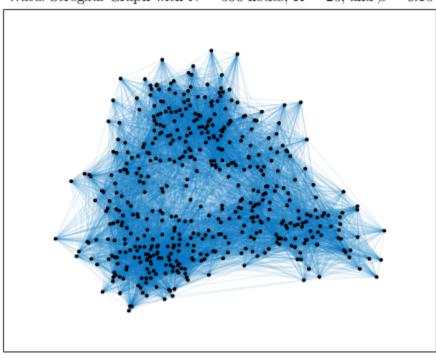
Watts-Strogatz Graph with N = 500 nodes, K = 25, and $\beta = 0$



Some Random Edges

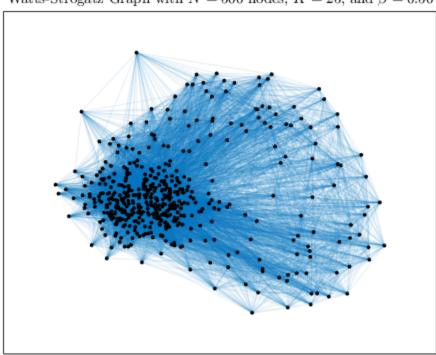
Increase the amount of randomness in the graph by raising beta to 0.15 and 0.50.

```
h2 = WattsStrogatz(500,25,0.15);
plot(h2,'NodeColor','k','EdgeAlpha',0.1);
title('Watts-Strogatz Graph with $N = 500$ nodes, $K = 25$, and $\beta = 0.15$', ...
    'Interpreter','latex')
```



Watts-Strogatz Graph with N=500 nodes, K=25, and $\beta=0.15$

```
h3 = WattsStrogatz(500,25,0.50);
plot(h3,'NodeColor','k','EdgeAlpha',0.1);
title('Watts-Strogatz Graph with $N = 500$ nodes, $K = 25$, and $\beta = 0.50$', ...
'Interpreter','latex')
```

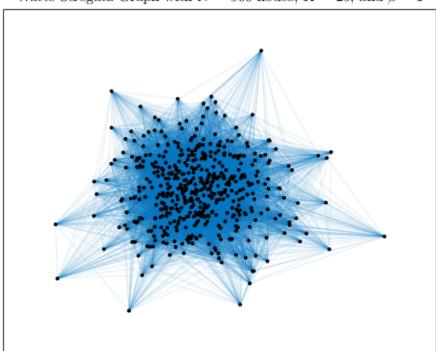


Watts-Strogatz Graph with N = 500 nodes, K = 25, and $\beta = 0.50$

Random Graph

Generate a completely random graph by increasing beta to its maximum value of 1.0. This rewires all of the edges.

```
h4 = WattsStrogatz(500,25,1);
plot(h4,'NodeColor','k','EdgeAlpha',0.1);
title('Watts-Strogatz Graph with $N = 500$ nodes, $K = 25$, and $\beta = 1$', ...
'Interpreter','latex')
```



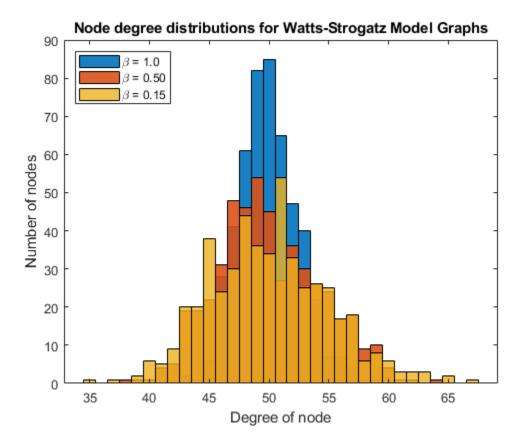
Watts-Strogatz Graph with N = 500 nodes, K = 25, and $\beta = 1$

Degree Distribution

The degree distribution of the nodes in the different Watts-Strogatz graphs varies. When beta is 0, the nodes all have the same degree, 2K, so the degree distribution is just a Dirac-delta function centered on 2K, $\delta(x-2K)$. However, as beta increases, the degree distribution changes.

This plot shows the degree distributions for the nonzero values of beta.

```
histogram(degree(h2), 'BinMethod', 'integers', 'FaceAlpha', 0.9);
hold on
histogram(degree(h3), 'BinMethod', 'integers', 'FaceAlpha', 0.9);
histogram(degree(h4), 'BinMethod', 'integers', 'FaceAlpha', 0.8);
hold off
title('Node degree distributions for Watts-Strogatz Model Graphs')
xlabel('Degree of node')
ylabel('Number of nodes')
legend('\beta = 1.0', '\beta = 0.50', '\beta = 0.15', 'Location', 'NorthWest')
```



Hub Formation

The Watts-Strogatz graph has a high clustering coefficient, so the nodes tend to form cliques, or small groups of closely interconnected nodes. As beta increases towards its maximum value of 1.0, you see an increasingly large number of hub nodes, or nodes of high relative degree. The hubs are a common connection between other nodes and between cliques in the graph. The existence of hubs is what permits the formation of cliques while preserving a short average path length.

Calculate the average path length and number of hub nodes for each value of beta. For the purposes of this example, the hub nodes are nodes with degree greater than or equal to 55. These are all of the nodes whose degree increased 10% or more compared to the original ring lattice.

```
n = 55;
d = [mean(mean(distances(h))), nnz(degree(h)>=n); ...
    mean(mean(distances(h2))), nnz(degree(h2)>=n); ...
    mean(mean(distances(h3))), nnz(degree(h3)>=n);
    mean(mean(distances(h4))), nnz(degree(h4)>=n)];
T = table([0 0.15 0.50 1]', d(:,1), d(:,2),...
    'VariableNames',{'Beta','AvgPathLength','NumberOfHubs'})
T =

4x3 table

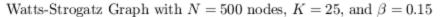
Beta AvgPathLength NumberOfHubs
```

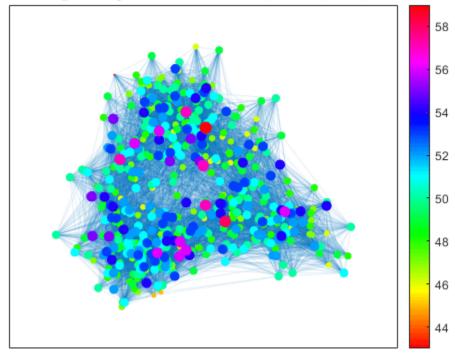
0	5.48	0
0.15	2.0715	20
0.5	1.9101	85
1	1.9008	92

As beta increases, the average path length in the graph quickly falls to its limiting value. This is due to the formation of the highly connected hub nodes, which become more numerous as beta increases.

Plot the $\beta=0.15$ Watts-Strogatz model graph, making the size and color of each node proportional to its degree. This is an effective way to visualize the formation of hubs.

```
colormap hsv
deg = degree(h2);
nSizes = 2*sqrt(deg-min(deg)+0.2);
nColors = deg;
plot(h2,'MarkerSize',nSizes,'NodeCData',nColors,'EdgeAlpha',0.1)
title('Watts-Strogatz Graph with $N = 500$ nodes, $K = 25$, and $\beta = 0.15$', ...
'Interpreter','latex')
colorbar
```





See Also

digraph | graph

Use PageRank Algorithm to Rank Websites

This example shows how to use a PageRank algorithm to rank a collection of websites. Although the PageRank algorithm was originally designed to rank search engine results, it also can be more broadly applied to the nodes in many different types of graphs. The PageRank score gives an idea of the relative importance of each graph node based on how it is connected to the other nodes.

Theoretically, the PageRank score is the limiting probability that someone randomly clicking links on each website will arrive at any particular page. So pages with a high score are highly connected and discoverable within the network, and it is more likely a random web surfer will visit that page.

Algorithm Description

At each step in the PageRank algorithm, the score of each page is updated according to,

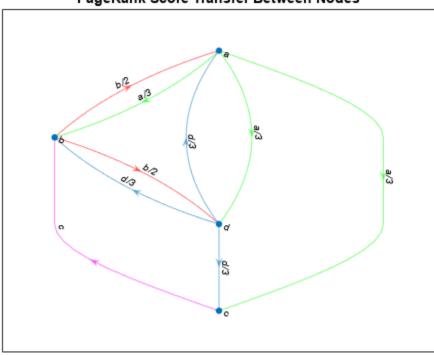
```
r = (1-P)/n + P*(A'*(r./d) + s/n);
```

- r is a vector of PageRank scores.
- P is a scalar damping factor (usually 0.85), which is the probability that a random surfer clicks on a link on the current page, instead of continuing on another random page.
- A' is the transpose of the adjacency matrix of the graph.
- d is a vector containing the out-degree of each node in the graph. d is set to 1 for nodes with no outgoing edges.
- n is the scalar number of nodes in the graph.
- s is the scalar sum of the PageRank scores for pages with no links.

In other words, the rank of each page is largely based on the ranks of the pages that link to it. The term A'*(r./d) picks out the scores of the source nodes that link to each node in the graph, and the scores are normalized by the total number of outbound links of those source nodes. This ensures that the sum of the PageRank scores is always 1. For example, if node 2 links to nodes 1, 3, and 4, then it transfers 1/3 of its PageRank score to each of those nodes during each iteration of the algorithm.

Create a graph that illustrates how each node confers its PageRank score to the other nodes in the graph.

```
s = {'a' 'a' 'a' 'b' 'b' 'c' 'd' 'd' 'd'};
t = {'b' 'c' 'd' 'd' 'a' 'b' 'c' 'a' 'b'};
G = digraph(s,t);
labels = {'a/3' 'a/3' 'a/3' 'b/2' 'b/2' 'c' 'd/3' 'd/3' 'd/3'};
p = plot(G, 'Layout', 'layered', 'EdgeLabel', labels);
highlight(p,[1 1 1],[2 3 4], 'EdgeColor', 'g')
highlight(p,[2 2],[1 4], 'EdgeColor', 'r')
highlight(p,3,2,'EdgeColor', 'm')
title('PageRank Score Transfer Between Nodes')
```

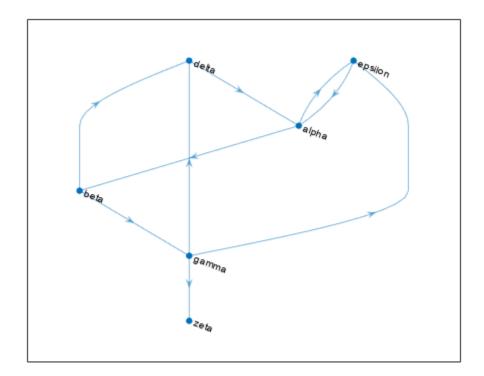


PageRank Score Transfer Between Nodes

The centrality function contains an option for calculating PageRank scores.

PageRank with 6 Nodes

Create and plot a directed graph containing six nodes representing fictitious websites.



Calculate the PageRank centrality score for this graph. Use a follow probability (otherwise known as a damping factor) of 0.85.

```
pr = centrality(G, 'pagerank', 'FollowProbability', 0.85)
pr = 6×1
     0.3210
     0.1706
     0.1066
     0.1368
     0.2008
     0.0643
```

View the PageRank scores and degree information for each page.

```
G.Nodes.PageRank = pr;
G.Nodes.InDegree = indegree(G);
G.Nodes.OutDegree = outdegree(G);
G.Nodes
ans=6×4 table
```

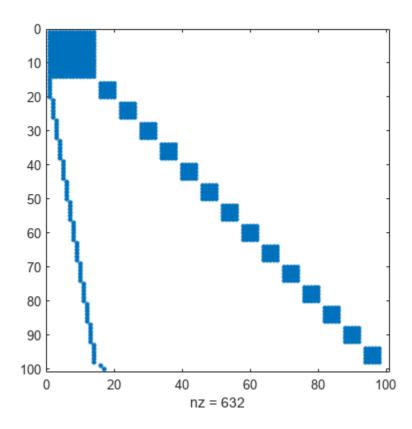
Name		PageRank	InDegree	OutDegree	
<pre>{'http://www.example.com/alpha'</pre>	}	0.32098	2	2	
{'http://www.example.com/beta'	}	0.17057	1	2	

The results show that it is not just the *number* of page links that determines the score, but also the *quality*. The alpha and gamma websites both have a total degree of 4, however alpha links to both epsilon and beta, which also are highly ranked. gamma is only linked to by one page, beta, which is in the middle of the list. Thus, alpha is scored higher than gamma by the algorithm.

PageRank of Websites on mathworks.com

Load the data in mathworks100.mat and view the adjacency matrix, A. This data was generated in 2015 using an automatic page crawler. The page crawler began at https://www.mathworks.com and followed links to subsequent web pages until the adjacency matrix contained information on the connections of 100 unique web pages.

```
load mathworks100.mat
spy(A)
```



Create a directed graph with the sparse adjacency matrix, A, using the URLs contained in U as node names.

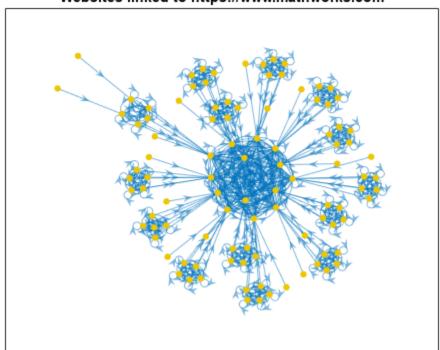
```
G = digraph(A,U)
G =
   digraph with properties:
```

```
Edges: [632x1 table]
Nodes: [100x1 table]
```

Plot the graph using the force layout.

```
plot(G,'NodeLabel',{},'NodeColor',[0.93 0.78 0],'Layout','force');
title('Websites linked to https://www.mathworks.com')
```

Websites linked to https://www.mathworks.com



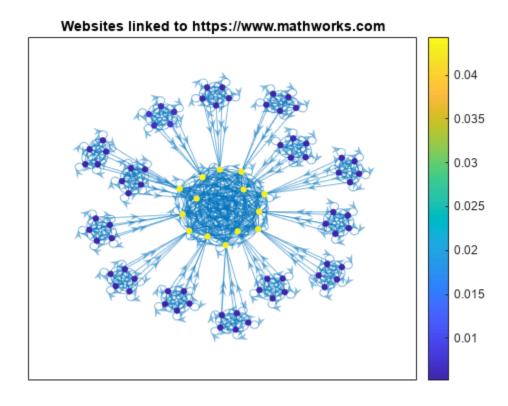
Compute the PageRank scores for the graph, G, using 200 iterations and a damping factor of 0.85. Add the scores and degree information to the nodes table of the graph.

```
pr = centrality(G,'pagerank','MaxIterations',200,'FollowProbability',0.85);
G.Nodes.PageRank = pr;
G.Nodes.InDegree = indegree(G);
G.Nodes.OutDegree = outdegree(G);
View the top 25 resulting scores.
G.Nodes(1:25,:)
ans=25×4 table
Name
```

```
{ 'https://cn.mathworks.com'
                                                                                    0.043085
{'https://jp.mathworks.com'
                                                                                    0.043085
{'https://kr.mathworks.com'
                                                                                    0.043085
                                                                                    0.043085
{'https://uk.mathworks.com'
{ 'https://au.mathworks.com'
                                                                                    0.043085
{'https://de.mathworks.com'
                                                                                    0.043085
{'https://es.mathworks.com'
                                                                                    0.043085
{ 'https://fr.mathworks.com'
                                                                                    0.043085
{ 'https://in.mathworks.com'
                                                                                    0.043085
{ 'https://it.mathworks.com'
                                                                                    0.043085
{'https://nl.mathworks.com'
                                                                                    0.043085
{'https://se.mathworks.com'
                                                                                    0.043085
{'https://www.mathworks.com/index.html%3Fnocookie%3Dtrue'
                                                                                      0.0015
{'https://www.mathworks.com/company/aboutus/policies statements/patents.html'}
                                                                                    0.007714
```

Extract and plot a subgraph containing all nodes whose score is greater than 0.005. Color the graph nodes based on their PageRank score.

```
H = subgraph(G,find(G.Nodes.PageRank > 0.005));
plot(H,'NodeLabel',{},'NodeCData',H.Nodes.PageRank,'Layout','force');
title('Websites linked to https://www.mathworks.com')
colorbar
```



The PageRank scores for the top websites are all quite similar, such that a random web surfer has about a 4.5% chance to land on each page. This small group of highly connected pages forms a clique

in the center of the plot. Connected to this central clique are several smaller cliques, which are highly connected amongst themselves.

References

Moler, C. Experiments with MATLAB. Chapter 7: Google PageRank. MathWorks, Inc., 2011.

See Also

digraph|graph|centrality

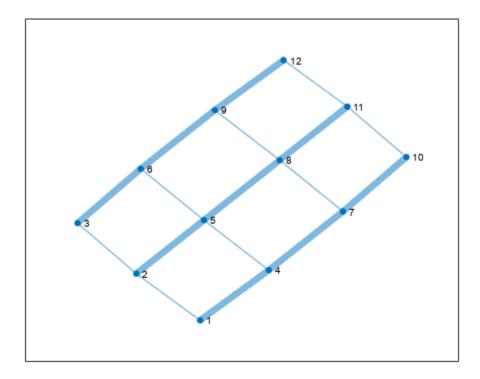
Label Graph Nodes and Edges

This example shows how to add and customize labels on graph nodes and edges.

Create and Plot Graph

Create a graph representing the gridded streets and intersections in a city. Add weights to the edges so that the main avenues and cross streets appear differently in the plot. Plot the graph with the edge line widths proportional to the weight of the edge.

```
s = [1 1 2 2 3 4 4 5 5 6 7 7 8 8 9 10 11];
t = [2 4 3 5 6 5 7 6 8 9 8 10 9 11 12 11 12];
weights = [1 5 1 5 5 1 5 1 5 5 1 5 1 5 5 1 1];
G = graph(s,t,weights);
P = plot(G,'LineWidth',G.Edges.Weight);
```

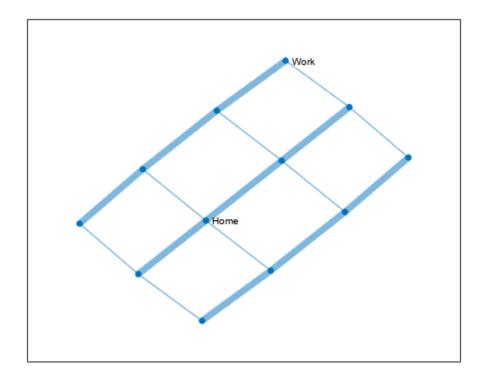


Add Node Labels

For graphs with 100 or fewer nodes, MATLAB® automatically labels the nodes using the numeric node indices or node names (larger graphs omit these labels by default). However, you can change the node labels by adjusting the NodeLabel property of the GraphPlot object P or by using the labelnode function. Therefore, even if the nodes have names, you can use labels that are different from the names.

Remove the default numeric node labels. Label one of the intersections as Home and another as Work.

```
labelnode(P,1:12,'')
labelnode(P,5,'Home')
labelnode(P,12,'Work')
```



Add Edge Labels

The edges in a plotted graph are *not* labeled automatically. You can add edge labels by changing the value of the EdgeLabel property of the GraphPlot object P or by using the labeledge function.

Add edge labels for streets in New York City. The order of the edges is defined in the G.Edges table of the graph, so the order of the labels you specify must respect that order. It is convenient to store edge labels directly in the G.Edges table, so that the edge name lives right next to the other edge information.

G.Edges

ans=	=17×2 EndNo	<i>table</i> odes	Weight
	1	2	1
	1	4	5
	2	3	1
	2	5	5
	3	6	5
	4	5	1
	4	7	5

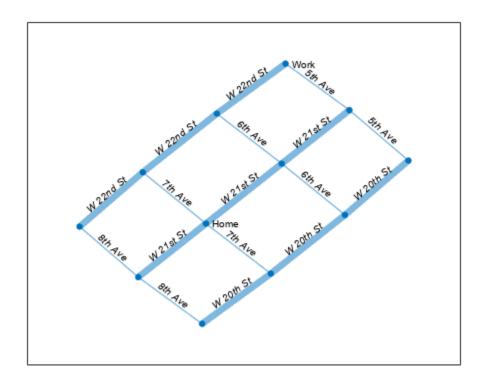
```
5
        6
                 1
 5
        8
                 5
 6
        9
                 5
 7
        8
                 1
 7
       10
                 5
8
                 1
       9
                 5
8
       11
9
                 5
       12
       11
                 1
10
```

This example has 17 edges but only 7 unique street names. Therefore, it makes sense to define the street names in a cell array and then index into the cell array to retrieve the desired street name for each edge. Add a variable to the G. Edges table containing the street names.

```
streets = {'8th Ave' '7th Ave' '6th Ave' '5th Ave' ...
    'W 20th St' 'W 21st St' 'W 22nd St'}';
inds = [1 5 1 6 7 2 5 2 6 7 3 5 3 6 7 4 4];
G.Edges.StreetName = streets(inds);
G.Edges
ans=17×3 table
    EndNodes
                Weight
                            StreetName
     1
           2
                  1
                           {'8th Ave' }
     1
                           {'W 20th St'}
           4
                  5
     2
           3
                  1
                          {'8th Ave'
     2
           5
                  5
                          {'W 21st St'}
     3
                  5
                          {'W 22nd St'}
           6
           5
                  1
                          {'7th Ave'
     4
           7
                  5
                           {'W 20th St'}
     4
                           {'7th Ave'
     5
           6
                  1
     5
                           {'W 21st St'}
           8
                  5
                  5
                           {'W 22nd St'}
     6
           9
     7
           8
                  1
                          {'6th Ave'
     7
          10
                  5
                          {'W 20th St'}
     8
                  1
          9
                           {'6th Ave'
     8
                  5
          11
                          {'W 21st St'}
     9
          12
                  5
                           {'W 22nd St'}
    10
          11
                  1
                           {'5th Ave' }
```

Update the EdgeLabel property to reference these street names.

P.EdgeLabel = G.Edges.StreetName;



Adjust Font Properties

The node and edge labels in a graph plot have their own properties that control the appearance and style of the labels. Since the properties are decoupled, you can use different styles for the node labels and the edge labels.

For **Node** labels, you can adjust:

- NodeLabel
- NodeLabelColor
- NodeFontName
- NodeFontSize
- NodeFontWeight
- NodeFontAngle

For **Edge** labels, you can adjust:

- EdgeLabel
- EdgeLabelColor
- EdgeFontName
- EdgeFontSize
- EdgeFontWeight

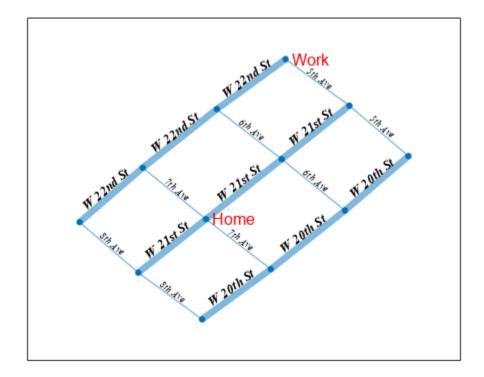
• EdgeFontAngle

Use these properties to adjust the fonts in this example with New York City Streets:

- Change NodeFontSize and NodeLabelColor so that the intersection labels are 12 pt. font and red.
- Change EdgeFontWeight, EdgeFontAngle, and EdgeFontSize to use a larger, bold font for streets in one direction and a smaller, italic font for streets in the other direction.
- Change EdgeFontName to use Times New Roman for the edge labels.

You can use the highlight function to change the graph properties of a subset of the graph edges. Create a logical index isAvenue that is true for edge labels containing the word 'Ave'. Using this logical vector as an input to highlight, label all of the Avenues in one way, and all of the non-Avenues another way.

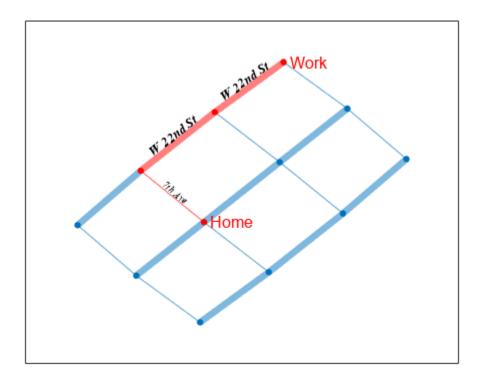
```
P.NodeFontSize = 12;
P.NodeLabelColor = 'r';
isAvenue = contains(P.EdgeLabel, 'Ave');
highlight(P, 'Edges', isAvenue, 'EdgeFontAngle', 'italic', 'EdgeFontSize', 7);
highlight(P, 'Edges', ~isAvenue, 'EdgeFontWeight', 'bold', 'EdgeFontSize', 10);
P.EdgeFontName = 'Times New Roman';
```



Highlight Edges

Find the shortest path between the Home and Work nodes and examine which streets are on the path. Highlight the nodes and edges on the path in red and remove the edge labels for all edges that are not on the path.

```
[path,d,pathEdges] = shortestpath(G,5,12)
path = 1 \times 4
      5 6 9 12
d = 11
pathEdges = 1 \times 3
      8
          10
                  15
G.Edges.StreetName(pathEdges,:)
ans = 3x1 cell
     {'7th Ave'
     {'W 22nd St'}
     {'W 22nd St'}
highlight(P,'Edges',pathEdges,'EdgeColor','r')
highlight(P,path,'NodeColor','r')
labeledge(P, setdiff(1:numedges(G), pathEdges), '')
```



See Also

GraphPlot

More About

- "Graph Plotting and Customization" on page 5-17
- "Add Node Properties to Graph Plot Data Tips" on page 5-36

Functions of One Variable

- "Create and Evaluate Polynomials" on page 6-2
- "Roots of Polynomials" on page 6-4
- "Integrate and Differentiate Polynomials" on page 6-9
- "Polynomial Curve Fitting" on page 6-11
- "Predicting the US Population" on page 6-13
- "Roots of Scalar Functions" on page 6-18

Create and Evaluate Polynomials

This example shows how to represent a polynomial as a vector in MATLAB® and evaluate the polynomial at points of interest.

Representing Polynomials

MATLAB® represents polynomials as row vectors containing coefficients ordered by descending powers. For example, the three-element vector

$$p = [p2 p1 p0];$$

represents the polynomial

$$p(x) = p_2 x^2 + p_1 x + p_0.$$

Create a vector to represent the quadratic polynomial $p(x) = x^2 - 4x + 4$.

$$p = [1 -4 4];$$

Intermediate terms of the polynomial that have a coefficient of 0 must also be entered into the vector, since the 0 acts as a placeholder for that particular power of x.

Create a vector to represent the polynomial $p(x) = 4x^5 - 3x^2 + 2x + 33$.

$$p = [4 \ 0 \ 0 \ -3 \ 2 \ 33];$$

Evaluating Polynomials

After entering the polynomial into MATLAB® as a vector, use the polyval function to evaluate the polynomial at a specific value.

Use polyval to evaluate p(2).

$$polyval(p,2)$$
 ans = 153

Alternatively, you can evaluate a polynomial in a matrix sense using polyvalm. The polynomial expression in one variable, $p(x) = 4x^5 - 3x^2 + 2x + 33$, becomes the matrix expression

$$p(X) = 4X^5 - 3X^2 + 2X + 33I,$$

where X is a square matrix and I is the identity matrix.

Create a square matrix, X, and evaluate p at X.

215378 111419 269614

See Also

polyval | polyvalm | poly | roots

More About

- "Roots of Polynomials" on page 6-4
- "Integrate and Differentiate Polynomials" on page 6-9
- "Polynomial Curve Fitting" on page 6-11

Roots of Polynomials

This example shows several different methods to calculate the roots of a polynomial.

```
"Numeric Roots" on page 6-4

"Roots Using Substitution" on page 6-4

"Roots in a Specific Interval" on page 6-5

"Symbolic Roots" on page 6-7
```

Numeric Roots

The roots function calculates the roots of a single-variable polynomial represented by a vector of coefficients.

For example, create a vector to represent the polynomial $x^2 - x - 6$, then calculate the roots.

```
p = [1 -1 -6];
r = roots(p)
r =
```

By convention, MATLAB returns the roots in a column vector.

The poly function converts the roots back to polynomial coefficients. When operating on vectors, poly and roots are inverse functions, such that poly(roots(p)) returns p (up to roundoff error, ordering, and scaling).

When operating on a matrix, the poly function computes the characteristic polynomial of the matrix. The roots of the characteristic polynomial are the eigenvalues of the matrix. Therefore, roots(poly(A)) and eig(A) return the same answer (up to roundoff error, ordering, and scaling).

Roots Using Substitution

You can solve polynomial equations involving trigonometric functions by simplifying the equation using a substitution. The resulting polynomial of one variable no longer contains any trigonometric functions.

For example, find the values of θ that solve the equation

```
3\cos^2(\theta) - \sin(\theta) + 3 = 0.
```

Use the fact that $\cos^2(\theta) = 1 - \sin^2(\theta)$ to express the equation entirely in terms of sine functions:

$$-3\sin^2(\theta) - \sin(\theta) + 6 = 0.$$

Use the substitution $x = \sin(\theta)$ to express the equation as a simple polynomial equation:

$$-3x^2 - x + 6 = 0$$
.

Create a vector to represent the polynomial.

```
p = [-3 -1 6];
```

Find the roots of the polynomial.

```
r = roots(p)

r = 2 \times 1

-1.5907

1.2573
```

To undo the substitution, use $\theta = \sin^{-1}(x)$. The asin function calculates the inverse sine.

```
theta = asin(r)
theta = 2×1 complex
-1.5708 + 1.0395i
1.5708 - 0.7028i
```

Verify that the elements in theta are the values of θ that solve the original equation (within roundoff error).

```
f = @(Z) 3*cos(Z).^2 - sin(Z) + 3;
f(theta)
ans = 2×1 complex
10<sup>-14</sup> ×
    -0.0888 + 0.0647i
    0.2665 + 0.0399i
```

Roots in a Specific Interval

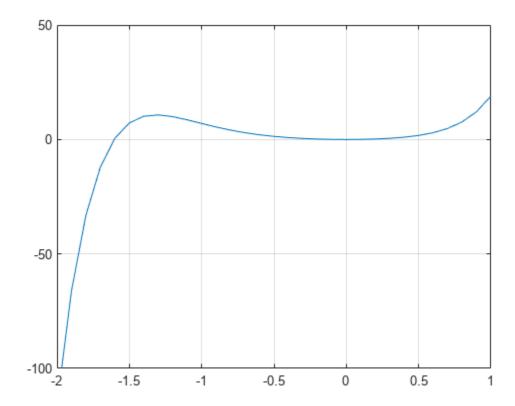
Use the fzero function to find the roots of a polynomial in a specific interval. Among other uses, this method is suitable if you plot the polynomial and want to know the value of a particular root.

For example, create a function handle to represent the polynomial $3x^7 + 4x^6 + 2x^5 + 4x^4 + x^3 + 5x^2$.

```
p = @(x) 3*x.^7 + 4*x.^6 + 2*x.^5 + 4*x.^4 + x.^3 + 5*x.^2;
```

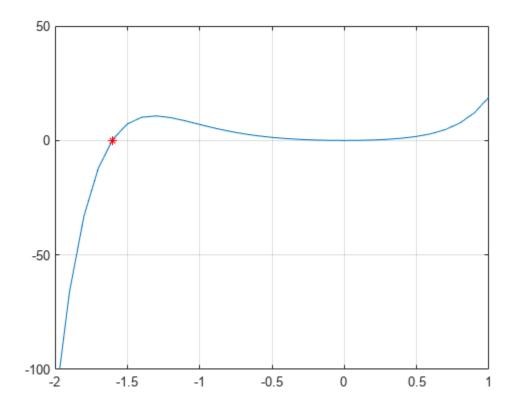
Plot the function over the interval [-2, 1].

```
x = -2:0.1:1;
plot(x,p(x))
ylim([-100 50])
grid on
hold on
```



From the plot, the polynomial has a trivial root at 0 and another near -1.5. Use fzero to calculate and plot the root that is near -1.5.

```
Z = fzero(p, -1.5)
Z = -1.6056
plot(Z,p(Z),'r*')
```



Symbolic Roots

If you have Symbolic Math $\mathsf{Toolbox}^{\scriptscriptstyle\mathsf{TM}}$, then there are additional options for evaluating polynomials symbolically. One way is to use the solve function.

Another way is to use the factor function to factor the polynomial terms.

```
F = factor(x^2-x-6)
F =
[ x + 2, x - 3]
```

See "Solve Algebraic Equations" (Symbolic Math Toolbox) for more information.

See Also

roots | poly | eig

More About

- "Create and Evaluate Polynomials" on page 6-2
- "Roots of Scalar Functions" on page 6-18
- "Integrate and Differentiate Polynomials" on page 6-9

Integrate and Differentiate Polynomials

This example shows how to use the polyint and polyder functions to analytically integrate or differentiate any polynomial represented by a vector of coefficients.

Use polyder to obtain the derivative of the polynomial $p(x) = x^3 - 2x - 5$. The resulting polynomial is $q(x) = \frac{d}{dx}p(x) = 3x^2 - 2$.

$$p = [1 \ 0 \ -2 \ -5];$$

 $q = polyder(p)$
 $q = 1 \times 3$

Similarly, use polyint to integrate the polynomial $p(x) = 4x^3 - 3x^2 + 1$. The resulting polynomial is $q(x) = \int p(x)dx = x^4 - x^3 + x$.

polyder also computes the derivative of the product or quotient of two polynomials. For example, create two vectors to represent the polynomials $a(x) = x^2 + 3x + 5$ and $b(x) = 2x^2 + 4x + 6$.

Calculate the derivative $\frac{d}{dx}[a(x)b(x)]$ by calling polyder with a single output argument.

$$c = polyder(a,b)$$

 $c = 1 \times 4$
8 30 56 38

Calculate the derivative $\frac{d}{dx} \left[\frac{a(x)}{b(x)} \right]$ by calling polyder with two output arguments. The resulting polynomial is

$$\frac{d}{dx} \left[\frac{a(x)}{b(x)} \right] = \frac{-2x^2 - 8x - 2}{4x^4 + 16x^3 + 40x^2 + 48x + 36} = \frac{q(x)}{d(x)}.$$
[q,d] = polyder(a,b)

$$q = 1 \times 3$$

- 2 -8 - 2 $d = 1 \times 5$ 4 16 40 48 36

See Also

polyder|polyint|conv|deconv

More About

- "Analytic Solution to Integral of Polynomial" on page 15-7
- "Create and Evaluate Polynomials" on page 6-2

Polynomial Curve Fitting

This example shows how to fit a polynomial curve to a set of data points using the polyfit function. You can use polyfit to find the coefficients of a polynomial that fits a set of data in a least-squares sense using the syntax

```
p = polyfit(x,y,n),
```

where:

- x and y are vectors containing the x and y coordinates of the data points
- n is the degree of the polynomial to fit

Create some *x*-*y* test data for five data points.

```
x = [1 2 3 4 5];

y = [5.5 43.1 128 290.7 498.4];
```

Use polyfit to find a third-degree polynomial that approximately fits the data.

```
p = polyfit(x,y,3)

p = 1 \times 4

-0.1917 \quad 31.5821 \quad -60.3262 \quad 35.3400
```

After you obtain the polynomial for the fit line using polyfit, you can use polyval to evaluate the polynomial at other points that might not have been included in the original data.

Compute the values of the polyfit estimate over a finer domain and plot the estimate over the real data values for comparison. Include an annotation of the equation for the fit line.

```
x2 = 1:.1:5;

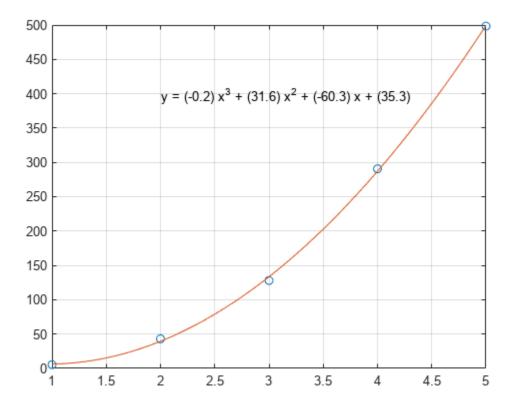
y2 = polyval(p,x2);

plot(x,y,'o',x2,y2)

grid on

s = sprintf('y = (%.1f) x^3 + (%.1f) x^2 + (%.1f) x + (%.1f)',p(1),p(2),p(3),p(4));

text(2,400,s)
```



See Also

polyfit|polyval

More About

- "Programmatic Fitting"
- "Create and Evaluate Polynomials" on page 6-2

Predicting the US Population

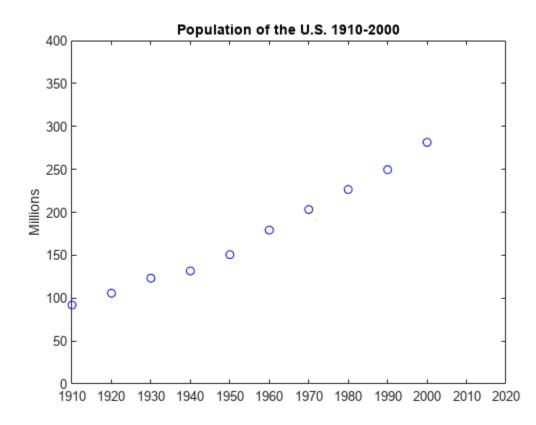
This example shows that extrapolating data using polynomials of even modest degree is risky and unreliable.

This example is older than MATLAB®. It started as an exercise in *Computer Methods for Mathematical Computations*, by Forsythe, Malcolm and Moler, published by Prentice-Hall in 1977.

Now, MATLAB makes it much easier to vary the parameters and see the results, but the underlying mathematical principles are unchanged.

Create and plot two vectors with US Census data from 1910 to 2000.

```
% Time interval
t = (1910:10:2000)';
% Population
p = [91.972 105.711 123.203 131.669 150.697...
179.323 203.212 226.505 249.633 281.422]';
% Plot
plot(t,p,'bo');
axis([1910 2020 0 400]);
title('Population of the U.S. 1910-2000');
ylabel('Millions');
```



What is your guess for the population in the year 2010?

```
p = 10×1

91.9720

105.7110

123.2030

131.6690

150.6970

179.3230

203.2120

226.5050

249.6330

281.4220
```

Fit the data with a polynomial in t and use it to extrapolate the population at t = 2010. Obtain the coefficients in the polynomial by solving a linear system of equations involving an 11-by-11 Vandermonde matrix, with elements as powers of scaled time, $A(i,j) = s(i)^{n-j}$.

```
n = length(t);
s = (t-1950)/50;
A = zeros(n);
A(:,end) = 1;
for j = n-1:-1:1
    A(:,j) = s .* A(:,j+1);
end
```

Obtain the coefficients c for a polynomial of degree d that fits the data p by solving a linear system of equations involving the last d+1 columns of the Vandermonde matrix:

```
A(:,n-d:n)*c \sim p
```

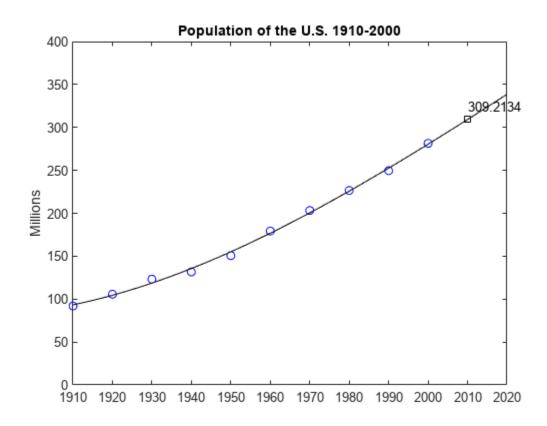
- If d < 10, then more equations than unknowns exist, and a least-squares solution is appropriate.
- If d == 10, then you can solve the equations exactly and the polynomial actually interpolates the
 data.

In either case, use the backslash operator to solve the system. The coefficients for the cubic fit are:

Now evaluate the polynomial at every year from 1910 to 2010 and plot the results.

```
v = (1910:2020)';
x = (v-1950)/50;
w = (2010-1950)/50;
y = polyval(c,x);
z = polyval(c,w);
```

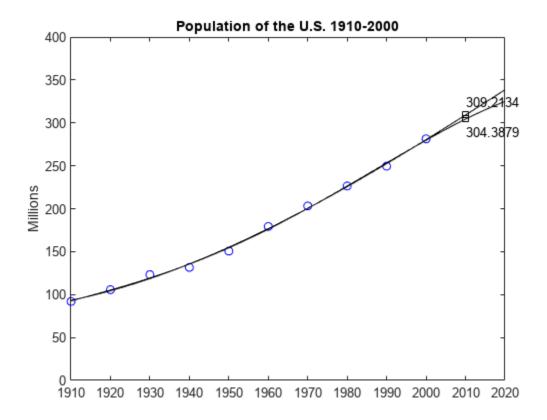
```
hold on
plot(v,y,'k-');
plot(2010,z,'ks');
text(2010,z+15,num2str(z));
hold off
```



Compare the cubic fit with the quartic. Notice that the extrapolated point is very different.

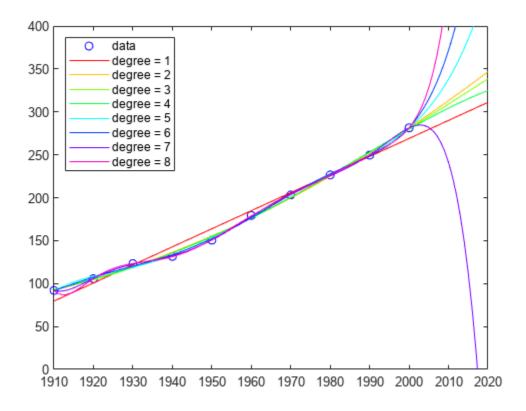
```
c = A(:,n-4:n)\p;
y = polyval(c,x);
z = polyval(c,w);

hold on
plot(v,y,'k-');
plot(2010,z,'ks');
text(2010,z-15,num2str(z));
hold off
```



As the degree increases, the extrapolation becomes even more erratic.

```
cla
plot(t,p,'bo')
hold on
axis([1910 2020 0 400])
colors = hsv(8);
labels = {'data'};
for d = 1:8
   [Q,R] = qr(A(:,n-d:n));
   R = R(1:d+1,:);
   Q = Q(:,1:d+1);
   c = R \setminus (Q'*p);
                    % Same as c = A(:,n-d:n)\p;
   y = polyval(c,x);
   z = polyval(c,11);
   plot(v,y,'color',colors(d,:));
   labels{end+1} = ['degree = ' int2str(d)];
legend(labels, 'Location', 'NorthWest')
hold off
```



See Also polyfit

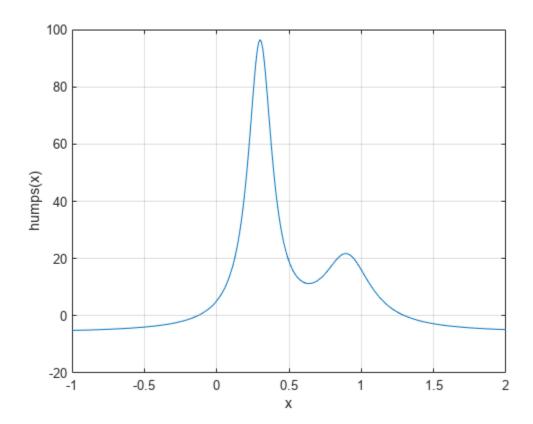
Roots of Scalar Functions

Solving a Nonlinear Equation in One Variable

The fzero function attempts to find a root of one equation with one variable. You can call this function with either a one-element starting point or a two-element vector that designates a starting interval. If you give fzero a starting point x0, fzero first searches for an interval around this point where the function changes sign. If the interval is found, fzero returns a value near where the function changes sign. If no such interval is found, fzero returns NaN. Alternatively, if you know two points where the function value differs in sign, you can specify this starting interval using a two-element vector; fzero is guaranteed to narrow down the interval and return a value near a sign change.

The following sections contain two examples that illustrate how to find a zero of a function using a starting interval and a starting point. The examples use the function humps.m, which is provided with MATLAB®. The following figure shows the graph of humps.

```
x = -1:.01:2;
y = humps(x);
plot(x,y)
xlabel('x');
ylabel('humps(x)')
grid on
```



Setting Options for fzero

You can control several aspects of the fzero function by setting options. You set options using optimset. Options include:

- Choosing the amount of display fzero generates see "Set Optimization Options" on page 9-10, Using a Starting Interval on page 6-19, and Using a Starting Point on page 6-20.
- Choosing various tolerances that control how fzero determines it is at a root see "Set Optimization Options" on page 9-10.
- Choosing a plot function for observing the progress of fzero towards a root see "Optimization Solver Plot Functions" on page 9-20.
- Using a custom-programmed output function for observing the progress of fzero towards a root

 see "Optimization Solver Output Functions" on page 9-14.

Using a Starting Interval

The graph of humps indicates that the function is negative at x = -1 and positive at x = 1. You can confirm this by calculating humps at these two points.

```
humps(1)
ans = 16
humps(-1)
ans = -5.1378
```

Consequently, you can use [-1 1] as a starting interval for fzero.

The iterative algorithm for fzero finds smaller and smaller subintervals of [-1 1]. For each subinterval, the sign of humps differs at the two endpoints. As the endpoints of the subintervals get closer and closer, they converge to zero for humps.

To show the progress of fzero at each iteration, set the Display option to iter using the optimset function.

```
options = optimset('Display','iter');
Then call fzero as follows:
```

```
a = fzero(@humps,[-1 1],options)
```

Func-count	Х	f(x)	Procedure
2	- 1	-5.13779	initial
3	-0.513876	-4.02235	interpolation
4	-0.513876	-4.02235	bisection
5	-0.473635	-3.83767	interpolation
6	-0.115287	0.414441	bisection
7	-0.115287	0.414441	interpolation
8	-0.132562	-0.0226907	interpolation
9	-0.131666	-0.0011492	interpolation
10	-0.131618	1.88371e-07	interpolation
11	-0.131618	-2.7935e-11	interpolation
12	-0.131618	8.88178e-16	interpolation
13	-0.131618	8.88178e-16	interpolation

```
Zero found in the interval [-1, 1]
a = -0.1316
```

Each value x represents the best endpoint so far. The Procedure column tells you whether each step of the algorithm uses bisection or interpolation.

You can verify that the function value at a is close to zero by entering

```
humps(a)
ans = 8.8818e-16
```

Using a Starting Point

Suppose you do not know two points at which the function values of humps differ in sign. In that case, you can choose a scalar x0 as the starting point for fzero. fzero first searches for an interval around this point on which the function changes sign. If fzero finds such an interval, it proceeds with the algorithm described in the previous section. If no such interval is found, fzero returns NaN.

For example, set the starting point to -0.2, the Display option to Iter, and call fzero:

```
options = optimset('Display', 'iter');
a = fzero(@humps, -0.2, options)
```

```
Search for an interval around -0.2 containing a sign change:
 Func-count
                          f(a)
                                                                    Procedure
                                            b
                                                       f(h)
    1
                 -0.2
                           -1.35385
                                              -0.2
                                                        -1.35385
                                                                    initial interval
    3
            -0.194343
                           -1.26077
                                         -0.205657
                                                        -1.44411
                                                                    search
    5
                           -1.22137
                                           -0.208
                                                         -1.4807
               -0.192
                                                                    search
   7
                           -1.16477
                                         -0.211314
                                                        -1.53167
            -0.188686
                                                                    search
   9
               -0.184
                           -1.08293
                                            -0.216
                                                         -1.60224
                                                                    search
   11
            -0.177373
                           -0.963455
                                         -0.222627
                                                         -1.69911
                                                                    search
   13
               -0.168
                          -0.786636
                                            -0.232
                                                         -1.83055
                                                                    search
   15
            -0.154745
                           -0.51962
                                         -0.245255
                                                         -2.00602
                                                                    search
   17
               -0.136
                          -0.104165
                                            -0.264
                                                         -2.23521
                                                                    search
             -0.10949
                           0.572246
                                                        -2.23521
   18
                                            -0.264
                                                                    search
Search for a zero in the interval [-0.10949, -0.264]:
 Func-count
                          f(x)
                                            Procedure
              X
   18
             -0.10949
                           0.572246
                                            initial
   19
            -0.140984
                          -0.219277
                                            interpolation
   20
            -0.132259
                         -0.0154224
                                            interpolation
   21
            -0.131617
                        3.40729e-05
                                            interpolation
   22
            -0.131618
                       -6.79505e-08
                                            interpolation
   23
            -0.131618
                       -2.98428e-13
                                            interpolation
   24
            -0.131618
                        8.88178e-16
                                            interpolation
            -0.131618
                        8.88178e-16
                                            interpolation
Zero found in the interval [-0.10949, -0.264]
```

```
The endpoints of the current subinterval at each iteration are listed under the headings a and b, while the corresponding values of humps at the endpoints are listed under f(a) and f(b), respectively.
```

a = -0.1316

Note: The endpoints a and b are not listed in any specific order: a can be greater than b or less than b.

For the first nine steps, the sign of humps is negative at both endpoints of the current subinterval, which is shown in the output. At the tenth step, the sign of humps is positive at a, -0.10949, but negative at b, -0.264. From this point on, the algorithm continues to narrow down the interval [-0.10949 -0.264], as described in the previous section, until it reaches the value -0.1316.

See Also

More About

- "Roots of Polynomials" on page 6-4
- "Optimizing Nonlinear Functions" on page 9-2
- "Systems of Nonlinear Equations" (Optimization Toolbox)

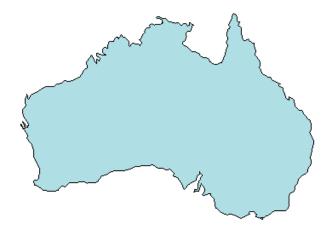
Computational Geometry

- "Triangulation Representations" on page 7-2
- "Working with Delaunay Triangulations" on page 7-14
- "Creating and Editing Delaunay Triangulations" on page 7-38
- "Spatial Searching" on page 7-53
- "Voronoi Diagrams" on page 7-58
- "Types of Region Boundaries" on page 7-65
- "Computing the Convex Hull" on page 7-71

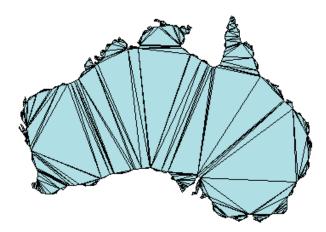
Triangulation Representations

2-D and 3-D Domains

Triangulations are often used to represent 2-D and 3-D geometric domains in application areas such as computer graphics, physical modeling, geographic information systems, medical imaging, and more. The map polygon shown here

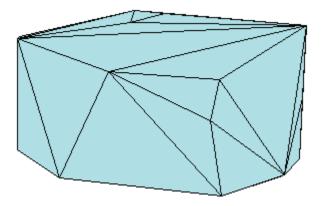


can be represented by the triangulation on the map shown below.



The triangulation decomposes a complex polygon into a collection of simpler triangular polygons. You can use these polygons for developing geometric-based algorithms or graphics applications.

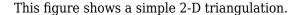
Similarly, you can represent the boundary of a 3-D geometric domain using a triangulation. The figure below shows the convex hull of a set of points in 3-D space. Each facet of the hull is a triangle.

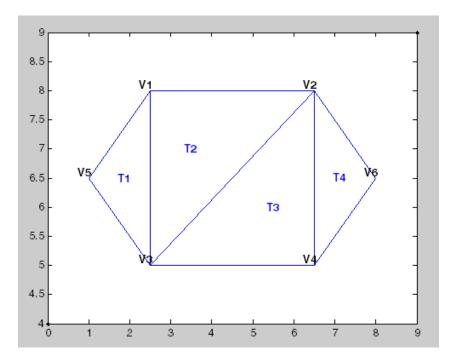


Triangulation Matrix Format

MATLAB uses a matrix format to represent triangulations. This format has two parts:

- The vertices, represented as a matrix in which each row contains the coordinates of a point in the triangulation.
- The triangulation connectivity, represented as a matrix in which each row defines a triangle or tetrahedron.





The following table shows the vertex information.

	Vertices	
Vertex ID	x-coordinate	<i>y</i> -coordinate

Vertices			
V1	2.5	8.0	
V2	6.5	8.0	
V3	2.5	5.0	
V4	6.5	5.0	
V5	1.0	6.5	
V6	8.0	6.5	

The data in the previous table is stored as a matrix in the MATLAB environment. The vertex IDs are labels used for identifying specific vertices. They are shown to illustrate the concept of a vertex ID, but they are not stored explicitly. Instead, the row numbers of the matrix serve as the vertex IDs.

The triangulation connectivity data is shown in this table.

Connectivity			
Triangle ID	IDs of Bounding Vertice	S	
T1	5	3	1
T2	3	2	1
T3	3	4	2
T4	4	6	2

The data in this table is stored as a matrix in the MATLAB environment. The triangle IDs are labels used for identifying specific triangles. They are shown to illustrate the concept of a triangle ID, but they are not stored explicitly. Instead, the row numbers of the matrix serve as the triangle IDs.

You can see that triangle T1 is defined by three vertices, $\{V5, V3, V1\}$. Similarly, T4 is defined by the vertices, $\{V4, V6, V2\}$. This format extends naturally to higher dimensions, which require additional columns of data. For example, a tetrahedron in 3-D space is defined by four vertices, each of which have three coordinates, (x, y, z).

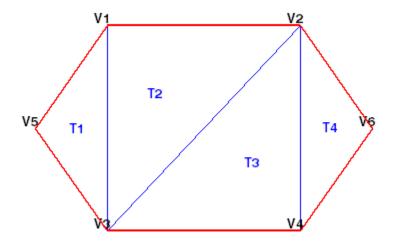
You can represent and query the following types of triangulations using MATLAB:

- 2-D triangulations consisting of triangles bounded by vertices and edges
- 3-D surface triangulations consisting of triangles bounded by vertices and edges
- 3-D triangulations consisting of tetrahedra bounded by vertices, edges, and faces

Querying Triangulations Using the triangulation Class

The matrix format provides a compact low-level, array-based representation for triangulations. When you use triangulations to develop algorithms, you might need more information about the geometric properties, topology, and adjacency information.

For example, you might compute the triangle incenters before plotting the annotated triangulation shown below. In this case, you use the incenters to display the triangle labels (T1, T2, etc.) within each triangle. If you want to plot the boundary in red, you need to determine the edges that are referenced by only one triangle.



The triangulation Class

You can use triangulation to create an in-memory representation of any 2-D or 3-D triangulation data that is in matrix format, such as the matrix output from the delaunay function or other software tools. When your data is represented using triangulation, you can perform topological and geometric queries, which you can use to develop geometric algorithms. For example, you can find the triangles or tetrahedra attached to a vertex, those that share an edge, their circumcenters, and other features.

You can create a triangulation in one of two ways:

- Pass existing data that you have in matrix format to triangulation. This data can be the output from a MATLAB function, such as delaunay or convhull. You also can import triangulation data that was created by another software application. When you work with imported data, be sure the connectivity data references the vertex array using 1-based indexing instead of 0-based indexing.
- Pass a set of points to delaunayTriangulation. The resulting Delaunay triangulation is a special kind of triangulation. This means you can perform any triangulation query on your data, as well as any Delaunay-specific query. In more formal MATLAB language terms, delaunayTriangulation is a subclass of triangulation.

Creating a triangulation from Matrix Data

This example shows how to use the triangulation matrix data to create a triangulation, explore what it is, and explore what it can do.

Create a matrix, P, that contains the vertex data.

```
P = [ 2.5 8.0
6.5 8.0
2.5 5.0
6.5 5.0
1.0 6.5
8.0 6.5];
```

Define the connectivity, T.

```
T = \begin{bmatrix} 5 & 3 & 1; \\ 3 & 2 & 1; \\ 3 & 4 & 2; \\ 4 & 6 & 2 \end{bmatrix};
```

Create a triangulation from this data.

Access the properties in a triangulation in the same way you access the fields of a struct. For example, examine the Points property, which contains the coordinates of the vertices.

TR.Points

```
ans = 6×2

2.5000 8.0000
6.5000 8.0000
2.5000 5.0000
6.5000 5.0000
1.0000 6.5000
8.0000 6.5000
```

Next, examine the connectivity.

TR.ConnectivityList

```
ans = 4 \times 3

5 3 1
3 2 1
3 4 2
4 6 2
```

The Points and ConnectivityList properties define the matrix data for the triangulation.

The triangulation class is a wrapper around the matrix data. The real benefit is the usefulness of the triangulation class methods. The methods are like functions that accept a triangulation and other relevant input data.

The triangulation class provides an easy way to index into the ConnectivityList property matrix. Access the first triangle in the triangulation.

```
TR.ConnectivityList(1,:) ans = 1 \times 3
```

```
5 3 1
```

Another way of getting the first triangle is TR(1,:).

Examine the first vertex of the first triangle.

```
TR(1,1)
```

ans = 5

Examine the second vertex of the first triangle.

```
TR(1,2)
```

ans = 3

Now, examine all the triangles in the triangulation.

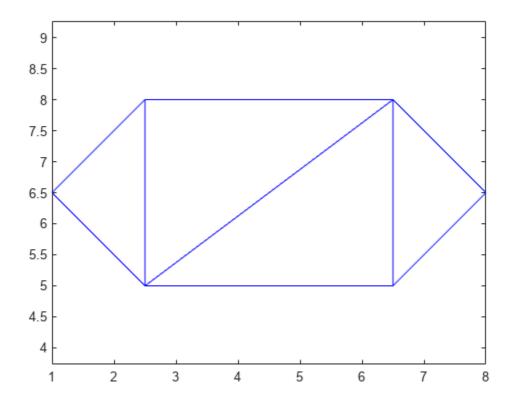
```
TR(:,:)
```

ans = 4×3

5	3	1
3	2	1
3	4	2
4	6	2

Use triplot to plot the triangulation. The triplot function is not a triangulation method, but it accepts and can plot a triangulation.

```
figure
triplot(TR)
axis equal
```

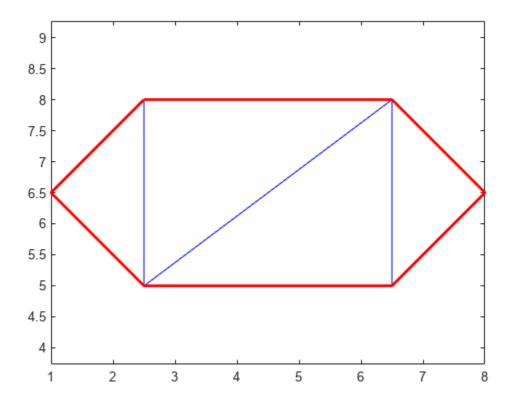


Use the triangulation method, freeBoundary, to query the free boundary and highlight it in a plot. This method returns the edges of the triangulation that are shared by only one triangle. The returned edges are expressed in terms of the vertex IDs.

```
boundaryedges = freeBoundary(TR)';
```

Now plot the boundary edges as a red line.

```
hold on
plot(P(boundaryedges,1),P(boundaryedges,2),'-r','LineWidth',2)
hold off
```



You can use the freeBoundary method to validate a triangulation. For example, if you observed red edges in the interior of the triangulation, then it would indicate a problem in how the triangles are connected.

Creating a triangulation Using delaunayTriangulation

This example shows how to create a Delaunay triangulation using delaunayTriangulation.

When you create a Delaunay triangulation using the delaunayTriangulation class, you automatically get access to the triangulation methods because delaunayTriangulation is a subclass of triangulation.

Create a delaunayTriangulation from a set of points.

DT = delaunayTriangulation(P)

```
DT =
  delaunayTriangulation with properties:
```

```
Points: [6x2 double]
ConnectivityList: [4x3 double]
Constraints: []
```

The resulting delaunayTriangulation object has the properties, Points and ConnectivityList, just like a triangulation object.

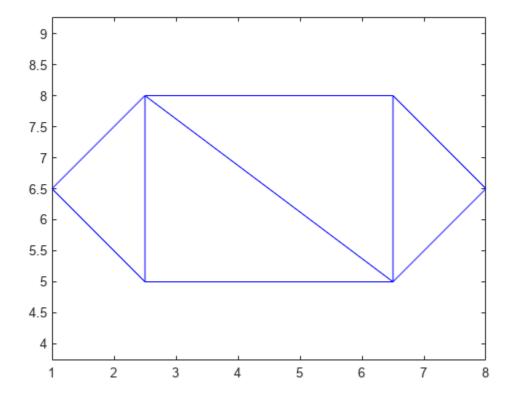
You can access the triangulation using direct indexing, just like triangulation. For example, examine the connectivity of the first triangle.

```
DT(1,:) ans = 1 \times 3 5 3 1
```

Next, examine the connectivity of the entire triangulation.

Use the triplot function to plot the triangulation.

```
triplot(DT)
axis equal
```



The parent class, triangulation, provides the incenter method to compute the incenters of each triangle.

```
IC = incenter(DT)

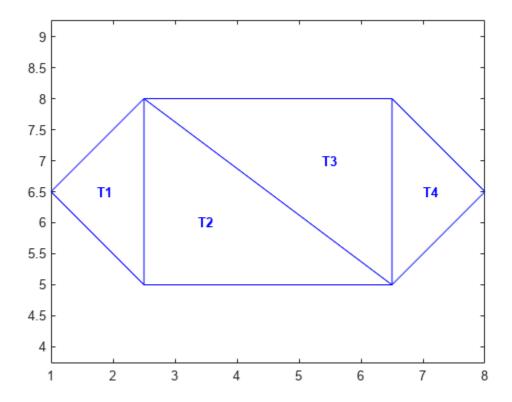
IC = 4×2

1.8787 6.5000
3.5000 6.0000
5.5000 7.0000
7.1213 6.5000
```

The returned value, IC, is an array of coordinates representing the incenters of the triangles.

Now, use the incenters to find the positions for placing triangle labels on the plot.

```
hold on
numtri = size(DT,1);
trilabels = arrayfun(@(P) {sprintf('T%d', P)}, (1:numtri)');
Htl = text(IC(:,1),IC(:,2),trilabels,'FontWeight','bold', ...
'HorizontalAlignment','center','Color','blue');
hold off
```



Instead of creating a Delaunay triangulation using delaunayTriangulation, you could use the delaunay function to create the triangulation connectivity data, and then pass the connectivity data to triangulation. For example,

T = delaunay(P);
TR = triangulation(T,P);
IC = incenter(TR);

Both approaches are valid in this example, but if you want to create a Delaunay triangulation and perform queries on it, then you should use delaunayTriangulation for these reasons:

- The delaunayTriangulation class provides additional methods that are useful for working with triangulations. For example, you can to perform nearest-neighbor and point-in-triangle searches.
- It allows you to edit the triangulation to add, move, or remove points.
- It allows you to create constrained Delaunay triangulations. This allows you to create a triangulation for a 2-D domain.

See Also

delaunay|delaunayTriangulation|freeBoundary|triangulation|triplot

More About

- "Working with Delaunay Triangulations" on page 7-14
- "Spatial Searching" on page 7-53

Working with Delaunay Triangulations

In this section...

"Definition of Delaunay Triangulation" on page 7-14

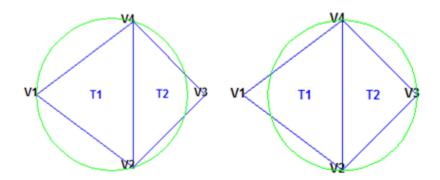
"Creating Delaunay Triangulations" on page 7-15

"Triangulation of Point Sets Containing Duplicate Locations" on page 7-35

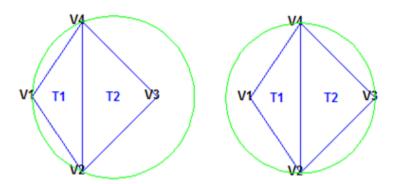
Definition of Delaunay Triangulation

Delaunay triangulations are widely used in scientific computing in many diverse applications. While there are numerous algorithms for computing triangulations, it is the favorable geometric properties of the Delaunay triangulation that make it so useful.

The fundamental property is the Delaunay criterion. In the case of 2-D triangulations, this is often called the empty circumcircle criterion. For a set of points in 2-D, a Delaunay triangulation of these points ensures the circumcircle associated with each triangle contains no other point in its interior. This property is important. In the illustration below, the circumcircle associated with T1 is empty. It does not contain a point in its interior. The circumcircle associated with T2 is empty. It does not contain a point in its interior. This triangulation is a Delaunay triangulation.



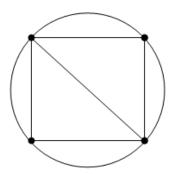
The triangles below are different. The circumcircle associated with T1 is not empty. It contains V3 in its interior. The circumcircle associated with T2 is not empty. It contains V1 in its interior. This triangulation is *not* a Delaunay triangulation.

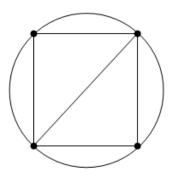


Delaunay triangles are said to be "well shaped" because in fulfilling the empty circumcircle property, triangles with large internal angles are selected over ones with small internal angles. The triangles in

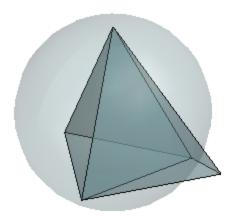
the non-Delaunay triangulation have sharp angles at vertices V2 and V4. If the edge {V2, V4} were replaced by an edge joining V1 and V3, the minimum angle would be maximized and the triangulation would become a Delaunay triangulation. Also, the Delaunay triangulation connects points in a nearest-neighbor manner. These two characteristics, well-shaped triangles and the nearest-neighbor relation, have important implications in practice and motivate the use of Delaunay triangulations in scattered data interpolation.

While the Delaunay property is well defined, the topology of the triangulation is not unique in the presence of degenerate point sets. In two dimensions, degeneracies arise when four or more unique points lie on the same circle. The vertices of a square, for example, have a nonunique Delaunay triangulation.





The properties of Delaunay triangulations extend to higher dimensions. The triangulation of a 3-D set of points is composed of tetrahedra. The next illustration shows a simple 3-D Delaunay triangulation made up of two tetrahedra. The circumsphere of one tetrahedron is shown to highlight the empty circumsphere criterion.



A 3-D Delaunay triangulation produces tetrahedra that satisfy the empty circumsphere criterion.

Creating Delaunay Triangulations

MATLAB provides two ways to create Delaunay triangulations:

• The functions delaunay and delaunayn

• The delaunayTriangulation class

The delaunay function supports the creation of 2-D and 3-D Delaunay triangulations. The delaunayn function supports creating Delaunay triangulations in 4-D and higher.

Tip Creating Delaunay triangulations in dimensions higher than 6-D is generally not practical for moderate to large point sets due to the exponential growth in required memory.

The delaunayTriangulation class supports creating Delaunay triangulations in 2-D and 3-D. It provides many methods that are useful for developing triangulation-based algorithms. These class methods are like functions, but they are restricted to work with triangulations created using delaunayTriangulation. The delaunayTriangulation class also supports the creation of related constructs such as the convex hull and Voronoi diagram. It also supports the creation of constrained Delaunay triangulations.

In summary:

- The delaunay function is useful when you only require the basic triangulation data, and that data is sufficiently complete for your application.
- The delaunayTriangulation class offers more functionality for developing triangulation-based applications. It is useful when you require the triangulation and you want to perform any of these operations:
 - Search the triangulation for triangles or tetrahedra enclosing a query point.
 - Use the triangulation to perform a nearest-neighbor point search.
 - Query the triangulation's topological adjacency or geometric properties.
 - Modify the triangulation to insert or remove points.
 - Constrain edges in the triangulation—this is called a constrained Delaunay triangulation.
 - Triangulate a polygon and optionally remove the triangles that are outside of the domain.
 - Use the Delaunay triangulation to compute the convex hull or Voronoi diagram.

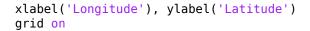
Using the delaunay and delaunayn functions

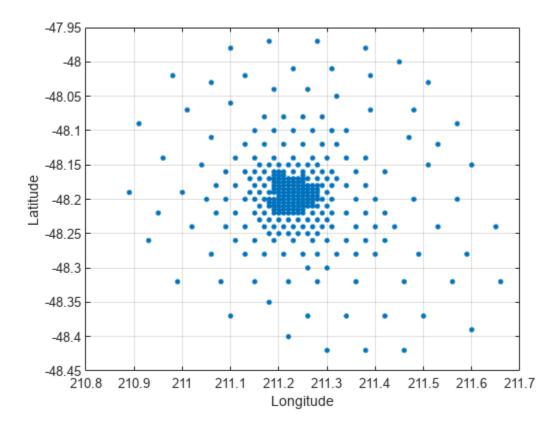
The delaunay and delaunayn functions take a set of points and produce a triangulation in matrix format. Refer to "Triangulation Matrix Format" on page 7-3 for more information on this data structure. In 2-D, the delaunay function is often used to produce a triangulation that can be used to plot a surface defined in terms of a set of scattered data points. In this application, it's important to note that this approach can only be used if the surface is single-valued. For example, it could not be used to plot a spherical surface because there are two z values corresponding to a single (x, y) coordinate. A simple example demonstrates how the delaunay function can be used to plot a surface representing a sampled data set.

This example shows how to use the delaunay function to create a 2-D Delaunay triangulation from the seamount data set. A *seamount* is an underwater mountain. The data set consists of a set of longitude (x) and latitude (y) locations, and corresponding seamount elevations (z) measured at those coordinates.

Load the seamount data set and view the (x, y) data as a scatter plot.

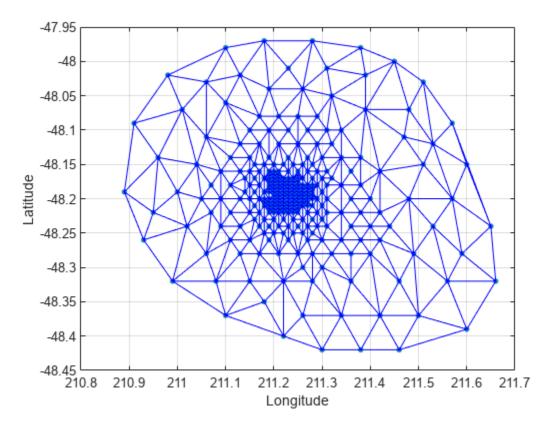
```
load seamount
plot(x,y,'.','markersize',12)
```





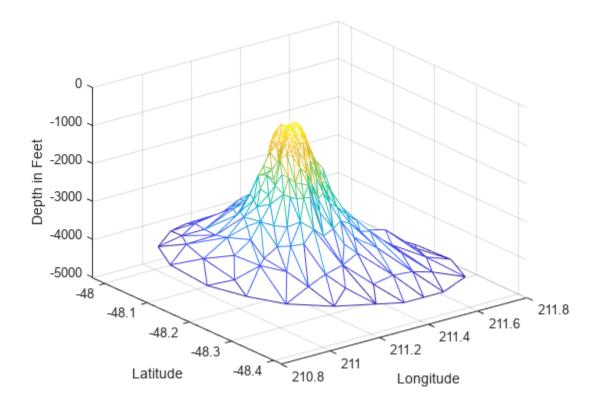
Construct a Delaunay triangulation from this point set and use triplot to plot the triangulation in the existing figure.

```
tri = delaunay(x,y);
hold on, triplot(tri,x,y), hold off
```



Add the depth data (z) from seamount to lift the vertices and create the surface. Create a new figure and use trimesh to plot the surface in wireframe mode.

```
figure
hidden on
trimesh(tri,x,y,z)
xlabel('Longitude'),ylabel('Latitude'),zlabel('Depth in Feet');
```

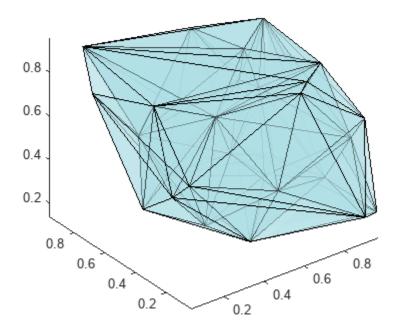


If you want to plot the surface in shaded mode, use trisurf instead of trimesh.

A 3-D Delaunay triangulation also can be created using the delaunay function. This triangulation is composed of tetrahedra.

This example shows how to create a 3-D Delaunay triangulation of a random data set. The triangulation is plotted using tetramesh, and the FaceAlpha option adds transparency to the plot.

```
rng('default')
X = rand([30 3]);
tet = delaunay(X);
faceColor = [0.6875 0.8750 0.8984];
tetramesh(tet,X,'FaceColor', faceColor,'FaceAlpha',0.3);
```



MATLAB provides the delaunayn function to support the creation of Delaunay triangulations in dimension 4-D and higher. Two complementary functions tsearchn and dsearchn are also provided to support spatial searching for N-D triangulations. See "Spatial Searching" on page 7-53 for more information on triangulation-based search.

Using the delaunayTriangulation Class

The delaunayTriangulation class provides another way to create Delaunay triangulations in MATLAB. While delaunay and delaunayTriangulation use the same underlying algorithm and produce the same triangulation, delaunayTriangulation provides complementary methods that are useful for developing Delaunay-based algorithms. These methods are like functions that are packaged together with the triangulation data into a container called a class. Keeping everything together in a class provides a more organized setup that improves ease of use. It also improves the performance of triangulation-based searches such as point-location and nearest-neighbor. delaunayTriangulation supports incremental editing of the Delaunay triangulation. You also can impose edge constraints in 2-D.

"Triangulation Representations" on page 7-2 introduces the triangulation class, which supports topological and geometric queries for 2-D and 3-D triangulations. A delaunayTriangulation is a special kind of triangulation. This means you can perform any triangulation query on a delaunayTriangulation in addition to the Delaunay-specific queries. In more formal MATLAB language terms, delaunayTriangulation is a subclass of triangulation.

This example shows how to create, query, and edit a Delaunay triangulation from the seamount data using delaunayTriangulation. The seamount data set contains (x, y) locations and corresponding elevations (z) that define the surface of the seamount.

Load and triangulate the (x, y) data.

The Constraints property is empty because there aren't any imposed edge constraints. The Points property represents the coordinates of the vertices, and the ConnectivityList property represents the triangles. Together, these two properties define the matrix data for the triangulation.

The delaunayTriangulation class is a wrapper around the matrix data, and it offers a set of complementary methods. You access the properties in a delaunayTriangulation in the same way you access the fields of a struct.

Access the vertex data.

```
DT.Points;
```

Access the connectivity data.

```
DT.ConnectivityList;
```

Access the first triangle in the ConnectivityList property.

```
DT.ConnectivityList(1,:) ans = 1 \times 3
```

```
230 205 152
```

delaunayTriangulation provides an easy way to index into the ConnectivityList property matrix.

Access the first triangle.

```
DT(1,:) ans = 1 \times 3
230 205 152
```

Examine the first vertex of the first triangle.

```
DT(1,1) ans = 230
```

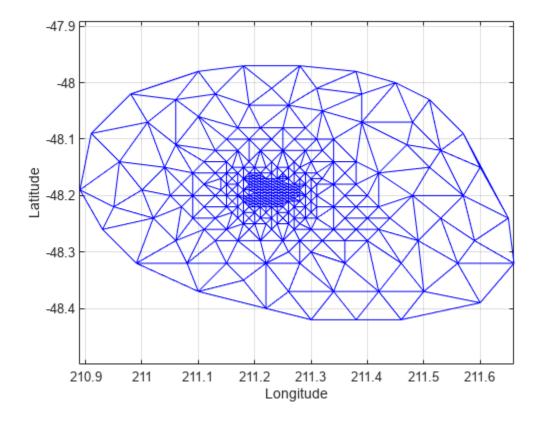
Examine all the triangles in the triangulation.

```
DT(:,:);
```

Indexing into the delaunayTriangulation output, DT, works like indexing into the triangulation array output from delaunay. The difference between the two are the extra methods that you can call on DT (for example, nearestNeighbor and pointLocation).

Use triplot to plot the delaunayTriangulation. The triplot function is not a delaunayTriangulation method, but it accepts and can plot a delaunayTriangulation.

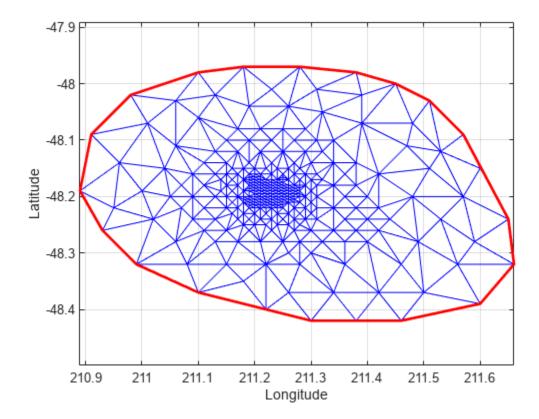
```
triplot(DT);
axis equal
xlabel('Longitude'), ylabel('Latitude')
grid on
```



Alternatively, you could use triplot(DT(:,:), DT.Points(:,1), DT.Points(:,2)); to get the same plot.

Use the delaunayTriangulation method, convexHull, to compute the convex hull and add it to the plot. Since you already have a Delaunay triangulation, this method allows you to derive the convex hull more efficiently than a full computation using convhull.

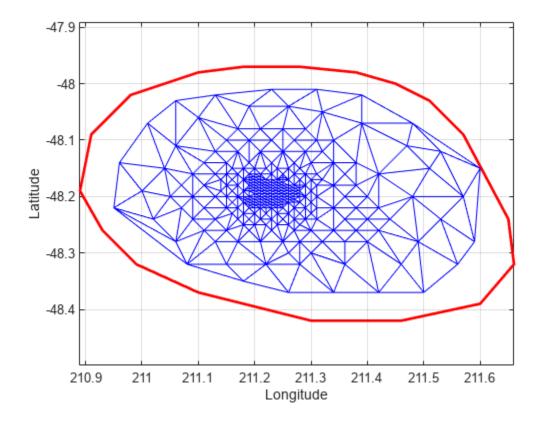
```
hold on
k = convexHull(DT);
xHull = DT.Points(k,1);
yHull = DT.Points(k,2);
plot(xHull,yHull,'r','LineWidth',2);
hold off
```



You can incrementally edit the delaunayTriangulation to add or remove points. If you need to add points to an existing triangulation, then an incremental addition is faster than a complete retriangulation of the augmented point set. Incremental removal of points is more efficient when the number of points to be removed is small relative to the existing number of points.

Edit the triangulation to remove the points on the convex hull from the previous computation.

```
% Plot the new triangulation.
hold on
triplot(DT);
hold off
```



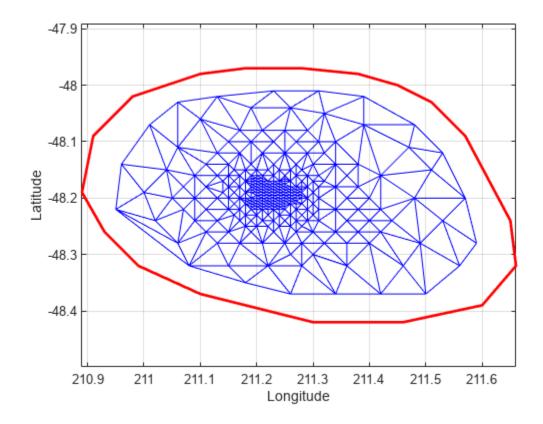
There is one vertex that is just inside the boundary of the convex hull that was not removed. The fact that it is interior to the hull can be seen using the Zoom-In tool in the figure. You could plot the vertex labels to determine the index of this vertex and remove it from the triangulation. Alternatively, you can use the nearestNeighbor method to identify the index more readily.

The point is close to location (211.6, -48.15). Use the nearestNeighbor method to find the nearest vertex.

vertexId = nearestNeighbor(DT, 211.6, -48.15)

Plot the new triangulation.

```
figure
plot(xHull,yHull,'r','LineWidth',2);
axis equal
xlabel('Longitude'),ylabel('Latitude')
grid on
hold on
triplot(DT);
hold off
```



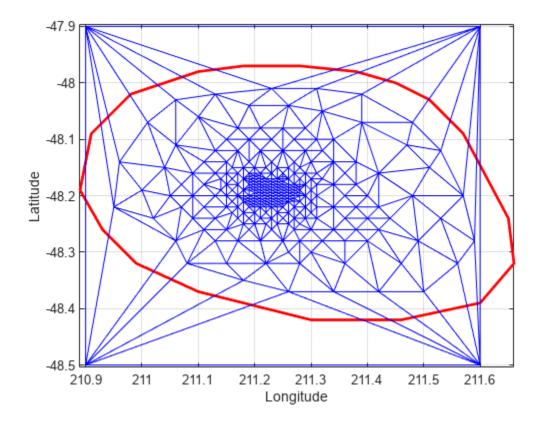
Add points to the existing triangulation. Add 4 points to form a rectangle around the triangulation.

Close all existing figures.

```
close all
```

Plot the new triangulation.

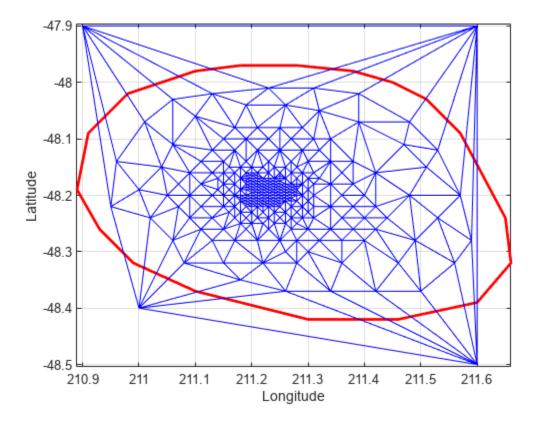
```
figure
plot(xHull,yHull,'r','LineWidth',2);
axis equal
xlabel('Longitude'),ylabel('Latitude')
grid on
hold on
triplot(DT);
hold off
```



You can edit the points in the triangulation to move them to a new location. Edit the first of the additional point set (the vertex ID 274).

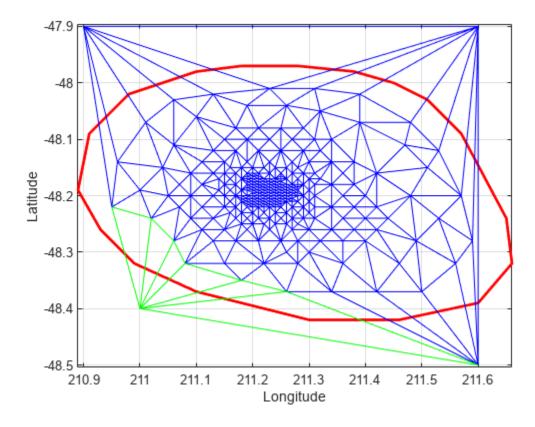
```
DT.Points(274,:) = [211 -48.4];
Close all existing figures.
close all
Plot the new triangulation
figure
plot(xHull,yHull,'r','LineWidth',2);
axis equal
xlabel('Longitude'),ylabel('Latitude')
grid on
hold on
```

triplot(DT);
hold off



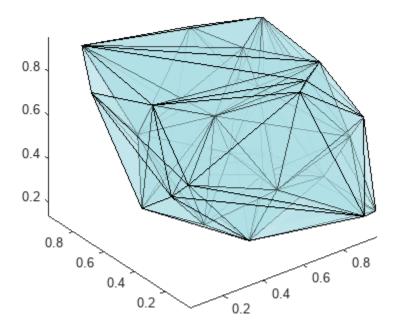
Use the a method of the triangulation class, vertexAttachments, to find the attached triangles. Since the number of triangles attached to a vertex is variable, the method returns the attached triangle IDs in a cell array. You need braces to extract the contents.

```
attTris = vertexAttachments(DT,274);
hold on
triplot(DT(attTris{:},:),DT.Points(:,1),DT.Points(:,2),'g')
hold off
```



delaunayTriangulation also can be used to triangulate points in 3-D space. The resulting triangulation is composed of tetrahedra.

This example shows how to use a delaunayTriangulation to create and plot the triangulation of 3-D points.

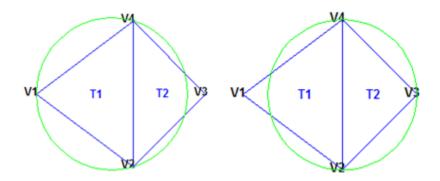


The tetramesh function plots both the internal and external faces of the triangulation. For large 3-D triangulations, plotting the internal faces might be an unnecessary use of resources. A plot of the boundary might be more appropriate. You can use the freeBoundary method to get the boundary triangulation in matrix format. Then pass the result to trimesh or trisurf.

Constrained Delaunay Triangulation

The delaunayTriangulation class allows you to constrain edges in a 2-D triangulation. This means you can choose a pair of points in the triangulation and constrain an edge to join those points. You can picture this as "forcing" an edge between one or more pairs of points. The following example shows how edge constraints can affect the triangulation.

The triangulation below is a Delaunay triangulation because it respects the empty circumcircle criterion.

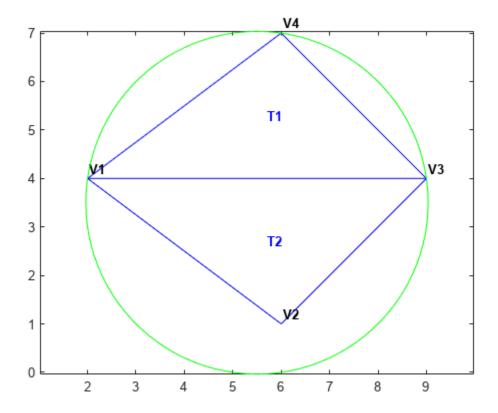


Triangulate a set of points with an edge constraint specified between vertex V1 and V3.

Define the point set.

```
P = [2 4; 6 1; 9 4; 6 7];
Define a constraint, C, between V1 and V3.
C = [1 \ 3];
DT = delaunayTriangulation(P,C);
Plot the triangulation and add annotations.
triplot(DT)
% Label the vertices.
hold on
numvx = size(P,1);
vxlabels = arrayfun(@(n) {sprintf('V%d', n)}, (1:numvx)');
Hpl = text(P(:,1)+0.2, P(:,2)+0.2, vxlabels, 'FontWeight', ...
  'bold', 'HorizontalAlignment', 'center', 'BackgroundColor', ...
  'none');
hold off
% Use the incenters to find the positions for placing triangle labels on the plot.
hold on
IC = incenter(DT);
numtri = size(DT,1);
trilabels = arrayfun(@(P) {sprintf('T%d', P)}, (1:numtri)');
Htl = text(IC(:,1),IC(:,2),trilabels,'FontWeight','bold', ...
'HorizontalAlignment', 'center', 'Color', 'blue');
hold off
% Plot the circumcircle associated with the triangle, T1.
hold on
[CC,r] = circumcenter(DT);
theta = 0:pi/50:2*pi;
xunit = r(1)*cos(theta) + CC(1,1);
yunit = r(1)*sin(theta) + CC(1,2);
plot(xunit, yunit, 'g');
axis equal
```

hold off



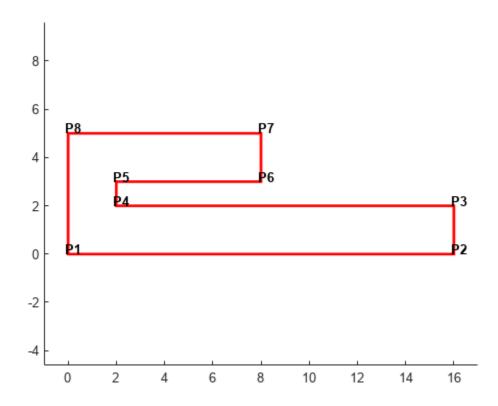
The constraint between vertices (V1, V3) was honored, however, the Delaunay criterion was invalidated. This also invalidates the nearest-neighbor relation that is inherent in a Delaunay triangulation. This means the nearestNeighbor search method provided by delaunayTriangulation cannot be supported if the triangulation has constraints.

In typical applications, the triangulation might be composed of many points, and a relatively small number of edges in the triangulation might be constrained. Such a triangulation is said to be locally non-Delaunay, because many triangles in the triangulation might respect the Delaunay criterion, but locally there might be some triangles that do not. In many applications, local relaxation of the empty circumcircle property is not a concern.

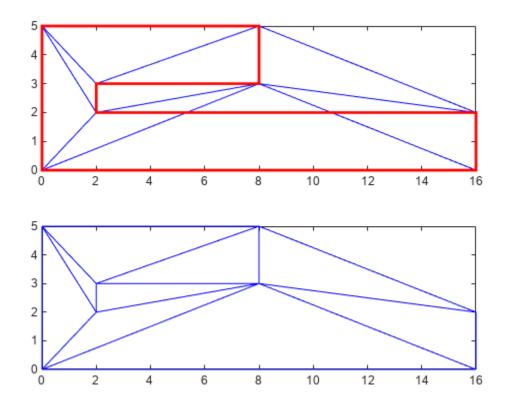
Constrained triangulations are generally used to triangulate a nonconvex polygon. The constraints give us a correspondence between the polygon edges and the triangulation edges. This relationship enables you to extract a triangulation that represents the region. The following example shows how to use a constrained delaunayTriangulation to triangulate a nonconvex polygon.

Define and plot a polygon.

```
hold on
numvx = size(P,1);
vxlabels = arrayfun(@(n) {sprintf('P%d', n)}, (1:numvx)');
Hpl = text(P(:,1)+0.2, P(:,2)+0.2, vxlabels, 'FontWeight', ...
   'bold', 'HorizontalAlignment','center', 'BackgroundColor', ...
   'none');
hold off
```



Create and plot the triangulation together with the polygon boundary.



This triangulation cannot be used to represent the domain of the polygon because some triangles cut across the boundary. You need to impose a constraint on the edges that are cut by triangulation edges. Since all edges have to be respected, you need to constrain all edges. The steps below show how to constrain all the edges.

Enter the constrained edge definition. Observe from the annotated figure where you need constraints (between (V1, V2), (V2, V3), and so on).

```
C = [1 \ 2; \ 2 \ 3; \ 3 \ 4; \ 4 \ 5; \ 5 \ 6; \ 6 \ 7; \ 7 \ 8; \ 8 \ 1];
```

In general, if you have N points in a sequence that define a polygonal boundary, the constraints can be expressed as C = [(1:(N-1))' (2:N)'; N 1];

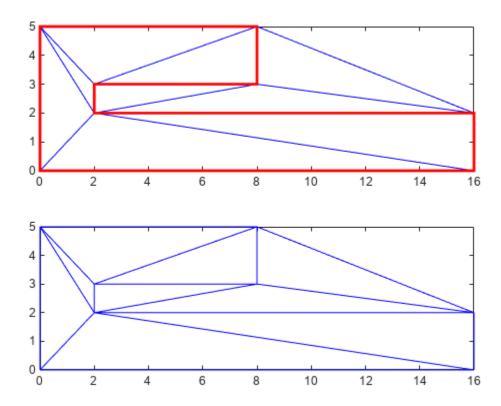
Specify the constraints when you create the delaunayTriangulation.

```
DT = delaunayTriangulation(P,C);
```

Alternatively, you can impose constraints on an existing triangulation by setting the Constraints property: DT.Constraints = C;

Plot the triangulation and polygon.

```
figure('Color','white')
subplot(2,1,1);
axis([-1 17 -1 6]);
axis equal
triplot(DT)
```

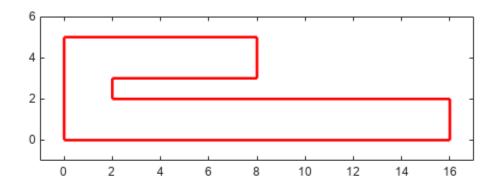


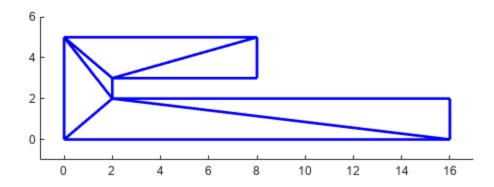
The plot shows that the edges of the triangulation respect the boundary of the polygon. However, the triangulation fills the concavities. What is needed is a triangulation that represents the polygonal domain. You can extract the triangles within the polygon using the delaunayTriangulation method, isInterior. This method returns a logical array whose true and false values that indicate whether the triangles are inside a bounded geometric domain. The analysis is based on the Jordan Curve theorem, and the boundaries are defined by the edge constraints. The ith triangle in the triangulation is considered to be inside the domain if the ith logical flag is true, otherwise it is outside.

Now use the isInterior method to compute and plot the set of domain triangles.

```
% Plot the constrained edges in red.
figure('Color','white')
subplot(2,1,1);
plot(P(C'),P(C'+size(P,1)),'-r','LineWidth', 2);
axis([-1 17 -1 6]);
```

```
% Compute the in/out status.
I0 = isInterior(DT);
subplot(2,1,2);
hold on;
axis([-1 17 -1 6]);
% Use triplot to plot the triangles that are inside.
% Uses logical indexing and dt(i,j) shorthand
% format to access the triangulation.
triplot(DT(IO, :),DT.Points(:,1), DT.Points(:,2),'LineWidth', 2)
hold off;
```





Triangulation of Point Sets Containing Duplicate Locations

The Delaunay algorithms in MATLAB construct a triangulation from a unique set of points. If the points passed to the triangulation function, or class, are not unique, the duplicate locations are detected and the duplicate point is ignored. This produces a triangulation that does not reference some points in the original input, namely the duplicate points. When you work with the delaunay and delaunayn functions, the presence of duplicates may be of little consequence. However, since many of the queries provided by the delaunayTriangulation class are index based, it is important to understand that delaunayTriangulation triangulates and works with the unique data set. Therefore, indexing based on the unique point set is the convention. This data is maintained by the Points property of delaunayTriangulation.

The following example illustrates the importance of referencing the unique data set stored within the Points property when working with delaunayTriangulation:

```
rng('default')
P = rand([25 2]);
P(18,:) = P(8,:)
P(16,:) = P(6,:)
P(12,:) = P(2,:)
DT = delaunayTriangulation(P)
```

When the triangulation is created, MATLAB issues a warning. The Points property shows that the duplicate points have been removed from the data.

```
DT =
   delaunayTriangulation with properties:
        Points: [22x2 double]
        ConnectivityList: [31x3 double]
        Constraints: []
```

If for example, the Delaunay triangulation is used to compute the convex hull, the indices of the points on the hull are indices with respect to the unique point set, DT.Points. Therefore, use the following code to compute and plot the convex hull:

```
K = DT.convexHull();
plot(DT.Points(:,1),DT.Points(:,2),'.');
hold on
plot(DT.Points(K,1),DT.Points(K,2),'-r');
```

If the original data set containing the duplicates were used in conjunction with the indices provided by delaunayTriangulation, then the result would be incorrect. The delaunayTriangulation works with indices that are based on the unique data set DT.Points. For example, the following would produce an incorrect plot, because K is indexed with respect to DT.Points and not P:

```
K = DT.convexHull();
plot(P(:,1),P(:,2),'.');
hold on
plot(P(K,1),P(K,2),'-r');
```

It's often more convenient to create a unique data set by removing duplicates prior to creating the delaunayTriangulation. Doing this eliminates the potential for confusion. This can be accomplished using the unique function as follows:

```
rng('default')
P = rand([25 2]);
P(18,:) = P(8,:)
P(16,:) = P(6,:)
P(12,:) = P(2,:)

[~, I, ~] = unique(P,'first','rows');
I = sort(I);
P = P(I,:);
DT = delaunayTriangulation(P) % The point set is unique
```

See Also

More About

• "Spatial Searching" on page 7-53

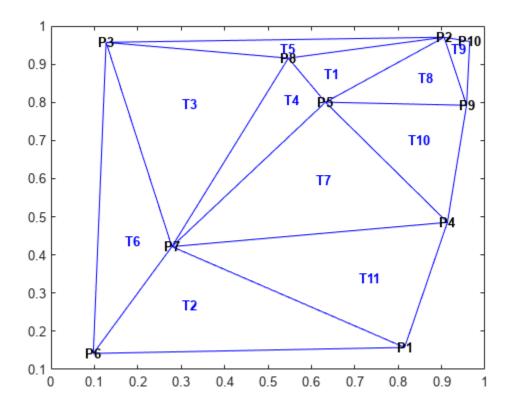
Creating and Editing Delaunay Triangulations

This example shows how to create, edit, and query Delaunay triangulations using the delaunayTriangulation class. The Delaunay triangulation is the most widely used triangulation in scientific computing. The properties associated with the triangulation provide a basis for solving a variety of geometric problems. Construction of constrained Delaunay triangulations is also shown, together with an applications covering medial axis computation and mesh morphing.

Example One: Create and Plot 2-D Delaunay Triangulation

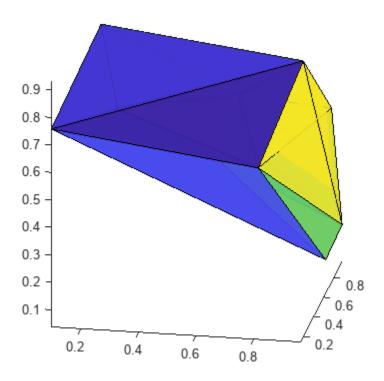
This example shows you how to compute a 2-D Delaunay triangulation and then plot the triangulation together with the vertex and triangle labels.

```
rng default
x = rand(10,1);
y = rand(10,1);
dt = delaunayTriangulation(x,y)
  delaunayTriangulation with properties:
              Points: [10x2 double]
    ConnectivityList: [11x3 double]
         Constraints: []
triplot(dt)
Display the vertex and triangle labels on the plot.
vxlabels = arrayfun(@(n) {sprintf('P%d', n)}, (1:10)');
Hpl = text(x,y,vxlabels,'FontWeight','bold','HorizontalAlignment',...
   'center', 'BackgroundColor', 'none');
ic = incenter(dt);
numtri = size(dt,1);
trilabels = arrayfun(@(x) {sprintf('T%d',x)}, (1:numtri)');
Htl = text(ic(:,1),ic(:,2),trilabels,'FontWeight','bold', ...
   'HorizontalAlignment','center','Color','blue');
hold off
```



Example Two: Create and Plot 3-D Delaunay Triangulation

This example shows you how to compute and plot a 3-D Delaunay triangulation.



To display large tetrahedral meshes, use the convexHull method to compute the boundary triangulation and plot it using trisurf. For example:

```
triboundary = convexHull(dt);
trisurf(triboundary, X(:,1), X(:,2), X(:,3), 'FaceColor', 'cyan')
```

Example Three: Access Triangulation Data Structure

There are two ways to access the triangulation data structure. One way is via the Triangulation property, the other way is using indexing.

Create a 2-D Delaunay triangulation from 10 random points.

One way to access the triangulation data structure is with the ConnectivityList property.

```
dt.ConnectivityList
```

```
ans = 11 \times 3
      2
             8
      7
             6
                     1
      3
             7
                     8
      8
             7
                     5
      3
                     2
             8
      6
             7
                     3
      7
                     5
             4
      5
                     2
             9
      2
             9
                    10
      5
             4
                     9
```

Indexing is a shorthand way to query the triangulation. The syntax is dt(i,j), where j is the jth vertex of the ith triangle. Standard indexing rules apply.

Query the triangulation data structure with indexing.

```
dt(:,:)
ans = 11 \times 3
     2
             8
                    5
     7
             6
                    1
     3
             7
                    8
     8
             7
                    5
                    2
     3
             8
     6
             7
                    3
      7
             4
                    5
     5
             9
                    2
      2
             9
                   10
     5
             4
                    9
```

The second triangle is:

```
dt(2,:) ans = 1 \times 3 7 6 1
```

The third vertex of the second triangle is:

```
dt(2,3) ans = 1 The first three triangles are:
```

dt(1:3,:) ans = 3×3

2 8

```
7 6 1
3 7 8
```

Example Four: Edit Delaunay Triangulation to Insert or Remove Points

This example shows you how to use index-based subscripting to insert or remove points. It is more efficient to edit a delaunayTriangulation to make minor modifications as opposed to recreating a new delaunayTriangulation from scratch, this is especially true if the data set is large.

Construct a Delaunay triangulation from 10 random points within a unit square.

```
rng default
x = rand(10,1);
y = rand(10,1);
dt = delaunayTriangulation(x,y)
dt =
  delaunayTriangulation with properties:
              Points: [10x2 double]
    ConnectivityList: [11x3 double]
         Constraints: []
Insert 5 additional random points.
dt.Points(end+(1:5),:) = rand(5,2)
dt =
  delaunayTriangulation with properties:
              Points: [15x2 double]
    ConnectivityList: [20x3 double]
         Constraints: []
Replace the fifth point.
dt.Points(5,:) = [0 \ 0]
  delaunayTriangulation with properties:
              Points: [15x2 double]
    ConnectivityList: [20x3 double]
         Constraints: []
Remove the fourth point.
dt.Points(4,:) = []
  delaunayTriangulation with properties:
              Points: [14x2 double]
    ConnectivityList: [18x3 double]
```

```
Constraints: []
```

Example Five: Create Constrained Delaunay Triangulation

This example shows you how to create a constrained Delaunay triangulation and illustrates the effect of the constraints.

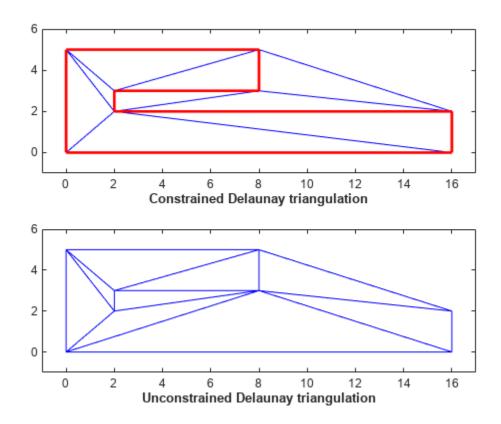
Create and plot a constrained Delaunay triangulation.

```
X = [0 0; 16 0; 16 2; 2 2; 2 3; 8 3; 8 5; 0 5];
C = [1 2; 2 3; 3 4; 4 5; 5 6; 6 7; 7 8; 8 1];
dt = delaunayTriangulation(X,C);
subplot(2,1,1)
triplot(dt)
axis([-1 17 -1 6])
xlabel('Constrained Delaunay triangulation','FontWeight','b')

Plot the constrained edges in red.
hold on
plot(X(C'),X(C'+size(X,1)),'-r','LineWidth',2)
hold off

Now delete the constraints and plot the unconstrained Delaunay triangulation.
dt.Constraints = [];
subplot(2,1,2)
triplot(dt)
axis([-1 17 -1 6])
```

xlabel('Unconstrained Delaunay triangulation','FontWeight','b')



Example Six: Create Constrained Delaunay Triangulation of Geographical Map

Load a map of the perimeter of the conterminous United States. Construct a constrained Delaunay triangulation representing the polygon. This triangulation spans a domain that is bounded by the convex hull of the set of points. Filter out the triangles that are within the domain of the polygon and plot them. Note: The data set contains duplicate data points; that is, two or more datapoints have the same location. The duplicate points are rejected and the delaunayTriangulation reformats the constraints accordingly.

```
clf
load usapolygon
```

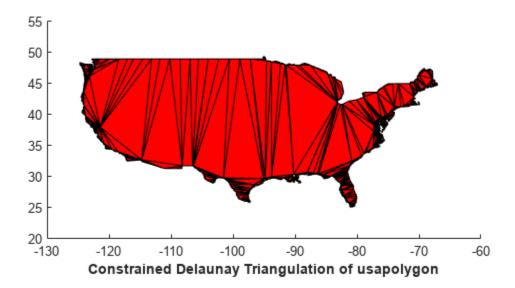
Define an edge constraint between two successive points that make up the polygonal boundary and create the Delaunay triangulation.

```
nump = numel(uslon);
C = [(1:(nump-1))' (2:nump)'; nump 1];
dt = delaunayTriangulation(uslon,uslat,C);

Warning: Duplicate data points have been detected and removed.
  The Triangulation indices and constraints are defined with respect to the unique set of points.

Warning: Intersecting edge constraints have been split, this may have added new points into the io = isInterior(dt);
patch('Faces',dt(io,:),'Vertices',dt.Points,'FaceColor','r')
axis equal
```

```
axis([-130 -60 20 55])
xlabel('Constrained Delaunay Triangulation of usapolygon', 'FontWeight', 'b')
```



Example Seven: Curve Reconstruction from Point Cloud

This example highlights the use of a Delaunay triangulation to reconstruct a polygonal boundary from a cloud of points. The reconstruction is based on the elegant Crust algorithm.

Reference: N. Amenta, M. Bern, and D. Eppstein. The crust and the beta-skeleton: combinatorial curve reconstruction. *Graphical Models and Image Processing*, 60:125-135, 1998.

Create a set of points representing the point cloud.

```
numpts = 192;
t = linspace( -pi, pi, numpts+1 )';
t(end) = [];
r = 0.1 + 5*sqrt( cos( 6*t ).^2 + (0.7).^2 );
x = r.*cos(t);
y = r.*sin(t);
ri = randperm(numpts);
x = x(ri);
y = y(ri);
Construct a Delaunay Triangulation of the point set.
dt = delaunayTriangulation(x,y);
```

tri = dt(:,:);

Insert the location of the Voronoi vertices into the existing triangulation.

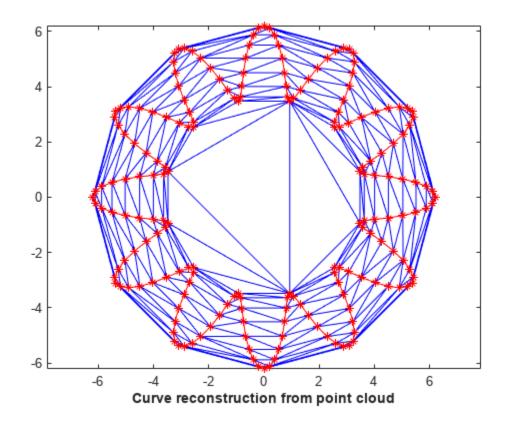
```
V = voronoiDiagram(dt);
```

Remove the infinite vertex and filter out duplicate points using unique.

```
V(1,:) = [];
numv = size(V,1);
dt.Points(end+(1:numv),:) = unique(V,'rows');
```

The Delaunay edges that connect pairs of sample points represent the boundary.

```
delEdges = edges(dt);
validx = delEdges(:,1) <= numpts;
validy = delEdges(:,2) <= numpts;
boundaryEdges = delEdges((validx & validy),:)';
xb = x(boundaryEdges);
yb = y(boundaryEdges);
clf
triplot(tri,x,y)
axis equal
hold on
plot(x,y,'*r')
plot(xb,yb,'-r')
xlabel('Curve reconstruction from point cloud','FontWeight','b')
hold off</pre>
```



Example Eight: Compute Approximate Medial Axis of Polygonal Domain

This example shows how to create an approximate Medial Axis of a polygonal domain using a constrained Delaunay triangulation. The *Medial Axis* of a polygon is defined by the locus of the center of a maximal disk within the polygon interior.

Construct a constrained Delaunay triangulation of a sample of points on the domain boundary.

```
load trimesh2d
dt = delaunayTriangulation(x,y,Constraints);
inside = isInterior(dt);
```

Construct a triangulation to represent the domain triangles.

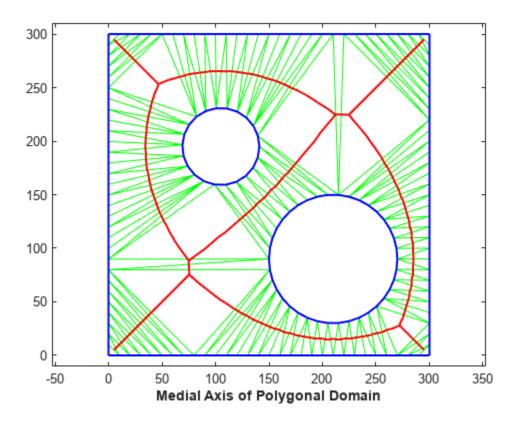
```
tr = triangulation(dt(inside,:),dt.Points);
```

Construct a set of edges that join the circumcenters of neighboring triangles. The additional logic constructs a unique set of such edges.

```
numt = size(tr,1);
T = (1:numt)';
neigh = neighbors(tr);
cc = circumcenter(tr);
xcc = cc(:,1);
ycc = cc(:,2);
idx1 = T < neigh(:,1);
idx2 = T < neigh(:,2);
idx3 = T < neigh(:,3);
neigh = [T(idx1) neigh(idx1,1); T(idx2) neigh(idx2,2); T(idx3) neigh(idx3,3)]';</pre>
```

Plot the domain triangles in green, the domain boundary in blue, and the medial axis in red.

```
clf
triplot(tr,'g')
hold on
plot(xcc(neigh), ycc(neigh), '-r','LineWidth',1.5)
axis([-10 310 -10 310])
axis equal
plot(x(Constraints'),y(Constraints'),'-b','LineWidth',1.5)
xlabel('Medial Axis of Polygonal Domain','FontWeight','b')
hold off
```

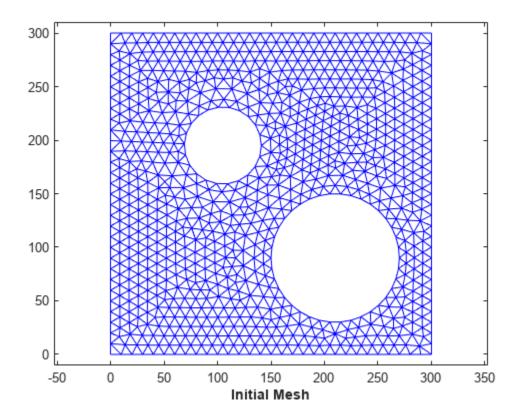


Example Nine: Morph 2-D Mesh to Modified Boundary

This example shows how to morph a mesh of a 2-D domain to accommodate a modification to the domain boundary.

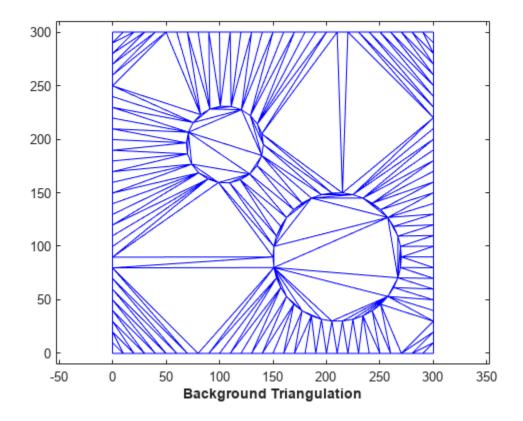
Step 1: Load the data. The mesh to be morphed is defined by trife, xfe, and yfe, which is a triangulation in face-vertex format.

```
load trimesh2d
clf
triplot(trife,xfe,yfe)
axis equal
axis([-10 310 -10 310])
axis equal
xlabel('Initial Mesh','FontWeight','b')
```



Step 2: Construct a background triangulation - a Constrained Delaunay triangulation of the set of points representing the mesh boundary. For each vertex of the mesh, compute a descriptor that defines its location with respect to the background triangulation. The descriptor is the enclosing triangle together with the barycentric coordinates with respect to that triangle.

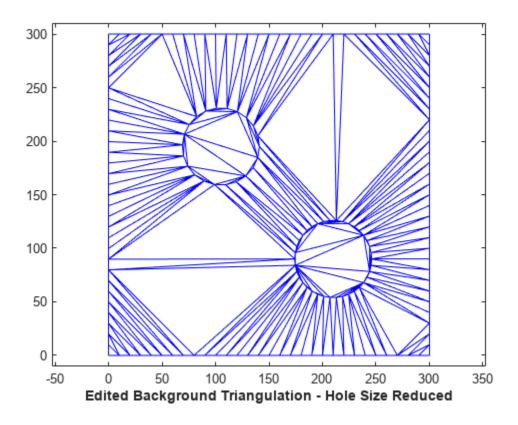
```
dt = delaunayTriangulation(x,y,Constraints);
clf
triplot(dt)
axis equal
axis([-10 310 -10 310])
axis equal
xlabel('Background Triangulation','FontWeight','b')
```



descriptors.tri = pointLocation(dt,xfe,yfe);
descriptors.baryCoords = cartesianToBarycentric(dt,descriptors.tri,[xfe yfe]);

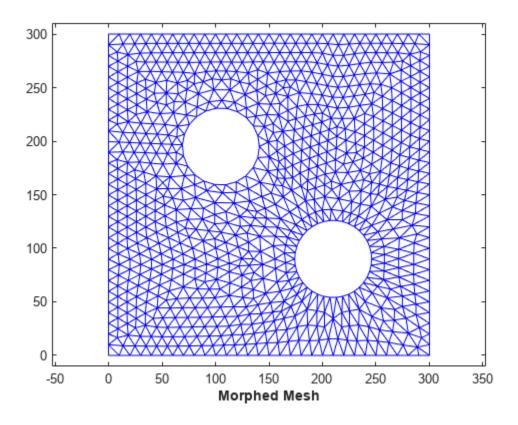
Step 3: Edit the background triangulation to incorporate the desired modification to the domain boundary.

```
ccl = [210 90];
circl = (143:180)';
x(circl) = (x(circl)-ccl(1))*0.6 + ccl(1);
y(circl) = (y(circl)-ccl(2))*0.6 + ccl(2);
tr = triangulation(dt(:,:),x,y);
clf
triplot(tr)
axis([-10 310 -10 310])
axis equal
xlabel('Edited Background Triangulation - Hole Size Reduced', 'FontWeight', 'b')
```



Step 4: Convert the descriptors back to Cartesian coordinates using the deformed background triangulation as a basis for evaluation.

```
Xnew = barycentricToCartesian(tr,descriptors.tri,descriptors.baryCoords);
tr = triangulation(trife,Xnew);
clf
triplot(tr)
axis([-10 310 -10 310])
axis equal
xlabel('Morphed Mesh','FontWeight','b')
```



Spatial Searching

Introduction

MATLAB® provides the necessary functions for performing a spatial search using either a Delaunay triangulation or a general triangulation. The search queries that MATLAB supports are:

- Nearest-neighbor search (sometimes called closest-point search or proximity search).
- Point-location search (sometimes called point-in-triangle search or point-in-simplex search, where a simplex is a triangle, tetrahedron or higher dimensional equivalent).

Given a set of points X and a query point q in Euclidean space, the nearest-neighbor search locates a point p in X that is closer to q than to any other point in X. Given a triangulation of X, the point-location search locates the triangle or tetrahedron that contains the query point q. Since these methods work for both Delaunay as well as general triangulations, you can use them even if a modification of the points violates the Delaunay criterion. You also can search a general triangulation represented in matrix format.

While MATLAB supports these search schemes in N dimensions, exact spatial searches usually become prohibitive as the number of dimensions extends beyond 3-D. You should consider approximate alternatives for large problems in up to 10 dimensions.

Nearest-Neighbor Search

There are a few ways to compute nearest-neighbors in MATLAB, depending on the dimensionality of the problem:

- For 2-D and 3-D searches, use the nearestNeighbor method provided by the triangulation class and inherited by the delaunayTriangulation class.
- For 4-D and higher, use the delaunayn function to construct the triangulation and the complementary dsearchn function to perform the search. While these N-D functions support 2-D and 3-D, they are not as general and efficient as the triangulation search methods.

This example shows how to perform a nearest-neighbor search in 2-D with delaunayTriangulation.

Begin by creating a random set of 15 points.

```
X = [3.5 \ 8.2; \ 6.8 \ 8.3; \ 1.3 \ 6.5; \ 3.5 \ 6.3; \ 5.8 \ 6.2; \ 8.3 \ 6.5; \dots \\ 1 \ 4; \ 2.7 \ 4.3; \ 5 \ 4.5; \ 7 \ 3.5; \ 8.7 \ 4.2; \ 1.5 \ 2.1; \ 4.1 \ 1.1; \dots \\ 7 \ 1.5; \ 8.5 \ 2.75];
```

Plot the points and add annotations to show the ID labels.

```
plot(X(:,1),X(:,2),'ob')
hold on
vxlabels = arrayfun(@(n) {sprintf('X%d', n)}, (1:15)');
Hpl = text(X(:,1)+0.2, X(:,2)+0.2, vxlabels, 'FontWeight', ...
    'bold', 'HorizontalAlignment','center', 'BackgroundColor', ...
    'none');
hold off
```

Create a Delaunay triangulation from the points.

```
dt = delaunayTriangulation(X);
```

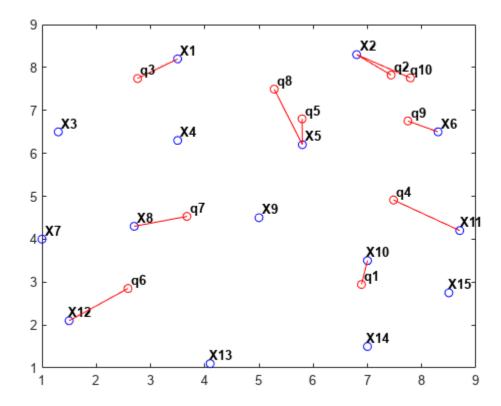
Create some query points and for each query point find the index of its corresponding nearest neighbor in X using the nearestNeighbor method.

```
numq = 10;
rng(0,'twister');
q = 2+rand(numq,2)*6;
xi = nearestNeighbor(dt, q);
```

Add the query points to the plot and add line segments joining the query points to their nearest neighbors.

```
xnn = X(xi,:);
hold on
plot(q(:,1),q(:,2),'or');
plot([xnn(:,1) q(:,1)]',[xnn(:,2) q(:,2)]','-r');

vxlabels = arrayfun(@(n) {sprintf('q%d', n)}, (1:numq)');
Hpl = text(q(:,1)+0.2, q(:,2)+0.2, vxlabels, 'FontWeight', ...
    'bold', 'HorizontalAlignment','center', ...
    'BackgroundColor','none');
hold off
```



Performing a nearest-neighbor search in 3-D is a direct extension of the 2-D example based on delaunayTriangulation.

For 4-D and higher, use the delaunayn and dsearchn functions as illustrated in the following example:

Create a random sample of points in 4-D and triangulate the points using delaunayn:

```
X = 20*rand(50,4) -10;
tri = delaunayn(X);
```

Create some query points and for each query point find the index of its corresponding nearest-neighbor in X using the dsearchn function:

```
q = rand(5,4);
xi = dsearchn(X,tri, q);
```

The nearestNeighbor method and the dsearchn function allow the Euclidean distance between the query point and its nearest-neighbor to be returned as an optional argument. In the 4-D example, you can compute the distances, dnn, as follows:

```
[xi,dnn] = dsearchn(X,tri,q);
```

Point-Location Search

A point-location search is a triangulation search algorithm that locates the simplex (triangle, tetrahedron, and so on) enclosing a query point. As in the case of the nearest-neighbor search, there are a few approaches to performing a point-location search in MATLAB, depending on the dimensionality of the problem:

- For 2-D and 3-D, use the class-based approach with the pointLocation method provided by the triangulation class and inherited by the delaunayTriangulation class.
- For 4-D and higher, use the delaunayn function to construct the triangulation and the complementary tsearchn function to perform the point-location search. Although supporting 2-D and 3-D, these N-D functions are not as general and efficient as the triangulation search methods.

This example shows how to use the delaunayTriangulation class to perform a point location search in 2-D.

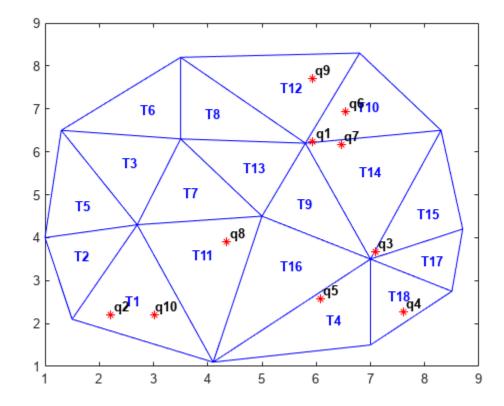
Begin with a set of 2-D points.

```
X = [3.5 \ 8.2; \ 6.8 \ 8.3; \ 1.3 \ 6.5; \ 3.5 \ 6.3; \ 5.8 \ 6.2; \ \dots \\ 8.3 \ 6.5; \ 1 \ 4; \ 2.7 \ 4.3; \ 5 \ 4.5; \ 7 \ 3.5; \ 8.7 \ 4.2; \ \dots \\ 1.5 \ 2.1; \ 4.1 \ 1.1; \ 7 \ 1.5; \ 8.5 \ 2.75];
```

Create the triangulation and plot it showing the triangle ID labels at the incenters of the triangles.

Now create some query points and add them to the plot. Then find the index of the corresponding enclosing triangles using the pointLocation method.

```
q = [5.9344]
               6.2363;
    2.2143
              2.1910;
    7.0948
              3.6615;
    7.6040
              2.2770;
    6.0724
              2.5828:
    6.5464
              6.9407;
    6.4588
              6.1690;
    4.3534
              3.9026;
    5.9329
              7.7013;
    3.0271
              2.2067];
hold on;
plot(q(:,1),q(:,2),'*r');
vxlabels = arrayfun(@(n) \{sprintf('q%d', n)\}, (1:10)');
Hpl = text(q(:,1)+0.2, q(:,2)+0.2, vxlabels, 'FontWeight', ...
    'bold', 'HorizontalAlignment', 'center', ...
    'BackgroundColor', 'none');
hold off
```



```
ti = pointLocation(dt,q);
```

Performing a point-location search in 3-D is a direct extension of performing a point-location search in 2-D with delaunayTriangulation.

For 4-D and higher, use the delaunayn and tsearchn functions as illustrated in the following example:

Create a random sample of points in 4-D and triangulate them using delaunayn:

```
X = 20*rand(50,4) -10;
tri = delaunayn(X);
```

Create some query points and find the index of the corresponding enclosing simplices using the tsearchn function:

```
q = rand(5,4);
ti = tsearchn(X,tri,q);
```

The pointLocation method and the tsearchn function allow the corresponding barycentric coordinates to be returned as an optional argument. In the 4-D example, you can compute the barycentric coordinates as follows:

```
[ti,bc] = tsearchn(X,tri,q);
```

The barycentric coordinates are useful for performing linear interpolation. These coordinates provide you with weights that you can use to scale the values at each vertex of the enclosing simplex. See "Interpolating Scattered Data" on page 8-17 for further details.

See Also

nearestNeighbor|delaunayTriangulation|triangulation|delaunayn|dsearchn|
pointLocation|triangulation|tsearchn|delaunay

Related Examples

- "Working with Delaunay Triangulations" on page 7-14
- "Triangulation Representations" on page 7-2
- "Interpolating Scattered Data" on page 8-17

Voronoi Diagrams

```
In this section...

"Plot 2-D Voronoi Diagram and Delaunay Triangulation" on page 7-58

"Computing the Voronoi Diagram" on page 7-61
```

The Voronoi diagram of a discrete set of points X decomposes the space around each point X(i) into a region of influence $R\{i\}$. This decomposition has the property that an arbitrary point P within the region $R\{i\}$ is closer to point i than any other point. The region of influence is called a Voronoi region and the collection of all the Voronoi regions is the Voronoi diagram.

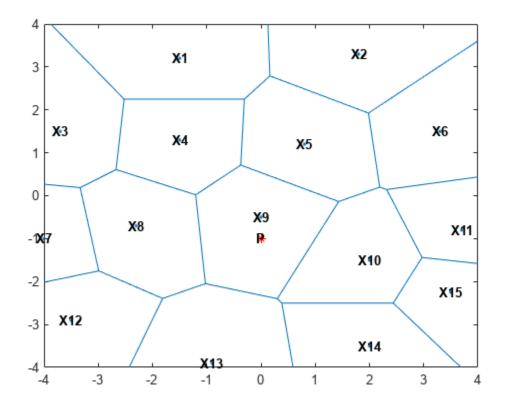
The Voronoi diagram is an N-D geometric construct, but most practical applications are in 2-D and 3-D space. The properties of the Voronoi diagram are best understood using an example.

Plot 2-D Voronoi Diagram and Delaunay Triangulation

This example shows the Voronoi diagram and the Delaunay triangulation on the same 2-D plot.

Use the 2-D voronoi function to plot the Voronoi diagram for a set of points.

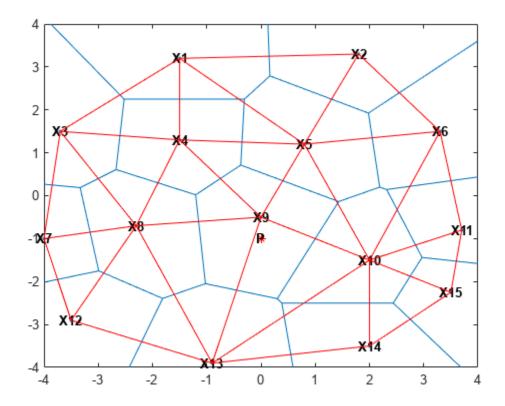
```
figure()
X = [-1.5 \ 3.2; \ 1.8 \ 3.3; \ -3.7 \ 1.5; \ -1.5 \ 1.3; \dots]
      0.8 1.2; 3.3 1.5; -4.0 -1.0; -2.3 -0.7; ...
      0 -0.5; 2.0 -1.5; 3.7 -0.8; -3.5 -2.9; ...
     -0.9 -3.9; 2.0 -3.5; 3.5 -2.25];
voronoi(X(:,1),X(:,2))
% Assign labels to the points.
nump = size(X,1);
plabels = arrayfun(@(n) {sprintf('X%d', n)}, (1:nump)');
Hpl = text(X(:,1), X(:,2), plabels, 'FontWeight', ...
      'bold', 'HorizontalAlignment', 'center', ...
      'BackgroundColor', 'none');
% Add a query point, P, at (0, -1.5).
P = [0 -1];
plot(P(1),P(2), '*r');
text(P(1), P(2), 'P', 'FontWeight', 'bold', ...
     'HorizontalAlignment','center', ...
     'BackgroundColor', 'none');
hold off
```



Observe that P is closer to X9 than to any other point in X, which is true for any point P within the region that bounds X9.

The Voronoi diagram of a set of points X is closely related to the Delaunay triangulation of X. To see this relationship, construct a Delaunay triangulation of the point set X and superimpose the triangulation plot on the Voronoi diagram.

```
dt = delaunayTriangulation(X);
hold on
triplot(dt,'-r');
hold off
```



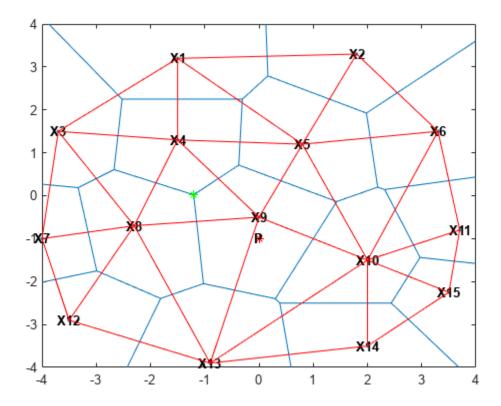
From the plot you can see that the Voronoi region associated with the point X9 is defined by the perpendicular bisectors of the Delaunay edges attached to X9. Also, the vertices of the Voronoi edges are located at the circumcenters of the Delaunay triangles. You can illustrate these associations by plotting the circumcenter of triangle {|X9|,|X4|,|X8|}.

To find the index of this triangle, query the triangulation. The triangle contains the location (-1, 0).

```
tidx = pointLocation(dt,-1,0);
```

Now, find the circumcenter of this triangle and plot it in green.

```
cc = circumcenter(dt,tidx);
hold on
plot(cc(1),cc(2),'*g');
hold off
```



The Delaunay triangulation and Voronoi diagram are geometric duals of each other. You can compute the Voronoi diagram from the Delaunay triangulation and vice versa.

Observe that the Voronoi regions associated with points on the convex hull are unbounded (for example, the Voronoi region associated with X13). The edges in this region "end" at infinity. The Voronoi edges that bisect Delaunay edges (X13, X12) and (X13, X14) extend to infinity. While the Voronoi diagram provides a nearest-neighbor decomposition of the space around each point in the set, it does not directly support nearest-neighbor queries. However, the geometric constructions used to compute the Voronoi diagram are also used to perform nearest-neighbor searches.

Computing the Voronoi Diagram

This example shows how to compute a 2-D and 3-D Voronoi diagram.

MATLAB provides functions to plot the Voronoi diagram in 2-D and to compute the topology of the Voronoi diagram in N-D. In practice, Voronoi computation is not practical in dimensions beyond 6-D for moderate to large data sets, due to the exponential growth in required memory.

The voronoi plot function plots the Voronoi diagram for a set of points in 2-D space. In MATLAB there are two ways to compute the topology of the Voronoi diagram of a point set:

- Using the function voronoin
- Using the delaunayTriangulation method, voronoiDiagram.

The voronoin function supports the computation of the Voronoi topology for discrete points in N-D ($N \ge 2$). The voronoiDiagram method supports computation of the Voronoi topology for discrete points 2-D or 3-D.

The voronoiDiagram method is recommended for 2-D or 3-D topology computations as it is more robust and gives better performance for large data sets. This method supports incremental insertion and removal of points and complementary queries, such as nearest-neighbor point search.

The voronoin function and the voronoiDiagram method represent the topology of the Voronoi diagram using a matrix format. See "Triangulation Matrix Format" on page 7-3 for further details on this data structure.

Given a set of points, X, obtain the topology of the Voronoi diagram as follows:

• Using the voronoin function

```
[V,R] = voronoin(X)
```

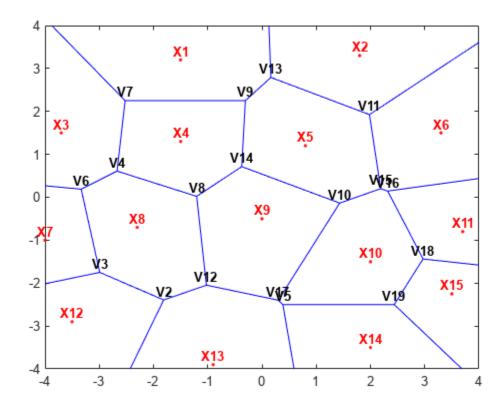
• Using the voronoiDiagram method

```
dt = delaunayTriangulation(X);
[V,R] = voronoiDiagram(dt)
```

V is a matrix representing the coordinates of the Voronoi vertices (the vertices are the end points of the Voronoi edges). By convention the first vertex in V is the infinite vertex. R is a vector cell array length size(X,1), representing the Voronoi region associated with each point. Hence, the Voronoi region associated with the point X(i) is $R\{i\}$.

Define and plot the voronoi diagram for a set of points

```
X = [-1.5 \ 3.2; \ 1.8 \ 3.3; \ -3.7 \ 1.5; \ -1.5 \ 1.3; \ 0.8 \ 1.2; \ \dots
      3.3 1.5; -4.0 -1.0; -2.3 -0.7; 0 -0.5; 2.0 -1.5; ...
      3.7 -0.8; -3.5 -2.9; -0.9 -3.9; 2.0 -3.5; 3.5 -2.25];
[VX,VY] = voronoi(X(:,1),X(:,2));
h = plot(VX, VY, '-b', X(:,1), X(:,2), '.r');
xlim([-4,4])
ylim([-4,4])
% Assign labels to the points X.
nump = size(X,1);
plabels = arrayfun(@(n) {sprintf('X%d', n)}, (1:nump)');
Hpl = text(X(:,1), X(:,2)+0.2, plabels, 'color', 'r', ...
      'FontWeight', 'bold', 'HorizontalAlignment',...
      'center', 'BackgroundColor', 'none');
% Compute the Voronoi diagram.
dt = delaunayTriangulation(X);
[V,R] = voronoiDiagram(dt);
% Assign labels to the Voronoi vertices V.
% By convention the first vertex is at infinity.
numv = size(V,1);
vlabels = arrayfun(@(n) {sprintf('V%d', n)}, (2:numv)');
hold on
```



R{9} gives the indices of the Voronoi vertices associated with the point site X9.

R{9}

ans =
$$1 \times 5$$

8 12 17 10 14

The indices of the Voronoi vertices are the indices with respect to the V array.

Similarly, R{4} gives the indices of the Voronoi vertices associated with the point site X4.

R{4}

ans =
$$1 \times 5$$
4 8 14 9 7

In 3-D a Voronoi region is a convex polyhedron, the syntax for creating the Voronoi diagram is similar. However the geometry of the Voronoi region is more complex. The following example illustrates the creation of a 3-D Voronoi diagram and the plotting of a single region.

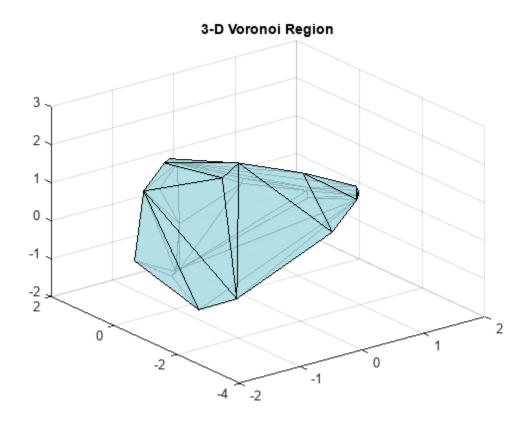
Create a sample of 25 points in 3-D space and compute the topology of the Voronoi diagram for this point set.

```
rng('default')
X = -3 + 6.*rand([25 3]);
dt = delaunayTriangulation(X);
```

Compute the topology of the Voronoi diagram.

```
[V,R] = voronoiDiagram(dt);
```

Find the point closest to the origin and plot the Voronoi region associated with this point.



See Also

More About

"Spatial Searching" on page 7-53

Types of Region Boundaries

```
In this section...

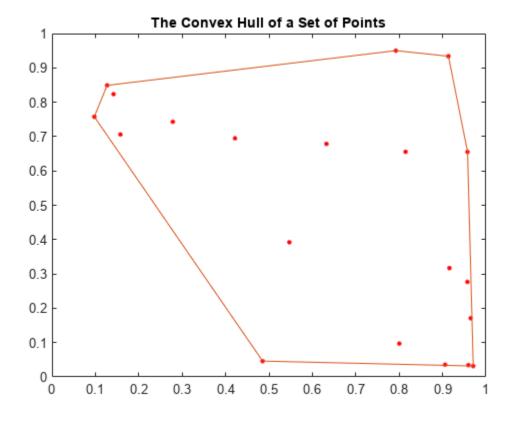
"Convex Hulls vs. Nonconvex Polygons" on page 7-65

"Alpha Shapes" on page 7-67
```

Convex Hulls vs. Nonconvex Polygons

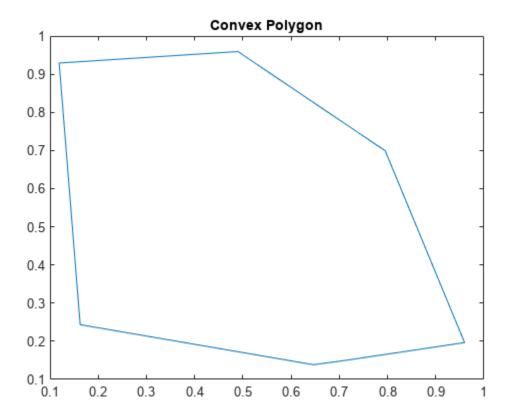
The convex hull of a set of points in N-D space is the smallest convex region enclosing all points in the set. If you think of a 2-D set of points as pegs in a peg board, the convex hull of that set would be formed by taking an elastic band and using it to enclose all the pegs.

```
rng('default')
x = rand(20,1);
y = rand(20,1);
plot(x,y,'r.','MarkerSize',10)
hold on
k = convhull(x,y);
plot(x(k),y(k))
title('The Convex Hull of a Set of Points')
hold off
```



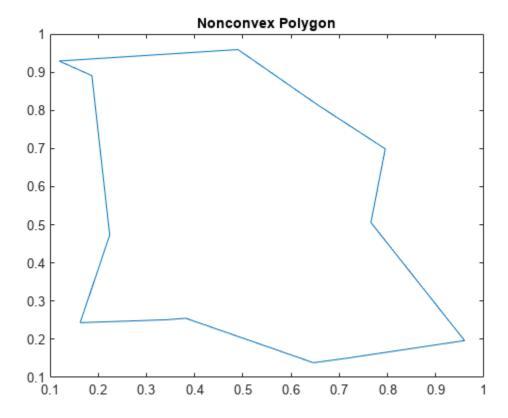
A convex polygon is a polygon that does not have concave vertices, for example:

```
x = rand(20,1);
y = rand(20,1);
k = convhull(x,y);
plot(x(k),y(k))
title('Convex Polygon')
```



You can also create a boundary of a point set that is nonconvex. If you shrink and tighten the convex hull from above, you can enclose all of the points in a nonconvex polygon with concave vertices:

```
k = boundary(x,y,0.9);
plot(x(k),y(k))
title('Nonconvex Polygon')
```



The convex hull has numerous applications. You can compute the upper bound on the area bounded by a discrete point set in the plane from the convex hull of the set. The convex hull simplifies the representation of more complex polygons or polyhedra. For instance, to determine whether two nonconvex bodies intersect, you could apply a series of fast rejection steps to avoid the penalty of a full intersection analysis:

- Check if the axis-aligned bounding boxes around each body intersect.
- If the bounding boxes intersect, you can compute the convex hull of each body and check intersection of the hulls.

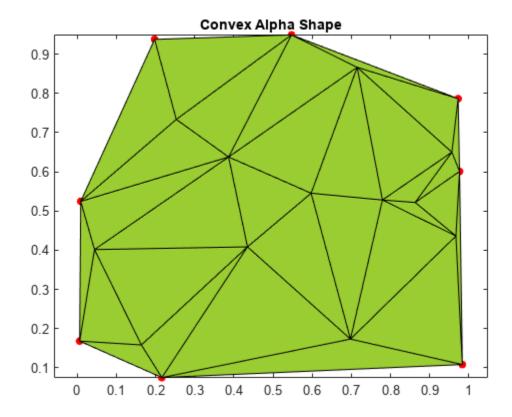
If the convex hulls did not intersect, this would avoid the expense of a more comprehensive intersection test.

While convex hulls and nonconvex polygons are convenient ways to represent relatively simple boundaries, they are in fact specific instances of a more general geometric construct called the alpha shape.

Alpha Shapes

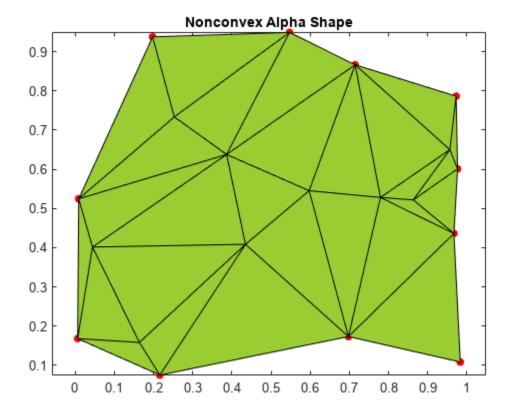
The alpha shape of a set of points is a *generalization* of the convex hull and a subgraph of the Delaunay triangulation. That is, the convex hull is just one type of alpha shape, and the full family of alpha shapes can be derived from the Delaunay triangulation of a given point set.

```
rng(4)
x = rand(20,1);
y = rand(20,1);
plot(x,y,'r.','MarkerSize',20)
hold on
shp = alphaShape(x,y,100);
plot(shp)
title('Convex Alpha Shape')
hold off
```



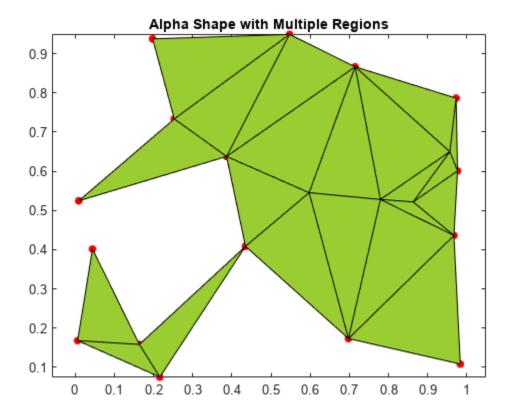
Unlike the convex hull, alpha shapes have a parameter that controls the level of detail, or how tightly the boundary fits around the point set. The parameter is called *alpha* or the *alpha radius*. Varying the alpha radius from 0 to Inf produces a set of different alpha shapes unique for that point set.

```
plot(x,y,'r.','MarkerSize',20)
hold on
shp = alphaShape(x,y,.5);
plot(shp)
title('Nonconvex Alpha Shape')
hold off
```



Varying the alpha radius can sometimes result in an alpha shape with multiple regions, which might or might not contain holes. However, the alphaShape function in MATLAB® always returns regularized alpha shapes, which prevents isolated or dangling points, edges, or faces.

```
plot(x,y,'r.','MarkerSize',20)
hold on
shp = alphaShape(x,y);
plot(shp)
title('Alpha Shape with Multiple Regions')
hold off
```



See Also convhull | alphaShape

More About

- "Using the delaunayTriangulation Class" on page 7-20
- "Triangulation Matrix Format" on page 7-3

Computing the Convex Hull

In this section...

"Computing the Convex Hull Using convhull and convhulln" on page 7-71

"Convex Hull Computation Using the delaunayTriangulation Class" on page 7-74

"Convex Hull Computation Using alphaShape" on page 7-75

MATLAB provides several ways to compute the convex hull:

- Using the MATLAB functions convhull and convhulln
- Using the convexHull method provided by the delaunayTriangulation class
- Using the alphaShape function with an alpha radius of Inf.

The convhull function supports the computation of convex hulls in 2-D and 3-D. The convhull function supports the computation of convex hulls in N-D ($N \ge 2$). The convhull function is recommended for 2-D or 3-D computations due to better robustness and performance.

The delaunayTriangulation class supports 2-D or 3-D computation of the convex hull from the Delaunay triangulation. This computation is not as efficient as the dedicated convhull and convhulln functions. However, if you have a delaunayTriangulation of a point set and require the convex hull, the convexHull method can compute the convex hull more efficiently from the existing triangulation.

The alphaShape function also supports the 2-D or 3-D computation of the convex hull by setting the alpha radius input parameter to Inf. Like delaunayTriangulation, however, computing the convex hull using alphaShape is less efficient than using convhull or convhulln directly. The exception is when you are working with a previously created alpha shape object.

Computing the Convex Hull Using convhull and convhulln

The convhull and convhulln functions take a set of points and output the indices of the points that lie on the boundary of the convex hull. The point index-based representation of the convex hull supports plotting and convenient data access. The following examples illustrate the computation and representation of the convex hull.

The first example uses a 2-D point set from the seamount dataset as input to the convhull function.

Load the data.

load seamount

Compute the convex hull of the point set.

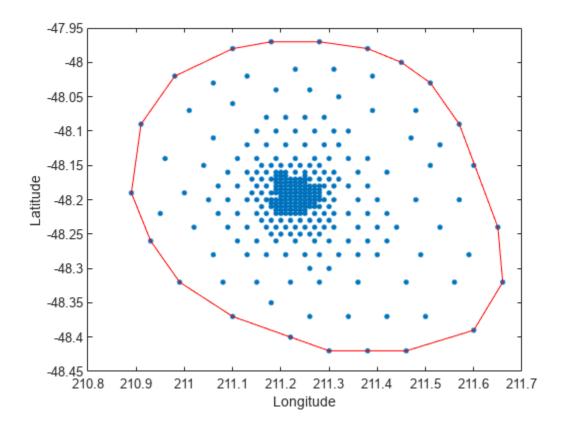
```
K = convhull(x,y);
```

K represents the indices of the points arranged in a counter-clockwise cycle around the convex hull.

Plot the data and its convex hull.

```
plot(x,y,'.','markersize',12)
xlabel('Longitude')
```

```
ylabel('Latitude')
hold on
plot(x(K),y(K),'r')
```



Add point labels to the points on the convex hull to observe the structure of K.

```
[K,A] = convhull(x,y);
```

convhull can compute the convex hull of both 2-D and 3-D point sets. You can reuse the seamount dataset to illustrate the computation of the 3-D convex hull.

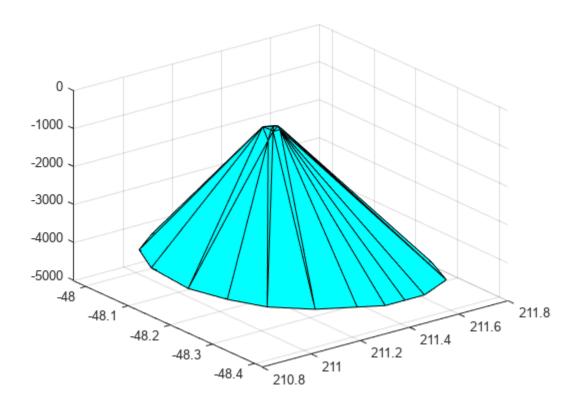
Include the seamount z-coordinate data elevations.

```
close(gcf)
K = convhull(x,y,z);
```

In 3-D the boundary of the convex hull, K, is represented by a triangulation. This is a set of triangular facets in matrix format that is indexed with respect to the point array. Each row of the matrix K represents a triangle.

Since the boundary of the convex hull is represented as a triangulation, you can use the triangulation plotting function trisurf.

```
trisurf(K,x,y,z,'Facecolor','cyan')
```



The volume bounded by the 3-D convex hull can optionally be returned by convhull, the syntax is as follows.

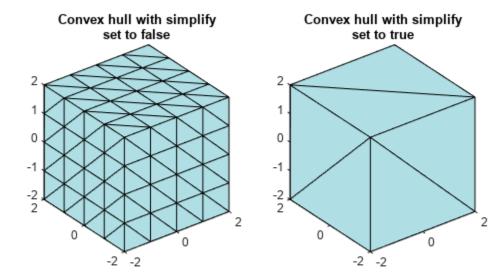
```
[K,V] = convhull(x,y,z);
```

The convhull function also provides the option of simplifying the representation of the convex hull by removing vertices that do not contribute to the area or volume. For example, if boundary facets of the convex hull are collinear or coplanar, you can merge them to give a more concise representation. The following example illustrates use of this option.

```
[x,y,z] = meshgrid(-2:1:2,-2:1:2,-2:1:2);
x = x(:);
y = y(:);
z = z(:);

K1 = convhull(x,y,z);
subplot(1,2,1)
defaultFaceColor = [0.6875 0.8750 0.8984];
trisurf(K1,x,y,z,'Facecolor',defaultFaceColor)
axis equal
title(sprintf('Convex hull with simplify\nset to false'))

K2 = convhull(x,y,z,'simplify',true);
subplot(1,2,2)
trisurf(K2,x,y,z,'Facecolor',defaultFaceColor)
axis equal
title(sprintf('Convex hull with simplify\nset to true'))
```



MATLAB provides the convhulln function to support the computation of convex hulls and hypervolumes in higher dimensions. Though convhulln supports N-D, problems in more than 10 dimensions present challenges due to the rapidly growing memory requirements.

The convhull function is superior to convhulln in 2-D and 3-D as it is more robust and gives better performance.

Convex Hull Computation Using the delaunay Triangulation Class

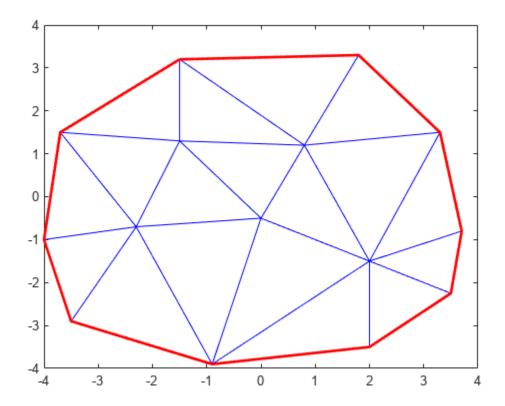
This example shows the relationship between a Delaunay triangulation of a set of points in 2-D and the convex hull of that set of points.

The delaunayTriangulation class supports computation of Delaunay triangulations in 2-D and 3-D space. This class also provides a convexHull method to derive the convex hull from the triangulation.

Create a Delaunay triangulation of a set of points in 2-D.

Plot the triangulation and highlight the edges that are shared only by a single triangle reveals the convex hull.

```
triplot(dt)
fe = freeBoundary(dt)';
hold on
plot(X(fe,1), X(fe,2), '-r', 'LineWidth',2)
hold off
```



In 3-D, the facets of the triangulation that are shared only by one tetrahedron represent the boundary of the convex hull.

The dedicated convhull function is generally more efficient than a computation based on the convexHull method. However, the triangulation based approach is appropriate if:

- You have a delaunayTriangulation of the point set already and the convex hull is also required.
- You need to add or remove points from the set incrementally and need to recompute the convex hull frequently after you have edited the points.

Convex Hull Computation Using alphaShape

This example shows how to compute the convex hull of a 2-D point set using the alphaShape function.

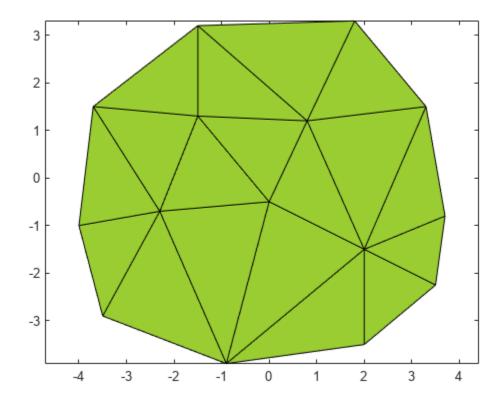
alphaShape computes a regularized alpha shape from a set of 2-D or 3-D points. You can specify the alpha radius, which determines how tightly or loosely the alpha shape envelops the point set. When the alpha radius is set to Inf, the resulting alpha shape is the convex hull of the point set.

Create a set of 2-D points.

```
X = [-1.5 \ 3.2; \ 1.8 \ 3.3; \ -3.7 \ 1.5; \ -1.5 \ 1.3; \ 0.8 \ 1.2; \ \dots \ 3.3 \ 1.5; \ -4.0 \ -1.0; \ -2.3 \ -0.7; \ 0 \ -0.5; \ 2.0 \ -1.5; \ \dots \ 3.7 \ -0.8; \ -3.5 \ -2.9; \ -0.9 \ -3.9; \ 2.0 \ -3.5; \ 3.5 \ -2.25];
```

Compute and plot the convex hull of the point set using an alpha shape with alpha radius equal to Inf.

```
shp = alphaShape(X,Inf);
plot(shp)
```



See Also

convhull | convhulln | convexHull | delaunayTriangulation | alphaShape

Related Examples

• "Working with Delaunay Triangulations" on page 7-14

Interpolation

- "Gridded and Scattered Sample Data" on page 8-2
- "Interpolating Gridded Data" on page 8-5
- "Interpolation of Multiple 1-D Value Sets" on page 8-13
- "Interpolation of 2-D Selections in 3-D Grids" on page 8-15
- "Interpolating Scattered Data" on page 8-17
- "Interpolation Using a Specific Delaunay Triangulation" on page 8-41
- "Extrapolating Scattered Data" on page 8-44
- "Normalize Data with Differing Magnitudes" on page 8-50
- "Resample Image with Gridded Interpolation" on page 8-53

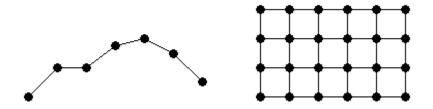
Gridded and Scattered Sample Data

Interpolation is a method to estimate the value of a function at a query location that lies within the domain of a set of sample data points. The function value is calculated based on the sample data points that are closest to the query point. MATLAB can perform two kinds of interpolation depending on the structure of the sample data. The sample data can form a grid, or can be scattered.

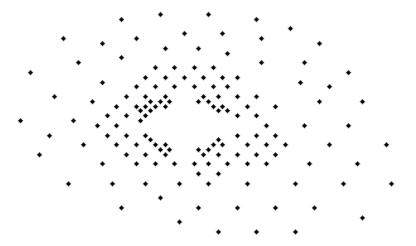
Gridded sample data makes interpolation more efficient, because the organized structure of the data makes it easy for MATLAB to find the sample data points closest to the query point. However, interpolating scattered data requires a "Delaunay Triangulation" of the data points, and this introduces an extra layer of computation. Therefore, if your data can be approximated as a grid, gridded interpolation provides substantial savings in computation time and memory usage compared to scattered interpolation.

The two approaches to interpolation are covered in the following topics:

• "Interpolating Gridded Data" on page 8-5 covers 1-D interpolation, and the N-D interpolation of sample data that is in axis-aligned grid format:



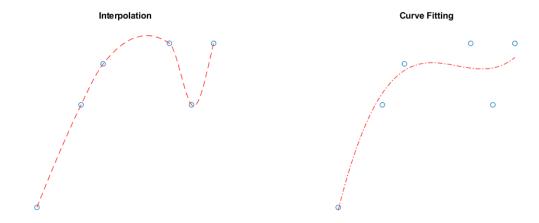
• "Interpolating Scattered Data" on page 8-17 covers the N-D interpolation of scattered data:



Interpolation versus Curve Fitting

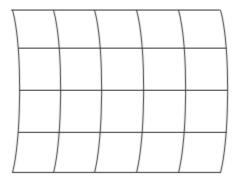
The interpolation methods available in MATLAB create interpolating functions that pass through the sample data points. That is, if you query the interpolation function at a sample location, you get back the exact sample data value and not an approximation. By contrast, curve and surface fitting

algorithms do not necessarily pass through the sample data points. For more information about curve fitting, see Curve Fitting Toolbox.

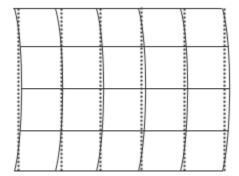


Grid Approximation Techniques

In some cases, you may need to approximate a grid for your data. For example, a grid can have points that lie along curved lines. A data set like this might occur if your data is longitude and latitude based:



With a curved grid, you are effectively dealing with a set of scattered data and must use more computationally expensive scattered interpolation functions to interpolate the values. However, although the input data cannot be gridded directly, it is sometimes feasible to approximate the curved grid with straight grid lines at appropriate intervals:



You can create an approximate grid by creating a set of grid vectors with appropriate spacing. Approximating a curved grid with straight lines allows you to get the performance benefits of grid-based interpolation, at the cost of slightly distorting the data. For more information about creating grid vectors, see "Grid Representations" on page 8-5.

See Also

griddedInterpolant|scatteredInterpolant

Related Examples

- "Interpolating Gridded Data" on page 8-5
- "Interpolating Scattered Data" on page 8-17

Interpolating Gridded Data

Gridded data consists of values or measurements at regularly spaced points that form a grid. Gridded data arises in many areas, such as meteorology, surveying, and medical imaging. In these areas, it is common to take measurements at regular spatial intervals, possibly over time. These ordered grids of data can range from 1-D (for simple time series) to 4-D (for measuring volumes over time) or higher. Some examples of gridded data are:

- 1-D: Stock prices over time
- 2-D: Temperature of a surface
- 3-D: MRI image of a brain
- 4-D: Ocean measurements in a volume of water over time

In all of these applications, grid-based interpolation efficiently extends the usefulness of the data to points where no measurement was taken. For example, if you have hourly price data for a stock, you can use interpolation to approximate the price every 15 minutes.

MATLAB Gridded Interpolation Functions

MATLAB provides several tools for grid-based interpolation:

Grid Creation Functions

The meshgrid and ndgrid functions create grids of various dimensionality. meshgrid can create 2-D or 3-D grids, while ndgrid can create grids with any number of dimensions. These functions return grids using different output formats. You can convert between these grid formats using the pagetranspose (as of R2020b) or permute functions to swap the first two dimensions of the grid.

Interpolation Functions

The interp family of functions includes interp1, interp2, interp3, and interpn. Each function is designed to interpolate data with a specific number of dimensions. interp2 and interp3 use grids in meshgrid format, while interpn uses grids in ndgrid format.

Interpolation Objects

griddedInterpolant objects support interpolation in any number of dimensions for data in ndgrid format. These objects also support multivalued interpolation (as of R2021a), where each grid point can have multiple values associated with it.

There are memory and performance benefits to using <code>griddedInterpolant</code> objects over the <code>interp</code> functions. <code>griddedInterpolant</code> offers substantial performance improvements for repeated queries of the interpolant object, whereas the <code>interp</code> functions perform a new calculation each time they are called. Also, <code>griddedInterpolant</code> stores the sample points in a memory-efficient format (as a compact grid on page 8-6) and is multithreaded to take advantage of multicore computer processors.

Grid Representations

MATLAB allows you to represent a grid in one of three representations: full grid, compact grid, or default grid. The default grid and compact grid are used primarily for convenience and improved efficiency, respectively.

Full Grid

A full grid is one in which all points are explicitly defined. The outputs of ndgrid and meshgrid define a full grid. You can create full grids that are uniform, in which points in each dimension have equal spacing, or nonuniform, in which the spacing varies in one or more of the dimensions. Uniform grids can have different spacing in each dimension, as long as the spacing is constant within each dimension.

Uniform	Uniform	Nonuniform

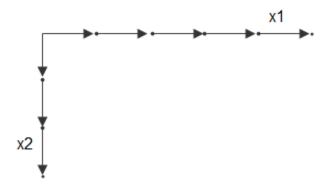
An example of a uniform full grid is:

```
[X,Y] = meshgrid([1 2 3],[3 6 9 12])
X =
     1
            2
                  3
     1
            2
     1
Y =
     3
            3
                  3
            6
     6
     9
            9
                  9
    12
           12
                 12
```

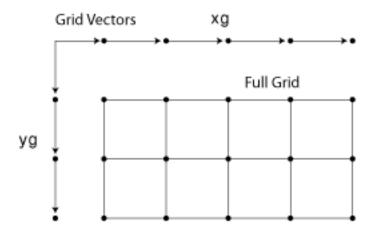
Compact Grid

Explicitly defining every point in a grid can consume a lot of memory when you are dealing with large grids. The compact grid representation is a way to dispense with the memory overhead of a full grid. The compact grid representation stores only grid vectors (one for each dimension) instead of the full grid. Together, the grid vectors implicitly define the grid. In fact, the inputs for meshgrid and ndgrid are grid vectors, and these functions replicate the grid vectors to form the full grid. The compact grid representation enables you to bypass grid creation and supply the grid vectors directly to the interpolation function.

For example, consider two vectors, x1 = 1:3 and x2 = 1:5. You can think of these vectors as a set of coordinates in the x1 direction and a set of coordinates in the x2 direction, like so:



Each arrow points to a location. You can use these two vectors to define a set of grid points, where one set of coordinates is given by x1 and the other set of coordinates is given by x2. When the grid vectors are replicated, they form two coordinate arrays that make up the full grid:



Your input grid vectors might be monotonic or nonmonotonic. Monotonic vectors contain values that either increase in that dimension or decrease in that dimension. Conversely, nonmonotonic vectors contain values that fluctuate. If the input grid vector is nonmonotonic, such as $[2\ 4\ 6\ 3\ 1]$, then $[X1,X2] = ndgrid([2\ 4\ 6\ 3\ 1])$ outputs a nonmonotonic grid. Your grid vectors should be monotonic if you intend to pass the grid to other MATLAB functions. The sort function is useful to ensure monotonicity.

Default Grid

In some applications, only the values at the grid points are important and not the distances between grid points. For example, most MRI scans gather data that is uniformly spaced in all directions. In cases like this, you can allow the interpolation function to automatically generate a default grid representation to use with the data. To do this, leave out the grid inputs to the interpolation function. When you leave out the grid inputs, the function automatically considers the data to be on a unit-spaced grid. The function creates this unit-spaced grid while it executes, saving you the trouble of creating a grid yourself.

Example: Temperature Interpolation on 2-D Grid

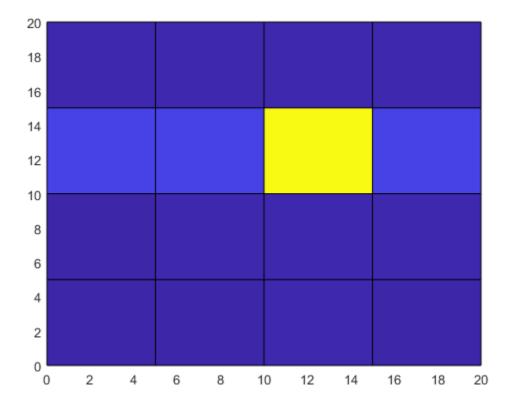
Consider temperature data collected on a surface at regular 5 cm intervals, extending 20 cm in each direction. Use meshgrid to create the full grid.

```
[X,Y] = meshgrid(0:5:20)
X =
             5
     0
                   10
                          15
                                 20
     0
             5
                   10
                          15
                                 20
     0
             5
                   10
                          15
                                 20
     0
             5
                   10
                          15
                                 20
     0
             5
                   10
                          15
                                 20
Y =
     0
             0
                    0
                           0
                                  0
     5
             5
                    5
                           5
                                  5
    10
            10
                   10
                          10
                                 10
    15
            15
                   15
                          15
                                 15
    20
           20
                   20
                          20
                                 20
```

The (x,y) coordinates of each grid point are represented as corresponding elements in the X and Y matrices. The first grid point is given by $[X(1) \ Y(1)]$, which is $[0 \ 0]$, the next grid point is given by $[X(2) \ Y(2)]$, which is $[0 \ 5]$, and so on.

Now, create a matrix to represent temperature measurements on the grid and then plot the data as a surface.

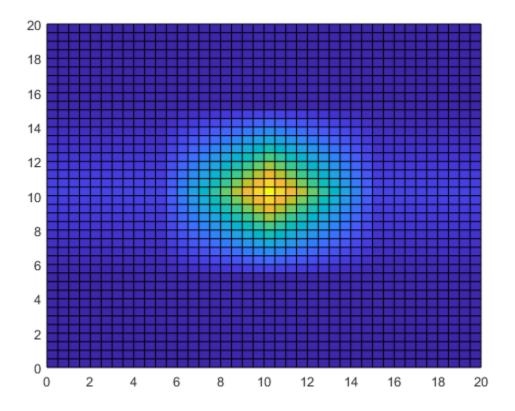
```
T = [1]
         1
             10
                  1
                      1;
     1
         10
             10
                  10
                      10;
     100 100 1000 100 100;
                  10 1;
     10
        10
             10
     1
             10
                  1
                      1];
         1
surf(X,Y,T)
view(2)
```



Although the temperature at the center grid point is large, its location and influence on surrounding grid points is not apparent from the raw data.

To improve the resolution of the data by a factor of 10, use interp2 to interpolate the temperature data onto a finer grid that uses 0.5 cm intervals. Use meshgrid again to create a finer grid represented by the matrices Xq and Yq. Then, use interp2 with the original grid, the temperature data, and the new grid points, and plot the resulting data. By default, interp2 uses linear interpolation in each dimension.

```
[Xq,Yq] = meshgrid(0:0.5:20);
Tq = interp2(X,Y,T,Xq,Yq);
surf(Xq,Yq,Tq)
view(2)
```



Interpolating the temperature data adds detail to the image and greatly improves the usefulness of the data within the area of measurements.

Gridded Interpolation Methods

The grid-based interpolation functions and objects in MATLAB offer several different methods for interpolation. When choosing an interpolation method, keep in mind that some require more memory or longer computation time than others. You may need to trade off these resources to achieve the desired smoothness in the result. The following table gives a preview of each interpolation method applied to the same 1-D data, and also provides an overview of the benefits, trade-offs, and requirements for each method.

Method	Description
Nearest Neighbor	The interpolated value at a query point is the value at the nearest sample grid point. Discontinuous Modest memory requirements Fastest computation time Requires 2 grid points in each dimension

Method	Description
Next Neighbor	The interpolated value at a query point is the value at the next sample grid point.
P P P P P P P P P P P P P P P P P P P	Discontinuous
	Same memory requirements and computation time as nearest neighbor
φ	Available for 1-D interpolation only
<u>_</u>	Requires at least 2 grid points
Previous Neighbor	The interpolated value at a query point is the value at the previous sample grid point.
g of the second	Discontinuous
م م	Same memory requirements and computation time as nearest neighbor
م م	Available for 1-D interpolation only
هي ا	Requires at least 2 grid points
Linear	The interpolated value at a query point is based on linear interpolation of the values at neighboring grid points in each respective dimension.
/ \ _ 9	C0 continuous
of god	Requires more memory and computation time than nearest neighbor
	Requires at least 2 grid points in each dimension
PChip	The interpolated value at a query point is based on a shape-preserving piece-wise cubic interpolation of the values at neighboring grid points.
9	C1 continuous
ad a sad	Requires more memory and computation time than linear
	Available for 1-D interpolation only
	Requires at least 4 grid points

Method	Description
Cubic	The interpolated value at a query point is based on cubic interpolation of the values at neighboring grid points in each respective dimension.
9	C1 continuous
	Requires more memory and computation time than linear
	Grid must have uniform spacing, though the spacing in each dimension does not have to be the same
	Requires at least 4 points in each dimension
Modified Akima	The interpolated value at a query point is based on a piecewise function of polynomials with degree at most three evaluated using the values of neighboring grid points in each respective dimension. The Akima formula is modified to avoid overshoots.
	C1 continuous
	Similar memory requirements as spline
	Requires more computation time than cubic, but typically less than spline
	Requires at least 2 grid points in each dimension
Spline	The interpolated value at a query point is based on a cubic interpolation of the values at neighboring grid points in each respective dimension.
/ \ ~ ?	C2 continuous
	Requires more memory and computation time than cubic
%	Requires at least 4 points in each dimension

See Also

 $\verb|interp1|| \verb|interp2|| \verb|interp3|| \verb|interpn|| \verb|griddedInterpolant||$

Related Examples

- "Resample Image with Gridded Interpolation" on page 8-53
- "Interpolation of Multiple 1-D Value Sets" on page 8-13
- "Interpolation of 2-D Selections in 3-D Grids" on page 8-15

Interpolation of Multiple 1-D Value Sets

This example shows how to interpolate three 1-D data sets in a single pass using <code>griddedInterpolant</code>. This is a faster alternative to looping over your data sets.

Define the *x*-coordinates that are common to all value sets.

```
x = (1:5)';
```

Define the sets of sample points along the columns of matrix V.

Create the interpolant F by passing the sample points and sample values to <code>griddedInterpolant</code>. With this setup, <code>griddedInterpolant</code> interprets V as containing three different 1-D data sets defined at the same x-values.

```
F = griddedInterpolant(x,V);
```

Create a vector of query points with 0.5 spacing.

```
qx = 1:0.5:5;
```

Evaluate the interpolant at the *x*-coordinates for each value set.

```
Vq = F(qx)
Vq = 9 \times 3
   1.0000
              2.0000
                        3.0000
   1.5000
             3.0000
                        4.5000
                        6.0000
   2.0000
             4.0000
   2.5000
              5.0000
                        7.5000
   3.0000
                       9.0000
              6.0000
   3.5000
             7.0000
                      10.5000
                       12.0000
   4.0000
             8.0000
   4.5000
                       13.5000
             9.0000
   5.0000
             10.0000
                       15.0000
```

See Also

griddedInterpolant

Related Examples

- "Interpolating Gridded Data" on page 8-5
- "Resample Image with Gridded Interpolation" on page 8-53

Interpolation of 2-D Selections in 3-D Grids

This example shows how to reduce the dimensionality of the grid plane arrays in 3-D to solve a 2-D interpolation problem.

In some application areas, it might be necessary to interpolate a lower dimensional plane of a grid; for example, interpolating a plane of a 3-D grid. When you extract the grid plane from the 3-D grid, the resulting arrays might be in 3-D format. You can use the squeeze function to reduce the dimensionality of the grid plane arrays to solve the problem in 2-D.

Create a 3-D sample grid and corresponding values.

```
[X,Y,Z] = ndgrid(1:5);
V = X.^2 + Y.^2 +Z;
```

Select a 2-D sample from the grid. In this case, the third column of samples.

```
x = X(:,3,:);

z = Z(:,3,:);

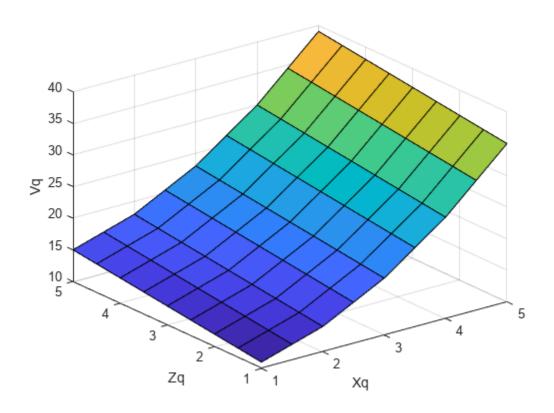
v = V(:,3,:);
```

zlabel('Vq');

The 2-D plane occurs at Y=3, so the Y dimension has been fixed. x, z, and v are 5-by-1-by-5 arrays. You must reduce them to 2-D arrays before evaluating the interpolant.

Reduce x, z, and v down to 2-D arrays using the squeeze function.

```
x = squeeze(x);
z = squeeze(z);
v = squeeze(v);
Interpolate the 2-D slice over a finer grid of query points.
[Xq,Zq] = ndgrid(1:0.5:5);
Vq = interpn(x,z,v,Xq,Zq);
Plot the results.
figure
surf(Xq,Zq,Vq);
xlabel('Xq');
ylabel('Zq');
```



See Also

interpn|squeeze

More About

- "Interpolating Gridded Data" on page 8-5
- "Interpolation of Multiple 1-D Value Sets" on page 8-13

Interpolating Scattered Data

```
"Scattered Data" on page 8-17

"Interpolating Scattered Data Using griddata and griddatan" on page 8-20

"scatteredInterpolant Class" on page 8-22

"Interpolating Scattered Data Using the scatteredInterpolant Class" on page 8-23

"Interpolation of Complex Scattered Data" on page 8-30

"Addressing Problems in Scattered Data Interpolation" on page 8-32
```

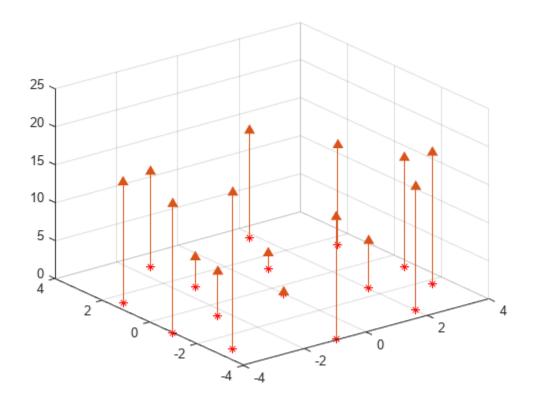
Scattered Data

Scattered data consists of a set of points X and corresponding values V, where the points have no structure or order between their relative locations. There are various approaches to interpolating scattered data. One widely used approach uses a Delaunay triangulation of the points.

This example shows how to construct an interpolating surface by triangulating the points and lifting the vertices by a magnitude V into a dimension orthogonal to X.

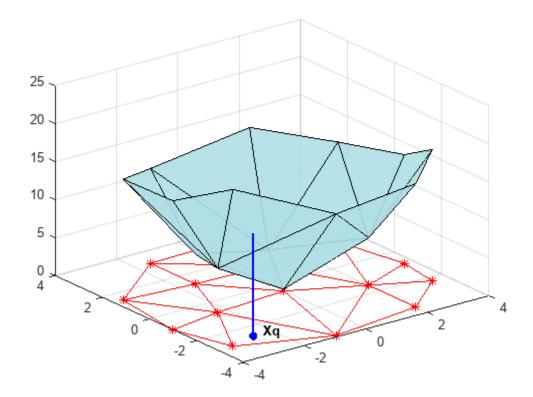
There are variations on how you can apply this approach. In this example, the interpolation is broken down into separate steps; typically, the overall interpolation process is accomplished with one function call.

Create a scattered data set on the surface of a paraboloid.



Create a Delaunay triangulation, lift the vertices, and evaluate the interpolant at the query point Xq.

```
figure('Color', 'white')
t = delaunay(X(:,1),X(:,2));
hold on
trimesh(t,X(:,1),X(:,2), zeros(15,1), ...
'EdgeColor','r', 'FaceColor','none')
defaultFaceColor = [0.6875 0.8750 0.8984];
trisurf(t,X(:,1),X(:,2), V, 'FaceColor', ...
     defaultFaceColor, 'FaceAlpha',0.9);
plot3(X(:,1),X(:,2),zeros(15,1), '*r')
axis([-4, 4, -4, 4, 0, 25]);
plot3(-2.6,-2.6,0,'*b','LineWidth', 1.6)
plot3([-2.6 -2.6]',[-2.6 -2.6]',[0 13.52]','-b','LineWidth',1.6)
hold off
view(322.5, 30);
text(-2.0, -2.6, 'Xq', 'FontWeight', 'bold', ...
'HorizontalAlignment','center', 'BackgroundColor', 'none');
```



This step generally involves traversing of the triangulation data structure to find the triangle that encloses the query point. Once you find the point, the subsequent steps to compute the value depend on the interpolation method. You could compute the nearest point in the neighborhood and use the value at that point (the nearest-neighbor interpolation method). You could also compute the weighted sum of values of the three vertices of the enclosing triangle (the linear interpolation method). These methods and their variants are covered in texts and references on scattered data interpolation.

Though the illustration highlights 2-D interpolation, you can apply this technique to higher dimensions. In more general terms, given a set of points X and corresponding values V, you can construct an interpolant of the form V = F(X). You can evaluate the interpolant at a query point Xq, to give Vq = F(Xq). This is a single-valued function; for any query point Xq within the convex hull of X, it will produce a unique value Vq. The sample data is assumed to respect this property in order to produce a satisfactory interpolation.

MATLAB provides two ways to perform triangulation-based scattered data interpolation:

- The functions griddata and griddatan
- The scatteredInterpolant class

The griddata function supports 2-D scattered data interpolation. The griddatan function supports scattered data interpolation in N-D; however, it is not practical in dimensions higher than 6-D for moderate to large point sets, due to the exponential growth in memory required by the underlying triangulation.

The scatteredInterpolant class supports scattered data interpolation in 2-D and 3-D space. Use of this class is encouraged as it is more efficient and readily adapts to a wider range of interpolation problems.

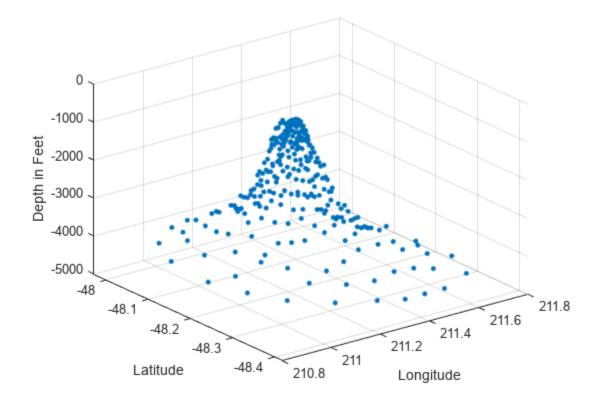
Interpolating Scattered Data Using griddata and griddatan

The griddata and griddatan functions take a set of sample points, X, corresponding values, V, and query points, Xq, and return the interpolated values, Vq. The calling syntax is similar for each function; the primary distinction is the 2-D / 3-D griddata function lets you define the points in terms of X, Y / X, Y, Z coordinates. These two functions interpolate scattered data at predefined gridpoint locations; the intent is to produce gridded data, hence the name. Interpolation is more general in practice. You might want to query at arbitrary locations within the convex hull of the points.

This example shows how the griddata function interpolates scattered data at a set of grid points and uses this gridded data to create a contour plot.

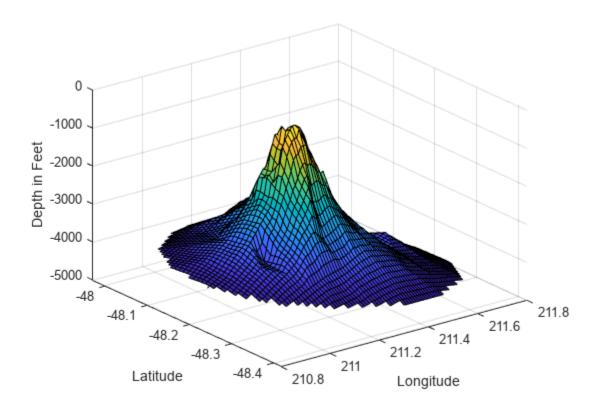
Plot the seamount data set (a *seamount* is an underwater mountain). The data set consists of a set of longitude (x) and latitude (y) locations, and corresponding seamount elevations (z) measured at those coordinates.

```
load seamount
plot3(x,y,z,'.','markersize',12)
xlabel('Longitude')
ylabel('Latitude')
zlabel('Depth in Feet')
grid on
```



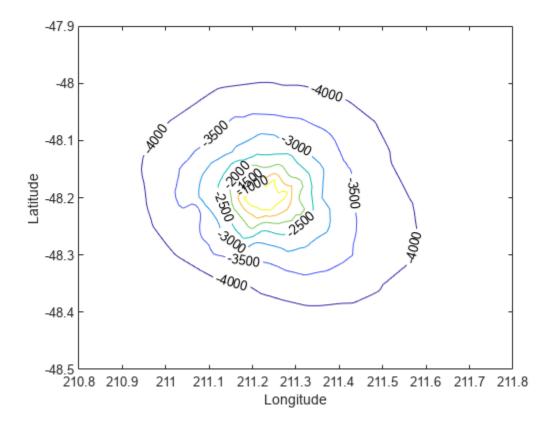
Use meshgrid to create a set of 2-D grid points in the longitude-latitude plane and then use griddata to interpolate the corresponding depth at those points.

```
figure
[xi,yi] = meshgrid(210.8:0.01:211.8, -48.5:0.01:-47.9);
zi = griddata(x,y,z,xi,yi);
surf(xi,yi,zi);
xlabel('Longitude')
ylabel('Latitude')
zlabel('Depth in Feet')
```



Now that the data is in a gridded format, compute and plot the contours.

```
figure
[c,h] = contour(xi,yi,zi);
clabel(c,h);
xlabel('Longitude')
ylabel('Latitude')
```



You can also use griddata to interpolate at arbitrary locations within the convex hull of the dataset. For example, the depth at coordinates (211.3, -48.2) is given by:

```
zi = griddata(x,y,z, 211.3, -48.2);
```

The underlying triangulation is computed each time the <code>griddata</code> function is called. This can impact performance if the same data set is interpolated repeatedly with different query points. The <code>scatteredInterpolant</code> class described in "Interpolating Scattered Data Using the scatteredInterpolant Class" on page 8-23 is more efficient in this respect.

MATLAB software also provides griddatan to support interpolation in higher dimensions. The calling syntax is similar to griddata.

scatteredInterpolant Class

The griddata function is useful when you need to interpolate to find the values at a set of predefined grid-point locations. In practice, interpolation problems are often more general, and the scatteredInterpolant class provides greater flexibility. The class has the following advantages:

- It produces an interpolating function that can be queried efficiently. That is, the underlying triangulation is created once and reused for subsequent queries.
- The interpolation method can be changed independently of the triangulation.
- The values at the data points can be changed independently of the triangulation.

- Data points can be incrementally added to the existing interpolant without triggering a complete recomputation. Data points can also be removed and moved efficiently, provided the number of points edited is small relative to the total number of sample points.
- It provides extrapolation functionality for approximating values at points that fall outside the convex hull. See "Extrapolating Scattered Data" on page 8-44 for more information.

scatteredInterpolant provides the following interpolation methods:

- 'nearest' Nearest-neighbor interpolation, where the interpolating surface is discontinuous.
- 'linear' Linear interpolation (default), where the interpolating surface is C0 continuous.
- 'natural' Natural-neighbor interpolation, where the interpolating surface is C1 continuous except at the sample points.

The scatteredInterpolant class supports scattered data interpolation in 2-D and 3-D space. You can create the interpolant by calling scatteredInterpolant and passing the point locations and corresponding values, and optionally the interpolation and extrapolation methods. See the scatteredInterpolant reference page for more information about the syntaxes you can use to create and evaluate a scatteredInterpolant.

Interpolating Scattered Data Using the scatteredInterpolant Class

This example shows how to use scatteredInterpolant to interpolate a scattered sampling of the peaks function.

Create the scattered data set.

rng default;

The Points property represents the coordinates of the data points, and the Values property represents the associated values. The Method property represents the interpolation method that performs the interpolation. The ExtrapolationMethod property represents the extrapolation method used when guery points fall outside the convex hull.

You can access the properties of F in the same way you access the fields of a struct. For example, use F.Points to examine the coordinates of the data points.

Evaluate the interpolant.

scatteredInterpolant provides subscripted evaluation of the interpolant. It is evaluated the same way as a function. You can evaluate the interpolant as follows. In this case, the value at the query location is given by Vq. You can evaluate at a single query point:

```
Vq = F([1.5 \ 1.25])
Vq = 1.4838
```

You can also pass individual coordinates:

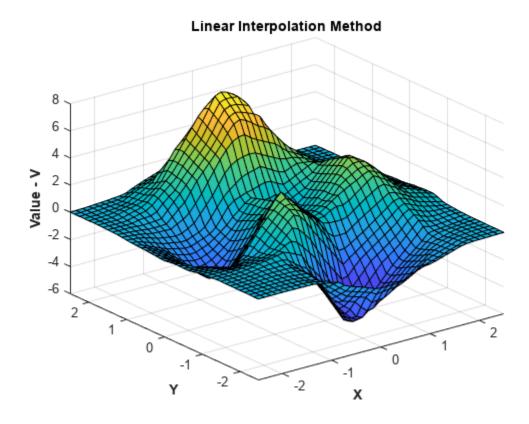
```
Vq = F(1.5, 1.25)
Vq = 1.4838
```

You can evaluate at a vector of point locations:

```
Xq = [0.5 0.25; 0.75 0.35; 1.25 0.85];
Vq = F(Xq)
Vq = 3×1
0.4057
1.2199
2.1639
```

You can evaluate F at grid point locations and plot the result.

```
[Xq,Yq] = meshgrid(-2.5:0.125:2.5);
Vq = F(Xq,Yq);
surf(Xq,Yq,Vq);
xlabel('X','fontweight','b'), ylabel('Y','fontweight','b');
zlabel('Value - V','fontweight','b');
title('Linear Interpolation Method','fontweight','b');
```



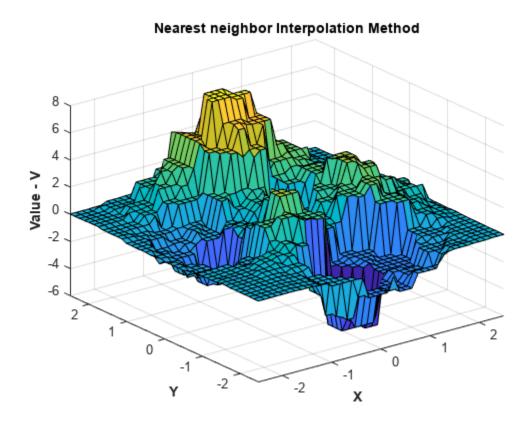
Change the interpolation method.

You can change the interpolation method on the fly. Set the method to 'nearest'.

```
F.Method = 'nearest';
```

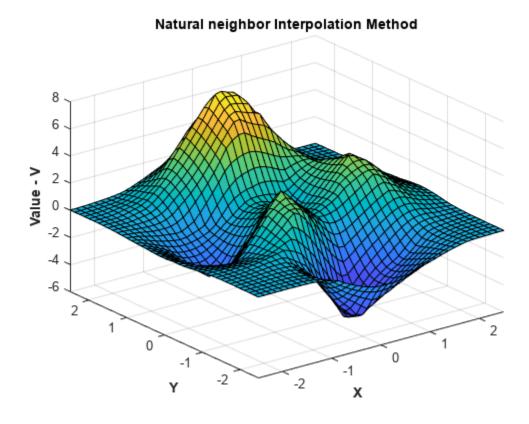
Reevaluate and plot the interpolant as before.

```
Vq = F(Xq,Yq);
figure
surf(Xq,Yq,Vq);
xlabel('X','fontweight','b'),ylabel('Y','fontweight','b')
zlabel('Value - V','fontweight','b')
title('Nearest neighbor Interpolation Method','fontweight','b');
```



Change the interpolation method to natural neighbor, reevaluate, and plot the results.

```
F.Method = 'natural';
Vq = F(Xq,Yq);
figure
surf(Xq,Yq,Vq);
xlabel('X','fontweight','b'),ylabel('Y','fontweight','b')
zlabel('Value - V','fontweight','b')
title('Natural neighbor Interpolation Method','fontweight','b');
```



Replace the values at the sample data locations.

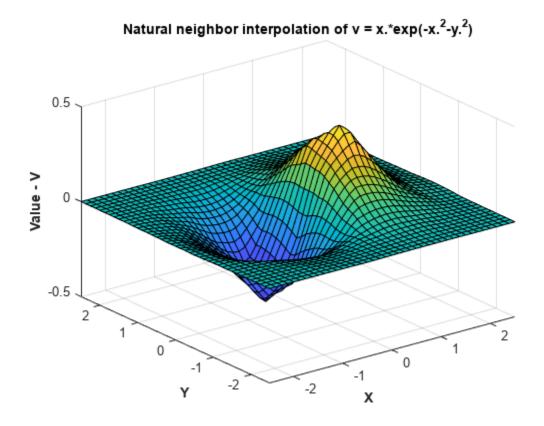
You can change the values V at the sample data locations, X, on the fly. This is useful in practice as some interpolation problems may have multiple sets of values at the same locations. For example, suppose you want to interpolate a 3-D velocity field that is defined by locations (x, y, z) and corresponding componentized velocity vectors (Vx, Vy, Vz). You can interpolate each of the velocity components by assigning them to the values property (V) in turn. This has important performance benefits, because it allows you to reuse the same interpolant without incurring the overhead of computing a new one each time.

The following steps show how to change the values in our example. You will compute the values using the expression, $v = xe^{-x^2 - y^2}$.

```
V = X(:,1).*exp(-X(:,1).^2-X(:,2).^2);
F.Values = V;
```

Evaluate the interpolant and plot the result.

```
Vq = F(Xq,Yq);
figure
surf(Xq,Yq,Vq);
xlabel('X','fontweight','b'), ylabel('Y','fontweight','b')
zlabel('Value - V','fontweight','b')
title('Natural neighbor interpolation of v = x.*exp(-x.^2-y.^2)')
```



Add additional point locations and values to the existing interpolant.

This performs an efficient update as opposed to a complete recomputation using the augmented data set.

When adding sample data, it is important to add both the point locations and the corresponding values.

Continuing the example, create new sample points as follows:

```
X = -1.5 + 3.*rand(100,2);

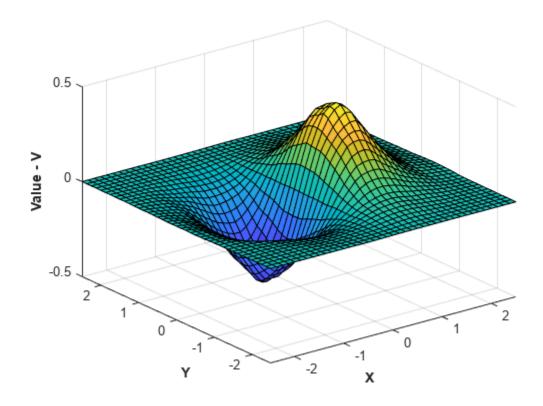
V = X(:,1).*exp(-X(:,1).^2-X(:,2).^2);
```

Add the new points and corresponding values to the triangulation.

```
F.Points(end+(1:100),:) = X;
F.Values(end+(1:100)) = V;
```

Evaluate the refined interpolant and plot the result.

```
Vq = F(Xq,Yq);
figure
surf(Xq,Yq,Vq);
xlabel('X','fontweight','b'), ylabel('Y','fontweight','b');
zlabel('Value - V','fontweight','b');
```



Remove data from the interpolant.

You can incrementally remove sample data points from the interpolant. You also can remove data points and corresponding values from the interpolant. This is useful for removing spurious outliers.

When removing sample data, it is important to remove both the point location and the corresponding value.

```
Remove the 25th point.

F.Points(25,:) = [];
F.Values(25) = [];

Remove points 5 to 15.

F.Points(5:15,:) = [];
F.Values(5:15) = [];

Retain 150 points and remove the rest.

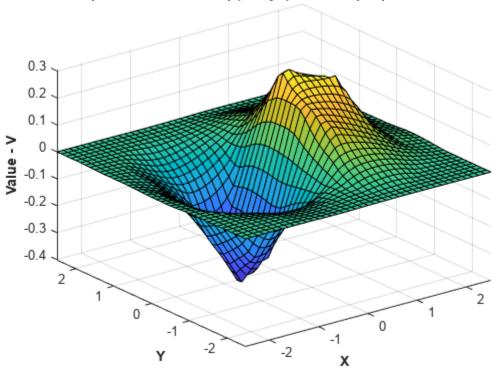
F.Points(150:end,:) = [];
F.Values(150:end) = [];

This creates a coarser surface when you evaluate and plot:

Vq = F(Xq,Yq);
figure
surf(Xq,Yq,Vq);
```

```
xlabel('X','fontweight','b'), ylabel('Y','fontweight','b');
zlabel('Value - V','fontweight','b');
title('Interpolation of v = x.*exp(-x.^2-y.^2) with sample points removed')
```

Interpolation of $v = x.*exp(-x.^2-y.^2)$ with sample points removed



Interpolation of Complex Scattered Data

This example shows how to interpolate scattered data when the value at each sample location is complex.

Create the sample data.

```
rng('default')
X = -3 + 6*rand([250 2]);
V = complex(X(:,1).*X(:,2), X(:,1).^2 + X(:,2).^2);
```

Create the interpolant.

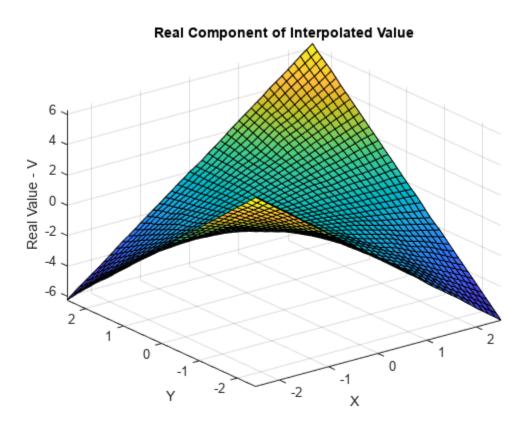
F = scatteredInterpolant(X,V);

Create a grid of query points and evaluate the interpolant at the grid points.

```
[Xq,Yq] = meshgrid(-2.5:0.125:2.5);
Vq = F(Xq,Yq);
```

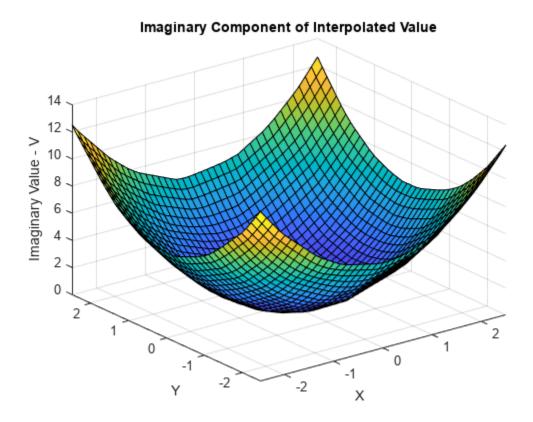
Plot the real component of Vq.

```
VqReal = real(Vq);
figure
surf(Xq,Yq,VqReal);
xlabel('X');
ylabel('Y');
zlabel('Real Value - V');
title('Real Component of Interpolated Value');
```



Plot the imaginary component of Vq.

```
VqImag = imag(Vq);
figure
surf(Xq,Yq,VqImag);
xlabel('X');
ylabel('Y');
zlabel('Imaginary Value - V');
title('Imaginary Component of Interpolated Value');
```



Addressing Problems in Scattered Data Interpolation

Many of the illustrative examples in the previous sections dealt with the interpolation of point sets that were sampled on smooth surfaces. In addition, the points were relatively uniformly spaced. For example, clusters of points were not separated by relatively large distances. In addition, the interpolant was evaluated well within the convex hull of the point locations.

When dealing with real-world interpolation problems the data may be more challenging. It may come from measuring equipment that is likely to produce inaccurate readings or outliers. The underlying data may not vary smoothly, the values may jump abruptly from point to point. This section provides you with some guidelines to identify and address problems with scattered data interpolation.

Input Data Containing NaNs

You should preprocess sample data that contains NaN values to remove the NaN values as this data cannot contribute to the interpolation. If a NaN is removed, the corresponding data values/ coordinates should also be removed to ensure consistency. If NaN values are present in the sample data, the constructor will error when called.

The following example illustrates how to remove NaNs.

Create some data and replace some entries with NaN:

```
x = rand(25,1)*4-2;

y = rand(25,1)*4-2;
```

```
x(5) = NaN; x(10) = NaN; y(12) = NaN; V(14) = NaN;
This code errors:
F = scatteredInterpolant(x,y,V);
Instead, find the sample point indices of the NaNs and then construct the interpolant:
nan flags = isnan(x) | isnan(y) | isnan(V);
x(nan flags) = [];
y(nan_flags) = [];
V(nan flags) = [];
F = scatteredInterpolant(x,y,V);
The following example is similar if the point locations are in matrix form. First, create data and
replace some entries with NaN values.
X = rand(25,2)*4-2;
V = X(:,1).^2 + X(:,2).^2;
X(5,1) = NaN; X(10,1) = NaN; X(12,2) = NaN; V(14) = NaN;
This code errors:
F = scatteredInterpolant(X,V);
Find the sample point indices of the NaN and then construct the interpolant:
nan flags = isnan(X(:,1)) \mid isnan(X(:,2)) \mid isnan(V);
X(nan flags,:) = [];
V(nan_flags) = [];
F = scatteredInterpolant(X,V);
```

Interpolant Outputs NaN Values

 $V = x.^2 + y.^2;$

griddata and griddatan return NaN values when you query points outside the convex hull using the 'linear' or 'natural' methods. However, you can expect numeric results if you query the same points using the 'nearest' method. This is because the nearest neighbor to a query point exists both inside and outside the convex hull.

If you want to compute approximate values outside the convex hull, you should use scatteredInterpolant. See "Extrapolating Scattered Data" on page 8-44 for more information.

Handling Duplicate Point Locations

Input data is rarely "perfect" and your application could have to handle duplicate data point locations. Two or more data points at the same location in your data set can have different corresponding values. In this scenario, scatteredInterpolant merges the points and computes the average of the corresponding values. This example shows how scatteredInterpolant performs an interpolation on a data set with duplicate points.

1 Create some sample data that lies on a planar surface:

```
x = rand(100,1)*6-3;

y = rand(100,1)*6-3;
```

V = x + y;

2 Introduce a duplicate point location by assigning the coordinates of point 50 to point 100:

```
x(50) = x(100);

y(50) = y(100);
```

3 Create the interpolant. Notice that F contains 99 unique data points:

```
F = scatteredInterpolant(x,y,V)
```

4 Check the value associated with the 50th point:

```
F.Values(50)
```

This value is the average of the original 50th and 100th value, as these two data points have the same location:

```
(V(50)+V(100))/2
```

In this scenario the interpolant resolves the ambiguity in a reasonable manner. However in some instances, data points can be close rather than coincident, and the values at those locations can be different.

In some interpolation problems, multiple sets of sample values might correspond to the same locations. For example, a set of values might be recorded at the same locations at different periods in time. For efficiency, you can interpolate one set of readings and then replace the values to interpolate the next set.

Always use consistent data management when replacing values in the presence of duplicate point locations. Suppose you have two sets of values associated with the 100 data point locations and you would like to interpolate each set in turn by replacing the values.

1 Consider two sets of values:

```
V1 = x + 4*y;

V2 = 3*x + 5*y
```

2 Create the interpolant. scatteredInterpolant merges the duplicate locations and the interpolant contains 99 unique sample points:

```
F = scatteredInterpolant(x,y,V1)
```

Replacing the values directly via F.Values = V2 means assigning 100 values to 99 samples. The context of the previous merge operation is lost; the number of sample locations will not match the number of sample values. The interpolant will require the inconsistency to be resolved to support queries.

In this more complex scenario, it is necessary to remove the duplicates prior to creating and editing the interpolant. Use the unique function to find the indices of the unique points. unique can also output arguments that identify the indices of the duplicate points.

```
[~, I, ~] = unique([x y],'first','rows');
I = sort(I);
x = x(I);
y = y(I);
```

```
V1 = V1(I);
V2 = V2(I);
F = scatteredInterpolant(x,y,V1)
```

Now you can use F to interpolate the first data set. Then you can replace the values to interpolate the second data set.

```
F. Values = V2:
```

Achieving Efficiency When Editing a scatteredInterpolant

scatteredInterpolant allows you to edit the properties representing the sample values (F.Values) and the interpolation method (F.Method). Since these properties are independent of the underlying triangulation, the edits can be performed efficiently. However, like working with a large array, you should take care not to accidentally create unnecessary copies when editing the data. Copies are made when more than one variable references an array and that array is then edited.

A copy is not made in the following:

```
A1 = magic(4)

A1(4,4) = 11
```

However, a copy is made in this scenario because the array is referenced by another variable. The arrays A1 and A2 can no longer share the same data once the edit is made:

```
A1 = magic(4)

A2 = A1

A1(4,4) = 32
```

Similarly, if you pass the array to a function and edit the array within that function, a deep copy may be made depending on how the data is managed. scatteredInterpolant contains data and it behaves like an array—in MATLAB language, it is called a value object. The MATLAB language is designed to give optimum performance when your application is structured into functions that reside in files. Prototyping at the command line may not yield the same level of performance.

The following example demonstrates this behavior, but it should be noted that performance gains in this example do not generalize to other functions in MATLAB.

This code does not produce optimal performance:

```
x = rand(1000000,1)*4-2;
y = rand(1000000,1)*4-2;
z = x.*exp(-x.^2-y.^2);
tic; F = scatteredInterpolant(x,y,z); toc
tic; F.Values = 2*z; toc
```

You can place the code in a function file to execute it more efficiently.

When MATLAB executes a program that is composed of functions that reside in files, it has a complete picture of the execution of the code; this allows MATLAB to optimize for performance. When you type the code at the command line, MATLAB cannot anticipate what you are going to type next, so it cannot perform the same level of optimization. Developing applications through the creation of reusable functions is general and recommended practice, and MATLAB will optimize the performance in this setting.

Interpolation Results Poor Near the Convex Hull

The Delaunay triangulation is well suited to scattered data interpolation problems because it has favorable geometric properties that produce good results. These properties are:

- The rejection of sliver-shaped triangles/tetrahedra in favor of more equilateral-shaped ones.
- The empty circumcircle property that implicitly defines a nearest-neighbor relation between the points.

The empty circumcircle property ensures the interpolated values are influenced by sample points in the neighborhood of the query location. Despite these qualities, in some situations the distribution of the data points may lead to poor results and this typically happens near the convex hull of the sample data set. When the interpolation produces unexpected results, a plot of the sample data and underlying triangulation can often provide insight into the problem.

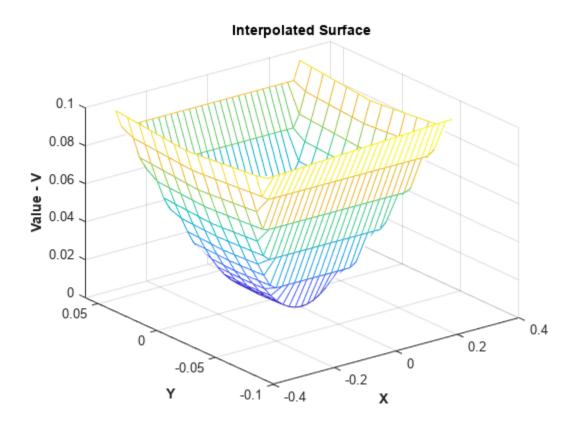
This example shows an interpolated surface that deteriorates near the boundary.

Create a sample data set that will exhibit problems near the boundary.

```
t = 0.4*pi:0.02:0.6*pi;
x1 = cos(t)';
y1 = sin(t)'-1.02;
x2 = x1;
y2 = y1*(-1);
x3 = linspace(-0.3,0.3,16)';
y3 = zeros(16,1);
x = [x1;x2;x3];
y = [y1;y2;y3];
```

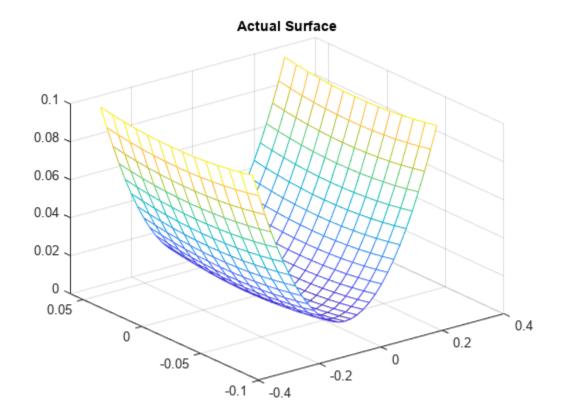
Now lift these sample points onto the surface $z = x^2 + y^2$ and interpolate the surface.

```
z = x.^2 + y.^2;
F = scatteredInterpolant(x,y,z);
[xi,yi] = meshgrid(-0.3:.02:0.3, -0.0688:0.01:0.0688);
zi = F(xi,yi);
mesh(xi,yi,zi)
xlabel('X','fontweight','b'), ylabel('Y','fontweight','b')
zlabel('Value - V','fontweight','b')
title('Interpolated Surface');
```



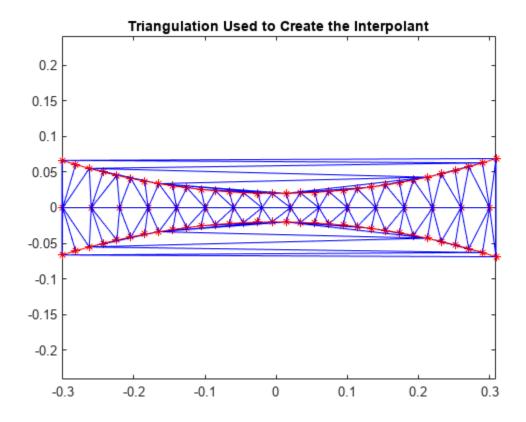
The actual surface is:

```
zi = xi.^2 + yi.^2;
figure
mesh(xi,yi,zi)
title('Actual Surface')
```



To understand why the interpolating surface deteriorates near the boundary, it is helpful to look at the underlying triangulation:

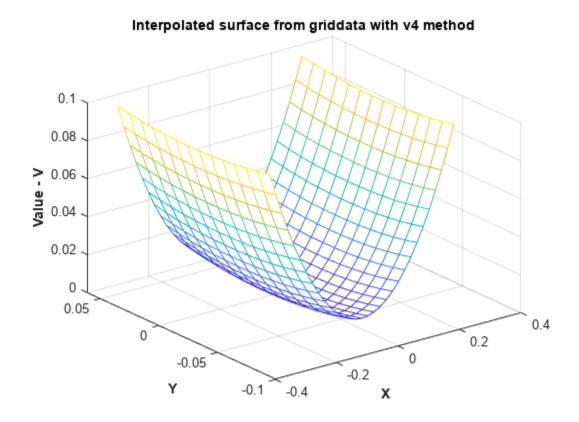
```
dt = delaunayTriangulation(x,y);
figure
plot(x,y,'*r')
axis equal
hold on
triplot(dt)
plot(x1,y1,'-r')
plot(x2,y2,'-r')
title('Triangulation Used to Create the Interpolant')
hold off
```



The triangles within the red boundaries are relatively well shaped; they are constructed from points that are in close proximity and the interpolation works well in this region. Outside the red boundary, the triangles are sliver-like and connect points that are remote from each other. There is not sufficient sampling to accurately capture the surface, so it is not surprising that the results in these regions are poor. In 3-D, visual inspection of the triangulation gets a bit trickier, but looking at the point distribution can often help illustrate potential problems.

The MATLAB® 4 griddata method, 'v4', is not triangulation-based and is not affected by deterioration of the interpolation surface near the boundary.

```
[xi,yi] = meshgrid(-0.3:.02:0.3, -0.0688:0.01:0.0688);
zi = griddata(x,y,z,xi,yi,'v4');
mesh(xi,yi,zi)
xlabel('X','fontweight','b'), ylabel('Y','fontweight','b')
zlabel('Value - V','fontweight','b')
title('Interpolated surface from griddata with v4 method','fontweight','b');
```



The interpolated surface from $\mbox{griddata}$ using the 'v4' method corresponds to the expected actual surface.

Interpolation Using a Specific Delaunay Triangulation

In this section...

"Nearest-Neighbor Interpolation Using a delaunayTriangulation Query" on page 8-41 "Linear Interpolation Using a delaunayTriangulation Query" on page 8-42

Nearest-Neighbor Interpolation Using a delaunayTriangulation Query

This example shows how to perform nearest-neighbor interpolation on a scattered set of points using a specific Delaunay triangulation.

Create a delaunayTriangulation of a set of scattered points in 2-D.

Sample a parabolic function, V(x,y), at the points specified in P.

```
V = P(:,1).^2 + P(:,2).^2;
```

Define 10 random query points.

```
Pq = -2 + 4*rand([10 2]);
```

Perform nearest-neighbor interpolation on V using the triangulation, DT. Use nearestNeighbor to find the indices of the nearest-neighbor vertices, vi, for the set of query points, Pq. Then examine the specific values of V at the indices.

```
vi = nearestNeighbor(DT,Pq);
Vq = V(vi)

Vq = 10×1

     2.7208
     3.7792
     1.8394
     3.5086
     1.8394
     3.5086
     1.4258
     5.4053
     4.0670
     0.5586
```

Linear Interpolation Using a delaunayTriangulation Query

This example shows how to perform linear interpolation on a scattered set of points with a specific Delaunay triangulation.

You can use the triangulation method, pointLocation, to compute the enclosing triangle of a query point and the magnitudes of the vertex weights. The weights are called barycentric coordinates, and they represent a partition of unity. That is, the sum of the three weights equals 1. The interpolated value of a function, V, at a query point is the sum of the weighted values of V at the three vertices. That is, if the function has values, V1, V2, V3 at the three vertices, and the weights are B1, B2, B3, then the interpolated value is (V1)(B1) + (V2)(B2) + (V3)(B3).

Create a delaunayTriangulation of a set of scattered points in 2-D.

Sample a parabolic function, V(x,y), at the points in P.

```
V = P(:,1).^2 + P(:,2).^2;
```

Define 10 random query points.

```
Pq = -2 + 4*rand([10 2]);
```

Find the triangle that encloses each query point using the pointLocation method. In the code below, ti contains the IDs of the enclosing triangles and bc contains the barycentric coordinates associated with each triangle.

```
[ti,bc] = pointLocation(DT,Pq);
```

Find the values of V(x,y) at the vertices of each enclosing triangle.

```
triVals = V(DT(ti,:));
```

Calculate the sum of the weighted values of V(x,y) using the dot product.

```
Vq = dot(bc',triVals')'
Vq = 10×1

2.2736
4.2596
2.1284
3.5372
4.6232
2.1797
1.2779
```

4.7644 3.6311

1.2196

See Also

delaunayTriangulation|pointLocation|nearestNeighbor

More About

• "Interpolating Scattered Data" on page 8-17

Extrapolating Scattered Data

```
#Factors That Affect the Accuracy of Extrapolation" on page 8-44

"Compare Extrapolation of Coarsely and Finely Sampled Scattered Data" on page 8-44

"Extrapolation of 3-D Data" on page 8-48
```

Factors That Affect the Accuracy of Extrapolation

scatteredInterpolant provides functionality for approximating values at points that fall outside the convex hull. The 'linear' extrapolation method is based on a least-squares approximation of the gradient at the boundary of the convex hull. The values it returns for query points outside the convex hull are based on the values and gradients at the boundary. The quality of the solution depends on how well you've sampled your data. If your data is coarsely sampled, the quality of the extrapolation is poor.

In addition, the triangulation near the convex hull boundary can have sliver-like triangles. These triangles can compromise your extrapolation results in the same way that they can compromise interpolation results. See "Interpolation Results Poor Near the Convex Hull" on page 8-35 for more information.

You should inspect your extrapolation results visually using your knowledge of the behavior outside the domain.

Compare Extrapolation of Coarsely and Finely Sampled Scattered Data

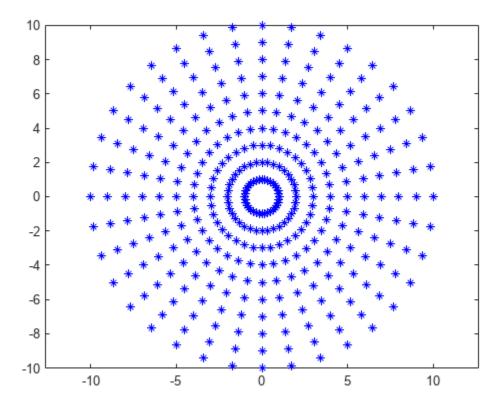
This example shows how to interpolate two different samplings of the same parabolic function. It also shows that a better distribution of sample points produces better extrapolation results.

Create a radial distribution of points spaced 10 degrees apart around 10 concentric circles. Use bsxfun to compute the coordinates, $x = \cos\theta$ and $y = \sin\theta$.

```
theta = 0:10:350;
c = cosd(theta);
s = sind(theta);
r = 1:10;

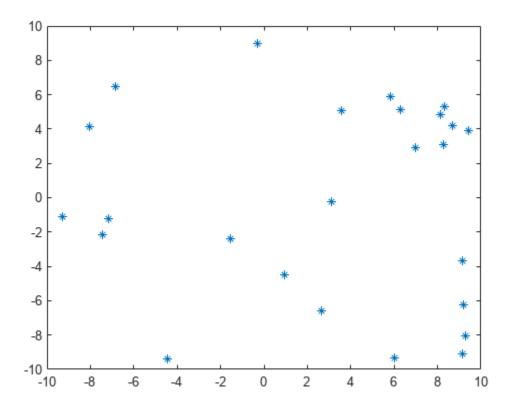
x1 = bsxfun(@times,r.',c);
y1 = bsxfun(@times,r.',s);

figure
plot(x1,y1,'*b')
axis equal
```



Create a second, more coarsely distributed set of points. Use the rand function to create random samplings in the range, [-10, 10].

```
rng default;
x2 = -10 + 20*rand([25 1]);
y2 = -10 + 20*rand([25 1]);
figure
plot(x2,y2,'*')
```



Sample a parabolic function, v(x,y), at both sets of points.

```
v1 = x1.^2 + y1.^2;

v2 = x2.^2 + y2.^2;
```

Create a scatteredInterpolant for each sampling of v(x,y).

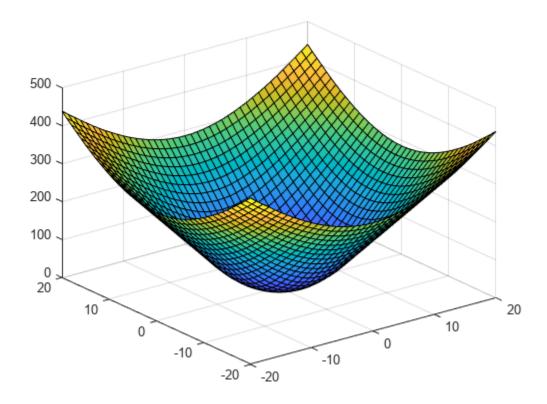
```
F1 = scatteredInterpolant(x1(:),y1(:),v1(:));
F2 = scatteredInterpolant(x2(:),y2(:),v2(:));
```

Create a grid of query points that extend beyond each domain.

```
[xq,yq] = ndgrid(-20:20);
```

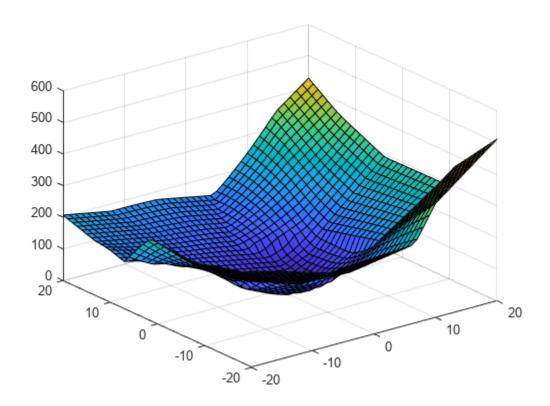
Evaluate F1 and plot the results.

```
figure
vq1 = F1(xq,yq);
surf(xq,yq,vq1)
```



Evaluate F2 and plot the results.

```
figure
vq2 = F2(xq,yq);
surf(xq,yq,vq2)
```



The quality of the extrapolation is not as good for F2 because of the coarse sampling of points in v2.

Extrapolation of 3-D Data

This example shows how to extrapolate a well sampled 3-D gridded dataset using scatteredInterpolant. The query points lie on a planar grid that is completely outside domain.

Create a 10-by-10-by-10 grid of sample points. The points in each dimension are in the range, [-10, 10].

```
[x,y,z] = ndgrid(-10:10);
```

Sample a function, v(x,y,z), at the sample points.

```
v = x.^2 + y.^2 + z.^2;
```

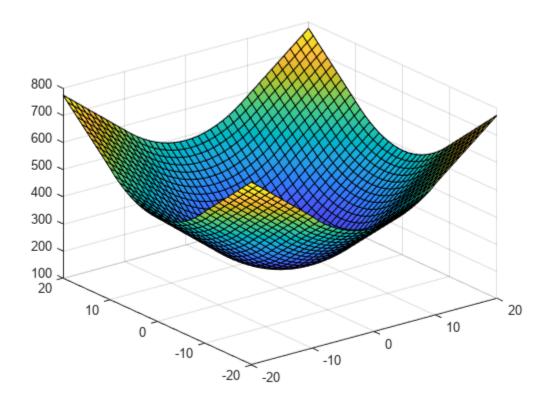
Create a scatteredInterpolant, specifying linear interpolation and extrapolation.

```
F = scatteredInterpolant(x(:),y(:),z(:),v(:),'linear','linear');
```

Evaluate the interpolant over an x-y grid spanning the range, [-20,20] at an elevation, z = 15.

```
[xq,yq,zq] = ndgrid(-20:20,-20:20,15);
vq = F(xq,yq,zq);
```

figure
surf(xq,yq,vq)



The extrapolation returned good results because the function is well sampled.

Normalize Data with Differing Magnitudes

This example shows how to use normalization to improve scattered data interpolation results with <code>griddata</code>. Normalization can improve the interpolation results in some cases, but in others it can compromise the accuracy of the solution. Whether to use normalization is a judgment made based on the nature of the data being interpolated.

- Benefits: Normalizing your data can potentially improve the interpolation result when the independent variables have different units and substantially different scales. In this case, scaling the inputs to have similar magnitudes might improve the numerical aspects of the interpolation. An example where normalization would be beneficial is if x represents engine speed in RPMs from 500 to 3500, and y represents engine load from 0 to 1. The scales of x and y differ by a few orders of magnitude, and they have different units.
- Cautions: Use caution when normalizing your data if the independent variables have the same units, even if the scales of the variables are different. With data of the same units, normalization distorts the solution by adding a directional bias, which affects the underlying triangulation and ultimately compromises the accuracy of the interpolation. An example where normalization is erroneous is if both x and y represent locations and have units of meters. Scaling x and y unequally is not recommended because 10 m due East should be spatially the same as 10 m due North.

Create some sample data where the values in y are a few orders of magnitude larger than those in x. Assume that x and y have different units.

```
x = rand(1,500)/100;

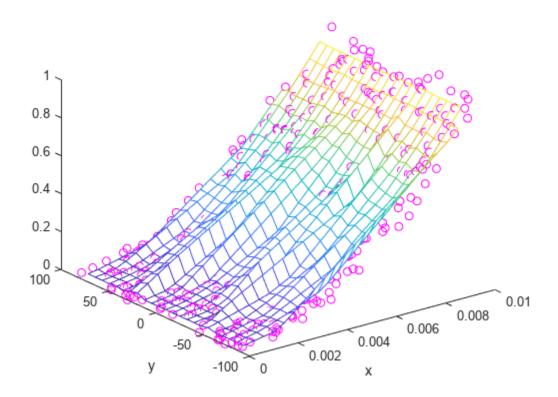
y = 2.*(rand(1,500)-0.5).*90;

z = (x.*1e2).^2;
```

Use the sample data to construct a grid of query points. Interpolate the sample data on the grid and plot the results.

```
X = linspace(min(x),max(x),25);
Y = linspace(min(y),max(y),25);
[xq, yq] = meshgrid(X,Y);
zq = griddata(x,y,z,xq,yq);

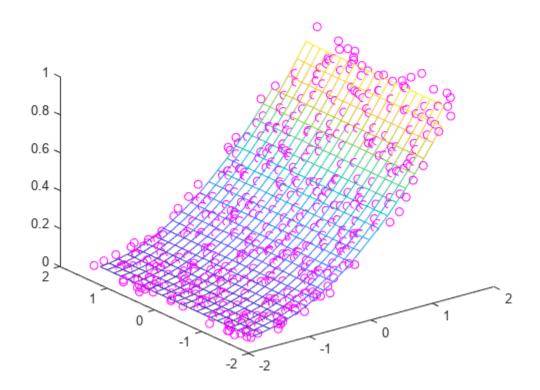
plot3(x,y,z,'mo')
hold on
mesh(xq,yq,zq)
xlabel('x')
ylabel('y')
hold off
```



The result produced by griddata is not very smooth and seems to be noisy. The differing scales in the independent variables contribute to this, since a small change in the size of one variable can lead to a much larger change in the size of the other variable.

Since x and y have different units, normalizing them so that they have similar magnitudes should help produce better results. Normalize the sample points using z-scores and regenerate the interpolation using qriddata.

```
% Normalize Sample Points
x = normalize(x);
y = normalize(y);
% Regenerate Grid
X = linspace(min(x),max(x),25);
Y = linspace(min(y),max(y),25);
[xq, yq] = meshgrid(X,Y);
% Interpolate and Plot
zq = griddata(x,y,z,xq,yq);
plot3(x,y,z,'mo')
hold on
mesh(xq,yq,zq)
```



In this case, normalizing the sample points permits griddata to compute a smoother solution.

See Also

griddata|griddatan|scatteredInterpolant

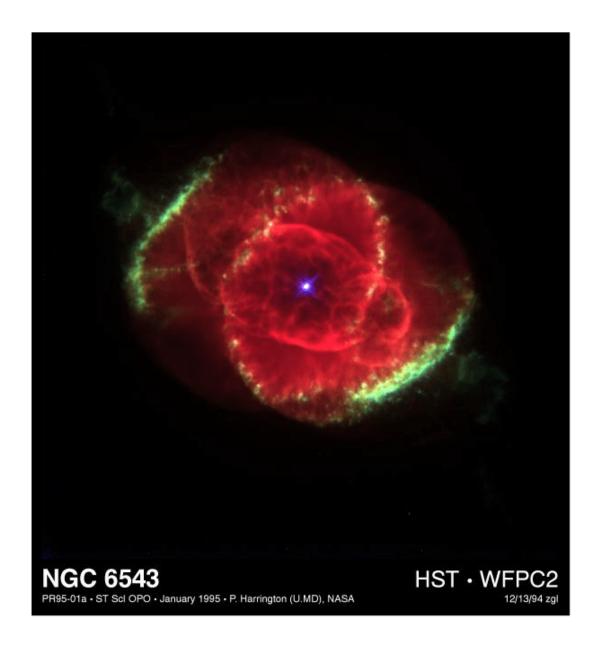
Resample Image with Gridded Interpolation

This example shows how to use <code>griddedInterpolant</code> to resample the pixels in an image. Resampling an image is useful for adjusting the resolution and size, and you also can use it to smooth out the pixels after zooming.

Load Image

Load and show the image ngc6543a.jpg, which is a Hubble Space Telescope image of the planetary nebulae NGC 6543. This image displays several interesting structures, such as concentric gas shells, jets of high-speed gas, and unusual knots of gas. The matrix A that represents the image is a 650-by-600-by-3 matrix of uint8 integers.

```
A = imread('ngc6543a.jpg');
imshow(A)
```



Create Interpolant

Create a gridded interpolant object for the image. griddedInterpolant only works for double-precision and single-precision matrices, so convert the uint8 matrix to double. To interpolate each RGB channel of the image, specify two grid vectors to describe the sample points in the first two dimensions. The grid vectors are grouped together as column vectors in a cell array $\{xg1, xg2, \ldots, xgN\}$. With this formulation, griddedInterpolant treats the 3-D matrix as containing multiple 2-D data sets defined on the same grid.

```
sz = size(A);
xg = 1:sz(1);
yg = 1:sz(2);
F = griddedInterpolant({xg,yg},double(A));
```

Resample Image Pixels

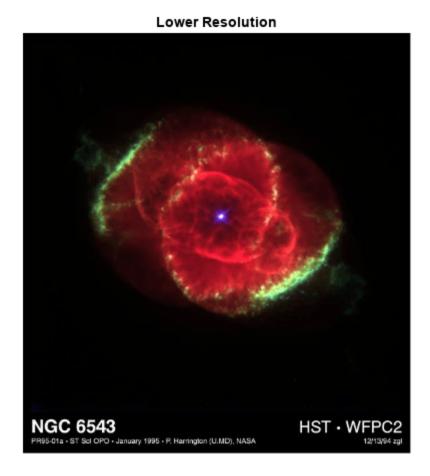
Use the sizes of the first two matrix dimensions to resample the image so that it is 120% the size. That is, for each 5 pixels in the original image, the interpolated image has 6 pixels. Evaluate the interpolant at the query points with the syntax $F(\{xq,yq\})$. griddedInterpolant evaluates each page in the 3-D image at the query points.

```
xq = (0:5/6:sz(1))';
yq = (0:5/6:sz(2))';
vq = uint8(F({xq,yq}));
imshow(vq)
title('Higher Resolution')
```



Similarly, reduce the size of the image by querying the interpolant with 55% fewer points than the original image. While you can simply index into the original image matrix to produce lower resolution images, interpolation enables you to resample the image at noninteger pixel locations.

```
xq = (0:1.55:sz(1))';
yq = (0:1.55:sz(2))';
vq = uint8(F({xq,yq}));
figure
imshow(vq)
title('Lower Resolution')
```

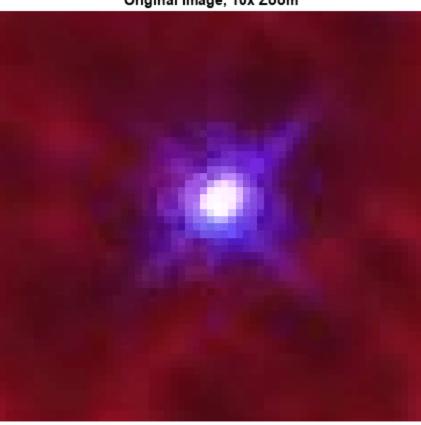


Smooth Out Zooming Artifacts

As you zoom in on an image, the pixels in the region of interest become larger and detail in the image is quickly lost. You can use image resampling to smooth out these zooming artifacts.

Zoom in on the bright spot in the center of the original image. (The indexing into A is to center this bright spot in the image so that subsequent zooming does not push it out of the frame.)

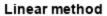
```
imshow(A(1:570,10:600,:),'InitialMagnification','fit')
zoom(10)
title('Original Image, 10x Zoom')
```

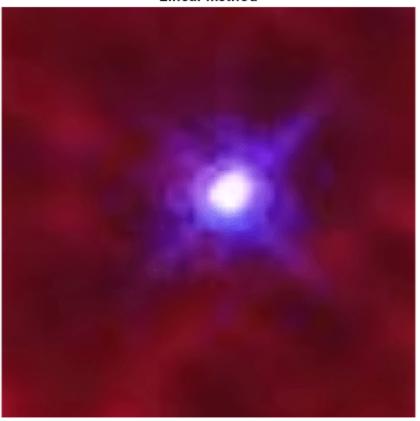


Original Image, 10x Zoom

Query the interpolant F to reproduce this zoomed image (approximately) with 10x higher resolution. Compare the results from several different interpolation methods.

```
xq = (1:0.1:sz(1))';
yq = (1:0.1:sz(2))';
F.Method = 'linear';
vq = uint8(F({xq,yq}));
imshow(vq(1:5700,150:5900,:),'InitialMagnification','fit')
zoom(10)
title('Linear method')
```



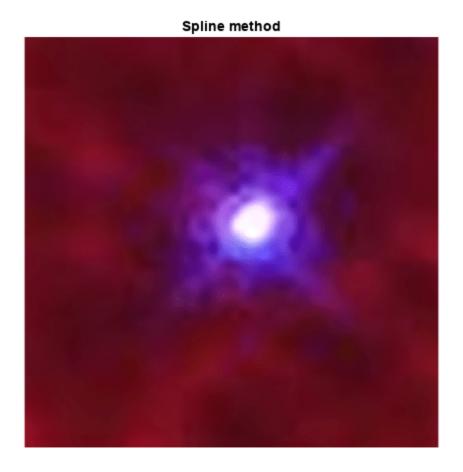


```
F.Method = 'cubic';
vq = uint8(F({xq,yq}));
imshow(vq(1:5700,150:5900,:),'InitialMagnification','fit')
zoom(10)
title('Cubic method')
```

Cubic method



```
F.Method = 'spline';
vq = uint8(F({xq,yq}));
imshow(vq(1:5700,150:5900,:),'InitialMagnification','fit')
zoom(10)
title('Spline method')
```



See Also griddedInterpolant|imshow

More About

• "Interpolating Gridded Data" on page 8-5

Optimization

- "Optimizing Nonlinear Functions" on page 9-2
- "Curve Fitting via Optimization" on page 9-7
- "Set Optimization Options" on page 9-10
- "Optimization Solver Iterative Display" on page 9-13
- "Optimization Solver Output Functions" on page 9-14
- "Optimization Solver Plot Functions" on page 9-20
- "Optimize Live Editor Task" on page 9-22
- "Optimization Troubleshooting and Tips" on page 9-28

Optimizing Nonlinear Functions

```
In this section...

"Minimizing Functions of One Variable" on page 9-2

"Minimizing Functions of Several Variables" on page 9-3

"Maximizing Functions" on page 9-4

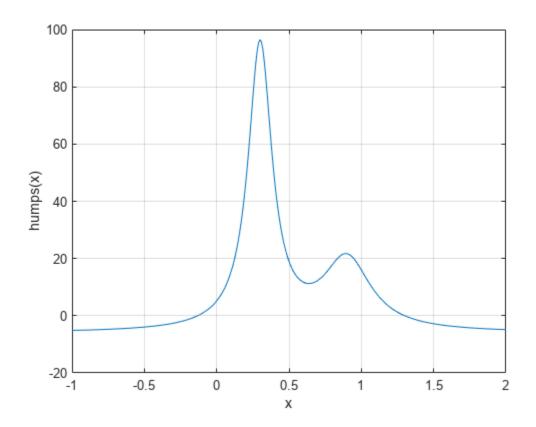
"fminsearch Algorithm" on page 9-4

"Reference" on page 9-6
```

Minimizing Functions of One Variable

Given a mathematical function of a single variable, you can use the fminbnd function to find a local minimizer of the function in a given interval. For example, consider the humps.m function, which is provided with MATLAB®. The following figure shows the graph of humps.

```
x = -1:.01:2;
y = humps(x);
plot(x,y)
xlabel('x')
ylabel('humps(x)')
grid on
```



To find the minimum of the humps function in the range (0.3,1), use

```
x = fminbnd(@humps, 0.3, 1)

x = 0.6370
```

You can see details of the solution process by using optimset to create options with the Display option set to 'iter'. Pass the resulting options to fminbnd.

```
options = optimset('Display','iter');
x = fminbnd(@humps,0.3,1,options)
```

Func-count	X	f(x)	Procedure
1	0.567376	12.9098	initial
2	0.732624	13.7746	golden
3	0.465248	25.1714	golden
4	0.644416	11.2693	parabolic
5	0.6413	11.2583	parabolic
6	0.637618	11.2529	parabolic
7	0.636985	11.2528	parabolic
8	0.637019	11.2528	parabolic
9	0.637052	11.2528	parabolic

```
Optimization terminated: the current x satisfies the termination criteria using OPTIONS.TolX of 1.000000e-04 x = 0.6370
```

The iterative display shows the current value of x and the function value at f(x) each time a function evaluation occurs. For fminbnd, one function evaluation corresponds to one iteration of the algorithm. The last column shows the procedure fminbnd uses at each iteration, a golden section search or a parabolic interpolation. For details, see "Optimization Solver Iterative Display" on page 9-13.

Note Optimization solvers apply to real-valued functions. Complex values cannot be optimized, except for a real-valued function of the complex values, such as the norm.

Minimizing Functions of Several Variables

The fminsearch function is similar to fminbnd except that it handles functions of many variables. Specify a starting vector x_0 rather than a starting interval. fminsearch attempts to return a vector x that is a local minimizer of the mathematical function near this starting vector.

To try fminsearch, create a function three var of three variables, x, y, and z.

```
function b = three_var(v)
x = v(1);
y = v(2);
z = v(3);
b = x.^2 + 2.5*sin(y) - z^2*x^2*y^2;
```

Now find a minimum for this function using x = -0.6, y = -1.2, and z = 0.135 as the starting values.

Note Optimization solvers apply to real-valued functions. Complex values cannot be optimized, except for a real-valued function of the complex values, such as the norm.

Maximizing Functions

The fminbnd and fminsearch solvers attempt to minimize an objective function. If you have a maximization problem, that is, a problem of the form

```
\max_{x} f(x),
```

then define g(x) = -f(x), and minimize g.

For example, to find the maximum of tan(cos(x)) near x = 5, evaluate:

```
[x fval] = fminbnd(@(x)-tan(cos(x)),3,8)
x =
    6.2832

fval =
    -1.5574
```

The maximum is 1.5574 (the negative of the reported fval), and occurs at x = 6.2832. This answer is correct since, to five digits, the maximum is tan(1) = 1.5574, which occurs at $x = 2\pi = 6.2832$.

fminsearch Algorithm

fminsearch uses the Nelder-Mead simplex algorithm as described in Lagarias et al. [1]. This algorithm uses a simplex of n+1 points for n-dimensional vectors x. The algorithm first makes a simplex around the initial guess x_0 by adding 5% of each component $x_0(i)$ to x_0 . The algorithm uses these n vectors as elements of the simplex in addition to x_0 . (The algorithm uses 0.00025 as component i if $x_0(i) = 0$.) Then, the algorithm modifies the simplex repeatedly according to the following procedure.

Note The keywords for the fminsearch iterative display appear in **bold** after the description of the step.

- **1** Let x(i) denote the list of points in the current simplex, i = 1,...,n + 1.
- Order the points in the simplex from lowest function value f(x(1)) to highest f(x(n+1)). At each step in the iteration, the algorithm discards the current worst point x(n+1), and accepts another point into the simplex. [Or, in the case of step 7 below, it changes all n points with values above f(x(1))].
- **3** Generate the reflected point

$$r = 2m - x(n+1), (9-1)$$

where

$$m = \sum x(i)/n, i = 1...n, \tag{9-2}$$

and calculate f(r).

- 4 If $f(x(1)) \le f(r) < f(x(n))$, accept r and terminate this iteration. **Reflect**
- **5** If f(r) < f(x(1)), calculate the expansion point s

$$s = m + 2(m - x(n+1)), \tag{9-3}$$

and calculate f(s).

- **a** If f(s) < f(r), accept s and terminate the iteration. **Expand**
- **b** Otherwise, accept *r* and terminate the iteration. **Reflect**
- If $f(r) \ge f(x(n))$, perform a contraction between m and either x(n+1) or r, depending on which has the lower objective function value.
 - **a** If f(r) < f(x(n + 1)) (that is, r is better than x(n + 1)), calculate

$$c = m + (r - m)/2$$
(9
4

and calculate f(c). If f(c) < f(r), accept c and terminate the iteration. **Contract outside**

Otherwise, continue with Step 7 (Shrink).

b If $f(r) \ge f(x(n+1))$, calculate

$$cc = m + (x(n + 1) - m)/2$$
(9
5

and calculate f(cc). If f(cc) < f(x(n + 1)), accept cc and terminate the iteration. **Contract inside**

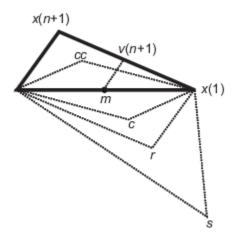
Otherwise, continue with Step 7 (Shrink).

7 Calculate the *n* points

$$v(i) = x(1) + (x(i) - x(1))/2 \tag{9-6}$$

and calculate f(v(i)), i = 2,...,n + 1. The simplex at the next iteration is x(1), v(2),...,v(n + 1). **Shrink**

The following figure shows the points that fminsearch can calculate in the procedure, along with each possible new simplex. The original simplex has a bold outline. The iterations proceed until they meet a stopping criterion.



Reference

[1] Lagarias, J. C., J. A. Reeds, M. H. Wright, and P. E. Wright. "Convergence Properties of the Nelder-Mead Simplex Method in Low Dimensions." SIAM Journal of Optimization, Vol. 9, Number 1, 1998, pp. 112–147.

See Also

- "Optimization Troubleshooting and Tips" on page 9-28
- "Nonlinear Optimization" (Optimization Toolbox)
- "Curve Fitting via Optimization" on page 9-7

Curve Fitting via Optimization

This example shows how to fit a nonlinear function to data. For this example, the nonlinear function is the standard exponential decay curve

```
y(t) = A \exp(-\lambda t)
```

where y(t) is the response at time t, and A and λ are the parameters to fit. Fitting the curve means finding parameters A and λ that minimize the sum of squared errors

$$\sum_{i=1}^{n} (y_i - A \exp(-\lambda t_i))^2,$$

where the times are t_i and the responses are y_i , i = 1, ..., n. The sum of squared errors is the objective function.

Create Sample Data

Usually, you have data from measurements. For this example, create artificial data based on a model with A = 40 and $\lambda = 0.5$, with normally distributed pseudorandom errors.

```
rng default % for reproducibility
tdata = 0:0.1:10;
ydata = 40*exp(-0.5*tdata) + randn(size(tdata));
```

Write Objective Function

Write a function that accepts parameters A and lambda and data tdata and ydata, and returns the sum of squared errors for the model y(t). Put all the variables to optimize (A and lambda) in a single vector variable (x). For more information, see "Minimizing Functions of Several Variables" on page 9-3.

```
type sseval
function sse = sseval(x,tdata,ydata)
A = x(1);
lambda = x(2);
sse = sum((ydata - A*exp(-lambda*tdata)).^2);
```

Save this objective function as a file named sseval.m on your MATLAB® path.

The fminsearch solver applies to functions of one variable, x. However, the sseval function has three variables. The extra variables tdata and ydata are not variables to optimize, but are data for the optimization. Define the objective function for fminsearch as a function of x alone:

```
fun = @(x)sseval(x,tdata,ydata);
```

For information about including extra parameters such as tdata and ydata, see "Parameterizing Functions" on page 10-2.

Find the Best Fitting Parameters

Start from a random positive set of parameters x0, and have fminsearch find the parameters that minimize the objective function.

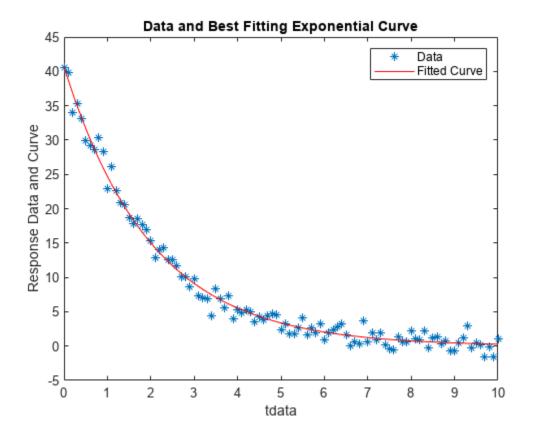
```
x0 = rand(2,1);
bestx = fminsearch(fun,x0)
bestx = 2×1
    40.6877
    0.4984
```

The result bestx is reasonably near the parameters that generated the data, A = 40 and lambda = 0.5.

Check the Fit Quality

To check the quality of the fit, plot the data and the resulting fitted response curve. Create the response curve from the returned parameters of your model.

```
A = bestx(1);
lambda = bestx(2);
yfit = A*exp(-lambda*tdata);
plot(tdata,ydata,'*');
hold on
plot(tdata,yfit,'r');
xlabel('tdata')
ylabel('Response Data and Curve')
title('Data and Best Fitting Exponential Curve')
legend('Data','Fitted Curve')
hold off
```



See Also

- "Optimizing Nonlinear Functions" on page 9-2
- "Nonlinear Data-Fitting" (Optimization Toolbox)
- "Nonlinear Regression" (Statistics and Machine Learning Toolbox)

Set Optimization Options

In this section... "How to Set Options" on page 9-10 "Options Table" on page 9-10 "Tolerances and Stopping Criteria" on page 9-11 "Output Structure" on page 9-12

How to Set Options

You can specify optimization parameters using an options structure that you create using the optimset function. You then pass options as an input to the optimization function, for example, by calling fminbnd with the syntax

```
x = fminbnd(fun,x1,x2,options)
or fminsearch with the syntax
x = fminsearch(fun,x0,options)
For example, to display output from the algorithm at each iteration, set the Display option to 'iter':
options = optimset('Display','iter');
```

Options Table

Option	Description	Solvers
Display	A flag indicating whether intermediate steps appear on the screen. • 'notify' (default) displays output only if the function does not converge.	fminbnd, fminsearch, fzero, lsqnonneg
	• 'iter' displays intermediate steps (not available with lsqnonneg). See "Optimization Solver Iterative Display" on page 9-13.	
	• 'off' or 'none' displays no intermediate steps.	
	• 'final' displays just the final output.	
FunValCheck	 Check whether objective function values are valid. 'on' displays an error when the objective function or constraints return a value that is complex or NaN. 	fminbnd, fminsearch, fzero
	• 'off' (default) displays no error.	
MaxFunEvals	The maximum number of function evaluations allowed. The default value is 500 for fminbnd and 200*length(x0) for fminsearch.	fminbnd, fminsearch

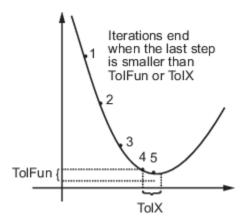
Option	Description	Solvers
MaxIter	The maximum number of iterations allowed. The default value is 500 for fminbnd and $200*length(x0)$ for fminsearch.	fminbnd, fminsearch
OutputFcn	Display information on the iterations of the solver. The default is [] (none). See "Optimization Solver Output Functions" on page 9-14.	fminbnd, fminsearch, fzero
PlotFcns	Plot information on the iterations of the solver. The default is [] (none). For available predefined functions, see "Optimization Solver Plot Functions" on page 9-20.	fminbnd, fminsearch, fzero
TolFun	The termination tolerance for the function value. The default value is 1.e-4. See "Tolerances and Stopping Criteria" on page 9-11.	fminsearch
TolX	The termination tolerance for x . The default value is 1.e-4, except for fzero, which has a default value of eps (= 2.2204e-16), and lsqnonneg, which has a default value of $10*eps*norm(c,1)*length(c)$. See "Tolerances and Stopping Criteria" on page 9-11.	fminbnd, fminsearch, fzero, lsqnonneg

Tolerances and Stopping Criteria

The number of iterations in an optimization depends on the stopping criteria for the solver. These criteria include several tolerances you can set. Generally, a tolerance is a threshold which, if crossed, stops the iterations of a solver.

Tip Generally, set the TolFun and TolX tolerances to well above eps, and usually above 1e-14. Setting small tolerances does not guarantee accurate results. Instead, a solver can fail to recognize when it has converged, and can continue futile iterations. A tolerance value smaller than eps effectively disables that stopping condition. This tip does not apply to fzero, which uses a default value of eps for TolX.

• TolX is a lower bound on the size of a step, meaning the norm of $(x_i - x_{i+1})$. If the solver attempts to take a step that is smaller than TolX, the iterations end. Solvers generally use TolX as a *relative* bound, meaning iterations end when $|(x_i - x_{i+1})| < \text{TolX*}(1 + |x_i|)$, or a similar relative measure.



- TolFun is a lower bound on the change in the value of the objective function during a step. If $|f(x_i) f(x_{i+1})| < \text{TolFun}$, the iterations end. Solvers generally use TolFun as a *relative* bound, meaning iterations end when $|f(x_i) f(x_{i+1})| < \text{TolFun}(1 + |f(x_i)|)$, or a similar relative measure.
- MaxIter is a bound on the number of solver iterations. MaxFunEvals is a bound on the number of function evaluations.

Note Unlike other solvers, fminsearch stops when it satisfies both TolFun and TolX.

Output Structure

The output structure includes the number of function evaluations, the number of iterations, and the algorithm. The structure appears when you provide fminbnd, fminsearch, or fzero with a fourth output argument, as in

[x,fval,exitflag,output] = fminbnd(@humps,0.3,1);

The details of the output structure for each solver are on the function reference pages.

The output structure is not an option that you choose with optimset. It is an optional output for fminbnd, fminsearch, and fzero.

See Also

- "Optimizing Nonlinear Functions" on page 9-2
- "Optimization Solver Output Functions" on page 9-14
- "Optimization Solver Plot Functions" on page 9-20

Optimization Solver Iterative Display

You obtain details of the steps solvers take by setting the Display option to 'iter' with optimset. The displayed output contains headings and items from the following list.

Heading	Information Displayed	Solvers	
Iteration	Iteration number, meaning the number of steps the algorithm has taken	fminsearch	
Func-count	Cumulative number of function evaluations	fminbnd, fminsearch, fzero	
Х	Current point	fminbnd, fzero	
f(x)	Current objective function value	fminbnd, fzero	
min f(x)	Smallest objective function value found	fminsearch	
Procedure	Algorithm used during the iteration		
	• initial	fminbnd	
	• golden (golden section search)		
	• parabolic (parabolic interpolation)		
	• initial simplex	fminsearch	
	• expand		
	• reflect		
	• shrink		
	• contract inside		
	• contract outside		
	For details, see "fminsearch Algorithm" on page 9-4.		
	• initial (initial point)	fzero	
	• search (search for an interval containing a zero)		
	• bisection		
	• interpolation (linear interpolation or inverse quadratic interpolation)		
a, f(a), b, f(b)	Search points and their function values while looking for an interval with function values of opposite signs	fzero	

See Also

- "Set Optimization Options" on page 9-10
- "Optimization Solver Output Functions" on page 9-14
- "Optimization Solver Plot Functions" on page 9-20

Optimization Solver Output Functions

```
In this section...

"What Is an Output Function?" on page 9-14

"Creating and Using an Output Function" on page 9-14

"Structure of the Output Function" on page 9-15

"Example of a Nested Output Function" on page 9-16

"Fields in optimValues" on page 9-17

"States of the Algorithm" on page 9-17

"Stop Flag" on page 9-18
```

What Is an Output Function?

An output function is a function that an optimization function calls at each iteration of its algorithm. Typically, you use an output function to generate graphical output, record the history of the data the algorithm generates, or halt the algorithm based on the data at the current iteration. You can create an output function as a function file, a local function, or a nested function.

You can use the OutputFcn option with the following MATLAB optimization functions:

- fminbnd
- fminsearch
- fzero

Creating and Using an Output Function

The following is a simple example of an output function that plots the points generated by an optimization function.

```
function stop = outfun(x, optimValues, state)
stop = false;
hold on;
plot(x(1),x(2),'.');
drawnow
```

You can use this output function to plot the points generated by fminsearch in solving the optimization problem

$$\min_x f(x) = \min_x e^{x_1} \left(4x_1^2 + 2x_2^2 + x_1x_2 + 2x_2 \right).$$

To do so,

- 1 Create a file containing the preceding code and save it as outfun.m in a folder on the MATLAB path.
- 2 Set the value of the Outputfon field of the options structure to a function handle to outfun.

```
options = optimset('OutputFcn', @outfun);
```

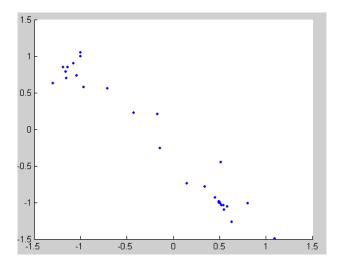
3 Enter the following commands:

```
hold on objfun=@(x) \exp(x(1))*(4*x(1)^2+2*x(2)^2+x(1)*x(2)+2*x(2)); [x fval] = fminsearch(objfun, [-1 1], options) hold off
```

These commands return the solution

```
x = 0.1290 -0.5323
fval = -0.5689
```

and display the following plot of the points generated by fminsearch:



Structure of the Output Function

The function definition line of the output function has the following form:

```
stop = outfun(x, optimValues, state)
```

where

- stop is a flag that is true or false depending on whether the optimization routine halts or continues. See "Stop Flag" on page 9-18.
- x is the point computed by the algorithm at the current iteration.
- optimValues is a structure containing data from the current iteration. "Fields in optimValues" on page 9-17 describes the structure in detail.
- state is the current state of the algorithm. "States of the Algorithm" on page 9-17 lists the possible values.

The optimization function passes the values of the input arguments to outfun at each iteration.

Example of a Nested Output Function

The example in "Creating and Using an Output Function" on page 9-14 does not require the output function to preserve data from one iteration to the next. When you do not need to save data between iterations, you can write the output function as a function file and call the optimization function directly from the command line. However, to have an output function to record data from one iteration to the next, write a single file that does the following:

- Contains the output function as a nested function—see "Nested Functions" in MATLAB Programming Fundamentals for more information.
- Calls the optimization function.

In the following example, the function file also contains the objective function as a local function. You can instead write the objective function as a separate file or as an anonymous function.

Nested functions have access to variables in the surrounding file. Therefore, this method enables the output function to preserve variables from one iteration to the next.

The following example uses an output function to record the fminsearch iterates in solving

$$\min_{x} f(x) = \min_{x} e^{x_1} \left(4x_1^2 + 2x_2^2 + x_1x_2 + 2x_2 \right).$$

The output function returns the sequence of points as a matrix called history.

To run the example, do the following steps:

- **1** Open a new file in the MATLAB Editor.
- **2** Copy and paste the following code into the file.

```
function [x fval history] = myproblem(x0)
  history = [];
  options = optimset('OutputFcn', @myoutput);
  [x fval] = fminsearch(@objfun, x0,options);

function stop = myoutput(x,optimvalues,state);
    stop = false;
    if isequal(state,'iter')
        history = [history; x];
    end
end

function z = objfun(x)
    z = exp(x(1))*(4*x(1)^2+2*x(2)^2+x(1)*x(2)+2*x(2));
    end
end
```

- **3** Save the file as myproblem.m in a folder on the MATLAB path.
- **4** At the MATLAB prompt, enter

```
[x fval history] = myproblem([-1 1]);
```

The function fminsearch returns x, the optimal point, and fval, the value of the objective function at x.

```
x,fval
```

```
x = 0.1290 -0.5323
fval = -0.5689
```

In addition, the output function myoutput returns the matrix history, which contains the points generated by the algorithm at each iteration, to the MATLAB workspace. The first four rows of history are

The final row of points in history is the same as the optimal point, x.

```
history(end,:)
ans =
     0.1290   -0.5323
objfun(history(end,:))
ans =
    -0.5689
```

Fields in optimValues

The following table lists the fields of the optimValues structure that are provided by the optimization functions fminbnd, fminsearch, and fzero.

The "Command-Line Display Headings" column of the table lists the headings that appear when you set the Display parameter of options to 'iter'.

optimValues Field (optimValues.field)	Description	Command-Line Display Heading
funccount	Cumulative number of function evaluations	Func-count
fval	Function value at current point	min f(x)
iteration	Iteration number — starts at 0	Iteration
procedure	Procedure messages	Procedure

States of the Algorithm

The following table lists the possible values for state:

State	Description
'init'	The algorithm is in the initial state before the first iteration.
'interrupt'	The algorithm is performing an iteration. In this state, the output function can halt the current iteration of the optimization. You might want the output function to halt the iteration to improve the efficiency of the computations. When state is set to 'interrupt', the values of x and optimValues are the same as at the last call to the output function, in which state is set to 'iter'.
'iter'	The algorithm is at the end of an iteration.
'done'	The algorithm is in the final state after the last iteration.

The following code illustrates how the output function uses the value of state to decide which tasks to perform at the current iteration.

```
switch state
    case 'init'
        % Setup for plots or dialog boxes
    case 'iter'
        % Make updates to plots or dialog boxes as needed
    case 'interrupt'
        % Check conditions to see whether optimization
        % should quit
    case 'done'
        % Cleanup of plots, dialog boxes, or final plot
end
```

Stop Flag

The output argument stop is a flag that is true or false. The flag tells the optimization function whether the optimization halts (true) or continues (false). The following examples show typical ways to use the stop flag.

Stopping an Optimization Based on Data in optimValues

The output function can stop an optimization at any iteration based on the current data in optimValues. For example, the following code sets stop to true if the objective function value is less than 5:

```
function stop = myoutput(x, optimValues, state)
stop = false;
% Check if objective function is less than 5.
if optimValues.fval < 5
    stop = true;
end</pre>
```

Stopping an Optimization Based on Dialog Box Input

If you design a UI to perform optimizations, you can have the output function stop an optimization with, for example, a **Stop** button. The following code shows how to do this callback. The code assumes that the **Stop** button callback stores the value true in the optimstop field of a handles structure called hObject stored in appdata.

```
function stop = myoutput(x, optimValues, state)
stop = false;
% Check if user has requested to stop the optimization.
stop = getappdata(hObject, 'optimstop');
```

See Also

- "Optimization Solver Plot Functions" on page 9-20
- "Set Optimization Options" on page 9-10
- "Optimization Solver Iterative Display" on page 9-13

Optimization Solver Plot Functions

```
In this section...

"What Is a Plot Function?" on page 9-20

"Example: Plot Function" on page 9-20
```

What Is a Plot Function?

The PlotFcns field of the options structure specifies one or more functions that an optimization function calls at each iteration to plot various measures of progress. Pass a function handle or cell array of function handles. The structure of a plot function is the same as the structure of an output function. For more information on this structure, see "Optimization Solver Output Functions" on page 9-14.

You can use the PlotFcns option with the following MATLAB optimization functions:

- fminbnd
- fminsearch
- fzero

The predefined plot functions for these optimization functions are:

- @optimplotx plots the current point
- @optimplotfval plots the function value
- @optimplotfunccount plots the function count (not available for fzero)

To view or modify a predefined plot function, open the function file in the MATLAB Editor. For example, to view the function file for plotting the current point, enter:

```
edit optimplotx.m
```

Example: Plot Function

View the progress of a minimization using fminsearch with the plot function @optimplotfval:

1 Write a file for the objective function. For this example, use:

```
function f = \text{onehump}(x)

r = x(1)^2 + x(2)^2;

s = \exp(-r);

f = x(1)*s+r/20;
```

2 Set the options to use the plot function:

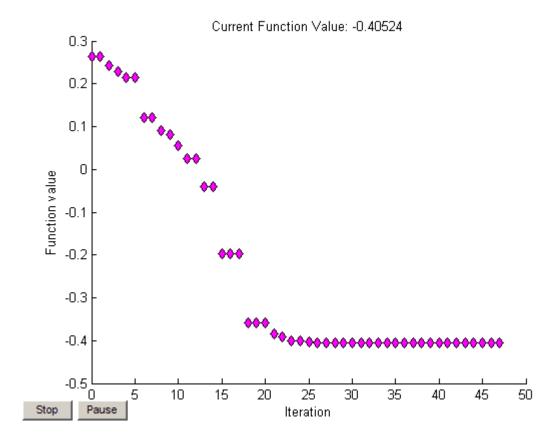
```
options = optimset('PlotFcns',@optimplotfval);
3 Call fminsearch starting from [2,1]:
```

[x ffinal] = fminsearch(@onehump,[2,1],options)

4 MATLAB returns the following:

```
x =
-0.6691 0.0000
```





See Also

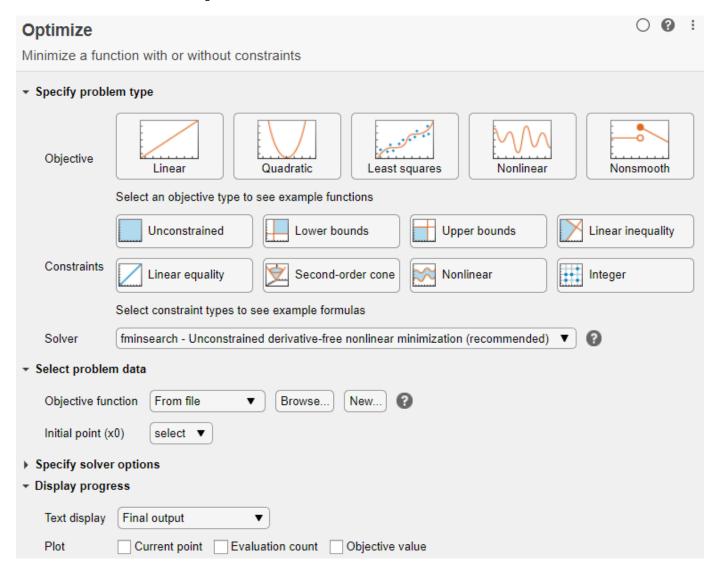
- "Optimization Solver Output Functions" on page 9-14
- "Set Optimization Options" on page 9-10
- "Optimization Solver Iterative Display" on page 9-13

Optimize Live Editor Task

In this section... "What Is the Optimize Live Editor Task?" on page 9-22 "Minimize a Nonlinear Function of Several Variables" on page 9-23 "Solve a Scalar Equation" on page 9-25

What Is the Optimize Live Editor Task?

The **Optimize** Live Editor task provides a visual interface for the fminbnd, fminsearch, fzero, and lsqnonneg solvers. To start the task, click the **New Live Script** button. Then click the **Insert** tab and select **Task > Optimize**.



Minimize a Nonlinear Function of Several Variables

This example shows how to minimize the function $f(x, y) = 100(y - x^2)^2 + (a - x)^2$ where the variable $a = \pi$ using the **Optimize** Live Editor task.

For a video describing a similar optimization problem, see How to Use the Optimize Live Editor Task.

- 1 On the **Home** tab, in the **File** section, click the **New Live Script** button.
- 2 Insert an Optimize Live Editor task. Click the Insert tab and then, in the Code section, select Task > Optimize.





- **3** For use in entering problem data, click the **Section Break** button. New sections appear above and below the task.
- **4** In the section above the **Optimize** task, enter the following code.

$$a = pi;$$

 $x0 = [-1 2];$

- **5** To place these variables into the workspace, press **Ctrl + Enter**.
- In the **Specify problem type** section of the task, click the **Objective > Nonlinear** button and the **Constraints > Unconstrained** button. The task shows that the recommended solver is fminsearch.

Note If you have Optimization Toolbox[™], your recommended solver at this point is different. Choose fminsearch to proceed with the example.

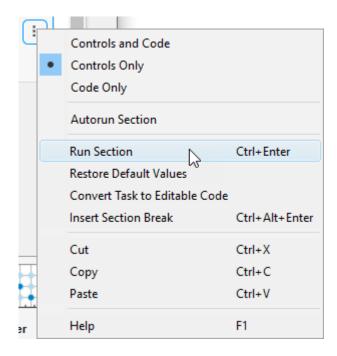
7 In the **Select problem data** section, select **Objective function > Local function** and then click the **New** button. A function script appears in a new section below the task. Edit the resulting code to contain the following uncommented lines.

```
function f = objectiveFcn(optimInput,a)
x = optimInput(1);
y = optimInput(2);
f = 100*(y - x^2)^2 + (a - x)^2;
end
```

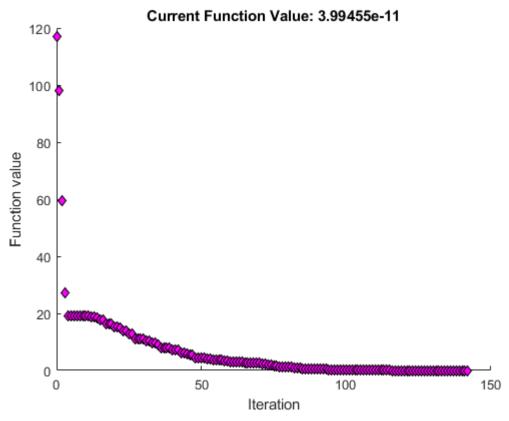
- 8 In the **Select problem data** section, select objectiveFcn as the local function.
- 9 In the **Select problem data** section, under **Function inputs**, select **Optimization input > optimInput** and **Fixed input:** a > a.



- **10** Select **Initial point (x0) > x0**.
- **11** In the **Display progress** section, select **Objective value** for the plot.
- 12 To run the solver, click the options button : at the top right of the task window, and select **Run** Section.



The following plot appears.



13 To view the solution point, look at the top of the **Optimize** task.

Optimize solution , objectiveValue = Minimize objectiveFcn using fminsearch solver

The solution and objectiveValue variables are returned to the workspace. To view their values, insert a section break below the task and enter this code.

```
disp(solution)
disp(objectiveValue)
```

14 Run the section by pressing **Ctrl+Enter**.

```
disp(solution)
     3.1416     9.8696
disp(objectiveValue)
     3.9946e-11
```

Solve a Scalar Equation

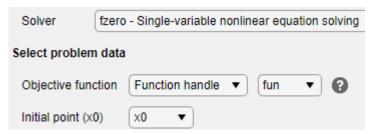
This example shows how to use the **Optimize** Live Editor task to find the point x where cos(x) = x.

On the **Home** tab, in the **File** section, click the **New Live Script** button. Enter these lines of code in the live script.

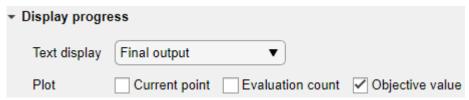
```
fun = @(x)\cos(x) - x;
 x0 = 0;
```

The first line defines the anonymous function fun, which takes the value 0 at the point x where $\cos(x) = x$. The second line defines the initial point $x\theta = 0$, where fzero begins its search for a solution.

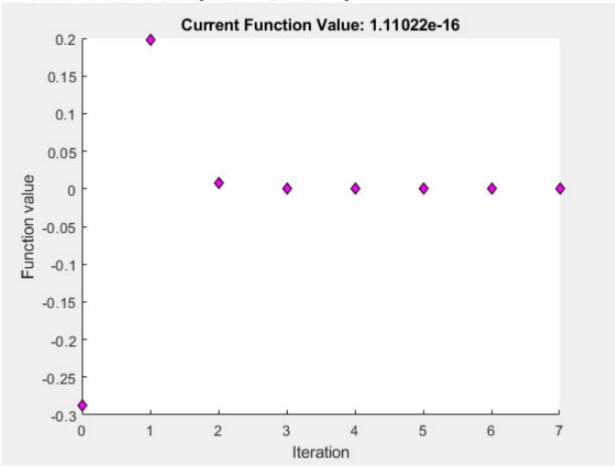
- **2** Put these variables in the MATLAB workspace by pressing **Ctrl+Enter**.
- 3 Insert an Optimize Live Editor task. Click the Insert tab and then, in the Code section, select Task > Optimize.
- 4 In the **Specify problem type** section of the task, select **Solver > fzero**.
- 5 In the **Select problem data** section, select **Objective function > Function handle** and then select fun. Select **Initial point (x0) > x0**.



6 In the Display progress section, select **Objective value** for the plot.



7 Run the solver by pressing **Ctrl+Enter**.



Zero found in the interval [-0.905097, 0.905097]

8 To see the solution value, insert a new section below the task by clicking the **Section Break** button on the **Insert** tab. In the new section, enter **solution** and press **Ctrl+Enter**.

solution

solution = 0.7391

See Also

Optimize | fzero | fminsearch

- "Optimization"
- "Add Interactive Tasks to a Live Script"
- How to Use the Optimize Live Editor Task

Optimization Troubleshooting and Tips

This table describes typical optimization problems and provides recommendations for handling them.

Problem	Recommendation
The solution found by fminbnd or fminsearch is not a global minimum. A global minimum has the smallest objective function value among all points in the search space.	There is no guarantee that a solution is a global minimum unless your problem is continuous and has only one minimum. To search for a global minimum, start the optimization from multiple starting points (or intervals, in the case of fminbnd).
It is impossible to evaluate the objective function f(x) at some points x. Such points are called infeasible.	Modify your function to return a large positive value for $f(x)$ at infeasible points x .
The minimization routine appears to enter an infinite loop or returns a solution that is not a minimum (or not a zero, in the case of fzero).	Perhaps your objective function returns NaN or complex values. Solvers expect only real objective function values. Any other values can cause unexpected results. To determine whether there are NaN or complex values, set
	<pre>options = optimset('FunValCheck','on')</pre>
	and call the optimization function with options as an input argument. If an objective function returns a NaN or complex value, this setting causes the solver to throw an error.
The solver takes a long time.	Most optimization problems benefit from good starting points. Try random starting points in a region that might be close to a solution, based on your problem characteristics.
	Sometimes you can solve a complicated problem using an evolutionary approach. First, solve problems with a smaller number of independent variables. Use solutions from these simpler problems as starting points for more complicated problems by using an appropriate mapping. Also, you can sometimes speed the solution by using simpler objective functions and less stringent stopping conditions in the initial stages of an optimization problem.
It is unclear what the solver is doing.	To see what the solver is doing as it iterates:
	• Monitor the iterations using a plot function such as @optimplotfval. Use optimset to set the PlotFcns option. See "Optimization Solver Plot Functions" on page 9-20.
	• Set the Display option to display information at the command line. See "Optimization Solver Iterative Display" on page 9-13.

Problem	Recommendation	
fminsearch fails to reach a solution.	 fminsearch can fail to reach a solution for various reasons. Poor scaling. If your problem is not adequately centered and scaled, the solver can fail to converge correctly. Try to have each coordinate give roughly the same effect on the objective function, and ensure that the scale of each coordinate near a possible solution is not too large or small. To do so, edit the objective function and add or multiply 	
	 appropriate constants for each coordinate. Inappropriate stopping criteria. If the value you specify for TolFun or TolX is too small, fminsearch can fail to realize when it has reached a solution. If the value is too large, fminsearch can halt far from a solution. Poor initial point. Try starting fminsearch from various 	
	 initial points. Insufficient iterations. If the solver runs out of iterations or gets stuck, try restarting fminsearch from its final point to reach a better solution. Sometimes fminsearch reaches 	
	a better solution. Sometimes infinsear ch reaches a better solution when you increase the value of the MaxFunEvals and MaxIter options from their default of 200*length(x0).	

Note Optimization solvers apply to real-valued functions. Complex values cannot be optimized, except for a real-valued function of the complex values, such as the norm.

See Also

More About

• "Optimizing Nonlinear Functions" on page 9-2

Function Handles

Parameterizing Functions

```
In this section...

"Overview" on page 10-2

"Parameterizing Using Nested Functions" on page 10-2

"Parameterizing Using Anonymous Functions" on page 10-3
```

Overview

This topic explains how to store or access extra parameters for mathematical functions that you pass to MATLAB function functions, such as fzero or integral.

MATLAB function functions evaluate mathematical expressions over a range of values. They are called function functions because they are functions that accept a function handle (a pointer to a function) as an input. Each of these functions expects that your objective function has a specific number of input variables. For example, fzero and integral accept handles to functions that have exactly one input variable.

Suppose you want to find the zero of the cubic polynomial $x^3 + bx + c$ for different values of the coefficients b and c. Although you could create a function that accepts three input variables (x, b, and c), you cannot pass a function handle that requires all three of those inputs to fzero. However, you can take advantage of properties of anonymous or nested functions to define values for additional inputs.

Parameterizing Using Nested Functions

One approach for defining parameters is to use a nested function—a function completely contained within another function in a program file. For this example, create a file named findzero.m that contains a parent function findzero and a nested function poly:

```
function y = findzero(b,c,x0)
y = fzero(@poly,x0);
  function y = poly(x)
  y = x^3 + b*x + c;
  end
end
```

The nested function defines the cubic polynomial with one input variable, x. The parent function accepts the parameters b and c as input values. The reason to nest poly within findzero is that nested functions share the workspace of their parent functions. Therefore, the poly function can access the values of b and c that you pass to findzero.

To find a zero of the polynomial with b = 2 and c = 3.5, using the starting point x0 = 0, you can call findzero from the command line:

```
x = findzero(2,3.5,0)
x =
    -1.0945
```

Parameterizing Using Anonymous Functions

Another approach for accessing extra parameters is to use an anonymous function. Anonymous functions are functions that you can define in a single command, without creating a separate program file. They can use any variables that are available in the current workspace.

For example, create a handle to an anonymous function that describes the cubic polynomial, and find the zero:

```
b = 2;
c = 3.5;
cubicpoly = @(x) x^3 + b*x + c;
x = fzero(cubicpoly,0)
x =
    -1.0945
```

Variable cubicpoly is a function handle for an anonymous function that has one input, x. Inputs for anonymous functions appear in parentheses immediately following the @ symbol that creates the function handle. Because b and c are in the workspace when you create cubicpoly, the anonymous function does not require inputs for those coefficients.

You do not need to create an intermediate variable, cubicpoly, for the anonymous function. Instead, you can include the entire definition of the function handle within the call to fzero:

```
b = 2;
c = 3.5;
x = fzero(@(x) x^3 + b*x + c,0)
x =
    -1.0945
```

You also can use anonymous functions to call more complicated objective functions that you define in a function file. For example, suppose you have a file named <code>cubicpoly.m</code> with this function definition:

```
function y = cubicpoly(x,b,c)
y = x^3 + b*x + c;
end
```

At the command line, define b and c, and then call fzero with an anonymous function that invokes cubicpoly:

```
b = 2;
c = 3.5;
x = fzero(@(x) cubicpoly(x,b,c),0)
x =
    -1.0945
```

Note To change the values of the parameters, you must create a new anonymous function. For example:

```
b = 10;

c = 25;

x = fzero(@(x) x^3 + b*x + c,0);
```

See Also

- "Create Function Handle"
- "Nested Functions"
- "Anonymous Functions"

Ordinary Differential Equations (ODEs)

- "Choose an ODE Solver" on page 11-2
- "Summary of ODE Options" on page 11-10
- "ODE Event Location" on page 11-13
- "Solve Nonstiff ODEs" on page 11-19
- "Solve Stiff ODEs" on page 11-23
- "Solve Differential Algebraic Equations (DAEs)" on page 11-30
- "Nonnegative ODE Solution" on page 11-35
- "Troubleshoot Common ODE Problems" on page 11-38
- "Differential Equations" on page 11-43
- "Solve Predator-Prey Equations" on page 11-52
- "Solve Equations of Motion for Baton Thrown into Air" on page 11-56
- "Solve ODE with Strongly State-Dependent Mass Matrix" on page 11-62
- "Solve Stiff Transistor Differential Algebraic Equation" on page 11-75
- "Solve System of ODEs with Multiple Initial Conditions" on page 11-80
- "Solve Celestial Mechanics Problem with High-Order Solvers" on page 11-88

Choose an ODE Solver

Ordinary Differential Equations

An ordinary differential equation (ODE) contains one or more derivatives of a dependent variable, y, with respect to a single independent variable, t, usually referred to as time. The notation used here for representing derivatives of y with respect to t is y' for a first derivative, y'' for a second derivative, and so on. The order of the ODE is equal to the highest-order derivative of y that appears in the equation.

For example, this is a second order ODE:

$$y'' = 9y$$

In an *initial value problem*, the ODE is solved by starting from an initial state. Using the initial condition, y_0 , as well as a period of time over which the answer is to be obtained, (t_0, t_f) , the solution is obtained iteratively. At each step the solver applies a particular algorithm to the results of previous steps. At the first such step, the initial condition provides the necessary information that allows the integration to proceed. The final result is that the ODE solver returns a vector of time steps $t = [t_0, t_1, t_2, ..., t_f]$ as well as the corresponding solution at each step $y = [y_0, y_1, y_2, ..., y_f]$.

Types of ODEs

The ODE solvers in MATLAB solve these types of first-order ODEs:

- Explicit ODEs of the form y' = f(t, y).
- Linearly implicit ODEs of the form M(t, y)y' = f(t, y), where M(t, y) is a nonsingular mass matrix. The mass matrix can be time- or state-dependent, or it can be a constant matrix. Linearly implicit ODEs involve linear combinations of the first derivative of y, which are encoded in the mass matrix.

Linearly implicit ODEs can always be transformed to an explicit form, $y' = M^{-1}(t, y)f(t, y)$. However, specifying the mass matrix directly to the ODE solver avoids this transformation, which is inconvenient and can be computationally expensive.

- If some components of y' are missing, then the equations are called *differential algebraic* equations, or DAEs, and the system of DAEs contains some algebraic variables. Algebraic variables are dependent variables whose derivatives do not appear in the equations. A system of DAEs can be rewritten as an equivalent system of first-order ODEs by taking derivatives of the equations to eliminate the algebraic variables. The number of derivatives needed to rewrite a DAE as an ODE is called the differential index. The ode15s and ode23t solvers can solve index-1 DAEs.
- Fully implicit ODEs of the form f(t, y, y') = 0. Fully implicit ODEs cannot be rewritten in an explicit form, and might also contain some algebraic variables. The ode15i solver is designed for fully implicit problems, including index-1 DAEs.

You can supply additional information to the solver for some types of problems by using the odeset function to create an options structure.

Systems of ODEs

You can specify any number of coupled ODE equations to solve, and in principle the number of equations is only limited by available computer memory. If the system of equations has n equations,

$$\begin{pmatrix} y_1' \\ y_2' \\ \vdots \\ y_n' \end{pmatrix} = \begin{pmatrix} f_1(t, y_1, y_2, ..., y_n) \\ f_2(t, y_1, y_2, ..., y_n) \\ \vdots \\ f_n(t, y_1, y_2, ..., y_n) \end{pmatrix},$$

then the function that encodes the equations returns a vector with n elements, corresponding to the values for y_1 , y_2 , ..., y_n . For example, consider the system of two equations

$$\begin{cases} y'_1 = y_2 \\ y'_2 = y_1 y_2 - 2 \end{cases}.$$

A function that encodes these equations is

```
function dy = myODE(t,y)
  dy(1) = y(2);
  dy(2) = y(1)*y(2)-2;
end
```

Higher-Order ODEs

The MATLAB ODE solvers only solve first-order equations. You must rewrite higher-order ODEs as an equivalent system of first-order equations using the generic substitutions

$$y_1 = y$$

 $y_2 = y'$
 $y_3 = y''$
:
:
:
:
:

The result of these substitutions is a system of n first-order equations

$$\begin{aligned} y'_1 &= y_2 \\ y'_2 &= y_3 \\ &\vdots \\ y'_n &= f(t, y_1, y_2, ..., y_n) \end{aligned}$$

For example, consider the third-order ODE

$$y''' - y''y + 1 = 0.$$

Using the substitutions

$$y_1 = y$$
$$y_2 = y'$$
$$y_3 = y''$$

results in the equivalent first-order system

```
y'_2 = y_3
```

The code for this system of equations is then

```
function dydt = f(t,y)
 dydt(1) = y(2);
 dydt(2) = y(3);
 dydt(3) = y(1)*y(3)-1;
```

Complex ODEs

Consider the complex ODE equation

```
y' = f(t, y),
```

where $y = y_1 + iy_2$. To solve it, separate the real and imaginary parts into different solution components, then recombine the results at the end. Conceptually, this looks like

```
yv = [Real(y) Imag(y)]
fv = [\text{Real}(f(t, y)) \text{ Imag}(f(t, y))].
```

For example, if the ODE is y' = yt + 2i, then you can represent the equation using the function file:

```
function f = complexf(t,y)
 f = y.*t + 2*i;
```

Then, the code to separate the real and imaginary parts is

```
function fv = imaginaryODE(t,yv)
 % Construct y from the real and imaginary components
 y = yv(1) + i*yv(2);
 % Evaluate the function
 yp = complexf(t,y);
 % Return real and imaginary in separate components
 fv = [real(yp); imag(yp)];
end
```

When you run a solver to obtain the solution, the initial condition y0 is also separated into real and imaginary parts to provide an initial condition for each solution component.

```
v0 = 1+i:
yv0 = [real(y0); imag(y0)];
tspan = [0 2];
[t,yv] = ode45(@imaginaryODE, tspan, yv0);
```

Once you obtain the solution, combine the real and imaginary components together to obtain the final result.

$$y = yv(:,1) + i*yv(:,2);$$

Basic Solver Selection

ode45 performs well with most ODE problems and should generally be your first choice of solver. However, ode23, ode78, ode89 and ode113 can be more efficient than ode45 for problems with looser or tighter accuracy requirements.

Some ODE problems exhibit *stiffness*, or difficulty in evaluation. Stiffness is a term that defies a precise definition, but in general, stiffness occurs when there is a difference in scaling somewhere in the problem. For example, if an ODE has two solution components that vary on drastically different time scales, then the equation might be stiff. You can identify a problem as stiff if nonstiff solvers (such as ode45) are unable to solve the problem or are extremely slow. If you observe that a nonstiff solver is very slow, try using a stiff solver such as ode15s instead. When using a stiff solver, you can improve reliability and efficiency by supplying the Jacobian matrix or its sparsity pattern.

This table provides general guidelines on when to use each of the different solvers.

Solver	Problem Type	Accuracy	When to Use
ode45	Nonstiff	Medium	Most of the time. ode45 should be the first solver you try.
ode23		Low	ode23 can be more efficient than ode45 at problems with crude tolerances, or in the presence of moderate stiffness.
ode113		Low to High	ode113 can be more efficient than ode45 at problems with stringent error tolerances, or when the ODE function is expensive to evaluate.
ode78		High	ode78 can be more efficient than ode45 at problems with smooth solutions that have high accuracy requirements.
ode89		High	ode89 can be more efficient than ode78 on very smooth problems, when integrating over long time intervals, or when tolerances are especially tight.

Solver	Problem Type	Accuracy	When to Use		
ode15s	Stiff	Low to Medium	Try ode15s when ode4 5 fails or is inefficient and you suspect that the problem is stiff. Also use ode15s when solving differential algebraic equations (DAEs).		
ode23s		Low	ode23s can be more efficient than ode15s at problems with crude error tolerances. It can solve some stiff problems for which ode15s is not effective. ode23s computes the Jacobian in each step, so it is beneficial to provide the Jacobian via odeset to maximize		
			efficiency and accuracy. If there is a mass matrix, it must be constant.		
ode23t		Low	Use ode23t if the problem is only moderately stiff and you need a solution without numerical damping. ode23t can solve		
			differential algebraic equations (DAEs).		
ode23tb		Low	Like ode23s, the ode23tb solver might be more efficient than ode15s at problems with crude error tolerances.		
ode15i	Fully implicit	Low	Use ode15i for fully implicit problems $f(t,y,y') = 0$ and for differential algebraic equations (DAEs) of index 1.		

For details and further recommendations about when to use each solver, see [5].

Summary of ODE Examples and Files

There are several example files available that serve as excellent starting points for most ODE problems. To run the **Differential Equations Examples** app, which lets you easily explore and run examples, type

odeexamples

To open an individual example file for editing, type

edit exampleFileName.m

To run an example, type

exampleFileName

This table contains a list of the available ODE and DAE example files as well as the solvers and options they use. Links are included for the subset of examples that are also published directly in the documentation.

Exampl e File	Solver Used	Options Specified	Description	Documentation Link
amp1da e	ode23t	• 'Mass'	Stiff DAE — electrical circuit with constant, singular mass matrix	"Solve Stiff Transistor Differential Algebraic Equation" on page 11-75
ballod e	ode23	'Events''OutputFcn''OutputSel''Refine''InitialStep''MaxStep'	Simple event location — bouncing ball	"ODE Event Location" on page 11-13
batono de	ode45	• 'Mass'	ODE with time- and state- dependent mass matrix — motion of a baton	"Solve Equations of Motion for Baton Thrown into Air" on page 11-56
brusso de	ode15s	'JPattern''Vectorized'	Stiff large problem — diffusion in a chemical reaction (the Brusselator)	"Solve Stiff ODEs" on page 11-23
burger sode	ode15s	 'Mass' 'MStateDepend ence' 'JPattern' 'MvPattern' 'RelTol' 'AbsTol' 	ODE with strongly state- dependent mass matrix — Burgers' equation solved using a moving mesh technique	"Solve ODE with Strongly State-Dependent Mass Matrix" on page 11-62

Exampl e File	Solver Used	Options Specified	Description	Documentation Link
femlod e	ode15s	'Mass''MStateDepend ence''Jacobian'	Stiff problem with a time- dependent mass matrix — finite element method	_
fem2od e	ode23s	• 'Mass'	Stiff problem with a constant mass matrix — finite element method	_
hb1ode	ode15s	_	Stiff ODE problem solved on a very long interval — Robertson chemical reaction	_
hb1dae	ode15s	'Mass''RelTol''AbsTol''Vectorized'	Stiff, linearly implicit DAE from a conservation law — Robertson chemical reaction	"Solve Robertson Problem as Semi-Explicit Differential Algebraic Equations (DAEs)"
ihb1da e	ode15i	'RelTol''AbsTol''Jacobian'	Stiff, fully implicit DAE — Robertson chemical reaction	"Solve Robertson Problem as Implicit Differential Algebraic Equations (DAEs)"
iburge rsode	ode15i	'RelTol''AbsTol''Jacobian''JPattern'	Implicit ODE system — Burgers' equation	
kneeod e	ode15s	• 'NonNegative'	The "knee problem" with nonnegativity constraints	"Nonnegative ODE Solution" on page 11-35
orbito de	ode45	'RelTol''AbsTol''Events''OutputFcn'	Advanced event location — restricted three body problem	"ODE Event Location" on page 11-13
rigido de	ode45	_	Nonstiff problem — Euler equations of a rigid body without external forces	"Solve Nonstiff ODEs" on page 11-19
vdpode	ode15s	• 'Jacobian'	Parameterizable van der Polequation (stiff for large μ)	"Solve Stiff ODEs" on page 11-23

References

- [1] Shampine, L. F. and M. K. Gordon, Computer Solution of Ordinary Differential Equations: the Initial Value Problem, W. H. Freeman, San Francisco, 1975.
- [2] Forsythe, G., M. Malcolm, and C. Moler, Computer Methods for Mathematical Computations, Prentice-Hall, New Jersey, 1977.

- [3] Kahaner, D., C. Moler, and S. Nash, *Numerical Methods and Software*, Prentice-Hall, New Jersey, 1989.
- [4] Shampine, L. F., Numerical Solution of Ordinary Differential Equations, Chapman & Hall, New York, 1994.
- [5] Shampine, L. F. and M. W. Reichelt, "The MATLAB ODE Suite," SIAM Journal on Scientific Computing, Vol. 18, 1997, pp. 1–22.
- [6] Shampine, L. F., Gladwell, I. and S. Thompson, *Solving ODEs with MATLAB*, Cambridge University Press, Cambridge UK, 2003.

See Also

odeset | odextend

More About

- "Solve Nonstiff ODEs" on page 11-19
- "Solve Stiff ODEs" on page 11-23
- "Solve Differential Algebraic Equations (DAEs)" on page 11-30

External Websites

• Ordinary Differential Equations

Summary of ODE Options

Solving ODEs frequently requires fine-tuning parameters, adjusting error tolerances, or passing additional information to the solver. This topic shows how to specify options, and which differential equation solvers each option is compatible with.

Options Syntax

Use the odeset function to create an options structure that you then pass to the solver as the fourth input argument. For example, to adjust the relative and absolute error tolerances:

```
opts = odeset('RelTol',1e-2,'AbsTol',1e-5);
[t,y] = ode45(@odefun,tspan,y0,opts);
```

If you use the command odeset with no inputs, then MATLAB displays a list of the possible values for each option, with default values indicated by curly braces {}.

The odeget function queries the value of an option in an existing structure, which you can use to dynamically change option values based on conditions. For example, this code detects whether Stats is set to 'on', and changes the value if necessary:

```
if isempty(odeget(opts,'Stats'))
 odeset(opts, 'Stats', 'on')
end
```

Compatibility of Options with Each Solver

Some options in odeset are generic and compatible with any solver, while others are solver-specific. This table summarizes the compatibility of each option with the different solvers.

Optio n Group	Optio n	ode45	ode23	ode78	ode89	ode11 3	ode15 s	ode23 s	ode23 t	ode23 tb	ode15
Error Contro	RelTo l	0	0	0	Ø	0	0	0	0	0	0
1	AbsTo l	0	0	Ø	Ø	0	0	0	0	0	0
	NormC ontro l	0	Ø	9	②	0	0	Ø	②	Ø	0
Solver Output	NonNe gativ e	0	Ø	9	②	0	0	¥	②	Ø	*
	Outpu tFcn	0	0	Ø	Ø	0	0	0	0	Ø	0
	Outpu tSel	0	②	②	②	Ø	Ø	Ø	Ø	Ø	0
	Refin e	0	Ø	Ø	Ø	Ø	Ø	Ø	Ø	Ø	0

Optio n Group	Optio n	ode45	ode23	ode78	ode89	ode11 3	ode15 s	ode23 s	ode23 t	ode23 tb	ode15
	Stats	0	0	0	0	0	0	Ø	0	0	0
Step Size	Initi alSte p	S	9	Ø	Ø	Ø	Ø	9	Ø	Ø	0
	MaxSt ep	Ø	Ø	Ø	Ø	Ø	②	Ø	Ø	0	0
Event Locati on	Event s	8	8	0	0	0	0	8	0	0	(3)
Jacobi an	Jacob ian	×	×	×	×	×	0	Ø	Ø	Ø	0
Matrix	JPatt ern	×	×	×	×	×	0	Ø	0	Ø	0
	Vecto rized	×	×	×	×	×	0	Ø	0	Ø	0
Mass	Mass	0	0	0	0	0	0	0	0	0	×
Matrix and DAEs	MStat eDepe ndenc e	Ø	Ø	②	❷	❷	Ø	*	Ø	Ø	**
	MvPat tern	¥	¥	×	×	×	②	¥	Ø	②	×
	MassS ingul ar	×	×	×	×	×	Ø	×	Ø	×	*
	Initi alSlo pe	×	×	×	¥	¥	0	×	Ø	¥	*
Algorit hm Option s for ode15 s and ode15 i	Max0r der	¥	¥	¥	×	×	0	¥	¥	×	0
	BDF	*	*	*	**	**	9	*	*	*	**

 $^{{}^*}$ Use the NonNegative parameter with ode15s, ode23t, and ode23tb only for those problems in which there is no mass matrix.

^{**} The events function for ode15i must accept a third input argument for yp.

Usage Examples

MATLAB includes several example files that show how to use various options. For example, type edit ballode to see an example that uses 'Events' to specify an events function, or edit batonode to see an example that uses 'Mass' to specify a mass matrix. For a complete summary of example files and which options they use, see "Summary of ODE Examples and Files" on page 11-7.

See Also

odeset | odeget

More About

- "Choose an ODE Solver" on page 11-2
- "ODE Event Location" on page 11-13
- "Nonnegative ODE Solution" on page 11-35

ODE Event Location

What is Event Location?

Part of the difficulty in solving some systems of ODEs is determining an appropriate time to stop the solution. The final time in the interval of integration might be defined by a specific event and not by a number. An example is an apple falling from a tree. The ODE solver should stop once the apple hits the ground, but you might not know when that event would occur beforehand. Similarly, some problems involve events that do not terminate the solution. An example is a moon orbiting a planet. In this case you might not want to stop the integration early, but you still want to detect each time the moon completes one period around the larger body.

Use event functions to detect when certain events occur during the solution of an ODE. Event functions take an expression that you specify, and detect an event when that expression is equal to zero. They can also signal the ODE solver to halt integration when they detect an event.

Writing an Event Function

Use the 'Events' option of the odeset function to specify an event function. The event function must have the general form

```
[value,isterminal,direction] = myEventsFcn(t,y)
```

In the case of ode15i, the event function must also accept a third input argument for yp.

The output arguments value, isterminal, and direction are vectors whose ith element corresponds to the ith event:

- value(i) is a mathematical expression describing the ith event. An event occurs when value(i) is equal to zero.
- isterminal(i) = 1 if the integration is to terminate when the ith event occurs. Otherwise, it is 0.
- direction(i) = 0 if all zeros are to be located (the default). A value of +1 locates only zeros where the event function is increasing, and -1 locates only zeros where the event function is decreasing. Specify direction = [] to use the default value of 0 for all events.

Again, consider the case of an apple falling from a tree. The ODE that represents the falling body is

$$y'' = -1 + y'^2,$$

with the initial conditions y(0) = 1 and y'(0) = 0. You can use an event function to determine when y(t) = 0, which is when the apple hits the ground. For this problem, an event function that detects when the apple hits the ground is

```
function [position,isterminal,direction] = appleEventsFcn(t,y)
  position = y(1); % The value that we want to be zero
  isterminal = 1; % Halt integration
  direction = 0; % The zero can be approached from either direction
end
```

Event Information

If you specify an events function, then call the ODE solver with three extra output arguments, as

```
[t,y,te,ye,ie] = odeXY(odefun,tspan,y0,options)
```

The three additional outputs returned by the solver correspond to the detected events:

- te is a column vector of the times at which events occurred.
- ve contains the solution value at each of the event times in te.
- ie contains indices into the vector returned by the event function. The values indicate which event the solver detected.

Alternatively, you can call the solver with a single output, as

```
sol = odeXY(odefun,tspan,y0,options)
```

In this case, the event information is stored in the structure as sol.te, sol.ye, and sol.ie.

Limitations

The root-finding mechanism employed by the ODE solver in conjunction with the event function has these limitations:

- If a terminal event occurs during the first step of the integration, then the solver registers the event as nonterminal and continues integrating.
- If more than one terminal event occurs during the first step, then only the first event registers and the solver continues integrating.
- Zeros are determined by sign crossings between steps. Therefore, zeros of functions with an even number of crossings between steps can be missed.

If the solver steps past events, try reducing RelTol and AbsTol to improve accuracy. Alternatively, set MaxStep to place an upper bound on the step size. Adjusting tspan does not change the steps taken by the solver.

Simple Event Location: A Bouncing Ball

This example shows how to write a simple event function for use with an ODE solver. The example file ballode models the motion of a bouncing ball. The events function halts the integration each time the ball bounces, and the integration then restarts with new initial conditions. As the ball bounces, the integration stops and restarts several times.

The equations for the bouncing ball are

$$y'_1 = y_2$$

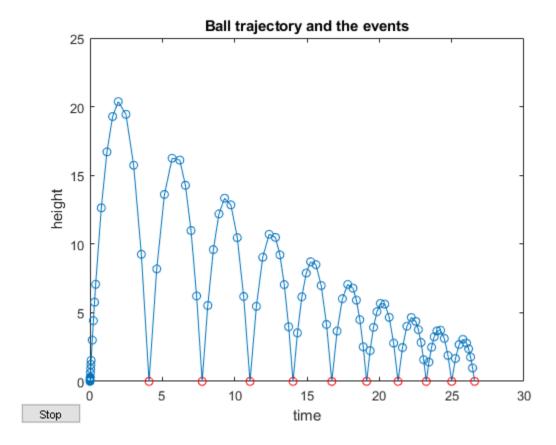
 $y'_2 = -9.8$.

A ball bounce occurs when the height of the ball $y_1(t)$ is equal to zero after decreasing. An events function that codes this behavior is

```
function [value,isterminal,direction] = bounceEvents(t,y)
```

Type ballode to run the example and illustrate the use of an events function to simulate the bouncing of a ball.

ballode



Advanced Event Location: Restricted Three Body Problem

This example shows how to use the directional components of an event function. The example file orbitode simulates a restricted three body problem where one body is orbiting two much larger bodies. The events function determines the points in the orbit where the orbiting body is closest and farthest away. Since the value of the events function is the same at the closest and farthest points of the orbit, the direction of zero crossing is what distinguishes them.

The equations for the restricted three body problem are

$$\begin{array}{ll} y_1' &= y_3 \\ y_2' &= y_4 \\ y_3' &= 2y_4 + y_1 - \frac{\mu^*(y_1 + \mu)}{r_1^3} - \frac{\mu(y_1 - \mu^*)}{r_2^3} \\ y_4' &= -2y_3 + y_2 - \frac{\mu^* y_2}{r_1^3} - \frac{\mu y_2}{r_2^3}, \end{array}$$

where

$$\mu = 1/82.45
\mu^* = 1 - \mu
r_1 = \sqrt{(y_1 + \mu)^2 + y_2^2}
r_2 = \sqrt{(y_1 - \mu^*)^2 + y_2^2}.$$

The first two solution components are coordinates of the body of infinitesimal mass, so plotting one against the other gives the orbit of the body.

The events function nested in orbitode.m searches for two events. One event locates the point of maximum distance from the starting point, and the other locates the point where the spaceship returns to the starting point. The events are located accurately, even though the step sizes used by the integrator are not determined by the locations of the events. In this example, the ability to specify the direction of the zero crossing is critical. Both the point of return to the starting point and the point of maximum distance from the starting point have the same event values, and the direction of the crossing is used to distinguish them. An events function that codes this behavior is

```
function [value,isterminal,direction] = orbitEvents(t,y)
st dDSQdt is the derivative of the equation for current distance. Local
% minimum/maximum occurs when this value is zero.
dDSQdt = 2 * ((y(1:2)-y0(1:2))' * y(3:4));
value = [dDSQdt; dDSQdt];
isterminal = [1; 0];
                              % stop at local minimum
direction = [1; -1];
                              % [local minimum, local maximum]
end
```

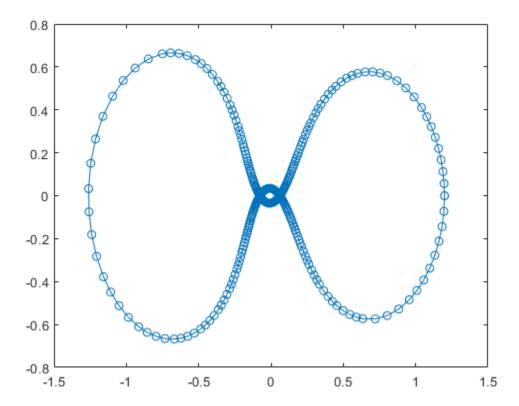
Type orbitode to run the example.

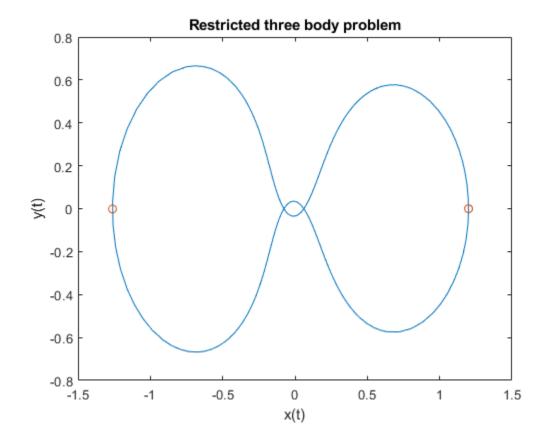
orbitode

This is an example of event location where the ability to specify the direction of the zero crossing is critical. Both the point of return to the initial point and the point of maximum distance have the same event function value, and the direction of the crossing is used to distinguish them.

Calling ODE45 with event functions active...

Note that the step sizes used by the integrator are NOT determined by the location of the events, and the events are still located accurately.





See Also

odeset | odeget

More About

- "Choose an ODE Solver" on page 11-2
- "Summary of ODE Options" on page 11-10
- "Parameterizing Functions" on page 10-2

Solve Nonstiff ODEs

This page contains two examples of solving nonstiff ordinary differential equations using ode45. MATLAB® has several solvers for nonstiff ODEs.

- ode45
- ode23
- ode78
- ode89
- ode113

For most nonstiff problems, ode45 performs best. However, ode23 is recommended for problems that permit a slightly cruder error tolerance or in the presence of moderate stiffness. Likewise, ode113 can be more efficient than ode45 for problems with more stringent error tolerances or when the ODE function is computationally expensive to evaluate. ode78 and ode89 are high-order solvers that excel with long integrations where accuracy is crucial for stability.

If the nonstiff solvers take a long time to solve the problem or consistently fail the integration, then the problem might be *stiff*. See "Solve Stiff ODEs" on page 11-23 for more information.

Example: Nonstiff van der Pol Equation

The van der Pol equation is a second order ODE

$$y_1'' - \mu \left(1 - y_1^2\right) y_1' + y_1 = 0,$$

where $\mu > 0$ is a scalar parameter. Rewrite this equation as a system of first-order ODEs by making the substitution $y'_1 = y_2$. The resulting system of first-order ODEs is

$$y'_1 = y_2$$

 $y'_2 = \mu(1 - y_1^2)y_2 - y_1.$

The system of ODEs must be coded into a function file that the ODE solver can use. The general functional signature of an ODE function is

```
dydt = odefun(t,y)
```

That is, the function must accept both t and y as inputs, even if it does not use t for any computations.

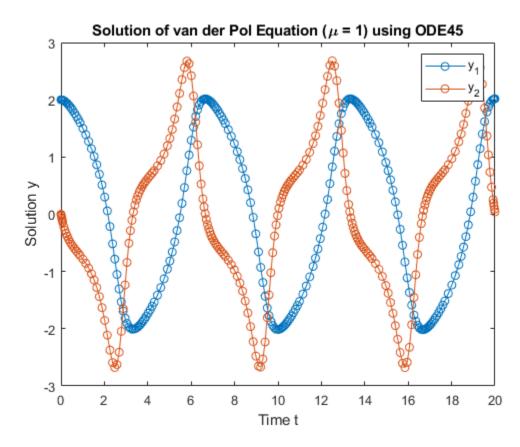
The function file vdp1.m codes the van der Pol equation using $\mu = 1$. The variables y_1 and y_2 are represented by y(1) and y(2), and the two-element column vector dydt contains the expressions for y_1' and y_2' .

```
function dydt = vdp1(t,y)
%VDP1 Evaluate the van der Pol ODEs for mu = 1
%
%    See also ODE113, ODE23, ODE45.
%    Jacek Kierzenka and Lawrence F. Shampine
```

```
Copyright 1984-2014 The MathWorks, Inc.
dydt = [y(2); (1-y(1)^2)*y(2)-y(1)];
```

Solve the ODE using the ode45 function on the time interval [0 20] with initial values [2 0]. The output is a column vector of time points t and a solution array y. Each row in y corresponds to a time returned in the corresponding row of t. The first column of y corresponds to 91, and the second column to y_2 .

```
[t,y] = ode45(@vdp1,[0 20],[2; 0]);
Plot the solutions for y_1 and y_2 against t.
plot(t,y(:,1),'-0',t,y(:,2),'-0')
title('Solution of van der Pol Equation (\mu = 1) using ODE45');
xlabel('Time t');
ylabel('Solution y');
legend('y 1','y 2')
```



The vdpode function solves the same problem, but it accepts a user-specified value for μ . The van der Pol equations become stiff as μ increases. For example, with the value $\mu=1000$ vou need to use a stiff solver such as ode15s to solve the system.

Example: Nonstiff Euler Equations

The Euler equations for a rigid body without external forces are a standard test problem for ODE solvers intended for nonstiff problems.

The equations are

```
y'_1 = y_2y_3

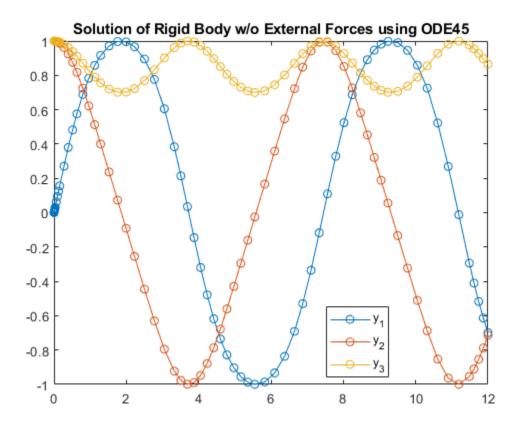
y'_2 = -y_1y_3

y'_3 = -0.51y_1y_2.
```

The function file rigidode defines and solves this first-order system of equations over the time interval [0 12], using the vector of initial conditions [0; 1; 1] corresponding to the initial values of y_1 , y_2 , and y_3 . The local function f(t,y) encodes the system of equations.

rigidode calls ode45 with no output arguments, so the solver uses the default output function odeplot to automatically plot the solution points after each step.

```
function rigidode
%RIGIDODE Euler equations of a rigid body without external forces.
   A standard test problem for non-stiff solvers proposed by Krogh. The
   analytical solutions are Jacobian elliptic functions, accessible in
%
   MATLAB. The interval here is about 1.5 periods; it is that for which
%
   solutions are plotted on p. 243 of Shampine and Gordon.
%
%
   L. F. Shampine and M. K. Gordon, Computer Solution of Ordinary
   Differential Equations, W.H. Freeman & Co., 1975.
%
%
   See also ODE45, ODE23, ODE113, FUNCTION HANDLE.
%
   Mark W. Reichelt and Lawrence F. Shampine, 3-23-94, 4-19-94
   Copyright 1984-2014 The MathWorks, Inc.
tspan = [0 12];
y0 = [0; 1; 1];
% solve the problem using ODE45
figure;
ode45(@f,tspan,y0);
                    _____
function dydt = f(t,y)
dydt = [ y(2)*y(3)
   -y(1)*y(3)
   -0.51*y(1)*y(2) ];
Solve the nonstiff Euler equations by calling the rigidode function.
rigidode
title('Solution of Rigid Body w/o External Forces using ODE45')
legend('y_1','y_2','y_3','Location','Best')
```



See Also ode45 | ode23 | ode78 | ode89 | ode113

More About

- "Choose an ODE Solver" on page 11-2
- "Parameterizing Functions" on page 10-2

External Websites

Qualitative Analysis of ODEs (MathWorks Teaching Resources)

Solve Stiff ODEs

This page contains two examples of solving stiff ordinary differential equations using ode15s. MATLAB® has four solvers designed for stiff ODEs.

- ode15s
- ode23s
- ode23t
- ode23tb

For most stiff problems, ode15s performs best. However, ode23s, ode23t, and ode23tb can be more efficient if the problem permits a crude error tolerance.

What is a Stiff ODE?

For some ODE problems, the step size taken by the solver is forced down to an unreasonably small level in comparison to the interval of integration, even in a region where the solution curve is smooth. These step sizes can be so small that traversing a short time interval might require millions of evaluations. This can lead to the solver failing the integration, but even if it succeeds it will take a very long time to do so.

Equations that cause this behavior in ODE solvers are said to be *stiff*. The problem that stiff ODEs pose is that explicit solvers (such as ode45) are untenably slow in achieving a solution. This is why ode45 is classified as a *nonstiff solver* along with ode23, ode78, ode89, and ode113.

Solvers that are designed for stiff ODEs, known as *stiff solvers*, typically do more work per step. The pay-off is that they are able to take much larger steps, and have improved numerical stability compared to the nonstiff solvers.

Solver Options

For stiff problems, specifying the Jacobian matrix using odeset is particularly important. Stiff solvers use the Jacobian matrix $\partial f_i/\partial y_i$ to estimate the local behavior of the ODE as the integration proceeds, so supplying the Jacobian matrix (or, for large sparse systems, its sparsity pattern) is critical for efficiency and reliability. Use the Jacobian, JPattern, or Vectorized options of odeset to specify information about the Jacobian. If you do not supply the Jacobian then the solver estimates it numerically using finite differences.

See odeset for a complete listing of other solver options.

Example: Stiff van der Pol Equation

The van der Pol equation is a second order ODE

$$y_1'' - \mu \left(1 - y_1^2\right) y_1' + y_1 = 0,$$

where $\mu > 0$ is a scalar parameter. When $\mu = 1$, the resulting system of ODEs is nonstiff and easily solved using ode45. However, if you increase μ to 1000, then the solution changes dramatically and exhibits oscillation on a much longer time scale. Approximating the solution of the initial value problem becomes more difficult. Because this particular problem is stiff, a solver intended for nonstiff problems, such as ode45, is too inefficient to be practical. Use a stiff solver such as ode15s for this problem instead.

Rewrite the van der Pol equation as a system of first-order ODEs by making the substitution $y_1 = y_2$. The resulting system of first-order ODEs is

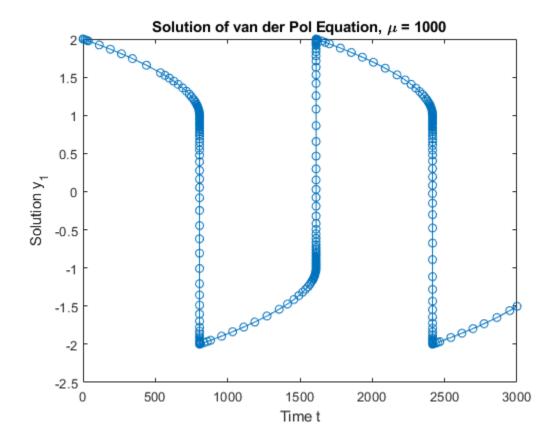
```
y'_1 = y_2
y_2' = \mu(1 - y_1^2)y_2 - y_1.
```

The vdp1000 function evaluates the van der Pol equation using $\mu = 1000$.

```
function dydt = vdp1000(t,y)
%VDP1000 Evaluate the van der Pol ODEs for mu = 1000.
%
   See also ODE15S, ODE23S, ODE23T, ODE23TB.
   Jacek Kierzenka and Lawrence F. Shampine
   Copyright 1984-2014 The MathWorks, Inc.
dydt = [y(2); 1000*(1-y(1)^2)*y(2)-y(1)];
```

Use the ode15s function to solve the problem with an initial conditions vector of [2; 0], over a time interval of [0 3000]. For scaling reasons, plot only the first component of the solution.

```
[t,y] = ode15s(@vdp1000,[0 3000],[2; 0]);
plot(t,y(:,1),'-o');
title('Solution of van der Pol Equation, \mu = 1000');
xlabel('Time t');
ylabel('Solution y 1');
```



The vdpode function also solves the same problem, but it accepts a user-specified value for μ . The equations become increasingly stiff as μ increases.

Example: Sparse Brusselator System

The classic Brusselator system of equations is potentially large, stiff, and sparse. The Brusselator system models diffusion in a chemical reaction, and is represented by a system of equations involving u, v, u', and v'.

$$\begin{array}{ll} u_i' &= 1 + u_i^2 v_i - 4 u_i + \alpha \left(N+1\right)^2 \left(u_{i-1} - 2_i + u_{i+1}\right) \\ v_i' &= 3 u_i - u_i^2 v_i + \alpha \left(N+1\right)^2 \left(v_{i-1} - 2 v_i + v_{i+1}\right) \end{array}$$

The function file brussode solves this set of equations on the time interval [0,10] with $\alpha = 1/50$. The initial conditions are

$$u_j(0) = 1 + \sin(2\pi x_j)$$

 $v_j(0) = 3,$

where $x_j=i/N+1$ for i=1,...,N. Therefore, there are 2N equations in the system, but the Jacobian $\partial f/\partial y$ is a banded matrix with a constant width of 5 if the equations are ordered as $u_1,v_1,u_2,v_2,...$. As N increases, the problem becomes increasingly stiff, and the Jacobian becomes increasingly sparse.

The function call brussode (N), for $N \geq 2$, specifies a value for N in the system of equations, corresponding to the number of grid points. By default, brussode uses N=20.

brussode contains a few subfunctions:

- The nested function f(t,y) encodes the system of equations for the Brusselator problem, returning a vector.
- The local function jpattern(N) returns a sparse matrix of 1s and 0s showing the locations of nonzeros in the Jacobian. This matrix is assigned to the JPattern field of the options structure. The ODE solver uses this sparsity pattern to generate the Jacobian numerically as a sparse matrix. Supplying this sparsity pattern in the problem significantly reduces the number of function evaluations required to generate the 2N-by-2N Jacobian, from 2N evaluations to just 4.

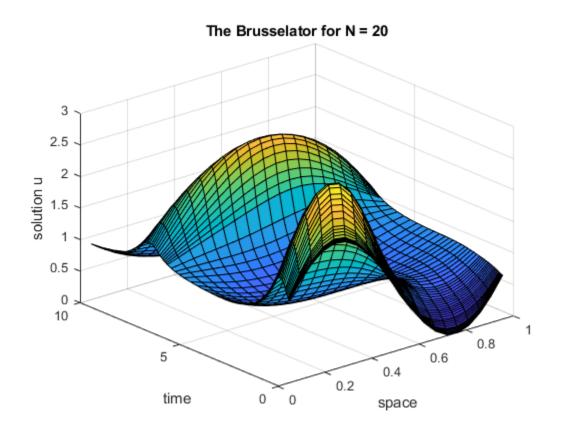
```
function brussode(N)
%BRUSSODE Stiff problem modelling a chemical reaction (the Brusselator).
    The parameter N \ge 2 is used to specify the number of grid points; the
    resulting system consists of 2N equations. By default, N is 20. The
    problem becomes increasingly stiff and increasingly sparse as N is
    increased. The Jacobian for this problem is a sparse constant matrix
    (banded with bandwidth 5).
%
%
    The property 'JPattern' is used to provide the solver with a sparse
%
%
    matrix of 1's and 0's showing the locations of nonzeros in the Jacobian
    df/dy. By default, the stiff solvers of the ODE Suite generate Jacobians
%
%
    numerically as full matrices. However, when a sparsity pattern is
%
    provided, the solver uses it to generate the Jacobian numerically as a
%
    sparse matrix. Providing a sparsity pattern can significantly reduce the
    number of function evaluations required to generate the Jacobian and can
%
%
    accelerate integration. For the BRUSSODE problem, only 4 evaluations of
%
    the function are needed to compute the 2N x 2N Jacobian matrix.
%
%
    Setting the 'Vectorized' property indicates the function f is
%
    vectorized.
%
%
    E. Hairer and G. Wanner, Solving Ordinary Differential Equations II,
%
    Stiff and Differential-Algebraic Problems, Springer-Verlag, Berlin,
%
    1991, pp. 5-8.
%
    See also ODE15S, ODE23S, ODE23T, ODE23TB, ODESET, FUNCTION HANDLE.
%
%
    Mark W. Reichelt and Lawrence F. Shampine, 8-30-94
    Copyright 1984-2014 The MathWorks, Inc.
% Problem parameter, shared with the nested function.
if nargin<1</pre>
   N = 20;
end
tspan = [0; 10];
y0 = [1+\sin((2*pi/(N+1))*(1:N)); repmat(3,1,N)];
options = odeset('Vectorized','on','JPattern',jpattern(N));
[t,y] = ode15s(@f,tspan,y0,options);
```

u = y(:,1:2:end);

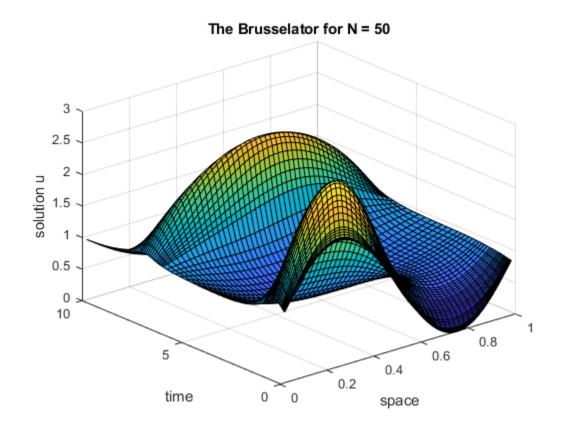
```
x = (1:N)/(N+1);
figure;
surf(x,t,u);
view(-40,30);
xlabel('space');
ylabel('time');
zlabel('solution u');
title(['The Brusselator for N = ' num2str(N)]);
% Nested function -- N is provided by the outer function.
   function dydt = f(t,y)
      % Derivative function
      c = 0.02 * (N+1)^2;
      % Evaluate the 2 components of the function at one edge of the grid
      % (with edge conditions).
      i = 1;
      dydt(i,:) = 1 + y(i+1,:).*y(i,:).^2 - 4*y(i,:) + c*(1-2*y(i,:)+y(i+2,:));
      dydt(i+1,:) = 3*y(i,:) - y(i+1,:).*y(i,:).^2 + c*(3-2*y(i+1,:)+y(i+3,:));
      % Evaluate the 2 components of the function at all interior grid points.
      i = 3:2:2*N-3;
      dydt(i,:) = 1 + y(i+1,:).*y(i,:).^2 - 4*y(i,:) + ...
         c*(y(i-2,:)-2*y(i,:)+y(i+2,:));
      dydt(i+1,:) = 3*y(i,:) - y(i+1,:).*y(i,:).^2 + ...
         c*(y(i-1,:)-2*y(i+1,:)+y(i+3,:));
      % Evaluate the 2 components of the function at the other edge of the grid
      % (with edge conditions).
      i = 2*N-1;
      \mathsf{dydt}(\mathtt{i},:) \ = \ 1 \ + \ \mathsf{y}(\mathtt{i}+1,:) \ .^*\mathsf{y}(\mathtt{i},:) \ .^2 \ - \ 4^*\mathsf{y}(\mathtt{i},:) \ + \ \mathsf{c}^*(\mathsf{y}(\mathtt{i}-2,:) \ - 2^*\mathsf{y}(\mathtt{i},:) + 1);
      dydt(i+1,:) = 3*y(i,:) - y(i+1,:).*y(i,:).^2 + c*(y(i-1,:)-2*y(i+1,:)+3);
   end
end % brussode
% Subfunction -- the sparsity pattern
function S = jpattern(N)
% Jacobian sparsity pattern
B = ones(2*N,5);
B(2:2:2*N,2) = zeros(N,1);
B(1:2:2*N-1,4) = zeros(N,1);
S = spdiags(B, -2:2, 2*N, 2*N);
```

Solve the Brusselator system for N=20 by running the function brussode.

brussode



Solve the system for N=50 by specifying an input to brussode. brussode(50)



See Also

ode15s | ode23s | ode23t | ode23tb

More About

- "Choose an ODE Solver" on page 11-2
- "Summary of ODE Options" on page 11-10
- "Parameterizing Functions" on page 10-2

Solve Differential Algebraic Equations (DAEs)

In this section...

"What is a Differential Algebraic Equation?" on page 11-30

"Consistent Initial Conditions" on page 11-31

"Differential Index" on page 11-31

"Imposing Nonnegativity" on page 11-32

"Solve Robertson Problem as Semi-Explicit Differential Algebraic Equations (DAEs)" on page 11-32

What is a Differential Algebraic Equation?

Differential algebraic equations are a type of differential equation where one or more derivatives of dependent variables are not present in the equations. Variables that appear in the equations without their derivative are called *algebraic*, and the presence of algebraic variables means that you cannot write down the equations in the explicit form y' = f(t, y). Instead, you can solve DAEs with these

The ode15s and ode23t solvers can solve index-1 linearly implicit problems with a singular mass matrix M(t, y)y' = f(t, y), including semi-explicit DAEs of the form

$$y' = f(t, y, z)$$
$$0 = g(t, y, z).$$

In this form, the presence of algebraic variables leads to a singular mass matrix, since there are one or more zeros on the main diagonal.

$$My' = \begin{pmatrix} y'_1 & 0 & \cdots & 0 \\ 0 & y'_2 & 0 & \vdots \\ \vdots & 0 & \ddots & 0 \\ 0 & \cdots & 0 & 0 \end{pmatrix}.$$

By default, solvers automatically test the singularity of the mass matrix to detect DAE systems. If you know about singularity ahead of time then you can set the MassSingular option of odeset to 'yes'. With DAEs, you can also provide the solver with a quess of the initial conditions for y_0 using the InitialSlope property of odeset. This is in addition to specifying the usual initial conditions for y_0 in the call to the solver.

The ode15i solver can solve more general DAEs in the fully implicit form

$$f(t, y, y') = 0.$$

In the fully implicit form, the presence of algebraic variables leads to a singular Jacobian matrix. This is because at least one of the columns in the matrix is guaranteed to contain all zeros, since the derivative of that variable does not appear in the equations.

$$J = \partial f / \partial y' = \begin{pmatrix} \frac{\partial f_1}{\partial y'_1} & \cdots & \frac{\partial f_1}{\partial y'_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial y'_1} & \cdots & \frac{\partial f_m}{\partial y'_n} \end{pmatrix}$$

The ode15i solver requires that you specify initial conditions for both y'_0 and y_0 . Also, unlike the other ODE solvers, ode15i requires the function encoding the equations to accept an extra input: odefun(t,y,yp).

DAEs arise in a wide variety of systems because physical conservation laws often have forms like x + y + z = 0. If x, x', y, and y' are defined explicitly in the equations, then this conservation equation is sufficient to solve for z without having an expression for z'.

Consistent Initial Conditions

When you are solving a DAE, you can specify initial conditions for both y_0 and y_0 . The ode15i solver requires both initial conditions to be specified as input arguments. For the ode15s and ode23t solvers, the initial condition for y_0 is optional (but can be specified using the InitialSlope option of odeset). In both cases, it is possible that the initial conditions you specify do not agree with the equations you are trying to solve. Initial conditions that conflict with one another are called *inconsistent*. The treatment of the initial conditions varies by solver:

- ode15s and ode23t If you do not specify an initial condition for y'_0 , then the solver automatically computes consistent initial conditions based on the initial condition you provide for y_0 . If you specify an inconsistent initial condition for y'_0 , then the solver treats the values as guesses, attempts to compute consistent values close to the guesses, and continues on to solve the problem.
- ode15i The initial conditions you supply to the solver must be consistent, and ode15i does not
 check the supplied values for consistency. The helper function decic computes consistent initial
 conditions for this purpose.

Differential Index

DAEs are characterized by their *differential index*, which is a measure of their singularity. By differentiating equations you can eliminate algebraic variables, and if you do this enough times then the equations take the form of a system of explicit ODEs. The differential index of a system of DAEs is the number of derivatives you must take to express the system as an equivalent system of explicit ODEs. Thus, ODEs have a differential index of 0.

An example of an index-1 DAE is

$$v(t) = k(t)$$
.

For this equation, you can take a single derivative to obtain the explicit ODE form

$$y'=k'(t) .$$

An example of an index-2 DAE is

$$y'_1 = y_2$$

0 = $k(t) - y_1$.

These equations require two derivatives to be rewritten in the explicit ODE form

$$y'_1 = k'(t)$$

$$y'_2 = k''(t) .$$

The ode15s and ode23t solvers only solve DAEs of index 1. If the index of your equations is 2 or higher, then you need to rewrite the equations as an equivalent system of index-1 DAEs. It is always possible to take derivatives and rewrite a DAE system as an equivalent system of index-1 DAEs. Be aware that if you replace algebraic equations with their derivatives, then you might have removed some constraints. If the equations no longer include the original constraints, then the numerical solution can drift.

If you have Symbolic Math Toolbox, then see "Solve Differential Algebraic Equations (DAEs)" (Symbolic Math Toolbox) for more information.

Imposing Nonnegativity

Most of the options in odeset on page 11-10 work as expected with the DAE solvers ode15s. ode23t, and ode15i. However, one notable exception is with the use of the NonNegative on page 11-35 option. The NonNegative option does not support implicit solvers (ode15s, ode23t, ode23tb) applied to problems with a mass matrix. Therefore, you cannot use this option to impose nonnegativity constraints on a DAE problem, which necessarily has a singular mass matrix. For more details, see [1].

Solve Robertson Problem as Semi-Explicit Differential Algebraic **Equations (DAEs)**

This example reformulates a system of ODEs as a system of differential algebraic equations (DAEs). The Robertson problem found in hb1ode.m is a classic test problem for programs that solve stiff ODEs. The system of equations is

$$\begin{array}{ll} y_1' &= -0.04y_1 + 10^4 y_2 y_3 \\ y_2' &= 0.04y_1 - 10^4 y_2 y_3 - (3 \times 10^7) y_2^2 \\ y_3' &= (3 \times 10^7) y_2^2. \end{array}$$

hblode solves this system of ODEs to steady state with the initial conditions $y_1 = 1$, $y_2 = 0$, and $y_3 = 0$. But the equations also satisfy a linear conservation law,

$$y_1' + y_2' + y_3' = 0.$$

In terms of the solution and initial conditions, the conservation law is

$$y_1 + y_2 + y_3 = 1$$
.

The system of equations can be rewritten as a system of DAEs by using the conservation law to determine the state of \(\mathcal{Y} \)3. This reformulates the problem as the DAE system

$$\begin{array}{ll} y_1' &= -0.04y_1 + 10^4 y_2 y_3 \\ y_2' &= 0.04y_1 - 10^4 y_2 y_3 - (3 \times 10^7) y_2^2 \\ 0 &= y_1 + y_2 + y_3 - 1. \end{array}$$

The differential index of this system is 1, since only a single derivative of \(\mathcal{Y} \) is required to make this a system of ODEs. Therefore, no further transformations are required before solving the system.

The function robertsdae encodes this DAE system. Save robertsdae.m in your current folder to run the example.

```
function out = robertsdae(t,y)
out = [-0.04*y(1) + 1e4*y(2).*y(3)
    0.04*y(1) - 1e4*y(2).*y(3) - 3e7*y(2).^2
    y(1) + y(2) + y(3) - 1 ];
```

The full example code for this formulation of the Robertson problem is available in hb1dae.m.

Solve the DAE system using ode15s. Consistent initial conditions for y0 are obvious based on the conservation law. Use odeset to set the options:

• Use a constant mass matrix to represent the left hand side of the system of equations.

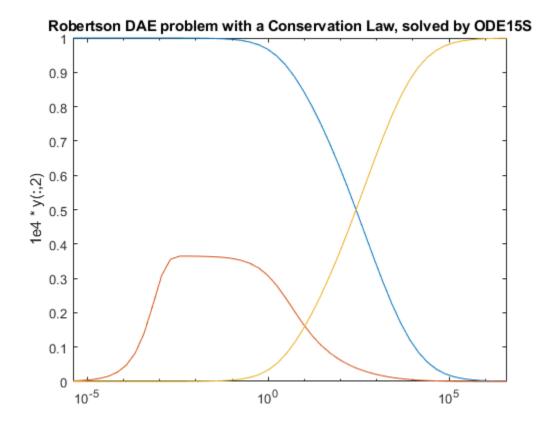
$$\left(\begin{array}{c} y_1' \\ y_2' \\ 0 \end{array}\right) = My' \to M = \left(\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{array}\right)$$

- Set the relative error tolerance to 1e-4.
- Use an absolute tolerance of 1e-10 for the second solution component, since the scale varies dramatically from the other components.
- Leave the 'MassSingular' option at its default value 'maybe' to test the automatic detection of a DAE.

```
y0 = [1; 0; 0];
tspan = [0 4*logspace(-6,6)];
M = [1 0 0; 0 1 0; 0 0 0];
options = odeset('Mass',M,'RelTol',1e-4,'AbsTol',[1e-6 1e-10 1e-6]);
[t,y] = ode15s(@robertsdae,tspan,y0,options);

Plot the solution.

y(:,2) = 1e4*y(:,2);
semilogx(t,y);
ylabel('1e4 * y(:,2)');
title('Robertson DAE problem with a Conservation Law, solved by ODE15S');
```



References

[1] Shampine, L.F., S. Thompson, J.A. Kierzenka, and G.D. Byrne. "Non-Negative Solutions of ODEs." Applied Mathematics and Computation 170, no. 1 (November 2005): 556-569. https://doi.org/ 10.1016/j.amc.2004.12.011.

See Also

ode15s | ode23t | ode15i | odeset

More About

- "Choose an ODE Solver" on page 11-2
- "Summary of ODE Options" on page 11-10
- "Equation Solving" (Symbolic Math Toolbox)

External Websites

Solving Index-1 DAEs in MATLAB and Simulink

Nonnegative ODE Solution

This topic shows how to constrain the solution of an ODE to be nonnegative. Imposing nonnegativity is not always trivial, but sometimes it is necessary due to the physical interpretation of the equations or due to the nature of the solution. You should only impose this constraint on the solution when necessary, such as in cases where the integration fails without it, or where the solution would be inapplicable.

If certain components of the solution must be nonnegative, then use odeset to set the NonNegative option for the indices of these components. This option is not available for ode23s, ode15i, or for implicit solvers (ode15s, ode23t, ode23tb) applied to problems with a mass matrix. In particular, you cannot impose nonnegativity constraints on a DAE problem, which necessarily has a singular mass matrix.

Example: Absolute Value Function

Consider the initial value problem

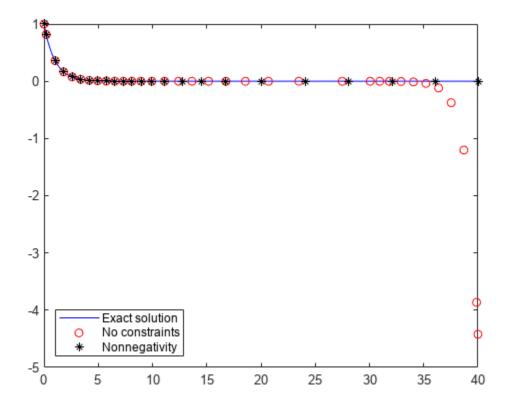
```
y' = -|y|,
```

solved on the interval [0,40] with the initial condition y(0)=1. The solution of this ODE decays to zero. If the solver produces a negative solution value, then it begins to track the solution of the ODE through this value, and the computation eventually fails as the calculated solution diverges to $-\infty$. Using the NonNegative option prevents this integration failure.

Compare the analytic solution of $y(t) = e^{-t}$ to a solution of the ODE using ode45 with no extra options, and to one with the NonNegative option set.

```
ode = @(t,y) -abs(y);
% Standard solution with |ode45|
options1 = odeset('Refine',1);
[t0,y0] = ode45(ode,[0 40],1,options1);
% Solution with nonnegative constraint
options2 = odeset(options1,'NonNegative',1);
[t1,y1] = ode45(ode,[0 40],1,options2);
% Analytic solution
t = linspace(0,40,1000);
y = exp(-t);
```

Plot the three solutions for comparison. Imposing nonnegativity is crucial to keep the solution from veering off toward $-\infty$.



Example: The Knee Problem

Another example of a problem that requires a nonnegative solution is the knee problem coded in the example file kneede. The equation is

$$\epsilon y' = (1 - x)y - y^2,$$

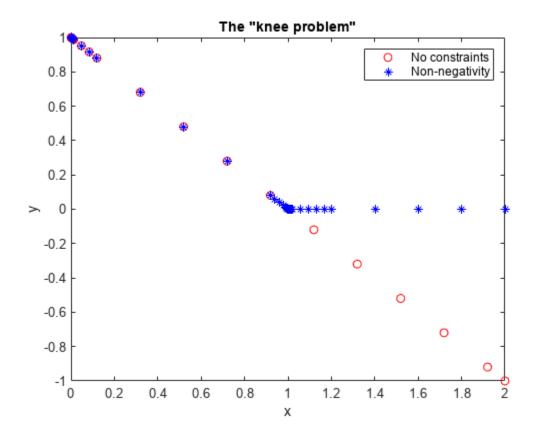
solved on the interval [0,2] with the initial condition y(0)=1. The parameter ϵ generally is taken to satisfy $0 < \epsilon \ll 1$, and this problem uses $\epsilon = 1 \times 10^{-6}$. The solution to this ODE approaches y = 1 - xfor x < 1 and y = 0 for x > 1. However, computing the numerical solution with default tolerances shows that the solution follows the y = 1 - x isocline for the whole interval of integration. Imposing nonnegativity constraints results in the correct solution.

Solve the knee problem with and without nonnegativity constraints.

```
epsilon = 1e-6;
y0 = 1;
xspan = [0 2];
odefcn = @(x,y,epsilon) ((1-x)*y - y^2)/epsilon;
% Solve without imposing constraints
[x1,y1] = ode15s(@(x,y) odefcn(x,y,epsilon), xspan, y0);
% Impose a nonnegativity constraint
options = odeset('NonNegative',1);
[x2,y2] = ode15s(@(x,y) odefcn(x,y,epsilon), xspan, y0, options);
```

Plot the solutions for comparison.

```
plot(x1,y1,'ro',x2,y2,'b*')
axis([0,2,-1,1])
title('The "knee problem"')
legend('No constraints','Non-negativity')
xlabel('x')
ylabel('y')
```



References

[1] Shampine, L.F., S. Thompson, J.A. Kierzenka, and G.D. Byrne, "Non-negative solutions of ODEs," *Applied Mathematics and Computation* Vol. 170, 2005, pp. 556-569.

See Also

odeset

More About

- "Choose an ODE Solver" on page 11-2
- "Summary of ODE Options" on page 11-10

Troubleshoot Common ODE Problems

Error Tolerances

Question or Problem	Answer
How do I choose the error thresholds RelTol and AbsTol?	RelTol, the relative accuracy tolerance, controls the number of correct digits in the computed answer. AbsTol, the absolute error tolerance, controls the difference between the computed answer and the true solution. At each step, the error e in component i of the solution satisfies
	<pre> e(i) ≤ max(RelTol*abs(y(i)),AbsTol(i))</pre>
	Roughly speaking, this means that you want RelTol correct digits in all solution components, excluding those smaller than the threshold AbsTol(i). Even if you are not interested in a component y(i) when it is small, you might have to specify a value for AbsTol(i) that is small enough to get some correct digits in y(i) so that you can accurately compute more interesting components.
I want answers that are correct to the precision of the computer. Why can I not simply set RelTol to eps?	You can get close to machine precision, but not that close. The solvers do not allow RelTol near eps because they try to approximate a continuous function. At tolerances comparable to eps, the machine arithmetic causes all functions to look discontinuous.
How do I tell the solver that I do not care about getting an accurate answer for one of the solution components?	You can increase the absolute error tolerance AbsTol for this solution component. If the tolerance is bigger than the solution component, this specifies that no digits in the component need to be correct. The solver might have to get some correct digits in this component to compute other components accurately, but it generally handles this automatically.

Problem Scale

Question or Problem	Answer
How large a problem can I solve with the ODE suite?	The primary constraints are memory and time. At each time step, the solvers for nonstiff problems allocate vectors of length n, where n is the number of equations in the system. The solvers for stiff problems allocate vectors of length n but also allocate an n-by-n Jacobian matrix. For these solvers, it might be advantageous to specify the Jacobian sparsity pattern using the JPattern option of odeset.
	If the problem is nonstiff, or if you are using the JPattern option, it might be possible to solve a problem with thousands of unknowns. In this case, however, storage of the result can be problematic. Ask the solver to evaluate the solution at specific points only, or call the solver with no output arguments and use an output function to monitor the solution.
I am solving a very large system, but only care about a few of the components of y. Is there any way to avoid storing all of the elements?	Yes. The OutputFcn option is designed specifically for this purpose. When you call the solver with no output arguments, the solver does not allocate storage to hold the entire solution history. Instead, the solver calls OutputFcn(t,y,flag) at each time step. To keep the history of specific elements, write an output function that stores or plots only the elements you care about.
What is the startup cost of the integration and how can I reduce it?	The biggest startup cost occurs as the solver attempts to find a step size appropriate to the scale of the problem. If you happen to know an appropriate step size, use the InitialStep option. For example, if you repeatedly call the integrator in an event location loop, the last step that was taken before the event is probably scaled correctly for the next integration. Type edit ballode to see an example.
The first step size that the integrator takes is too large, and it misses important behavior.	You can specify the first step size with the InitialStep option. The integrator tries this step size, then reduces it if necessary.

Solution Components

Question or Problem	Answer
The solution does not look like what I expected.	If your expectations are correct, then reduce the error tolerances from their default values. A smaller relative error tolerance is needed to accurately solve problems integrated over "long" intervals, as well as problems that are moderately unstable. Check whether there are solution components that stay smaller than their absolute error
	tolerance for some time. If so, you are not requiring any correct digits in these components. This might be acceptable for these components, but failing to compute them accurately might degrade the accuracy of other components that depend on them.
My plots are not smooth enough.	Increase the value of Refine from its default value of 4 in ode45, 8 in ode78 and ode89, and 1 in the other solvers. The larger the value of Refine, the more output points the solver generates. Execution speed is not affected much by increasing the value of Refine from its default value.
I am plotting the solution as it is computed and it looks fine, but the code gets stuck at some point.	First verify that the ODE function is smooth near the point where the code gets stuck. If it is not, then the solver must take small steps to deal with this. It might help to break the integration interval into pieces over which the ODE function is smooth.
	If the function is smooth and the code is taking extremely small steps, you are probably trying to solve a stiff problem with a solver not intended for that purpose. Switch to using one of the stiff solvers ode15s, ode23s, ode23t, or ode23tb.
What if I have the final and not the initial value?	All the solvers of the ODE suite allow you to solve backward or forward in time. The syntax for the solvers is [t,y] = ode45(odefun,[t0 tf],y0); and the syntax accepts t0 > tf.

Question or Problem	Answer
My integration proceeds very slowly, using too many time steps.	First, check that tspan is not too long. Remember that the solver uses as many time points as necessary to produce a smooth solution. If the ODE function changes on a time scale that is very short compared to tspan, then the solver uses a lot of time steps. Long-time integration is a hard problem. Break tspan into smaller pieces.
	If the ODE function does not change noticeably on the tspan interval, it could be that your problem is stiff. Try using one of the stiff solvers ode15s, ode23s, ode23t, or ode23tb.
	Finally, make sure that the ODE function is written in an efficient way. The solvers evaluate the derivatives in the ODE function many times. The cost of numerical integration depends critically on the expense of evaluating the ODE function. Rather than recomputing complicated constant parameters at each evaluation, store them in global variables, or calculate them once and pass them to nested functions.
I know that the solution undergoes a radical change at time t, where t0 <= t <= tf , but the integrator steps past without "seeing" it.	If you know that there is a sharp change at time t, try breaking the tspan interval into two pieces, [t0 t] and [t tf], and call the integrator twice or continue the integration using odextend.
	If the differential equation has periodic coefficients or solutions, ensure the solver does not step over periods by restricting the maximum step size to the length of the period.

Problem Type

Can the solvers handle partial differential equations (PDEs) that have been discretized by the method of lines?	Yes, because the discretization produces a system of ODEs. Depending on the discretization, you might have a form involving mass matrices, which the ODE solvers provide for. Often the system is stiff. This is to be expected if the PDE is parabolic, or when there are phenomena that happen on very different time scales such as a chemical reaction in a fluid flow. In such cases, use one of the four stiff solvers ode15s, ode23s, ode23t, or ode23tb.
	If there are many equations, use the JPattern option to specify the Jacobian sparsity pattern. This can make the difference between success and failure as it prevents the computation from being too expensive. Type edit burgersode to see an example that uses JPattern. If the system is not stiff, or not very stiff, then ode23 and ode45 are more efficient than the stiff
	Solvers ode15s, ode23s, ode23t, and ode23tb. You can solve parabolic-elliptic partial differential equations in 1-D directly with the MATLAB PDE solver pdepe.
Can I integrate a set of sampled data?	Not directly. Instead, represent the data as a function by interpolation or some other scheme for fitting data. The smoothness of this function is critical. A piecewise polynomial fit such as a spline can look smooth to the eye, but rough to a solver; the solver takes small steps where the derivatives of the fit have jumps. Either use a smooth function to represent the data or use one of the lower-order solvers (ode23, ode23s, ode23t, ode23tb) that is less sensitive to smoothness. See "ODE with Time-Dependent Terms" for an example.

See Also

odeset | odeget | deval | odextend

More About

- "Choose an ODE Solver" on page 11-2
- "Summary of ODE Options" on page 11-10
- "ODE Event Location" on page 11-13
- "Nonnegative ODE Solution" on page 11-35

Differential Equations

This example shows how to use MATLAB® to formulate and solve several different types of differential equations. MATLAB offers several numerical algorithms to solve a wide variety of differential equations:

- Initial value problems
- · Boundary value problems
- Delay differential equations
- · Partial differential equations

Initial Value Problem

vanderpoldemo is a function that defines the van der Pol equation

$$\frac{d^2y}{dt^2} - \mu(1 - y^2)\frac{dy}{dt} + y = 0.$$

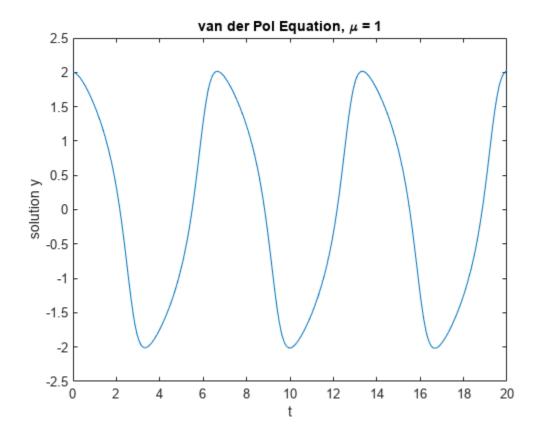
type vanderpoldemo

```
function dydt = vanderpoldemo(t,y,Mu) %VANDERPOLDEMO Defines the van der Pol equation for ODEDEMO. % Copyright 1984-2014 The MathWorks, Inc. dydt = [y(2); Mu*(1-y(1)^2)*y(2)-y(1)];
```

The equation is written as a system of two first-order ordinary differential equations (ODEs). These equations are evaluated for different values of the parameter μ . For faster integration, you should choose an appropriate solver based on the value of μ .

For $\mu=1$, any of the MATLAB ODE solvers can solve the van der Pol equation efficiently. The ode45 solver is one such example. The equation is solved in the domain [0,20] with the initial conditions y(0)=2 and $\frac{\mathrm{d}y}{\mathrm{d}t}\Big|_{t=0}=0$.

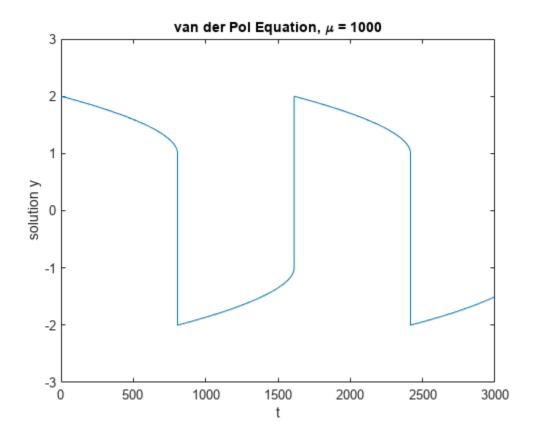
```
tspan = [0 20];
y0 = [2; 0];
Mu = 1;
ode = @(t,y) vanderpoldemo(t,y,Mu);
[t,y] = ode45(ode, tspan, y0);
% Plot solution
plot(t,y(:,1))
xlabel('t')
ylabel('solution y')
title('van der Pol Equation, \mu = 1')
```



For larger magnitudes of μ , the problem becomes *stiff*. This label is for problems that resist attempts to be evaluated with ordinary techniques. Instead, special numerical methods are needed for fast integration. The ode15s, ode23s, ode23t, and ode23tb functions can solve stiff problems efficiently.

This solution to the van der Pol equation for $\mu = 1000$ uses ode15s with the same initial conditions. You need to stretch out the time span drastically to [0, 3000] to be able to see the periodic movement of the solution.

```
tspan = [0, 3000];
y0 = [2; 0];
Mu = 1000;
ode = @(t,y) vanderpoldemo(t,y,Mu);
[t,y] = ode15s(ode, tspan, y0);
plot(t,y(:,1))
title('van der Pol Equation, \mu = 1000')
axis([0 3000 -3 3])
xlabel('t')
ylabel('solution y')
```



Boundary Value Problems

bvp4c and bvp5c solve boundary value problems for ordinary differential equations.

The example function twoode has a differential equation written as a system of two first-order ODEs. The differential equation is

$$\frac{d^2y}{dt^2} + |y| = 0.$$

```
type twoode
```

```
function dydx = twoode(x,y)
%TWOODE Evaluate the differential equations for TWOBVP.
%
    See also TWOBC, TWOBVP.
%    Lawrence F. Shampine and Jacek Kierzenka
%    Copyright 1984-2014 The MathWorks, Inc.
dydx = [ y(2); -abs(y(1)) ];
```

The function twobc has the boundary conditions for the problem: y(0) = 0 and y(4) = -2.

```
type twobc
```

```
function res = twobc(ya,yb)
%TWOBC Evaluate the residual in the boundary conditions for TWOBVP.
```

```
%
%
    See also TWOODE, TWOBVP.
%
    Lawrence F. Shampine and Jacek Kierzenka
    Copyright 1984-2014 The MathWorks, Inc.
res = [ ya(1); yb(1) + 2 ];
```

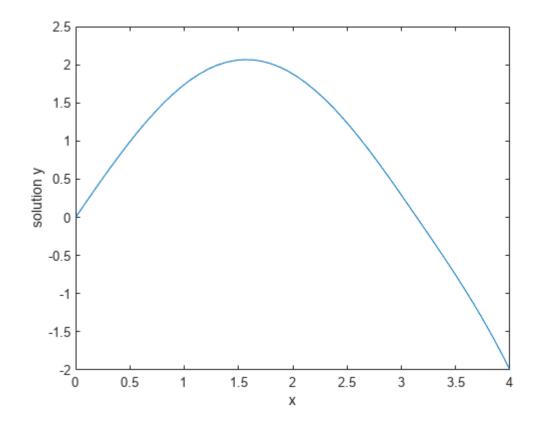
Prior to calling bvp4c, you have to provide a guess for the solution you want represented at a mesh. The solver then adapts the mesh as it refines the solution.

The bvpinit function assembles the initial guess in a form you can pass to the solver bvp4c. For a mesh of [0 1 2 3 4] and constant guesses of y(x) = 1 and y'(x) = 0, the call to bypinit is:

```
solinit = bvpinit([0 1 2 3 4],[1; 0]);
```

With this initial guess, you can solve the problem with bvp4c. Evaluate the solution returned by bvp4c at some points using deval, and then plot the resulting values.

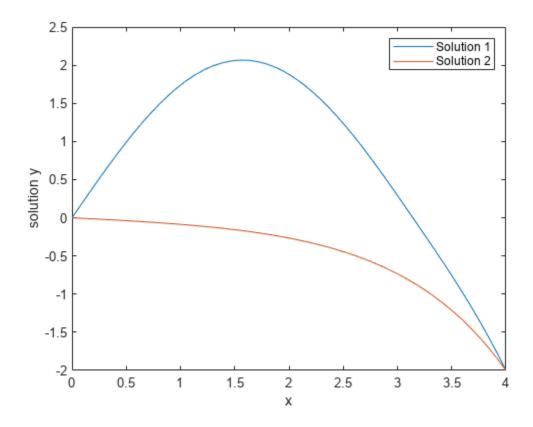
```
sol = bvp4c(@twoode, @twobc, solinit);
xint = linspace(0, 4, 50);
yint = deval(sol, xint);
plot(xint, yint(1,:));
xlabel('x')
ylabel('solution y')
hold on
```



This particular boundary value problem has exactly two solutions. You can obtain the other solution by changing the initial guesses to y(x) = -1 and y'(x) = 0.

```
solinit = bvpinit([0 1 2 3 4],[-1; 0]);
sol = bvp4c(@twoode,@twobc,solinit);

xint = linspace(0,4,50);
yint = deval(sol,xint);
plot(xint,yint(1,:));
legend('Solution 1','Solution 2')
hold off
```



Delay Differential Equations

dde23, ddesd, and ddensd solve delay differential equations with various delays. The examples ddex1, ddex2, ddex3, ddex4, and ddex5 form a mini tutorial on using these solvers.

The ddex1 example shows how to solve the system of differential equations

$$y'_1(t) = y_1(t-1)$$

 $y'_2(t) = y_1(t-1) + y_2(t-0.2)$
 $y'_3(t) = y_2(t)$.

You can represent these equations with the anonymous function

```
ddex1fun = @(t,y,Z) [Z(1,1); Z(1,1)+Z(2,2); y(2)];
```

The history of the problem (for $t \le 0$) is constant:

```
y_1(t) = 1
```

$$y_2(t) = 1$$

$$y_3(t) = 1$$
.

You can represent the history as a vector of ones.

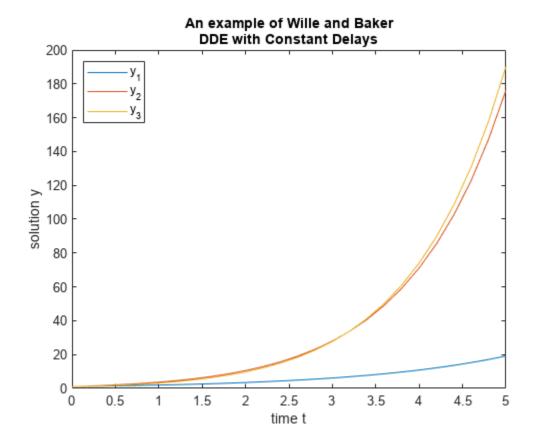
```
ddex1hist = ones(3,1);
```

A two-element vector represents the delays in the system of equations.

```
lags = [1 \ 0.2];
```

Pass the function, delays, solution history, and interval of integration [0, 5] to the solver as inputs. The solver produces a continuous solution over the whole interval of integration that is suitable for plotting.

```
sol = dde23(ddex1fun, lags, ddex1hist, [0 5]);
plot(sol.x,sol.y);
title({'An example of Wille and Baker', 'DDE with Constant Delays'});
xlabel('time t');
ylabel('solution y');
legend('y_1','y_2','y_3','Location','NorthWest');
```



Partial Differential Equations

pdepe solves partial differential equations in one space variable and time. The examples pdex1, pdex2, pdex3, pdex4, and pdex5 form a mini tutorial on using pdepe.

This example problem uses the functions pdex1pde, pdex1ic, and pdex1bc.

pdex1pde defines the differential equation

$$\pi^2 \frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} \right).$$

```
type pdex1pde
```

```
function [c,f,s] = pdex1pde(x,t,u,DuDx)
%PDEX1PDE Evaluate the differential equations components for the PDEX1 problem.
%
    See also PDEPE, PDEX1.
%    Lawrence F. Shampine and Jacek Kierzenka
%    Copyright 1984-2014 The MathWorks, Inc.

c = pi^2;
f = DuDx;
s = 0;
```

pdexlic sets up the initial condition

```
u(x,0) = \sin \pi x.
```

```
type pdexlic
```

```
function u0 = pdexlic(x)
%PDEXIIC Evaluate the initial conditions for the problem coded in PDEX1.
%
    See also PDEPE, PDEX1.
%    Lawrence F. Shampine and Jacek Kierzenka
%    Copyright 1984-2014 The MathWorks, Inc.
u0 = sin(pi*x);
```

pdex1bc sets up the boundary conditions

$$u(0,t) = 0,$$

$$\pi e^{-t} + \frac{\partial}{\partial x} u(1,t) = 0.$$

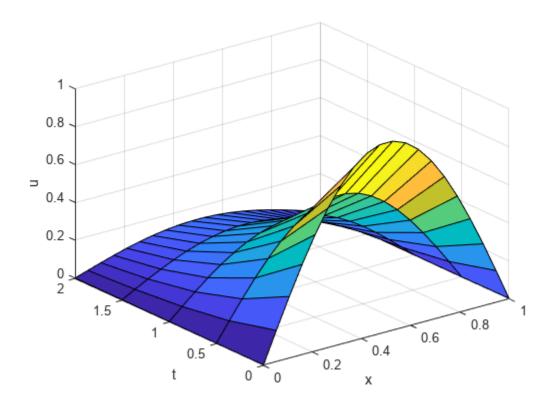
type pdex1bc

```
function [pl,ql,pr,qr] = pdex1bc(xl,ul,xr,ur,t)
%PDEX1BC Evaluate the boundary conditions for the problem coded in PDEX1.
%    See also PDEPE, PDEX1.
%    Lawrence F. Shampine and Jacek Kierzenka
%    Copyright 1984-2014 The MathWorks, Inc.
```

```
pl = ul;
ql = 0;
pr = pi * exp(-t);
qr = 1;
```

pdepe requires the spatial discretization x and a vector of times t (at which you want a snapshot of the solution). Solve the problem using a mesh of 20 nodes and request the solution at five values of t. Extract and plot the first component of the solution.

```
x = linspace(0,1,20);
t = [0 \ 0.5 \ 1 \ 1.5 \ 2];
sol = pdepe(0,@pdex1pde,@pdex1ic,@pdex1bc,x,t);
u1 = sol(:,:,1);
surf(x,t,u1);
xlabel('x');
ylabel('t');
zlabel('u');
```



See Also

ode45 | bvp4c | pdepe

More About

- "Choose an ODE Solver" on page 11-2
- "Solving Boundary Value Problems" on page 12-2
- "Solving Partial Differential Equations" on page 13-2

Solve Predator-Prey Equations

This example shows how to solve a differential equation representing a predator/prey model using both ode23 and ode45. These functions are for the numerical solution of ordinary differential equations using variable step size Runge-Kutta integration methods. ode23 uses a simple 2nd and 3rd order pair of formulas for medium accuracy and ode45 uses a 4th and 5th order pair for higher accuracy.

Consider the pair of first-order ordinary differential equations known as the Lotka-Volterra equations, or predator-prev model:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = x - \alpha xy$$
$$\frac{\mathrm{d}y}{\mathrm{d}t} = -y + \beta xy.$$

The variables x and y measure the sizes of the prey and predator populations, respectively. The quadratic cross term accounts for the interactions between the species. The prey population increases when no predators are present, and the predator population decreases when prey are scarce.

Code Equations

To simulate the system, create a function that returns a column vector of state derivatives, given state and time values. The two variables x and y can be represented in MATLAB® as the first two values in a vector y. Similarly, the derivatives are the first two values in a vector yp. The function must accept values for t and y and return the values produced by the equations in yp.

```
yp(1) = (1 - alpha*y(2))*y(1)
yp(2) = (-1 + beta*y(1))*y(2)
```

In this example, the equations are contained in a file called lotka.m. This file uses parameter values of $\alpha = 0.01$ and $\beta = 0.02$.

```
type lotka
function yp = lotka(t,y)
%LOTKA Lotka-Volterra predator-prey model.
   Copyright 1984-2014 The MathWorks, Inc.
yp = diag([1 - .01*y(2), -1 + .02*y(1)])*y;
```

Simulate System

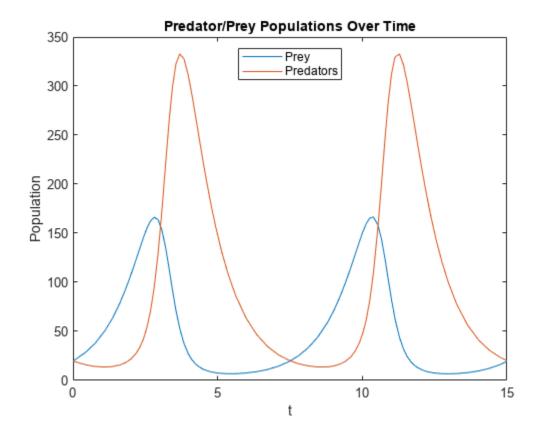
Use ode23 to solve the differential equation defined in lotka over the interval 0 < t < 15. Use an initial condition of x(0) = y(0) = 20 so that the populations of predators and prey are equal.

```
t0 = 0;
tfinal = 15;
y0 = [20; 20];
[t,y] = ode23(@lotka,[t0 tfinal],y0);
```

Plot Results

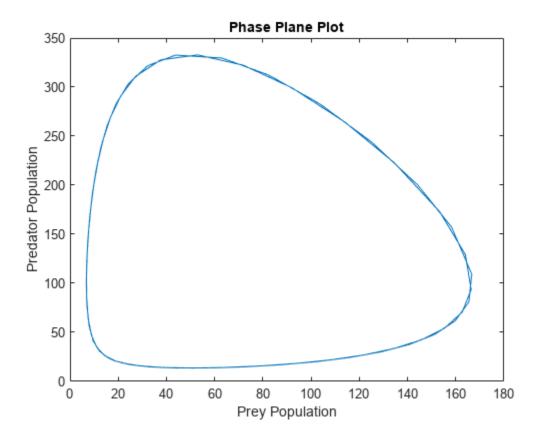
Plot the resulting populations against time.

```
plot(t,y)
title('Predator/Prey Populations Over Time')
xlabel('t')
ylabel('Population')
legend('Prey','Predators','Location','North')
```



Now plot the populations against each other. The resulting phase plane plot makes the cyclic relationship between the populations very clear.

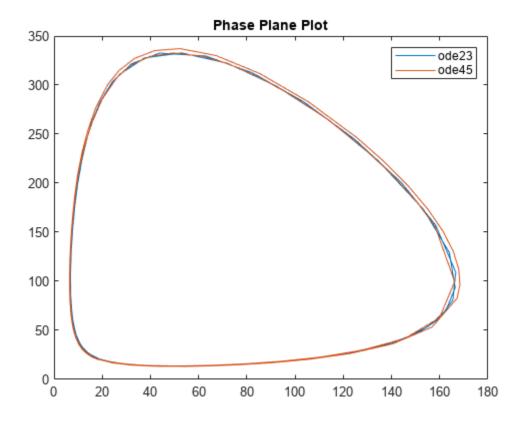
```
plot(y(:,1),y(:,2))
title('Phase Plane Plot')
xlabel('Prey Population')
ylabel('Predator Population')
```



Compare Results of Different Solvers

Solve the system a second time using ode45, instead of ode23. The ode45 solver takes longer for each step, but it also takes larger steps. Nevertheless, the output of ode45 is smooth because by default the solver uses a continuous extension formula to produce output at four equally spaced time points in the span of each step taken. (You can adjust the number of points with the 'Refine' option.) Plot both solutions for comparison.

```
[T,Y] = ode45(@lotka,[t0 tfinal],y0);
plot(y(:,1),y(:,2),'-',Y(:,1),Y(:,2),'-');
title('Phase Plane Plot')
legend('ode23','ode45')
```



The results show that solving differential equations using different numerical methods can produce slightly different answers.

See Also

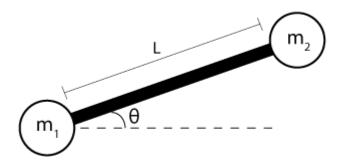
ode45 | ode23

More About

- "Choose an ODE Solver" on page 11-2
- "Solve Nonstiff ODEs" on page 11-19

Solve Equations of Motion for Baton Thrown into Air

This example solves a system of ordinary differential equations that model the dynamics of a baton thrown into the air [1]. The baton is modeled as two particles with masses m_1 and m_2 connected by a rod of length L. The baton is thrown into the air and subsequently moves in the vertical xy-plane subject to the force due to gravity. The rod forms an angle θ with the horizontal and the coordinates of the first mass are (x, y). With this formulation, the coordinates of the second mass are $(x + L \cos \theta, y + L \sin \theta)$.





The equations of motion for the system are obtained by applying Lagrange's equations for each of the three coordinates, x, y, and θ :

$$(m_1 + m_2)\ddot{x} - m_2 L \, \ddot{\theta} \sin \theta - m_2 L \, \dot{\theta}^2 \cos \theta = 0,$$

$$(m_1 + m_2)\ddot{y} - m_2 L \, \ddot{\theta} \cos \theta - m_2 L \, \dot{\theta}^2 \sin \theta + (m_1 + m_2)g = 0,$$

$$L^2 \ddot{\theta} - L \, \ddot{x} \sin \theta + L \, \ddot{y} \cos \theta + g \, L \cos \theta = 0.$$

To solve this system of ODEs in MATLAB®, code the equations into a function before calling the solver ode45. You can either include the required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Code Equations

The ode45 solver requires the equations to be written in the form $\dot{q} = f(t, q)$, where \dot{q} is the first derivative of each coordinate. In this problem, the solution vector has six components: x, y, the angle θ , and their first derivatives:

$$q = \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \\ q_5 \\ q_6 \end{bmatrix} = \begin{bmatrix} x \\ \dot{x} \\ y \\ \dot{y} \\ \theta \\ \dot{\theta} \end{bmatrix}$$

With this notation, you can rewrite the equations of motion entirely in terms of the elements of q:

$$\begin{split} (m_1+m_2)\dot{q}_2 - m_2L\ \dot{q}_6\sin q_5 &= m_2L\ q_6^2\cos q_5,\\ (m_1+m_2)\dot{q}_4 - m_2L\ \dot{q}_6\cos q_5 &= m_2L\ q_6^2\sin q_5 - (m_1+m_2)g,\\ L^2\dot{q}_6 - L\ \dot{q}_2\sin q_5 + L\ \dot{q}_4\cos q_5 &= -g\ L\cos q_5\,. \end{split}$$

Unfortunately, the equations of motion do not fit into the form $\dot{q} = f(t, q)$ required by the solver, since there are several terms on the left with first derivatives. When this occurs, you must use a mass matrix to represent the left side of the equation.

With matrix notation, you can rewrite the equations of motion as a system of six equations using a mass matrix in the form $M(t, q) \dot{q} = f(t, q)$. The mass matrix expresses the linear combinations of first derivatives on the left side of the equation with a matrix-vector product. In this form, the system of equations becomes:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & m_1 + m_2 & 0 & 0 & 0 & -m_2L\sin q_5 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & m_1 + m_2 & 0 & m_2L\cos q_5 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & -L\sin q_5 & 0 & L\cos q_5 & 0 & L^2 \end{bmatrix} \begin{bmatrix} \dot{q}_1 \\ \dot{q}_2 \\ \dot{q}_3 \\ \dot{q}_4 \\ \dot{q}_5 \\ \dot{q}_6 \end{bmatrix} = \begin{bmatrix} q_2 \\ m_2L & q_6^2\cos q_5 \\ q_4 \\ m_2L & q_6^2\sin q_5 - (m_1 + m_2)g \\ q_6 \\ -gL\cos q_5 \end{bmatrix}$$

From this expression, you can write a function that calculates the nonzero elements of the mass matrix. The function takes three inputs: t and the solution vector q are required (you must specify these inputs even if they are not used in the body of the function), and P is an optional extra input used to pass in parameter values. To pass the parameters for this problem to the function, create P as a structure that holds the parameter values and then use the technique described in "Parameterizing Functions" on page 10-2 to pass the structure to the function as an extra input.

```
function M = mass(t,q,P)
% Extract parameters
m1 = P.m1;
m2 = P.m2;
L = P.L;
g = P.g;
% Mass matrix function
M = zeros(6,6);
M(1,1) = 1;
M(2,2) = m1 + m2;
M(2,6) = -m2*L*sin(q(5));
```

```
M(3,3) = 1;
M(4,4) = m1 + m2;
M(4,6) = m2*L*cos(q(5));
M(5,5) = 1;
M(6,2) = -L*sin(q(5));
M(6,4) = L*cos(q(5));
M(6,6) = L^2;
end
```

Next, you can write a function for the right side of each of the equations in the system $M(t,q)\dot{q}=f(t,q)$. Like the mass matrix function, this function takes two required inputs for t and q, and one optional input for parameter values P.

```
function dydt = f(t,q,P)
% Extract parameters
m1 = P.m1;
m2 = P.m2;
L = P.L;
g = P.g;
% Equation to solve
dydt = [q(2)]
        m2*L*q(6)^2*cos(q(5))
        a(4)
        m2*L*q(6)^2*sin(q(5))-(m1+m2)*q
        q(6)
        -g*L*cos(q(5))];
end
```

Solve System of Equations

First, create a structure P of parameter values for m_1 , m_2 , g, and L by setting appropriately named fields in a structure. The structure P is passed to the mass matrix and ODE functions as an extra input.

```
P.m1 = 0.1:
P.m2 = 0.1;
P.L = 1;
P.g = 9.81
P = struct with fields:
    m1: 0.1000
    m2: 0.1000
    L: 1
     g: 9.8100
```

Create a vector with 25 points between 0 and 4 for the time span of the integration. When you specify a vector of times, ode45 returns interpolated solutions at the requested times.

```
tspan = linspace(0,4,25);
```

Set the initial conditions of the problem. Since the baton is thrown upward at an angle, use nonzero values for the initial velocities, $\dot{x_0} = 4$, $\dot{y_0} = 20$, and $\dot{\theta_0} = 2$. For the initial positions, the baton begins in an upright position, so $\theta_0 = -\pi/2$, $x_0 = 0$, and $y_0 = L$.

```
y0 = [0; 4; P.L; 20; -pi/2; 2];
```

Use odeset to create an options structure that references the mass matrix function. Since the solver expects the mass matrix function to have only two inputs, use an anonymous function to pass in the parameters P from the workspace.

```
opts = odeset('Mass',@(t,q) mass(t,q,P));
```

Finally, solve the system of equations using ode45 with these inputs:

- An anonymous function for the equations Q(t,q) f(t,q,P)
- The vector tspan of times where the solution is requested
- The vector y0 of initial conditions
- The options structure opts that references the mass matrix

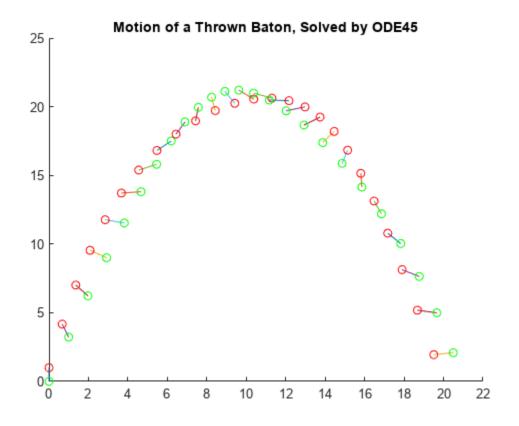
```
[t,q] = ode45(@(t,q) f(t,q,P),tspan,y0,opts);
```

Plot Results

The outputs from ode45 contain the solutions of the equations of motion at each requested time step. To examine the results, plot the motion of the baton over time.

Loop through each row of the solution, and at each time step, plot the position of the baton. Color each end of the baton differently so that you can see its rotation over time.

```
figure
title('Motion of a Thrown Baton, Solved by ODE45');
axis([0 22 0 25])
hold on
for j = 1:length(t)
    theta = q(j,5);
    X = q(j,1);
    Y = q(j,3);
    xvals = [X X+P.L*cos(theta)];
    yvals = [Y Y+P.L*sin(theta)];
    plot(xvals,yvals,xvals(1),yvals(1),'ro',xvals(2),yvals(2),'go')
end
hold off
```



References

[1] Wells, Dare A. Schaum's Outline of Theory and Problems of Lagrangian Dynamics: With a Treatment of Euler's Equations of Motion, Hamilton's Equations and Hamilton's Principle. Schaum's Outline Series. New York: Schaum Pub. Co, 1967.

Local Functions

Listed here are the local helper functions that the ODE solver calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

```
function dydt = f(t,q,P) % Equations to solve
% Extract parameters
m1 = P.m1;
m2 = P.m2;
L = P.L;
g = P.g;
% RHS of system of equations
dydt = [q(2)]
        m2*L*q(6)^2*cos(q(5))
        m2*L*q(6)^2*sin(q(5))-(m1+m2)*g
        q(6)
        -g*L*cos(q(5))];
end
```

```
function M = mass(t,q,P) % Mass matrix function
% Extract parameters
m1 = P.m1;
m2 = P.m2;
L = P.L;
g = P.g;
% Set nonzero elements in mass matrix
M = zeros(6,6);
M(1,1) = 1;

M(2,2) = m1 + m2;
M(2,6) = -m2*L*sin(q(5));
M(3,3) = 1;
M(4,4) = m1 + m2;
M(4,6) = m2*L*cos(q(5));
M(5,5) = 1;
M(6,2) = -L*sin(q(5));
M(6,4) = L*cos(q(5));
M(6,6) = L^2;
end
```

See Also

ode45

More About

- "Choose an ODE Solver" on page 11-2
- "Solve Nonstiff ODEs" on page 11-19

Solve ODE with Strongly State-Dependent Mass Matrix

This example shows how to solve Burgers' equation using a moving mesh technique [1]. The problem includes a mass matrix, and options are specified to account for the strong state dependence and sparsity of the mass matrix, making the solution process more efficient.

Problem Setup

Burgers' equation is a convection-diffusion equation given by the PDE

$$\frac{\partial u}{\partial t} = \epsilon \frac{\partial^2 u}{\partial x^2} - \frac{\partial}{\partial x} \left(\frac{u^2}{2} \right), \quad 0 < x < 1, \quad t > 0, \ \epsilon = 1 \times 10^{-4}.$$

Applying a coordinate transformation (Eq. 18 in [1]) leads to an extra term on the left-hand side:

$$\frac{\partial u}{\partial t} - \frac{\partial u}{\partial x} \frac{\partial x}{\partial t} = \epsilon \frac{\partial^2 u}{\partial x^2} - \frac{\partial}{\partial x} \left(\frac{u^2}{2} \right).$$

Converting the PDE into an ODE of one variable is accomplished by using finite differences to approximate the partial derivatives taken with respect to x. If the finite differences are written as Δ , then the PDE can be rewritten as an ODE that only contains derivatives taken with respect to t:

$$\frac{du}{dt} - \Delta u \frac{dx}{dt} = \epsilon \Delta^2 u - \Delta \left(\frac{u^2}{2} \right).$$

In this form, you can use an ODE solver such as ode15s to solve for u and x over time.

For this example, the problem is formulated on a moving mesh of N points, and the moving mesh technique described in [1] positions the mesh points at each time step so that they are concentrated in areas of change. The boundary and initial conditions are

$$u(0,t) = u(1,t) = 0,$$

 $u(x,0) = \sin(2\pi x) + \frac{1}{2}\sin(\pi x).$

For a given initial mesh of N points, there are 2N equations to solve: N equations corresponding to Burgers' equation, and N equations determining the movement of each mesh point. So, the final system of equations is:

$$\frac{du_1}{dt} - \Delta u_1 \frac{dx_1}{dt} = \epsilon \Delta^2 u_1 - \Delta \left(\frac{u_1^2}{2}\right),$$

$$\vdots$$

$$\frac{du_N}{dt} - \Delta u_N \frac{dx_N}{dt} = \epsilon \Delta^2 u_N - \Delta \left(\frac{u_N^2}{2}\right),$$

$$\frac{d^2 \dot{x_1}}{dt^2} = \frac{1}{\tau} \frac{d}{dt} \left(B(x_1, t) \frac{dx_1}{dt}\right),$$

$$\vdots$$

$$\frac{d^2 \dot{x_N}}{dt^2} = \frac{1}{\tau} \frac{d}{dt} \left(B(x_N, t) \frac{dx_N}{dt}\right).$$

The terms for the moving mesh correspond to MMPDE6 in [1]. The parameter τ represents a timescale for forcing the mesh toward equidistribution. The term B(x,t) is a monitor function given by Eq. 21 in [1]:

$$B(x,t) = \sqrt{1 + \left(\frac{du_i}{dx_i}\right)^2}.$$

The approach used in this example to solve Burgers' equation with moving mesh points demonstrates several techniques:

- The system of equations is expressed using a mass matrix formulation, M y' = f(t, y). The mass matrix is provided to the ode15s solver as a function.
- The derivative function not only includes the equations for Burgers' equation, but also a set of equations governing the moving mesh selection.
- The sparsity patterns of the Jacobian dF/dy and the derivative of the mass matrix multiplied with a vector d(Mv)/dy are supplied to the solver as functions. Supplying these sparsity patterns helps the solver operate more efficiently.
- Finite differences are used to approximate several partial derivatives.

To solve this equation in MATLAB®, write a derivative function, a mass matrix function, a function for the sparsity pattern of the Jacobian dF/dy, and a function for the sparsity pattern of d(Mv)/dy. You can either include the required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Code Mass Matrix

The left side of the system of equations involves linear combinations of first derivatives, so a mass matrix is required to represent all of the terms. Set the left side of the system of equations equal to M y to extract the form of the mass matrix. The mass matrix is composed of four blocks, each of which is a square matrix of order N:

$$\begin{bmatrix} \frac{\partial u_1}{\partial t} - \frac{\partial u_1}{\partial x_1} \frac{\partial x_1}{\partial t} \\ \vdots \\ \frac{\partial u_N}{\partial t} - \frac{\partial u_N}{\partial x_N} \frac{\partial x_N}{\partial t} \\ \frac{\partial^2 \dot{x_1}}{\partial t^2} \\ \vdots \\ \frac{\partial^2 \dot{x_N}}{\partial t^2} \end{bmatrix} = M \ y' = \begin{bmatrix} M_1 \ M_2 \\ M_3 \ M_4 \end{bmatrix} \begin{bmatrix} \dot{u_1} \\ \vdots \\ \dot{u_N} \\ \dot{x_1} \\ \vdots \\ \dot{x_N} \end{bmatrix}.$$

This formulation shows that M_1 and M_2 form the left side of Burgers' equations (the first N equations in the system), while M_3 and M_4 form the left side of the mesh equations (the last N equations in the system). The block matrices are:

$$\begin{split} M_1 &= I_N, \\ M_2 &= -\frac{\partial u_i}{\partial x_i} I_N, \\ M_3 &= 0_N, \\ M_4 &= \frac{\partial^2}{\partial t^2} I_N \,. \end{split}$$

 I_N is the $N \times N$ identity matrix. The partial derivatives in M_2 are estimated using finite differences, while the partial derivative in M_4 uses a Laplacian matrix. Notice that M_3 contains only zeros because none of the equations for the mesh movement depend on \dot{u} .

Now you can write a function that computes the mass matrix. The function must accept two inputs for time t and the solution vector y. Since the solution vector y contains half \dot{u} components and half \dot{x} components, the function extracts these first. Then, the function forms all of the block matrices (taking the boundary values of the problem into account) and assembles the mass matrix using the four blocks.

```
function M = mass(t,y)
% Extract the components of y for the solution u and mesh x
N = length(y)/2;
u = y(1:N);
x = y(N+1:end);
% Boundary values of solution u and mesh x
u0 = 0;
uNP1 = 0;
x0 = 0;
xNP1 = 1;
% M1 and M2 are the portions of the mass matrix for Burgers' equation.
% The derivative du/dx is approximated with finite differences, using
% single-sided differences on the edges and centered differences in between.
M1 = speve(N);
M2 = sparse(N,N);
M2(1,1) = - (u(2) - u0)/(x(2) - x0);
for i = 2:N-1
    M2(i,i) = -(u(i+1) - u(i-1))/(x(i+1) - x(i-1));
M2(N,N) = - (uNP1 - u(N-1))/(xNP1 - x(N-1));
% M3 and M4 define the equations for mesh point evolution, corresponding to
\% MMPDE6 in the reference paper. Since the mesh functions only involve \mathsf{d}/\mathsf{dt}(\mathsf{dx}/\mathsf{dt}) ,
st the M3 portion of the mass matrix is all zeros. The second derivative in M4 is
% approximated using a finite difference Laplacian matrix.
M3 = sparse(N,N);
e = ones(N,1);
M4 = spdiags([e -2*e e], -1:1,N,N);
% Assemble mass matrix
M = [M1 M2]
     M3 M4];
end
```

Note: All functions are included as local functions at the end of the example.

Code Derivative Function

The derivative function for this problem returns a vector with 2N elements. The first N elements correspond to Burgers' equations, while the last N elements are for the moving mesh equations. The function movingMeshODE goes through these steps to evaluate the right-hand sides of all the equations in the system:

- **1** Evaluate Burgers' equations using finite differences (first N elements).
- **2** Evaluate monitor function (last *N* elements).
- **3** Apply spatial smoothing to monitor function and evaluate moving mesh equations.

The first N equations in the derivative function encode the right side of Burgers' equations. Burgers' equations can be considered as a differential operator involving spatial derivatives of the form:

$$f(u) = \epsilon \frac{\partial^2 u}{\partial x^2} - \frac{\partial}{\partial x} \left(\frac{u^2}{2} \right).$$

The reference paper [1] describes the process of approximating the differential operator f using centered finite differences by

$$f_i = \epsilon \left[\frac{\left(\frac{u_i + 1 - u_i}{x_i + 1 - x_i}\right) - \left(\frac{u_i - u_i - 1}{x_i - x_i - 1}\right)}{\frac{1}{2}(x_{i+1} - x_{i-1})} \right] - \frac{1}{2} \left(\frac{u_{i+1}^2 - u_{i-1}^2}{x_{i+1} - x_{i-1}}\right).$$

On the edges of the mesh (for which i = 1 and i = N), only single-sided differences are used instead. This example uses $\epsilon = 1 \times 10^{-4}$.

The equations governing the mesh (comprising the last N equations in the derivative function) are

$$\frac{\partial^2 \dot{x}}{\partial t^2} = \frac{1}{\tau} \frac{\partial}{\partial t} \Big(B(x, t) \frac{\partial x}{\partial t} \Big).$$

Just as with Burgers' equations, you can use finite differences to approximate the monitor function B(x, t):

$$B(x,t) = \sqrt{1 + \left(\frac{\partial u_i}{\partial x_i}\right)^2} = \sqrt{1 + \left(\frac{u_{i+1} - u_{i-1}}{x_{i+1} - x_{i-1}}\right)^2}.$$

Once the monitor function is evaluated, spatial smoothing is applied (Equations 14 and 15 in [1]). This example uses $\gamma = 2$ and p = 2 for the spatial smoothing parameters.

The function encoding the system of equations is

```
function g = movingMeshODE(t,y)
% Extract the components of y for the solution u and mesh x
N = length(y)/2;
u = y(1:N);
x = y(N+1:end);
% Boundary values of solution u and mesh x
u0 = 0;
uNP1 = 0;
x0 = 0;
```

```
xNP1 = 1;
% Preallocate g vector of derivative values.
g = zeros(2*N,1);
% Use centered finite differences to approximate the RHS of Burgers'
% equations (with single-sided differences on the edges). The first N
% elements in g correspond to Burgers' equations.
for i = 2:N-1
    delx = x(i+1) - x(i-1);
    q(i) = 1e-4*((u(i+1) - u(i))/(x(i+1) - x(i)) - ...
        (u(i) - u(i-1))/(x(i) - x(i-1)))/(0.5*delx) \dots
        -0.5*(u(i+1)^2 - u(i-1)^2)/delx;
end
delx = x(2) - x0;
q(1) = 1e-4*(u(2) - u(1))/(x(2) - x(1)) - (u(1) - u(0))/(x(1) - x(0))/(0.5*delx) ...
    - 0.5*(u(2)^2 - u0^2)/delx;
delx = xNP1 - x(N-1);
g(N) = 1e-4*((uNP1 - u(N))/(xNP1 - x(N)) - ...
    (u(N) - u(N-1))/(x(N) - x(N-1)))/delx - ...
    0.5*(uNP1^2 - u(N-1)^2)/delx;
% Evaluate the monitor function values (Eq. 21 in reference paper), used in
% RHS of mesh equations. Centered finite differences are used for interior
% points, and single-sided differences are used on the edges.
M = zeros(N,1);
for i = 2:N-1
    M(i) = sqrt(1 + ((u(i+1) - u(i-1))/(x(i+1) - x(i-1)))^2);
M0 = sqrt(1 + ((u(1) - u0)/(x(1) - x0))^2);
M(1) = sqrt(1 + ((u(2) - u0)/(x(2) - x0))^2);
M(N) = sqrt(1 + ((uNP1 - u(N-1))/(xNP1 - x(N-1)))^2);
MNP1 = sqrt(1 + ((uNP1 - u(N))/(xNP1 - x(N)))^2);
% Apply spatial smoothing (Eqns. 14 and 15) with gamma = 2, p = 2.
SM = zeros(N,1);
for i = 3:N-2
    SM(i) = sqrt((4*M(i-2)^2 + 6*M(i-1)^2 + 9*M(i)^2 + ...
        6*M(i+1)^2 + 4*M(i+2)^2)/29;
SM0 = sqrt((9*M0^2 + 6*M(1)^2 + 4*M(2)^2)/19);
SM(1) = sqrt((6*M0^2 + 9*M(1)^2 + 6*M(2)^2 + 4*M(3)^2)/25);
SM(2) = sart((4*M0^2 + 6*M(1)^2 + 9*M(2)^2 + 6*M(3)^2 + 4*M(4)^2)/29);
SM(N-1) = sqrt((4*M(N-3)^2 + 6*M(N-2)^2 + 9*M(N-1)^2 + 6*M(N)^2 + 4*MNP1^2)/29);
SM(N) = sqrt((4*M(N-2)^2 + 6*M(N-1)^2 + 9*M(N)^2 + 6*MNP1^2)/25);
SMNP1 = sqrt((4*M(N-1)^2 + 6*M(N)^2 + 9*MNP1^2)/19);
for i = 2:N-1
    g(i+N) = (SM(i+1) + SM(i))*(x(i+1) - x(i)) - ...
        (SM(i) + SM(i-1))*(x(i) - x(i-1));
g(1+N) = (SM(2) + SM(1))*(x(2) - x(1)) - (SM(1) + SM0)*(x(1) - x0);
g(N+N) = (SMNP1 + SM(N))*(xNP1 - x(N)) - (SM(N) + SM(N-1))*(x(N) - x(N-1));
% Form final discrete approximation for Eq. 12 in reference paper, the equation governing
% the mesh points.
tau = 1e-3;
g(1+N:end) = - g(1+N:end)/(2*tau);
end
```

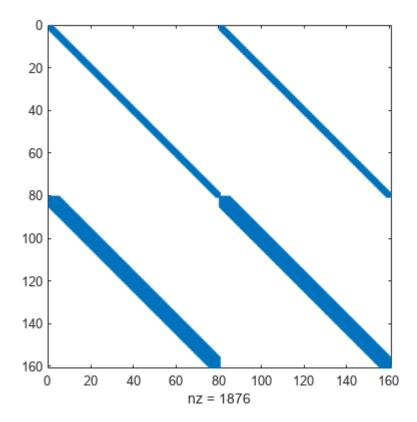
Code Functions for Sparsity Patterns

The Jacobian dF/dy for the derivative function is a $2N \times 2N$ matrix containing all of the partial derivatives of the derivative function, movingMeshODE. ode15s estimates the Jacobian using finite differences when the matrix is not supplied in the options structure. You can supply the sparsity pattern of the Jacobian to help ode15s calculate it more quickly.

The function for the sparsity pattern of the Jacobian is

Plot the sparsity pattern of dF/dy for N = 80 using spy.

```
spy(JPat(80))
```



Another way to make the calculation more efficient is to provide the sparsity pattern of d(Mv)/dy. You can find this sparsity pattern by examining which terms of u_i and x_i are present in the finite differences calculated in the mass matrix function.

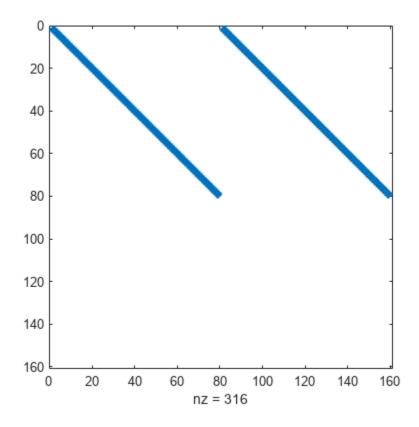
The function for the sparsity pattern of d(Mv)/dv is

```
function S = MvPat(N)
S = sparse(2*N,2*N);
```

```
S(1,2) = 1;
S(1,2+N) = 1;
for i = 2:N-1
    S(i,i-1) = 1;
    S(i,i+1) = 1;
    S(i,i-1+N) = 1;
    S(i,i+1+N) = 1;
end
S(N,N-1) = 1;
S(N,N-1+N) = 1;
```

Plot the sparsity pattern of d(Mv)/dy for N = 80 using spy.

spy(MvPat(80))



Solve System of Equations

Solve the system with the value N = 80. For the initial conditions, initialize x with a uniform grid and evaluate u(x, 0) on the grid.

```
N = 80;
h = 1/(N+1);
xinit = h*(1:N);
uinit = sin(2*pi*xinit) + 0.5*sin(pi*xinit);
y0 = [uinit xinit];
```

Use odeset to create an options structure that sets several values:

- A function handle for the mass matrix
- The state-dependence of the mass matrix, which for this problem is 'strong' since the mass matrix is a function of both t and y
- A function handle that calculates the Jacobian sparsity pattern
- A function handle that calculates the sparsity pattern of the derivative of the mass matrix multiplied by a vector
- The absolute and relative error tolerances

```
opts = odeset('Mass',@mass,'MStateDependence','strong','JPattern',JPat(N),...
'MvPattern',MvPat(N),'RelTol',1e-5,'AbsTol',1e-4);
```

Finally, call ode15s to solve the system on the interval [0, 1] using the movingMeshODE derivative function, the time span, the initial conditions, and the options structure.

```
tspan = [0 1];
sol = ode15s(@movingMeshODE,tspan,y0,opts);
```

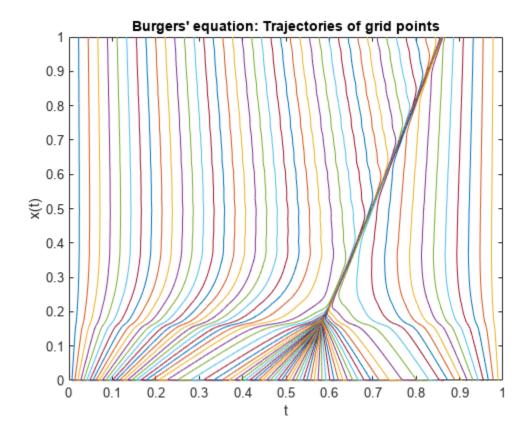
Plot Results

The result of the integration is a structure sol that contains the time steps t, the mesh points x(t), and the solution u(x, t). Extract these values from the structure.

```
t = sol.x;
x = sol.y(N+1:end,:);
u = sol.y(1:N,:);
```

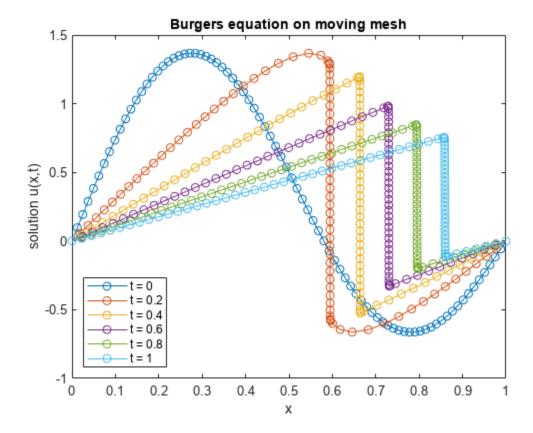
Plot the movement of the mesh points over time. The plot shows that the mesh points retain a reasonably even spacing over time (due to the monitor function), but they are able to cluster near the discontinuity in the solution as it moves.

```
plot(x,t)
xlabel('t')
ylabel('x(t)')
title('Burgers'' equation: Trajectories of grid points')
```



Now, sample u(x, t) at a few values of t and plot the evolution of the solution over time. The mesh points at the ends of the interval are fixed, so x(0) = 0 and x(N+1) = 1. The boundary values are u(t,0) = 0 and u(t,1) = 0, which you must add to the known values computed for the figure.

```
tint = 0:0.2:1;
yint = deval(sol,tint);
figure
labels = \{\};
for j = 1:length(tint)
   solution = [0; yint(1:N,j); 0];
   location = [0; yint(N+1:end,j); 1];
   labels{j} = ['t = ' num2str(tint(j))];
   plot(location, solution, '-o')
   hold on
end
xlabel('x')
ylabel('solution u(x,t)')
legend(labels{:},'Location','SouthWest')
title('Burgers equation on moving mesh')
hold off
```



The plot shows that u(x, 0) is a smooth wave that develops a steep gradient over time as it moves towards x = 1. The mesh points track the movement of the discontinuity so that extra evaluation points are in the appropriate position in each time step.

References

[1] Huang, Weizhang, et al. "Moving Mesh Methods Based on Moving Mesh Partial Differential Equations." *Journal of Computational Physics*, vol. 113, no. 2, Aug. 1994, pp. 279–90. https://doi.org/10.1006/jcph.1994.1135.

Local Functions

Listed here are the local helper functions that the solver ode15s calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

```
function g = movingMeshODE(t,y)
% Extract the components of y for the solution u and mesh x
N = length(y)/2;
u = y(1:N);
x = y(N+1:end);
% Boundary values of solution u and mesh x
u0 = 0;
uNP1 = 0;
x0 = 0;
xNP1 = 1;
```

```
% Preallocate g vector of derivative values.
g = zeros(2*N,1);
% Use centered finite differences to approximate the RHS of Burgers'
% equations (with single-sided differences on the edges). The first N
% elements in g correspond to Burgers' equations.
for i = 2:N-1
    delx = x(i+1) - x(i-1);
    g(i) = 1e-4*((u(i+1) - u(i))/(x(i+1) - x(i)) - ...
        (u(i) - u(i-1))/(x(i) - x(i-1)))/(0.5*delx) \dots
        - 0.5*(u(i+1)^2 - u(i-1)^2)/delx;
end
delx = x(2) - x0;
g(1) = 1e-4*(u(2) - u(1))/(x(2) - x(1)) - (u(1) - u(0))/(x(1) - x(0))/(0.5*delx) ...
    -0.5*(u(2)^2 - u0^2)/delx;
delx = xNP1 - x(N-1);
g(N) = 1e-4*((uNP1 - u(N))/(xNP1 - x(N)) - ...
    (u(N) - u(N-1))/(x(N) - x(N-1)))/delx - ...
    0.5*(uNP1^2 - u(N-1)^2)/delx;
% Evaluate the monitor function values (Eq. 21 in reference paper), used in
% RHS of mesh equations. Centered finite differences are used for interior
% points, and single-sided differences are used on the edges.
M = zeros(N,1);
for i = 2:N-1
    M(i) = sqrt(1 + ((u(i+1) - u(i-1))/(x(i+1) - x(i-1)))^2);
M0 = sqrt(1 + ((u(1) - u0)/(x(1) - x0))^2);
M(1) = sqrt(1 + ((u(2) - u0)/(x(2) - x0))^2);
M(N) = sqrt(1 + ((uNP1 - u(N-1))/(xNP1 - x(N-1)))^2);
MNP1 = sqrt(1 + ((uNP1 - u(N))/(xNP1 - x(N)))^2);
% Apply spatial smoothing (Eqns. 14 and 15) with gamma = 2, p = 2.
SM = zeros(N,1);
for i = 3:N-2
    SM(i) = sqrt((4*M(i-2)^2 + 6*M(i-1)^2 + 9*M(i)^2 + ...
        6*M(i+1)^2 + 4*M(i+2)^2)/29;
end
SM0 = sqrt((9*M0^2 + 6*M(1)^2 + 4*M(2)^2)/19);
SM(1) = sqrt((6*M0^2 + 9*M(1)^2 + 6*M(2)^2 + 4*M(3)^2)/25);
SM(2) = sqrt((4*M0^2 + 6*M(1)^2 + 9*M(2)^2 + 6*M(3)^2 + 4*M(4)^2)/29);
SM(N-1) = sqrt((4*M(N-3)^2 + 6*M(N-2)^2 + 9*M(N-1)^2 + 6*M(N)^2 + 4*MNP1^2)/29);
SM(N) = sart((4*M(N-2)^2 + 6*M(N-1)^2 + 9*M(N)^2 + 6*MNP1^2)/25);
SMNP1 = sgrt((4*M(N-1)^2 + 6*M(N)^2 + 9*MNP1^2)/19);
for i = 2:N-1
    q(i+N) = (SM(i+1) + SM(i))*(x(i+1) - x(i)) - ...
        (SM(i) + SM(i-1))*(x(i) - x(i-1));
g(1+N) = (SM(2) + SM(1))*(x(2) - x(1)) - (SM(1) + SM0)*(x(1) - x0);
g(N+N) = (SMNP1 + SM(N))*(xNP1 - x(N)) - (SM(N) + SM(N-1))*(x(N) - x(N-1));
% Form final discrete approximation for Eq. 12 in reference paper, the equation governing
% the mesh points.
tau = 1e-3;
g(1+N:end) = - g(1+N:end)/(2*tau);
end
```

```
function M = mass(t,y)
% Extract the components of y for the solution u and mesh x
N = length(y)/2;
u = y(1:N);
x = y(N+1:end);
% Boundary values of solution u and mesh x
u0 = 0;
uNP1 = 0;
x0 = 0:
xNP1 = 1:
\% M1 and M2 are the portions of the mass matrix for Burgers' equation.
% The derivative du/dx is approximated with finite differences, using
% single-sided differences on the edges and centered differences in between.
M1 = speye(N);
M2 = sparse(N,N);
M2(1,1) = - (u(2) - u0)/(x(2) - x0);
for i = 2:N-1
    M2(i,i) = -(u(i+1) - u(i-1))/(x(i+1) - x(i-1));
M2(N,N) = - (uNP1 - u(N-1))/(xNP1 - x(N-1));
% M3 and M4 define the equations for mesh point evolution, corresponding to
% MMPDE6 in the reference paper. Since the mesh functions only involve d/dt(dx/dt),
% the M3 portion of the mass matrix is all zeros. The second derivative in M4 is
% approximated using a finite difference Laplacian matrix.
M3 = sparse(N,N);
e = ones(N,1);
M4 = spdiags([e -2*e e], -1:1,N,N);
% Assemble mass matrix
M = [M1 M2]
     M3 M41:
end
function out = JPat(N) % Jacobian sparsity pattern
S1 = spdiags(ones(N,3),-1:1,N,N);
S2 = spdiags(ones(N,9), -4:4,N,N);
out = [S1 S1]
    S2 S21;
end
function S = MvPat(N) % Sparsity pattern for the derivative of the Mass matrix times a vector
S = sparse(2*N, 2*N);
S(1,2) = 1;
S(1,2+N) = 1;
for i = 2:N-1
    S(i,i-1) = 1;
    S(i,i+1) = 1;
    S(i,i-1+N) = 1;
    S(i,i+1+N) = 1;
end
S(N,N-1) = 1;
S(N,N-1+N) = 1;
```

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See Also

ode15s | odeset

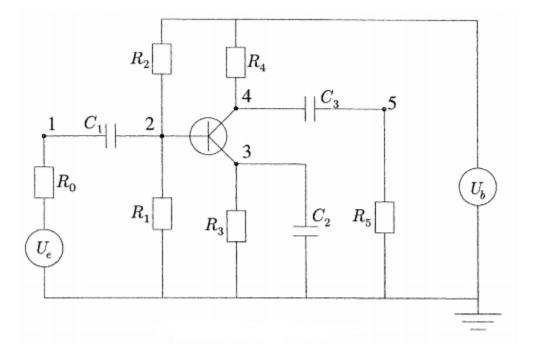
More About

- "Choose an ODE Solver" on page 11-2
- "Summary of ODE Options" on page 11-10
- "Solve Equations of Motion for Baton Thrown into Air" on page $11\mbox{-}56$

Solve Stiff Transistor Differential Algebraic Equation

This example shows how to use ode23t to solve a stiff differential algebraic equation (DAE) that describes an electrical circuit [1]. The one-transistor amplifier problem coded in the example file amp1dae.m can be rewritten in semi-explicit form, but this example solves it in its original form $Mu' = \phi(u)$. The problem includes a constant, singular mass matrix M.

The transistor amplifier circuit contains six resistors, three capacitors, and a transistor.



- The initial voltage signal is $U_e(t) = 0.4\sin(200\pi t)$.
- The operating voltage is $U_b = 6$.
- The voltages at the nodes are given by $U_i(t)$ (i = 1, 2, 3, 4, 5).
- The values of the resistors R_i (i = 1, 2, 3, 4, 5, 6) are constant, and the current through each resistor satisfies I = U/R.
- The values of the capacitors C_i (i = 1, 2, 3) are constant, and the current through each capacitor satisfies $I = C \cdot dU/dt$.

The goal is to solve for the output voltage through node 5, $U_5(t)$.

To solve this equation in MATLAB®, you need to code the equations, code a mass matrix, and set the initial conditions and interval of integration before calling the solver ode23t. You can either include the required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Code Mass Matrix

Using Kirchoff's law to equalize the current through each node (1 through 5), you can obtain a system of five equations describing the circuit:

node 1:
$$\frac{U_e(t)}{R_0} - \frac{U_1}{R_0} + C_1(U_2' - U_1') = 0$$
,
node 2: $\frac{U_b}{R_2} - U_2(\frac{1}{R_1} + \frac{1}{R_2}) + C_1(U_1' - U_2') - 0 \cdot 01f(U_2 - U_3) = 0$,
node 3: $f(U_2 - U_3) - \frac{U_3}{R_3} - C_2U_3' = 0$,
node 4: $\frac{U_b}{R_4} - \frac{U_4}{R_4} + C_3(U_5' - U_4') - 0 \cdot 99f(U_2 - U_3) = 0$,
node 5: $-\frac{U_5}{R_5} + C_3(U_4' - U_5') = 0$.

The mass matrix of this system, found by collecting the derivative terms on the left side of the equations, has the form

$$M = \begin{pmatrix} -c_1 & c_1 & 0 & 0 & 0 \\ c_1 & -c_1 & 0 & 0 & 0 \\ 0 & 0 & -c_2 & 0 & 0 \\ 0 & 0 & 0 & -c_3 & c_3 \\ 0 & 0 & 0 & c_3 & -c_3 \end{pmatrix},$$

where $c_k = k \times 10^{-6}$ for k = 1, 2, 3.

Create a mass matrix with the appropriate constants c_k , and then use the odeset function to specify the mass matrix. Even though it is apparent that the mass matrix is singular, leave the 'MassSingular' option at its default value of 'maybe' to test the automatic detection of a DAE problem by the solver.

```
c = 1e-6 * (1:3);
M = zeros(5,5);
M(1,1) = -c(1);
M(1,2) = c(1);
M(2,1) = c(1);
M(2,2) = -c(1);
M(3,3) = -c(2);
M(4,4) = -c(3);
M(4,5) = c(3);
M(5,4) = c(3);
M(5,5) = -c(3);
opts = odeset('Mass',M);
```

Code Equations

The function transampdae contains the system of equations for this example. The function defines values for all of the voltages and constant parameters. The derivatives gathered on the left side of the equations are coded in the mass matrix, and transampdae codes the right side of the equations.

```
function dudt = transampdae(t,u)
% Define voltages and parameters
Ue = @(t) 0.4*sin(200*pi*t);
Ub = 6;
R0 = 1000;
```

```
R15 = 9000;

alpha = 0.99;

beta = 1e-6;

Uf = 0.026;

% Define system of equations

f23 = beta*(exp((u(2) - u(3))/Uf) - 1);

dudt = [ -(Ue(t) - u(1))/R0

        -(Ub/R15 - u(2)*2/R15 - (1-alpha)*f23)

        -(f23 - u(3)/R15)

        -((Ub - u(4))/R15 - alpha*f23)

        (u(5)/R15) ];

end
```

Note: This function is included as a local function at the end of the example.

Code Initial Conditions

Set the initial conditions. This example uses the consistent initial conditions for the current through each node computed in [1].

```
\begin{array}{lll} Ub &=& 6;\\ u0(1) &=& 0;\\ u0(2) &=& Ub/2;\\ u0(3) &=& Ub/2;\\ u0(4) &=& Ub;\\ u0(5) &=& 0; \end{array}
```

Solve System of Equations

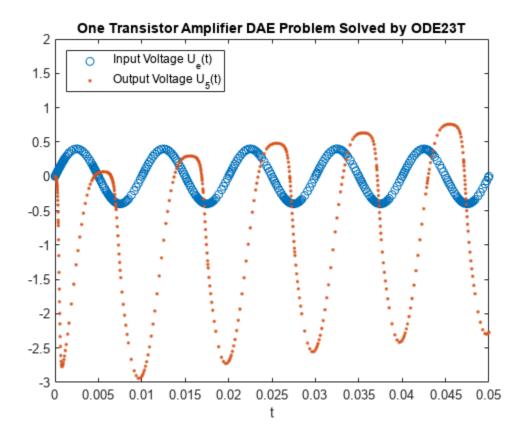
Solve the DAE system over the time interval [0 0.05] using ode23t.

```
tspan = [0 0.05];
[t,u] = ode23t(@transampdae,tspan,u0,opts);
```

Plot Results

Plot the initial voltage $U_e(t)$ and output voltage $U_5(t)$.

```
Ue = @(t) 0.4*sin(200*pi*t);
plot(t,Ue(t),'o',t,u(:,5),'.')
axis([0 0.05 -3 2]);
legend('Input Voltage U_e(t)','Output Voltage U_5(t)','Location','NorthWest');
title('One Transistor Amplifier DAE Problem Solved by ODE23T');
xlabel('t');
```



References

[1] Hairer, E., and Gerhard Wanner. Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems. Springer Berlin Heidelberg, 1991, p. 377.

Local Functions

Listed here is the local helper function that the ODE solver ode23t calls to calculate the solution. Alternatively, you can save this function as its own file in a directory on the MATLAB path.

```
function dudt = transampdae(t,u)
% Define voltages and parameters
Ue = @(t) 0.4*sin(200*pi*t);
Ub = 6;
R0 = 1000;
R15 = 9000;
alpha = 0.99;
beta = 1e-6;
Uf = 0.026;
% Define system of equations
f23 = beta*(exp((u(2) - u(3))/Uf) - 1);
dudt = [ -(Ue(t) - u(1))/R0 ]
    -(Ub/R15 - u(2)*2/R15 - (1-alpha)*f23)
    -(f23 - u(3)/R15)
    -((Ub - u(4))/R15 - alpha*f23)
```

```
(u(5)/R15)];
```

See Also

ode23t | ode15s

More About

- "Choose an ODE Solver" on page 11-2
- "Summary of ODE Options" on page 11-10
- "Solve Differential Algebraic Equations (DAEs)" on page 11-30
- "Solve ODE with Strongly State-Dependent Mass Matrix" on page 11-62

Solve System of ODEs with Multiple Initial Conditions

This example compares two techniques to solve a system of ordinary differential equations with multiple sets of initial conditions. The techniques are:

- Use a for-loop to perform several simulations, one for each set of initial conditions. This technique is simple to use but does not offer the best performance for large systems.
- Vectorize the ODE function to solve the system of equations for all sets of initial conditions simultaneously. This technique is the faster method for large systems but requires rewriting the ODE function so that it reshapes the inputs properly.

The equations used to demonstrate these techniques are the well-known Lotka-Volterra equations. which are first-order nonlinear differential equations that describe the populations of predators and prey.

Problem Description

The Lotka-Volterra equations are a system of two first-order, nonlinear ODEs that describe the populations of predators and prey in a biological system. Over time, the populations of the predators and prey change according to the equations

$$\frac{\mathrm{dx}}{\mathrm{dt}} = \alpha x - \beta x y,$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = \delta xy - \gamma y.$$

The variables in these equations are

- *x* is the population size of the prey
- y is the population size of the predators
- t is time
- α , β , δ , and γ are constant parameters that describe the interactions between the two species. This example uses the parameter values $\alpha = \gamma = 1$, $\beta = 0.01$, and $\delta = 0.02$.

For this problem, the initial values for x and y are the initial population sizes. Solving the equations then provides information about how the populations change over time as the species interact.

Solve Equations with One Initial Condition

To solve the Lotka-Volterra equations in MATLAB®, write a function that encodes the equations, specify a time interval for the integration, and specify the initial conditions. Then you can use one of the ODE solvers, such as ode45, to simulate the system over time.

A function that encodes the equations is

```
function dpdt = lotkaODE(t,p)
% LOTKA Lotka-Volterra predator-prey model
delta = 0.02;
beta = 0.01;
dpdt = [p(1) .* (1 - beta*p(2));
        p(2) .* (-1 + delta*p(1))];
end
```

(This function is included as a local function at the end of the example.)

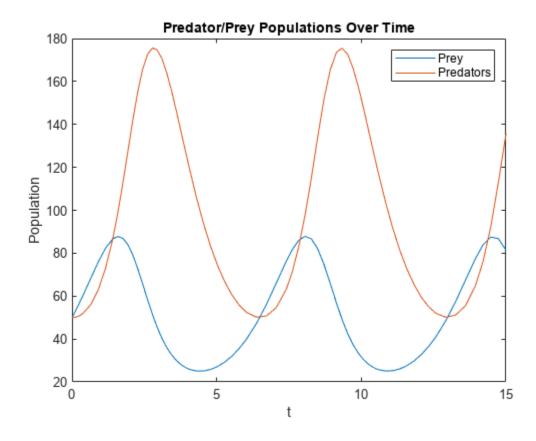
Since there are two equations in the system, dpdt is a vector with one element for each equation. Also, the solution vector p has one element for each solution component: p(1) represents x in the original equations, and p(2) represents y in the original equations.

Next, specify the time interval for integration as [0, 15] and set the initial population sizes for x and y to 50.

```
t0 = 0;
tfinal = 15;
p0 = [50; 50];
```

Solve the system with ode45 by specifying the ODE function, the time span, and the initial conditions. Plot the resulting populations versus time.

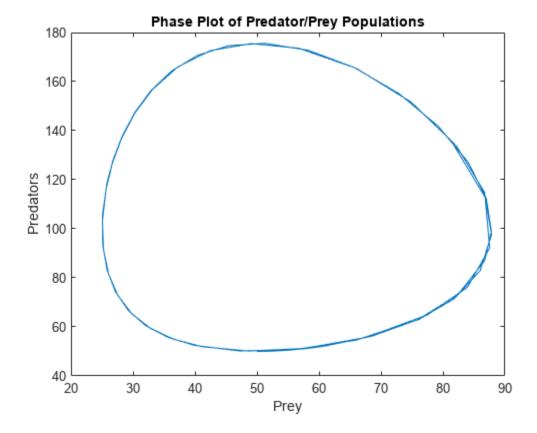
```
[t,p] = ode45(@lotka0DE,[t0 tfinal],p0);
plot(t,p)
title('Predator/Prey Populations Over Time')
xlabel('t')
ylabel('Population')
legend('Prey','Predators')
```



Since the solutions exhibit periodicity, plot the solutions against each other in a phase plot.

```
plot(p(:,1),p(:,2))
title('Phase Plot of Predator/Prey Populations')
```

```
xlabel('Prey')
ylabel('Predators')
```



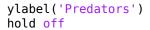
The resulting plots show the solution for the given initial population sizes. To solve the equations for different initial population sizes, change the values in p0 and rerun the simulation. However, this method only solves the equations for one initial condition at a time. The next two sections describe techniques to solve for many different initial conditions.

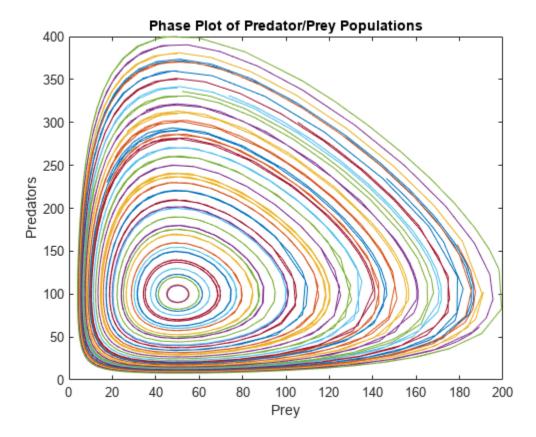
Method 1: Compute Multiple Initial Conditions with for-loop

The simplest way to solve a system of ODEs for multiple initial conditions is with a for-loop. This technique uses the same ODE function as the single initial condition technique, but the for-loop automates the solution process.

For example, you can hold the initial population size for x constant at 50, and use the for-loop to vary the initial population size for y between 10 and 400. Create a vector of population sizes for y0, and then loop over the values to solve the equations for each set of initial conditions. Plot a phase plot with the results from all iterations.

```
y0 = 10:10:400;
for k = 1:length(y0)
    [t,p] = ode45(@lotkaODE,[t0 tfinal],[50 y0(k)]);
    plot(p(:,1),p(:,2))
    hold on
title('Phase Plot of Predator/Prey Populations')
xlabel('Prey')
```





The phase plot shows all of the computed solutions for the different sets of initial conditions.

Method 2: Compute Multiple Initial Conditions with Vectorized ODE Function

Another method to solve a system of ODEs for multiple initial conditions is to rewrite the ODE function so that all of the equations are solved simultaneously. The steps to do this are:

- Provide all of the initial conditions to ode45 as a matrix. The size of the matrix is s-by-n, where s is the number of solution components and n is the number of initial conditions being solved for. Each column in the matrix then represents one complete set of initial conditions for the system.
- The ODE function must accept an extra input parameter for n, the number of initial conditions.
- Inside the ODE function, the solver passes the solution components p as a column vector. The ODE function must reshape the vector into a matrix with size s-by-n. Each row of the matrix then contains all of the initial conditions for each variable.
- The ODE function must solve the equations in a vectorized format, so that the expression accepts vectors for the solution components. In other words, $f(t,[y1\ y2\ y3\ ...])$ must return $[f(t,y1)\ f(t,y2)\ f(t,y3)\ ...]$.
- Finally, the ODE function must reshape its output back into a vector so that the ODE solver receives a vector back from each function call.

If you follow these steps, then the ODE solver can solve the system of equations using a vector for the solution components, while the ODE function reshapes the vector into a matrix and solves each

solution component for all of the initial conditions. The result is that you can solve the system for all of the initial conditions in one simulation.

To implement this method for the Lotka-Volterra system, start by finding the number of initial conditions n, and then form a matrix of initial conditions.

```
n = length(y0);
p0_all = [50*ones(n,1) y0(:)]';
```

Next, rewrite the ODE function so that it accepts n as an input. Use n to reshape the solution vector into a matrix, then solve the vectorized system and reshape the output back into a vector. A modified ODE function that performs these tasks is

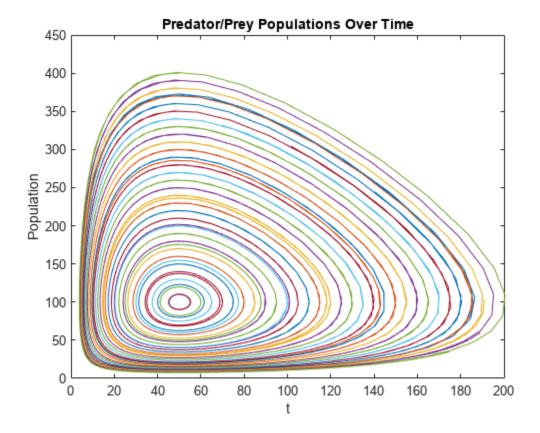
```
function dpdt = lotkasystem(t,p,n)
%LOTKA Lotka-Volterra predator-prey model for system of inputs p.
delta = 0.02;
beta = 0.01;
% Change the size of p to be: Number of equations-by-number of initial
% conditions.
p = reshape(p,[],n);
% Write equations in vectorized form.
dpdt = [p(1,:) .* (1 - beta*p(2,:));
        p(2,:) .* (-1 + delta*p(1,:))];
% Linearize output.
dpdt = dpdt(:);
end
```

Solve the system of equations for all of the initial conditions using ode45. Since ode45 requires the ODE function to accept two inputs, use an anonymous function to pass in the value of n from the workspace to lotkasystem.

```
[t,p] = ode45(@(t,p) lotkasystem(t,p,n),[t0 tfinal],p0 all);
```

Reshape the output vector into a matrix with size (numTimeSteps*s)-by-n. Each column of the output p(:,k) contains the solutions for one set of initial conditions. Plot a phase plot of the solution components.

```
p = reshape(p,[],n);
nt = length(t);
for k = 1:n
    plot(p(1:nt,k),p(nt+1:end,k))
    hold on
title('Predator/Prey Populations Over Time')
xlabel('t')
ylabel('Population')
hold off
```



The results are comparable to those obtained by the for-loop technique. However, there are some properties of the vectorized solution technique that you should keep in mind:

- The calculated solutions can be slightly different than those computed from a single initial input. The difference arises because the ODE solver applies norm checks to the entire system to calculate the size of the time steps, so the time-stepping behavior of the solution is slightly different. The change in time steps generally does not affect the accuracy of the solution, but rather which times the solution is evaluated at.
- For stiff ODE solvers (ode15s, ode23s, ode23t, ode23tb) that automatically evaluate the numerical Jacobian of the system, specifying the block diagonal sparsity pattern of the Jacobian using the JPattern option of odeset can improve the efficiency of the calculation. The block diagonal form of the Jacobian arises from the input reshaping performed in the rewritten ODE function.

Compare Timing Results

Time each of the previous methods using timeit. The timing for solving the equations with one set of initial conditions is included as a baseline number to see how the methods scale.

```
% Time one IC
baseline = timeit(@() ode45(@lotkaODE,[t0 tfinal],p0),2);
% Time for-loop
for k = 1:length(y0)
    loop_timing(k) = timeit(@() ode45(@lotkaODE,[t0 tfinal],[50 y0(k)]),2);
end
```

```
loop_timing = sum(loop_timing);
% Time vectorized fcn
vectorized_timing = timeit(@() ode45(@(t,p) lotkasystem(t,p,n),[t0 tfinal],p0_all),2);
```

Create a table with the timing results. Multiply all of the results by 1e3 to express the times in milliseconds. Include a column with the time per solution, which divides each time by the number of initial conditions being solved for.

```
TimingTable = table(1e3.*[baseline; loop_timing; vectorized_timing], 1e3.*[baseline; loop_timing,
                                       'VariableNames', {'TotalTime (ms)', 'TimePerSolution (ms)'}, 'RowNames', {'One IC', 'Multi ICs: Formula | TotalTime (ms) | TimePerSolution (ms) | TimePerSolutio
TimingTable=3×2 table
                                                                                                                                                                                                                                                        TotalTime (ms) TimePerSolution (ms)
```

	TOTALITINE (IIIS)	TIMEPEL SOCULION (1	115)
One IC	0.95787	0.95787	
Multi ICs: For-loop	24.599	0.61497	
Mult ICs: Vectorized	3.1137	0.077842	

The TimePerSolution column shows that the vectorized technique is the fastest of the three methods.

Local Functions

Listed here are the local functions that ode45 calls to calculate the solutions.

```
function dpdt = lotkaODE(t,p)
% LOTKA Lotka-Volterra predator-prey model
delta = 0.02:
beta = 0.01;
dpdt = [p(1) .* (1 - beta*p(2));
        p(2) \cdot * (-1 + delta*p(1))];
end
function dpdt = lotkasystem(t,p,n)
%LOTKA Lotka-Volterra predator-prey model for system of inputs p.
delta = 0.02;
beta = 0.01;
% Change the size of p to be: Number of equations-by-number of initial
% conditions.
p = reshape(p,[],n);
% Write equations in vectorized form.
dpdt = [p(1,:) .* (1 - beta*p(2,:));
        p(2,:) .* (-1 + delta*p(1,:))];
% Linearize output.
dpdt = dpdt(:);
end
```

See Also

ode45 | odeset

More About

- "Choose an ODE Solver" on page 11-2
- "Solve Predator-Prey Equations" on page 11-52

Solve Celestial Mechanics Problem with High-Order Solvers

This example shows how to use ode78 and ode89 to solve a celestial mechanics problem that requires high accuracy in each step from the ODE solver for a successful integration. Both ode45 and ode113 are unable to solve the problem using the default error tolerances. Even with more stringent error thresholds, ode89 performs best on the problem due to the high accuracy of the Runge-Kutta formulas it uses in each step.

Problem Description

The *Pleiades problem* is a celestial mechanics problem describing the gravitational interactions of seven stars [1]. This cluster of stars is also referred to as The Seven Sisters, and it is visible to the human eye in the night sky due to its proximity to Earth [2]. The system of equations describing the motion of the stars in the cluster consists of 14 nonstiff second-order differential equations, which produce a system of 28 equations when rewritten in first-order form.

Newton's second law of motion relates the force applied to a body to its rate of change in momentum over time,

$$F_i = \frac{\mathrm{d}}{\mathrm{d}t} p_i.$$

The momentum $(p_i = m_i v_i)$ has separate x- and y-components. At the same time, the universal law of gravitation describes the force working on body *i* from body *j* as

$$F_{ij} = g \frac{m_i m_j}{\|p_i - p_j\|^2} d_{ij}.$$

The term $d_{ij} = \frac{p_j - p_i}{\|p_j - p_i\|}$ gives the direction of the distance between the bodies, and the masses of the bodies are $m_i = i$ for i = 1, 2, ..., 7. For a system with many bodies, the force applied to any individual body is the sum of its interactions with all others, so

$$F_i = \sum_{i \neq j} F_{ij}.$$

Setting the gravitational constant q equal to 1 and solving yields a system of second-order equations describing the evolution of the x- and y-components over time.

$$x_i'' = f_i(x, y) = \sum_{j \neq i} \frac{m_j(x_j - x_i)}{r_{ij}^{3/2}},$$

$$y_i'' = h_i(x, y) = \sum_{j \neq i} \frac{m_j(y_j - y_i)}{r_{ij}^{3/2}},$$

where $r_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$. Because these two equations apply for each of the seven stars in the system, 14 second-order differential equations (i = 1, 2, ..., 7) describe the entire system.

The initial conditions for the system, as given in [1], are:

$$\begin{cases} x_0 = (3, 3, -1, -3, 2, -2, 2) \\ y_0 = (3, -3, 2, 0, 0, -4, 4) \\ x_0' = (0, 0, 0, 0, 0, 1.75, -1.5) \\ y_0' = (0, 0, 0, 0, -1.25, 1, 0, 0) \end{cases}$$

To solve this system of ODEs in MATLAB®, you must code the equations into a function before calling the solvers ode78 and ode89. You can either include the required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Code Equations

The ODE solvers in MATLAB require equations to be written in first-order form, q' = u(t, q). For this problem, the system of equations can be rewritten in first-order form using the substitutions w = x' and z = y'. With these substitutions, the system contains 28 first-order equations organized into four groups of seven equations:

$$\begin{bmatrix} x_i' \\ y_i' \\ w_i' \\ z_i' \end{bmatrix} = \begin{bmatrix} w_i \\ z_i \\ f_i(x, y) \\ h_i(x, y) \end{bmatrix}.$$

The solution vector produced by solving the system has the form

$$q = \begin{bmatrix} x_i \\ y_i \\ w_i \\ z_i \end{bmatrix}$$

Therefore, writing the original equations in terms of the solution vector q yields

$$\begin{bmatrix} x_i' \\ y_i' \\ w_i' \\ z_i' \end{bmatrix} = \begin{bmatrix} (q_{15}, q_{16}, \dots, q_{21}) \\ (q_{22}, q_{23}, \dots, q_{28}) \\ f_i(x, y) \\ h_i(x, y) \end{bmatrix},$$

where $x = (q_1, q_2, \ldots, q_7)$ and $y = (q_8, q_9, \ldots, q_{14})$. With the equations written in the first-order form q' = u(t, q), you can now write a function that calculates the components during each time step of the solution process. A function that codes this system of equations is:

In this function, the x and y values are extracted directly from the solution vector q, as are the first 14 components of the output. Then, the function uses the position values to calculate the distances between all seven stars, and these distances are used in the code for $f_i(x, y)$ and $h_i(x, y)$.

Set Optional Parameters

Use the odeset function to set the value of several optional parameters:

- Specify stringent error tolerances of 1e-13 and 1e-15 for the relative and absolute error tolerances, respectively.
- Turn on the display of solver statistics.

```
opts = odeset("RelTol", 1e-13, "AbsTol", 1e-15, "Stats", "on");
```

Solve System of Equations

Create a column vector with the initial conditions and a time vector with regularly spaced points in the range [0, 15]. When you specify a time vector with more than two elements, the solver returns solutions at the time points you specify.

```
init = [3 \ 3 \ -1 \ -3 \ 2 \ -2 \ 2 \ ...
         3 -3 2 0 0 -4 4 ...
         0 0 0 0 0 1.75 -1.5 ...
         0 0 0 -1.25 1 0 0]';
tspan = linspace(1,15,200);
```

Now, solve the equations using both ode78 and ode89 by specifying the equations, time span, initial values, and options. Use tic and toc to time each solver for comparison (note that timings can differ depending on your computer).

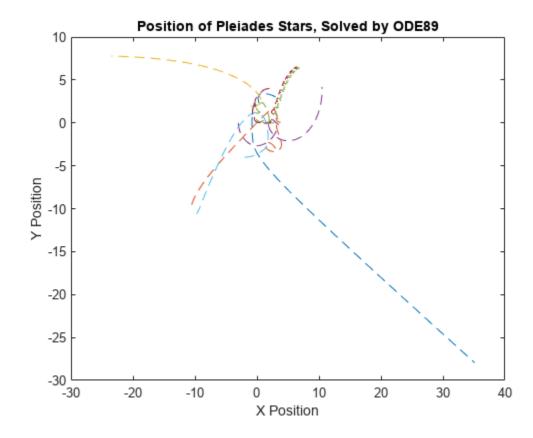
```
tic
[t78,q78] = ode78(@pleiades,tspan,init,opts);
14963 successful steps
549 failed attempts
201899 function evaluations
toc
Elapsed time is 7.457172 seconds.
[t89,q89] = ode89(@pleiades,tspan,init,opts);
4181 successful steps
56 failed attempts
68726 function evaluations
Elapsed time is 2.640665 seconds.
```

The output indicates that ode89 is best suited for solving the problem, because it is faster and has fewer failed steps.

Plot Solution Curves

The first 14 components of q89 contain the x and y positions for each of the seven stars, as obtained by ode89. Plot these solution components to see the trajectories of all the stars over time.

```
plot(q89(:,1),q89(:,8),'--',...
    q89(:,2),q89(:,9),'--',...
    q89(:,3),q89(:,10),'--',...
    q89(:,4),q89(:,11),'--',...
    q89(:,5),q89(:,12),'--',...
    q89(:,6),q89(:,13),'--',...
    q89(:,7),q89(:,14),'--')
title('Position of Pleiades Stars, Solved by ODE89')
xlabel('X Position')
ylabel('Y Position')
```



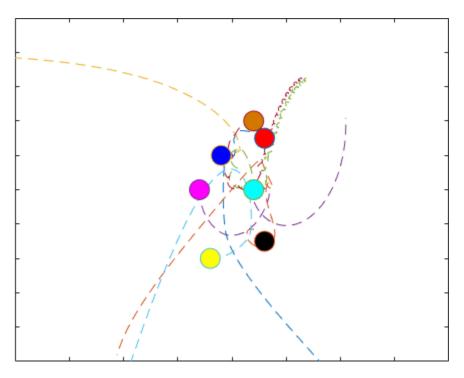
Create Animation of Results

Because the trajectories of the stars overlap considerably, a better way to visualize the results is to create an animation showing the stars move over time. The function AnimateOrbits, included as a local function at the end of this example, accepts the output from a solver for this problem and creates an animated GIF file in the current folder that shows the stars move along their trajectories.

For example, you can generate an animation with the output from the ode89 solver using the command

AnimateOrbits(t89,q89);

The following is a sample output GIF.



References

- [1] Hairer, E., et al. Solving Ordinary Differential Equations I: Nonstiff Problems. 2nd rev. ed, Springer, 2009.
- [2] "Pleiades." Wikipedia, 21 June 2021. Wikipedia, https://en.wikipedia.org/wiki/Pleiades.

Local Functions

This section includes the local functions called by the ODE solver to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

```
function dqdt = pleiades(t,q)
  x = q(1:7);
  y = q(8:14);
  xDist = (x - x.');
  yDist = (y - y.');
  r = (xDist.^2+yDist.^2).^(3/2);
  m = (1:7)';
  dqdt = [q(15:28);
             sum(xDist.*m./r,1,'omitnan').';
             sum(yDist.*m./r,1,'omitnan').'];
end
function AnimateOrbits(t,q)
for k = 1:length(t)
     plot(q(:,1),q(:,8),'--',q(:,2),q(:,9),'--',...

q(:,3),q(:,10),'--',q(:,4),q(:,11),'--',...

q(:,5),q(:,12),'--',q(:,6),q(:,13),'--',...

q(:,7),q(:,14),'--')
     hold on
     xlim([-20 20])
     ylim([-10 10])
```

```
sz = 15;
       plot(q(k,1),q(k,8),'o','MarkerSize',sz,'MarkerFaceColor','r')
       plot(q(k,1),q(k,0), 0 , MarkerSize ,sz, MarkerFaceColor','k')
plot(q(k,2),q(k,9),'o','MarkerSize',sz,'MarkerFaceColor','k')
plot(q(k,3),q(k,10),'o','MarkerSize',sz,'MarkerFaceColor','b')
plot(q(k,4),q(k,11),'o','MarkerSize',sz,'MarkerFaceColor','m')
plot(q(k,5),q(k,12),'o','MarkerSize',sz,'MarkerFaceColor','c')
plot(q(k,6),q(k,13),'o','MarkerSize',sz,'MarkerFaceColor','y')
plot(q(k,7),q(k,14),'o','MarkerSize',sz,'MarkerFaceColor',[210 120 0]./255)
       hold off
       drawnow
       M(k) = getframe(gca);
       im\{k\} = frame2im(M(k));
end
filename = "orbits.gif";
for idx = 1:length(im)
       [A,map] = rgb2ind(im{idx},256);
       if idx == 1
               imwrite(A, map, filename, 'gif', 'LoopCount', Inf, 'DelayTime', 0);
               imwrite(A,map,filename,'gif','WriteMode','append','DelayTime',0);
       end
end
close all
end
```

See Also

ode78 | ode89 | odeset

Related Examples

- "Choose an ODE Solver" on page 11-2
- "Summary of ODE Options" on page 11-10
- "Solve Equations of Motion for Baton Thrown into Air" on page 11-56

Boundary Value Problems (BVPs)

- "Solving Boundary Value Problems" on page 12-2
- "Solve BVP with Two Solutions" on page 12-8
- "Solve BVP with Unknown Parameter" on page 12-11
- "Solve BVP Using Continuation" on page 12-15
- "Verify BVP Consistency Using Continuation" on page 12-20
- "Solve BVP with Singular Term" on page 12-25
- "Solve BVP with Multiple Boundary Conditions" on page 12-29

Solving Boundary Value Problems

In a boundary value problem (BVP), the goal is to find a solution to an ordinary differential equation (ODE) that also satisfies certain specified boundary conditions. The boundary conditions specify a relationship between the values of the solution at two or more locations in the interval of integration. In the simplest case, the boundary conditions apply at the beginning and end (or boundaries) of the interval.

The MATLAB BVP solvers byp4c and byp5c are designed to handle systems of ODEs of the form

$$y' = f(x, y)$$

where:

- *x* is the independent variable
- y is the dependent variable
- y' represents the derivative of y with respect to x, also written as dy/dx

Boundary Conditions

In the simplest case of a two-point BVP, the solution to the ODE is sought on an interval [a, b], and must satisfy the boundary conditions

```
g(y(a), y(b)) = 0.
```

To specify the boundary conditions for a given BVP, you must:

 Write a function of the form res = bcfun(ya,yb), or use the form res = bcfun(ya,yb,p) if there are unknown parameters involved. You supply this function to the solver as the second input argument. The function returns res, which is the residual value of the solution at the boundary point. For example, if y(a) = 1 and y(b) = 0, then the boundary condition function is

```
function res = bcfun(ya,yb)
res = [ya(1)-1]
       yb(1)];
end
```

In the initial guess for the solution, the first and last points in the mesh specify the points at which the boundary conditions are enforced. For the above boundary conditions, you can specify bvpinit(linspace(a, b, 5), yinit) to enforce the boundary conditions at a and b.

The BVP solvers in MATLAB also can accommodate other types of problems that have:

- Unknown parameters p
- Singularities in the solutions
- Multipoint conditions (internal boundaries that separate the integration interval into several regions)

In the case of multipoint boundary conditions, the boundary conditions apply at more than two points in the interval of integration. For example, the solution might be required to be zero at the beginning, middle, and end of the interval. See bypinit for details on how to specify multiple boundary conditions.

Initial Guess of Solution

Unlike initial value problems, a boundary value problem can have:

- No solution
- A finite number of solutions
- · Infinitely many solutions

An important part of the process of solving a BVP is providing a guess for the required solution. The quality of this guess can be critical for the solver performance and even for a successful computation.

Use the bvpinit function to create a structure for the initial guess of the solution. The solvers bvp4c and bvp5c accept this structure as the third input argument.

Creating a good initial guess for the solution is more an art than a science. However, some general guidelines include:

- Have the initial guess satisfy the boundary conditions, since the solution is required to satisfy them as well. If the problem contains unknown parameters, then the initial guess for the parameters also should satisfy the boundary conditions.
- Try to incorporate as much information about the physical problem or expected solution into the initial guess as possible. For example, if the solution is supposed to oscillate or have a certain number of sign changes, then the initial guess should as well.
- Consider the placement of the mesh points (the x-coordinates of the initial guess of the solution). The BVP solvers adapt these points during the solution process, so you do not need to specify too many mesh points. Best practice is to specify a few mesh points placed near where the solution changes rapidly.
- If there is a known, simpler solution on a smaller interval, then use it as an initial guess on a larger interval. Often you can solve a problem as a series of relatively simpler problems, a practice called *continuation*. With continuation, a series of simple problems are connected by using the solution of one problem as the initial guess to solve the next problem.

Finding Unknown Parameters

Often BVPs involve unknown parameters p that have to be determined as part of solving the problem. The ODE and boundary conditions become

```
y' = f(x, y, p)
g(y(a), y(b), p) = 0
```

In this case, the boundary conditions must suffice to determine the values of the parameters p.

You must provide the solver with an initial guess for any unknown parameters. When you call bvpinit to create the structure solinit, specify the initial guess as a vector in the third input argument parameters.

```
solinit = bvpinit(x,v,parameters)
```

Additionally, the functions odefun and bcfun that encode the ODE equations and boundary conditions must each have a third argument.

```
dydx = odefun(x,y,parameters)
res = bcfun(ya,yb,parameters)
```

While solving the differential equations, the solver adjusts the value of the unknown parameters to satisfy the boundary conditions. The solver returns the final values of these unknown parameters in sol.parameters.

Singular BVPs

bvp4c and bvp5c can solve a class of singular BVPs of the form

$$y' = \frac{1}{x}Sy + f(x, y),$$

 $0 = g(y(0), y(b)).$

The solvers can also accommodate unknown parameters for problems of the form

$$y' = \frac{1}{x}Sy + f(x, y, p),$$

0 = $g(y(0), y(b), p)$.

Singular problems must be posed on an interval [0,b] with b > 0. Use bypset to pass the constant matrix S to the solver as the value of the 'SingularTerm' option. Boundary conditions at x = 0 must be consistent with the necessary condition for a smooth solution, Sy(0) = 0. The initial guess of the solution also should satisfy this condition.

When you solve a singular BVP, the solver requires that your function odefun(x,y) return only the value of the f(x, y) term in the equation. The term involving S is handled by the solver separately using the 'SingularTerm' option.

BVP Solver Selection

MATLAB includes the solvers bvp4c and bvp5c to solve BVPs. In most cases you can use the solvers interchangeably. The main difference between the solvers is that bvp4c implements a fourth-order formula, while bvp5c implements a fifth-order formula.

The bvp5c function is used exactly like bvp4c, with the exception of the meaning of error tolerances between the two solvers. If S(x) approximates the solution y(x), bvp4c controls the residual |S'(x) - f(x,S(x))|. This approach indirectly controls the true error |y(x) - S(x)|. Use bvp5c to control the true error directly.

Solver	Description
bvp4c	bvp4c is a finite difference code that implements the 3-stage Lobatto IIIa formula. This is a collocation formula, and the collocation polynomial provides a C¹-continuous solution that is fourth-order accurate uniformly in the interval of integration. Mesh selection and error control are based on the residual of the continuous solution.
	The collocation technique uses a mesh of points to divide the interval of integration into subintervals. The solver determines a numerical solution by solving a global system of algebraic equations resulting from the boundary conditions and the collocation conditions imposed on all the subintervals. The solver then estimates the error of the numerical solution on each subinterval. If the solution does not satisfy the tolerance criteria, then the solver adapts the mesh and repeats the process. You <i>must</i> provide the points of the initial mesh, as well as an initial approximation of the solution at the mesh points.
bvp5c	bvp5c is a finite difference code that implements the four-stage Lobatto IIIa formula. This is a collocation formula and the collocation polynomial provides a C¹-continuous solution that is fifth-order accurate uniformly in [a,b]. The formula is implemented as an implicit Runge-Kutta formula. bvp5c solves the algebraic equations directly, whereas bvp4c uses analytical condensation. bvp4c handles unknown parameters directly, while bvp5c augments the system with trivial differential equations for unknown parameters.

Evaluating the Solution

The collocation methods implemented in bvp4c and bvp5c produce C^1 -continuous solutions over the interval of integration [a,b]. You can evaluate the approximate solution, S(x), at any point in [a,b] using the helper function deval and the structure sol returned by the solver. For example, to evaluate the solution sol at the mesh of points xint, use the command

Sxint = deval(sol,xint)

The deval function is vectorized. For a vector xint, the ith column of Sxint approximates the solution y(xint(i)).

BVP Examples and Files

Several available example files serve as excellent starting points for most common BVP problems. To easily explore and run examples, simply use the Differential Equations Examples app. To run this app, type

odeexamples

To open an individual example file for editing, type

edit exampleFileName.m

To run an example, type

exampleFileName

This table contains a list of the available BVP example files, as well as the solvers and the options they use.

Example File	Solver Used	Options Specified	Description	Example Link
emdenbv p	bvp4c or bvp5c	• 'SingularTer m'	Emden's equation, a singular BVP	"Solve BVP with Singular Term" on page 12-25
fsbvp	bvp4c or bvp5c	_	Falkner-Skan BVP on an infinite interval	"Verify BVP Consistency Using Continuation" on page 12-20
mat4bvp	bvp4c or bvp5c	_	Fourth eigenfunction of Mathieu's equation	"Solve BVP with Unknown Parameter" on page 12-11
rcbvp	bvp4c and bvp5c	'FJacobian''AbsTol''RelTol''Stats'	Example comparing the errors controlled by bvp4c and bvp5c	"Compare bvp4c and bvp5c Solvers" (bvp4c) "Compare bvp4c and bvp5c Solvers" (bvp5c)
shockbv p	bvp4c or bvp5c	'FJacobian''BCJacobian''Vectorized'	Solution with a shock layer near $x = 0$	"Solve BVP Using Continuation" on page 12-15
twobvp	bvp4c	_	BVP with exactly two solutions	"Solve BVP with Two Solutions" on page 12-8
threebv p	bvp4c or bvp5c	_	Three-point boundary value problem	"Solve BVP with Multiple Boundary Conditions" on page 12-29

References

- [1] Ascher, U., R. Mattheij, and R. Russell. "Numerical Solution of Boundary Value Problems for Ordinary Differential Equations." Philadelphia, PA: SIAM, 1995, p. 372.
- [2] Shampine, L.F., and J. Kierzenka. "A BVP Solver based on residual control and the MATLAB PSE." *ACM Trans. Math. Softw.* Vol. 27, Number 3, 2001, pp. 299–316.
- [3] Shampine, L.F., M.W. Reichelt, and J. Kierzenka. "Solving Boundary Value Problems for Ordinary Differential Equations in MATLAB with bvp4c." *MATLAB File Exchange*, 2004.
- [4] Shampine, L.F., and J. Kierzenka. "A BVP Solver that Controls Residual and Error." *J. Numer. Anal. Ind. Appl. Math.* Vol. 3(1-2), 2008, pp. 27-41.

See Also

bvp4c | bvp5c | bvpinit | bvpset | pdepe | ode45

Solve BVP with Two Solutions

This example uses byp4c with two different initial quesses to find both solutions to a BVP problem.

Consider the differential equation

$$y'' + e^y = 0.$$

This equation is subject to the boundary conditions

$$y(0) = y(1) = 0.$$

To solve this equation in MATLAB®, you need to code the equation and boundary conditions, then generate a suitable initial guess for the solution before calling the boundary value problem solver bvp4c. You either can include the required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Code Equation

Create a function to code the equation. This function should have the signature dydx =bvpfun(x,y) or dydx = bvpfun(x,y,parameters), where:

- x is the independent variable.
- y is the solution (dependent variable).
- parameters is a vector of unknown parameter values (optional).

These inputs are automatically passed to the function by the solver, but the variable names determine how you code the equations. In this case, you can rewrite the second-order equation as a system of first-order equations

```
y_1' = y_2,
v_{2}' = -e^{y_1}.
The function encoding these equations is
function dydx = bvpfun(x,y)
dydx = [y(2)]
```

Code Boundary Conditions

-exp(y(1))];

For two-point boundary value conditions like the ones in this problem, the boundary conditions function should have the signature res = bcfun(ya,yb) or res = bcfun(ya,yb,parameters), depending on whether unknown parameters are involved. ya and yb are column vectors that the solver automatically passes to the function, and bcfun returns the residual in the boundary conditions.

For the boundary conditions y(0) = y(1) = 0, the bcfun function specifies that the residual value is zero at both boundaries. These residual values are enforced at the first and last points of the mesh that you specify to bypinit in your initial guess. The initial mesh in this problem should have x(1) = 0 and x(end) = 1.

```
function res = bcfun(ya,yb)
res = [ya(1)
          yb(1)];
end
```

Form Initial Guess

Call bvpinit to generate an initial guess of the solution. The mesh for x does not need to have a lot of points, but the first point must be 0. Then the last point must be 1 so that the boundary conditions are properly specified. Use an initial guess for y where the first component is slightly positive and the second component is zero.

```
xmesh = linspace(0,1,5);
solinit = bvpinit(xmesh, [0.1 0]);
```

Solve Equation

Solve the BVP using the bvp4c solver.

```
sol1 = bvp4c(@bvpfun, @bcfun, solinit);
```

Use Different Initial Guess

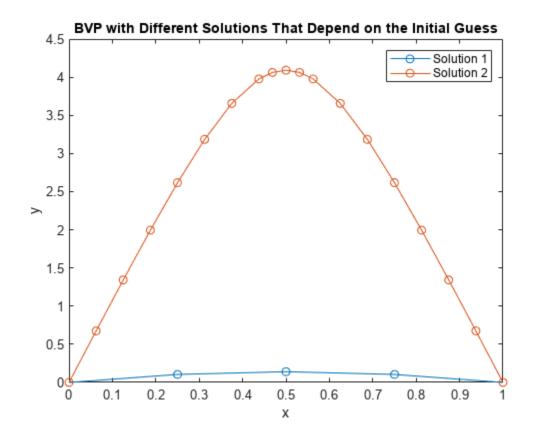
Solve the BVP a second time using a different initial guess for the solution.

```
solinit = bvpinit(xmesh, [3 0]);
sol2 = bvp4c(@bvpfun, @bcfun, solinit);
```

Compare Solutions

Plot the solutions that bvp4c calculates for the different initial conditions. Both solutions satisfy the stated boundary conditions, but have different behaviors inbetween. Since the solution is not always unique, the different behaviors show the importance of giving a good initial guess for the solution.

```
plot(sol1.x,sol1.y(1,:),'-o',sol2.x,sol2.y(1,:),'-o')
title('BVP with Different Solutions That Depend on the Initial Guess')
xlabel('x')
ylabel('y')
legend('Solution 1','Solution 2')
```



Local Functions

Listed here are the local helper functions that the BVP solver bvp4c calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

```
function dydx = bvpfun(x,y) % equation being solved
dydx = [y(2)]
        -exp(y(1))];
end
function res = bcfun(ya,yb) % boundary conditions
res = [ya(1)]
       yb(1)];
end
```

See Also

bvp4c | bvp5c | bvpinit

More About

"Solving Boundary Value Problems" on page 12-2

Solve BVP with Unknown Parameter

This example shows how to use bvp4c to solve a boundary value problem with an unknown parameter.

Mathieu's equation is defined on the interval $[0, \pi]$ by

$$y'' + (\lambda - 2q\cos(2x))y = 0.$$

When the parameter q = 5, the boundary conditions are

$$y'(0) = 0,$$

$$y'(\pi) = 0.$$

However, this only determines y(x) up to a constant multiple, so a third condition is required to specify a particular solution,

$$y(0) = 1$$
.

To solve this system of equations in MATLAB®, you need to code the equations, boundary conditions, and initial guess before calling the boundary value problem solver bvp4c. You can either include the required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Code Equation

Create a function to code the equations. This function should have the signature dydx = mat4ode(x,y,lambda), where:

- x is the independent variable.
- y is the dependent variable.
- lambda is an unknown parameter representing an eigenvalue.

You can write Mathieu's equation as a first-order system using the substitutions $y_1 = y$ and $y_2 = y'$,

```
y_1' = y_2,

y_2' = -(\lambda - 2q\cos(2x))y_1.
```

The corresponding function is then

Note: All functions are included as local functions at the end of the example.

Code Boundary Conditions

Now, write a function that returns the residual value of the boundary conditions at the boundary points. This function should have the signature res = mat4bc(ya,yb,lambda), where:

- ya is the value of the boundary condition at the beginning of the interval [a, b].
- yb is the value of the boundary condition at the end of the interval [a, b].
- lambda is an unknown parameter representing an eigenvalue.

This problem has three boundary conditions in the interval $[0, \pi]$. To calculate the residual values, you need to put the boundary conditions into the form g(x, y) = 0. In this form the boundary conditions are

Create Initial Guess

Lastly, create an initial guess of the solution. You must provide an initial guess for both solution components $y_1 = y(x)$ and $y_2 = y'(x)$, as well as the unknown parameter λ . Only eigenvalues and eigenfunctions that are close to the initial guesses can be computed. To increase the likelihood that the computed eigenfunction corresponds to the fourth eigenvalue, you should choose an initial guess that has the correct qualitative behavior.

For this problem, a cosine function makes for a good initial guess since it satisfies the three boundary conditions. Code the initial guess for y_1 and y_2 .

Call bypinit using a mesh of 10 points in the interval $[0, \pi]$, the initial guess function, and a guess of 15 for the value of λ .

```
lambda = 15;
solinit = bvpinit(linspace(0,pi,10),@mat4init,lambda);
```

Solve Equation

Call byp4c with the ODE function, boundary condition function, and initial guess.

```
sol = bvp4c(@mat4ode, @mat4bc, solinit);
```

Value of Parameter

Print the value of the unknown parameter λ found by bvp4c. This value is the fourth eigenvalue (q = 5) of Mathieu's equation.

Fourth eigenvalue is approximately 17.097.

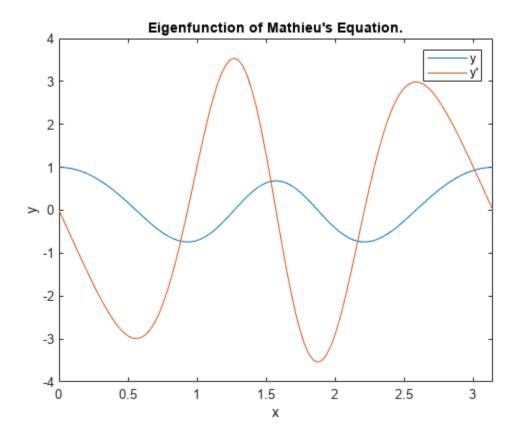
Plot Solution

Use deval to evaluate the solution computed by bvp4c at 100 points in the interval $[0, \pi]$.

```
xint = linspace(0,pi);
Sxint = deval(sol,xint);
```

Plot both solution components. The plot shows the eigenfunction (and its derivative) associated with the fourth eigenvalue $\lambda_4 = 17.097$.

```
plot(xint,Sxint)
axis([0 pi -4 4])
title('Eigenfunction of Mathieu''s Equation.')
xlabel('x')
ylabel('y')
legend('y','y''')
```



Local Functions

Listed here are the local helper functions that the BVP solver bvp4c calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

```
end
function res = mat4bc(ya,yb,lambda) % boundary conditions
res = [ya(2)]
       yb(2)
       ya(1)-1];
end
function yinit = mat4init(x) % initial guess function
yinit = [\cos(4*x)]
        -4*sin(4*x)];
end
```

See Also

bvp4c|bvp5c|bvpinit

More About

"Solving Boundary Value Problems" on page 12-2

Solve BVP Using Continuation

This example shows how to solve a numerically difficult boundary value problem using continuation, which effectively breaks the problem up into a sequence of simpler problems.

For $0 < e \ll 1$, consider the differential equation

$$ey'' + xy' = -e\pi^2 \cos(\pi x) - \pi x \sin(\pi x).$$

The problem is posed on the interval [-1, 1] and is subject to the boundary conditions

$$y(-1) = -2,$$

$$y(1) = 0$$
.

When $e = 10^{-4}$, the solution to the equation undergoes a rapid transition near x = 0, so it is difficult to solve numerically. Instead, this example uses continuation to iterate through several values of e until $e = 10^{-4}$. The intermediate solutions are each used as the initial guess for the next problem.

To solve this system of equations in MATLAB®, you need to code the equations, boundary conditions, and initial guess before calling the boundary value problem solver bvp4c. You either can include the required functions as local functions at the end of a file (as done here), or you can save them as separate, named files in a directory on the MATLAB path.

Code Equation

Using the substitutions $y_1 = y$ and $y_2 = y'$, you can rewrite the equation as the system of first-order equations

$$y_1' = y_2$$
,

$$y_2' = -\frac{x}{e}y' - \pi^2 \cos(\pi x) - \frac{\pi x}{e}\sin(\pi x).$$

Write a function to code the equations with the signature dydx = shockode(x,y), where:

- x is the independent variable.
- y is the dependent variable.
- dydx(1) gives the equation for y_1 , and dydx(2) gives the equation for y_2 .

Make the function vectorized, so that $shockode([x1 \ x2 \ ...],[y1 \ y2 \ ...])$ returns $[shockode(x1,y1) \ shockode(x2,y2) \ ...]$. This approach improves solver performance.

The corresponding function is

Note: All functions are included as local functions at the end of the example.

Code Boundary Conditions

The BVP solver requires the boundary conditions to be in the form g(y(a), y(b)) = 0. In this form the boundary conditions are:

$$y(-1) + 2 = 0,$$

 $y(1) = 0.$

Write a function to code the boundary conditions with the signature res = shockbc(ya,yb),

- ya is the value of the boundary condition at the beginning of the interval [a, b].
- yb is the value of the boundary condition at the end of the interval [a, b].

The corresponding function is

```
function res = shockbc(ya,yb) % boundary conditions
res = [ya(1)+2]
      yb(1)];
end
```

Code Jacobians

The analytical Jacobians for the ODE function and boundary conditions can be calculated easily in this problem. Providing the Jacobians makes the solver more efficient, since the solver no longer needs to approximate them with finite differences.

For the ODE function, the Jacobian matrix is

$$J_{\text{ODE}} = \frac{\partial f}{\partial y} = \begin{bmatrix} \frac{\partial f_1}{\partial y_1} & \frac{\partial f_1}{\partial y_2} \\ \frac{\partial f_2}{\partial y_1} & \frac{\partial f_2}{\partial y_2} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & -\frac{x}{e} \end{bmatrix}.$$

The corresponding function is

```
function jac = shockjac(x,y,e)
jac = [0 1
      0 -x/e];
```

Similarly, for the boundary conditions, the Jacobian matrices are

$$J_{y(a)} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, J_{y(b)} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}.$$

The corresponding function is

```
function [dBCdya,dBCdyb] = shockbcjac(ya,yb)
dBCdya = [1 0; 0 0];
dBCdyb = [0 \ 0; \ 1 \ 0];
end
```

Form Initial Guess

Use a constant guess for the solution on a mesh of five points in [-1, 1].

```
sol = bvpinit([-1 -0.5 0 0.5 1],[1 0]);
```

Solve Equation

If you try to solve the equation directly using $e = 10^{-4}$, then the solver is not able to overcome the poor conditioning of the problem near the x = 0 transition point. Instead, to obtain the solution for $e = 10^{-4}$, this example uses continuation by solving a sequence of problems for 10^{-2} , 10^{-3} , and 10^{-4} . The output from the solver in each iteration acts as the guess for the solution in the next iteration (this is why the variable for the initial guess from bvpinit is sol, and the output from the solver is also named sol).

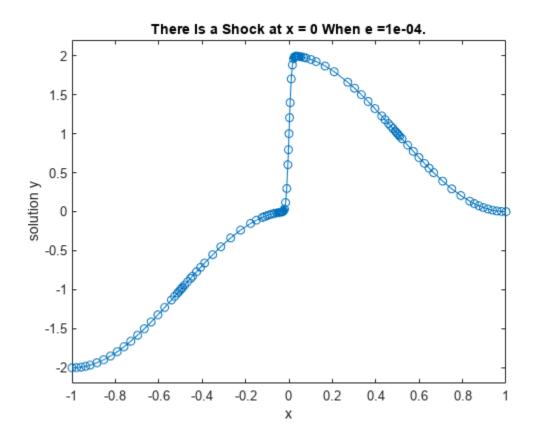
Since the value of the Jacobian depends on the value of *e*, set the options in the loop specifying the shockjac and shockbcjac functions for the Jacobians. Also, turn vectorization on since shockode is coded to handle vectors of values.

```
e = 0.1;
for i = 2:4
    e = e/10;
    options = bvpset('FJacobian',@(x,y) shockjac(x,y,e),'BCJacobian',@shockbcjac,'Vectorized','on
    sol = bvp4c(@(x,y) shockode(x,y,e),@shockbc, sol, options);
end
```

Plot Solution

Plot the results from bvp4c for the mesh x and solution y(x). With continuation, the solver is able to handle the discontinuity at x = 0.

```
plot(sol.x,sol.y(1,:),'-o');
axis([-1 1 -2.2 2.2]);
title(['There Is a Shock at x = 0 When e =' sprintf('%.e',e) '.']);
xlabel('x');
ylabel('solution y');
```



Local Functions

Listed here are the local functions that the BVP solver bvp4c calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

```
function dydx = shockode(x,y,e) % equation to solve
pix = pi*x;
dydx = [y(2,:)
       -x/e.*y(2,:) - pi^2*cos(pix) - pix/e.*sin(pix)];
end
function res = shockbc(ya,yb) % boundary conditions
res = [ya(1)+2]
       vb(1)1;
end
function jac = shockjac(x,y,e) % jacobian of shockode
jac = [0]
           1
       0
         -x/e];
end
function [dBCdya,dBCdyb] = shockbcjac(ya,yb) % jacobian of shockbc
dBCdya = [1 0; 0 0];
dBCdyb = [0 \ 0; \ 1 \ 0];
```

end																																	
%	 	 -	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	 	-	-	-	-	-	-	-	-	-	-	-	

See Also

bvp4c|bvpinit|bvpset

More About

- "Solving Boundary Value Problems" on page 12-2
- "Verify BVP Consistency Using Continuation" on page 12-20

Verify BVP Consistency Using Continuation

This example shows how to use continuation to gradually extend a BVP solution to larger intervals.

Falkner-Skan boundary value problems [1] arise from similarity solutions of a viscous, incompressible, laminar flow over a flat plate. An example equation is

$$f''' + f f'' + \beta (1 - f'^2) = 0.$$

The problem is posed on the infinite interval $[0, \infty]$ with $\beta = 0.5$, subject to the boundary conditions

$$f(0) = 0$$
,

$$f'(0) = 0$$
,

$$f'(\infty) = 1.$$

The BVP cannot be solved on the infinite interval, and it is impractical to solve the BVP in a very large finite interval. Instead, this example solves a sequence of problems posed on the smaller interval [0, a] to verify that the solution has consistent behavior as $a \to \infty$. This practice of breaking the problem up into simpler problems, with the solution of each problem feeding back in as the initial guess for the next problem, is called *continuation*.

To solve this system of equations in MATLAB®, you need to code the equations, boundary conditions, and options before calling the boundary value problem solver byp4c. You either can include the required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Code Equation

Create a function to code the equations. This function should have the signature dfdx =fsode(x,f), where:

- x is the independent variable.
- f is the dependent variable.

You can rewrite the third-order equation as a system of first-order equations using the substitutions $f_1 = f$, $f_2 = f'$, and $f_3 = f''$. The equations become

$$f_1' = f_2$$

$$f_2' = f_3$$
,

$$f_3' = -f_1 f_3 - \beta (1 - f_2^2).$$

The corresponding function is

```
function dfdeta = fsode(x,f)
b = 0.5;
dfdeta = [f(2)]
          -f(1)*f(3) - b*(1 - f(2)^2);
end
```

Note: All functions are included as local functions at the end of the example.

Code Boundary Conditions

Now, write a function that returns the residual value of the boundary conditions at the boundary points. This function should have the signature res = fsbc(f0, finf), where:

- f0 is the value of the boundary condition at the beginning of the interval.
- finf is the value of the boundary condition at the end of the interval.

To calculate the residual values, you need to put the boundary conditions in the form g(x, y) = 0. In this form, the boundary conditions are

```
f(0) = 0,
f'(0) = 0,
f'(\infty) - 1 = 0.
The corresponding function is
function res = fsbc(f0, finf)
res = [f0(1) \\ f0(2) \\ finf(2) - 1];
end
```

Create Initial Guess

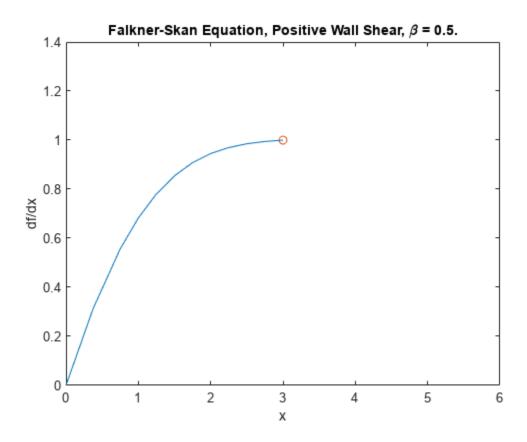
Lastly, you must provide an initial guess for the solution. A crude mesh of five points and a constant guess that satisfies the boundary conditions are good enough to get convergence on the interval [0, 3]. The variable infinity denotes the right-hand limit of the interval of integration. As the value of infinity increases on subsequent iterations from 3 to its maximum value of 6, the solution from each previous iteration acts as the initial guess for the next iteration.

```
infinity = 3;
maxinfinity = 6;
solinit = bvpinit(linspace(0,infinity,5),[0 0 1]);
```

Solve Equation and Plot Solutions

Solve the problem in the initial interval [0, 3]. Plot the solution, and compare the value of f''(0) to the analytic value [1].

```
sol = bvp4c(@fsode,@fsbc,solinit);
x = sol.x;
f = sol.y;
plot(x,f(2,:),x(end),f(2,end),'o');
axis([0 maxinfinity 0 1.4]);
title('Falkner-Skan Equation, Positive Wall Shear, \beta = 0.5.')
xlabel('x')
ylabel('df/dx')
hold on
```



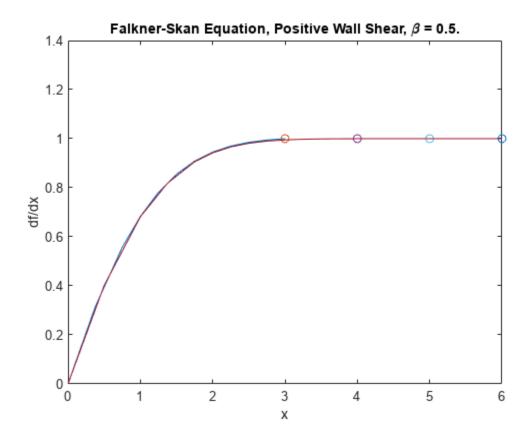
```
fprintf('Cebeci & Keller report that f''''(0) = 0.92768.\n')
Cebeci & Keller report that f''(0) = 0.92768.
fprintf('Value computed using infinity = %g is %7.5f.\n', ...
         infinity, f(3,1)
Value computed using infinity = 3 is 0.92915.
```

Now, solve the problem on progressively larger intervals by increasing the value of infinity for each iteration. The bypinit function extrapolates each solution to the new interval to act as the initial guess for the next value of infinity. Each iteration prints the calculated value of f''(0) and superimposes the plot of the solution over the previous solutions. When infinity = 6, the consistent behavior of the solution becomes evident and the value of f''(0) is very close to the predicted value.

```
for Bnew = infinity+1:maxinfinity
 solinit = bvpinit(sol,[0 Bnew]); % Extend solution to new interval
 sol = bvp4c(@fsode,@fsbc,solinit);
 x = sol.x;
 f = sol.y;
 fprintf('Value computed using infinity = %g is %7.5f.\n', ...
           Bnew, f(3,1))
 plot(x,f(2,:),x(end),f(2,end),'o');
 drawnow
end
```

```
Value computed using infinity = 4 is 0.92774. Value computed using infinity = 5 is 0.92770. Value computed using infinity = 6 is 0.92770.
```

hold off



Local Functions

Listed here are the local helper functions that the BVP solver bvp4c calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

References

[1] Cebeci, T. and H. B. Keller. "Shooting and Parallel Shooting Methods for Solving the Falkner-Skan Boundary-layer Equation." $J.\ Comp.\ Phys.$, Vol. 7, 1971, pp. 289-300.

See Also

bvp4c | bvp5c | bvpinit

More About

- "Solving Boundary Value Problems" on page 12-2
- "Solve BVP Using Continuation" on page 12-15

Solve BVP with Singular Term

This example shows how to solve Emden's equation, which is a boundary value problem with a singular term that arises in modeling a spherical body of gas.

After reducing the PDE of the model using symmetry, the equation becomes a second-order ODE defined on the interval [0, 1],

$$y'' + \frac{2}{x}y' + y^5 = 0.$$

At x=0, the (2/x) term is singular, but symmetry implies the boundary condition y'(0)=0. With this boundary condition, the term (2/x)y' is well defined as $x\to 0$. For the boundary condition $y(1)=\sqrt{3}/2$, the BVP has an analytical solution that you can compare to a numeric solution calculated in MATLAB®,

$$y(x) = \left[\sqrt{1 + \frac{x^2}{3}}\right]^{-1}.$$

The BVP solver bvp4c can solve singular BVPs that have the form

$$y' = S\frac{y}{x} + f(x, y).$$

The matrix S must be constant and the boundary conditions at x=0 must be consistent with the necessary condition $S \cdot y(0) = 0$. Use the 'SingularTerm' option of bypset to pass the S matrix to the solver.

You can rewrite Emden's equation as a system of first-order equations using $y_1 = y$ and $y_2 = y'$ as

$$y_1' = y_2$$

$$y_2' = -\frac{2}{x}y_2 - y_1^5.$$

The boundary conditions become

$$y_2(0) = 0$$
,

$$y_1(1) = \sqrt{3}/2$$
.

In the required matrix form, the system is

$$\begin{bmatrix} y_1' \\ y_2' \end{bmatrix} = \frac{1}{x} \begin{bmatrix} 0 & 0 \\ 0 & -2 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} + \begin{bmatrix} y_2 \\ -y_1^5 \end{bmatrix}.$$

In matrix form it is clear that
$$S = \begin{bmatrix} 0 & 0 \\ 0 & -2 \end{bmatrix}$$
 and $f(x, y) = \begin{bmatrix} y_2 \\ -y_1^5 \end{bmatrix}$.

To solve this system of equations in MATLAB, you need to code the equations, boundary conditions, and options before calling the boundary value problem solver bvp4c. You either can include the

required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Code Equation

Create a function to code the equations for f(x, y). This function should have the signature dydx = emdenode(x, y), where:

- x is the independent variable.
- y is the dependent variable.
- dydx(1) gives the equation for y_1 , and dydx(2) the equation for y_2 .

These inputs are automatically passed to the function by the solver, but the variable names determine how you code the equations. In this case:

The term that contains S is passed to the solver using options, so that term is not included in the function.

Code Boundary Conditions

Now, write a function that returns the residual value of the boundary conditions at the boundary points. This function should have the signature res = emdenbc(ya,yb), where:

- ya is the value of the boundary condition at the beginning of the interval.
- yb is the value of the boundary condition at the end of the interval.

For this problem, one of the boundary conditions is for y_1 , and the other is for y_2 . To calculate the residual values, you need to put the boundary conditions into the form g(x, y) = 0.

In this form the boundary conditions are

```
y_2(0) = 0,

y_1(1) - \sqrt{3}/2 = 0.
```

The corresponding function is then

```
function res = emdenbc(ya,yb)
res = [ya(2)
          yb(1) - sqrt(3)/2];
end
```

Create Initial Guess

Lastly, create an initial guess of the solution. For this problem, use a constant initial guess that satisfies the boundary conditions, and a simple mesh of five points between 0 and 1. Using many mesh points is unnecessary since the BVP solver adapts these points during the solution process.

$$y_1 = \sqrt{3}/2$$
,

```
y_2 = 0.

guess = [sqrt(3)/2; 0];

xmesh = linspace(0,1,5);

solinit = bvpinit(xmesh, guess);
```

Solve Equation

Create a matrix for S and pass it to bvpset as the value of the 'SingularTerm' option. Finally, call bvp4c with the ODE function, boundary condition function, initial guess, and option structure.

```
S = [0 0; 0 -2];
options = bvpset('SingularTerm',S);
sol = bvp4c(@emdenode, @emdenbc, solinit, options);
```

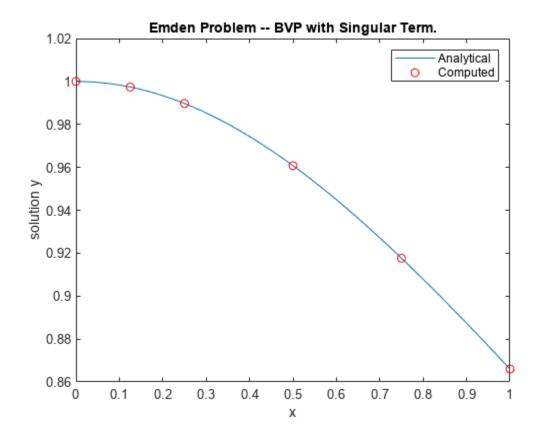
Plot Solution

Calculate the value of the analytical solution in [0, 1].

```
x = linspace(0,1);
truy = 1 ./ sqrt(1 + (x.^2)/3);
```

Plot the analytical solution and the solution calculated by bvp4c for comparison.

```
plot(x,truy,sol.x,sol.y(1,:),'ro');
title('Emden Problem -- BVP with Singular Term.')
legend('Analytical','Computed');
xlabel('x');
ylabel('solution y');
```



Local Functions

Listed here are the local helper functions that the BVP solver bvp4c calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

```
function dydx = emdenode(x,y) % equation being solved
dydx = [y(2)]
     -y(1)^5];
end
function res = emdenbc(ya,yb) % boundary conditions
res = [ya(2)]
     yb(1) - sqrt(3)/2];
end
%-----
```

See Also

bvp4c|bvp5c|bvpinit|bvpset

More About

"Solving Boundary Value Problems" on page 12-2

Solve BVP with Multiple Boundary Conditions

This example shows how to solve a multipoint boundary value problem, where the solution of interest satisfies conditions inside the interval of integration.

For x in $[0, \lambda]$, consider the equations

$$\mathbf{v}' = \frac{C-1}{n},$$

$$C' = \frac{\text{vC} - \min(x, 1)}{\eta}.$$

The known parameters of the problem are n, κ , $\lambda > 1$, and $\eta = \frac{\lambda^2}{n \cdot \kappa^2}$.

The term min(x, 1) in the equation for C'(x) is not smooth at x = 1, so the problem cannot be solved directly. Instead, you can break the problem into two: one set in the interval [0, 1], and the other set in the interval $[1, \lambda]$. The connection between the two regions is that the solutions must be continuous at x = 1. The solution must also satisfy the boundary conditions

$$v(0)=0,$$

$$C(\lambda) = 1$$
.

The equations for each region are

Region 1: $0 \le x \le 1$

$$\mathbf{v}'=\frac{C-1}{n},$$

$$C' = \frac{vC - x}{\eta}.$$

Region 2: $1 \le x \le \lambda$

$$\mathbf{v}' = \frac{C-1}{n},$$

$$C' = \frac{\text{vC} - 1}{n}.$$

The interface point x = 1 is included in both regions. At this point, the solver produces both *left* and *right* solutions, which must be equal to ensure continuity of the solution.

To solve this system of equations in MATLAB®, you need to code the equations, boundary conditions, and initial guess before calling the boundary value problem solver bvp5c. You either can include the required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Code Equations

The equations for v'(x) and C'(x) depend on the region being solved. For multipoint boundary value problems the derivative function must accept a third input argument region, which is used to

identify the region where the derivative is being evaluated. The solver numbers the regions from left to right, starting with 1.

Create a function to code the equations with the signature dydx = f(x,y,region,p), where:

- x is the independent variable.
- y is the dependent variable.
- dydx(1) gives the equation for v'(x), and dydx(2) the equation for C'(x).
- region is the number of the region where the derivative is being computed (in this two-region problem, region is 1 or 2).
- p is a vector containing the values of the constant parameters $[n, \kappa, \lambda, \eta]$.

Use a switch statement to return different equations depending on the region being solved. The function is

```
function dydx = f(x,y,region,p) % equations being solved
n = p(1);
eta = p(4);

dydx = zeros(2,1);
dydx(1) = (y(2) - 1)/n;

switch region
    case 1 % x in [0 1]
        dydx(2) = (y(1)*y(2) - x)/eta;
    case 2 % x in [1 lambda]
        dydx(2) = (y(1)*y(2) - 1)/eta;
end
end
```

Note: All functions are included as local functions at the end of the example.

Code Boundary Conditions

Solving two first-order differential equations in two regions requires four boundary conditions. Two of these conditions come from the original problem:

```
v(0) = 0,
C(\lambda) - 1 = 0.
```

The other two conditions enforce the continuity of the left and right solutions at the interface point x = 1:

```
v_L(1) - v_R(1) = 0,

C_L(1) - C_R(1) = 0.
```

For multipoint BVPs, the arguments of the boundary conditions function YL and YR become matrices. In particular, the kth column YL(:,k) is the solution at the left boundary of the kth region. Similarly, YR(:,k) is the solution at the right boundary of the kth region.

In this problem, y(0) is approximated by YL(:,1), while $y(\lambda)$ is approximated by YR(:,end). Continuity of the solution at x=1 requires that YR(:,1) = YL(:,2).

The function that encodes the residual value of the four boundary conditions is

```
\begin{array}{lll} \text{function res} &=& bc(YL,YR) \\ \text{res} &=& [YL(1,1) & \% \ v(0) = 0 \\ & YR(1,1) - YL(1,2) & \% \ \text{Continuity of } v(x) \ \text{at } x{=}1 \\ & YR(2,1) - YL(2,2) & \% \ \text{Continuity of } C(x) \ \text{at } x{=}1 \\ & YR(2,\text{end}) - 1]; & \% \ C(\text{lambda}) = 1 \end{array}
```

Form Initial Guess

For multipoint BVPs, the boundary conditions are automatically applied at the beginning and end of the interval of integration. However, you must specify double entries in xmesh for the other interface points. A simple guess that satisfies the boundary conditions is the constant guess y = [1; 1].

```
xc = 1;
xmesh = [0 0.25 0.5 0.75 xc xc 1.25 1.5 1.75 2];
yinit = [1; 1];
sol = bvpinit(xmesh,yinit);
```

Solve Equation

Define the values of the constant parameters and put them in the vector p. Provide the function to bvp5c with the syntax @(x,y,r) f(x,y,r,p) to provide the vector of parameters.

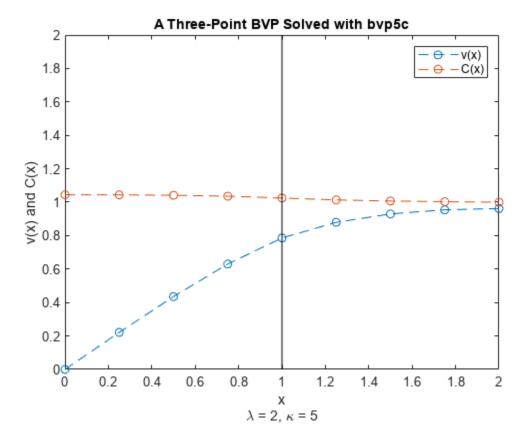
Calculate the solution for several values of κ , using each solution as the initial guess for the next. For each value of κ , calculate the value of the osmolarity Os = $\frac{1}{\nu(\lambda)}$. For each iteration of the loop, compare the computed value with the approximate analytical solution.

```
lambda = 2;
n = 5e-2;
for kappa = 2:5
   eta = lambda^2/(n*kappa^2);
   p = [n kappa lambda eta];
   sol = bvp5c(@(x,y,r) f(x,y,r,p), @bc, sol);
   K2 = lambda*sinh(kappa/lambda)/(kappa*cosh(kappa));
   approx = 1/(1 - K2);
   computed = 1/sol.y(1,end);
   fprintf(' %2i
                                %10.3f \n', kappa, computed, approx);
                     %10.3f
end
             1.462
                            1.454
   3
             1.172
                            1.164
             1.078
                             1.071
             1.039
                             1.034
```

Plot Solution

Plot the solution components for v(x) and C(x) and a vertical line at the interface point x = 1. The displayed solution for $\kappa = 5$ results from the final iteration of the loop.

```
\label{eq:continuous_sol_v(1,:),'--o',sol_x,sol_y(2,:),'--o'} \\ line([1 1], [0 2], 'Color', 'k') \\ legend('v(x)', 'C(x)') \\ title('A Three-Point BVP Solved with bvp5c') \\ xlabel(\{'x', '\lambda = 2, \kappa = 5'\}) \\ ylabel('v(x) and C(x)') \\ \end{aligned}
```



Local Functions

Listed here are the local helper functions that the BVP solver bvp5c calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

```
function dydx = f(x,y,region,p) % equations being solved
n = p(1);
eta = p(4);
dydx = zeros(2,1);
dydx(1) = (y(2) - 1)/n;
switch region
              % x in [0 1]
    case 1
        dydx(2) = (y(1)*y(2) - x)/eta;
              % x in [1 lambda]
    case 2
        dydx(2) = (y(1)*y(2) - 1)/eta;
end
end
function res = bc(YL,YR) % boundary conditions
res = [YL(1,1)]
                              % V(0) = 0
       YR(1,1) - YL(1,2)
YR(2,1) - YL(2,2)
                              % Continuity of v(x) at x=1
                              % Continuity of C(x) at x=1
       YR(2,end) - 1];
                              % C(lambda) = 1
```

en	d																																					
%-	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_	_				_	_	_	_	_	_	

See Also

bvp4c|bvp5c|bvpinit

More About

• "Solving Boundary Value Problems" on page 12-2

Partial Differential Equations (PDEs)

- "Solving Partial Differential Equations" on page 13-2
- "Solve Single PDE" on page 13-9
- "Solve PDE with Discontinuity" on page 13-16
- "Solve PDE and Compute Partial Derivatives" on page 13-23
- "Solve System of PDEs" on page 13-32
- "Solve System of PDEs with Initial Condition Step Functions" on page 13-39

Solving Partial Differential Equations

In a partial differential equation (PDE), the function being solved for depends on several variables, and the differential equation can include partial derivatives taken with respect to each of the variables. Partial differential equations are useful for modelling waves, heat flow, fluid dispersion, and other phenomena with spatial behavior that changes over time.

What Types of PDEs Can You Solve with MATLAB?

The MATLAB PDE solver pdepe solves initial-boundary value problems for systems of PDEs in one spatial variable x and time t. You can think of these as ODEs of one variable that also change with respect to time.

pdepe uses an informal classification for the 1-D equations it solves:

- Equations with a time derivative are parabolic. An example is the heat equation $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$.
- Equations without a time derivative are elliptic. An example is the Laplace equation $\frac{\partial^2 u}{\partial x^2} = 0$.

pdepe requires at least one parabolic equation in the system. In other words, at least one equation in the system must include a time derivative.

pdepe also solves certain 2-D and 3-D problems that reduce to 1-D problems due to angular symmetry (see the argument description for the symmetry constant m for more information).

Partial Differential Equation Toolbox extends this functionality to generalized problems in 2-D and 3-D with Dirichlet and Neumann boundary conditions.

Solving 1-D PDEs

A 1-D PDE includes a function u(x,t) that depends on time t and one spatial variable x. The MATLAB PDE solver pdepe solves systems of 1-D parabolic and elliptic PDEs of the form

$$c\left(x,t,u,\frac{\partial u}{\partial x}\right)\frac{\partial u}{\partial t}=x^{-m}\frac{\partial}{\partial x}\left(x^{m}f\left(x,t,u,\frac{\partial u}{\partial x}\right)\right)+s\left(x,t,u,\frac{\partial u}{\partial x}\right).$$

The equation has the properties:

- The PDEs hold for $t_0 \le t \le t_f$ and $a \le x \le b$.
- The spatial interval [a, b] must be finite.
- m can be 0, 1, or 2, corresponding to slab, cylindrical, or spherical symmetry, respectively. If m > 0, then $a \ge 0$ must also hold.
- The coefficient $f(x, t, u, \frac{\partial u}{\partial x})$ is a flux term and $s(x, t, u, \frac{\partial u}{\partial x})$ is a source term.
- The flux term must depend on the partial derivative $\partial u/\partial x$.

The coupling of the partial derivatives with respect to time is restricted to multiplication by a diagonal matrix $c(x, t, u, \frac{\partial u}{\partial x})$. The diagonal elements of this matrix are either zero or positive. An

element that is zero corresponds to an elliptic equation, and any other element corresponds to a parabolic equation. There must be at least one parabolic equation. An element of c that corresponds to a parabolic equation can vanish at isolated values of x if they are mesh points (points where the solution is evaluated). Discontinuities in c and s due to material interfaces are permitted provided that a mesh point is placed at each interface.

Solution Process

To solve PDEs with pdepe, you must define the equation coefficients for c, f, and s, the initial conditions, the behavior of the solution at the boundaries, and a mesh of points to evaluate the solution on. The function call sol = pdepe(m,pdefun,icfun,bcfun,xmesh,tspan) uses this information to calculate a solution on the specified mesh:

- m is the symmetry constant.
- pdefun defines the equations being solved.
- · icfun defines the initial conditions.
- · bcfun defines the boundary conditions.
- xmesh is a vector of spatial values for x.
- tspan is a vector of time values for t.

Together, the xmesh and tspan vectors form a 2-D grid that pdepe evaluates the solution on.

Equations

You must express the PDEs in the standard form expected by pdepe. Written in this form, you can read off the values of the coefficients c, f, and s.

In MATLAB you can code the equations with a function of the form

```
function [c,f,s] = pdefun(x,t,u,dudx)
c = 1;
f = dudx;
s = 0;
end
```

In this case pdefun defines the equation $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$. If there are multiple equations, then c, f, and s are vectors with each element corresponding to one equation.

Initial Conditions

At the initial time $t = t_0$, for all x, the solution components satisfy initial conditions of the form

```
u(x,t_0)=u_0(x).
```

In MATLAB you can code the initial conditions with a function of the form

```
function u0 = icfun(x)
u0 = 1;
end
```

In this case u0 = 1 defines an initial condition of $u_0(x,t_0) = 1$. If there are multiple equations, then u0 is a vector with each element defining the initial condition of one equation.

Boundary Conditions

At the boundary x = a or x = b, for all t, the solution components satisfy boundary conditions of the form

$$p(x,t,u)+q(x,t)f\Big(x,t,u,\frac{\partial u}{\partial x}\Big)=0.$$

q(x,t) is a diagonal matrix with elements that are either zero or never zero. Note that the boundary conditions are expressed in terms of the flux f, rather than the partial derivative of u with respect to x. Also, of the two coefficients p(x,t,u) and q(x,t), only p can depend on u.

In MATLAB you can code the boundary conditions with a function of the form

```
function [pL,qL,pR,qR] = bcfun(xL,uL,xR,uR,t)
pL = uL;
qL = 0;
pR = uR - 1;
qR = 0;
end
```

pL and qL are the coefficients for the left boundary, while pR and qR are the coefficients for the right boundary. In this case bcfun defines the boundary conditions

$$u_L(x_L, t) = 0$$

$$u_R(x_R, t) = 1$$

If there are multiple equations, then the outputs pL, qL, pR, and qR are vectors with each element defining the boundary condition of one equation.

Integration Options

The default integration properties in the MATLAB PDE solver are selected to handle common problems. In some cases, you can improve solver performance by overriding these default values. To do this, use odeset to create an options structure. Then, pass the structure to pdepe as the last input argument:

```
sol = pdepe(m,pdefun,icfun,bcfun,xmesh,tspan,options)
```

Of the options for the underlying ODE solver ode15s, only those shown in the following table are available for pdepe.

Category	Option Name
Error control	RelTol, AbsTol, NormControl
Step-size	InitialStep, MaxStep
Event logging	Events

Evaluating the Solution

After you solve an equation with pdepe, MATLAB returns the solution as a 3-D array sol, where sol(i,j,k) contains the kth component of the solution evaluated at t(i) and x(j). In general, you can extract the kth solution component with the command u = sol(:,:,k).

The time mesh you specify is used purely for output purposes, and does not affect the internal time steps taken by the solver. However, the spatial mesh you specify can affect the quality and speed of

the solution. After solving an equation, you can use pdeval to evaluate the solution structure returned by pdepe with a different spatial mesh.

Example: The Heat Equation

An example of a parabolic PDE is the heat equation in one dimension:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}.$$

This equation describes the dissipation of heat for $0 \le x \le L$ and $t \ge 0$. The goal is to solve for the temperature u(x, t). The temperature is initially a nonzero constant, so the initial condition is

$$u(x,0) = T_0$$
.

Also, the temperature is zero at the left boundary, and nonzero at the right boundary, so the boundary conditions are

$$u(0,t) = 0,$$

 $u(L,t) = 1.$

To solve this equation in MATLAB®, you need to code the equation, initial conditions, and boundary conditions, then select a suitable solution mesh before calling the solver pdepe. You either can include the required functions as local functions at the end of a file (as in this example), or save them as separate, named files in a directory on the MATLAB path.

Code Equation

Before you can code the equation, you need to make sure that it is in the form that the pdepe solver expects:

$$c\left(x,t,u,\frac{\partial u}{\partial x}\right)\frac{\partial u}{\partial t} = x^{-m}\frac{\partial}{\partial x}\left(x^{m}f\left(x,t,u,\frac{\partial u}{\partial x}\right)\right) + s\left(x,t,u,\frac{\partial u}{\partial x}\right).$$

In this form, the heat equation is

$$1 \cdot \frac{\partial u}{\partial t} = x^0 \frac{\partial}{\partial x} \left(x^0 \frac{\partial u}{\partial x} \right) + 0.$$

So the values of the coefficients are as follows:

- m = 0
- c = 1
- $f = \frac{\partial u}{\partial x}$
- s = 0

The value of m is passed as an argument to pdepe, while the other coefficients are encoded in a function for the equation, which is

```
function [c,f,s] = heatpde(x,t,u,dudx)
c = 1;
```

```
f = dudx;
s = 0;
end
```

(Note: All functions are included as local functions at the end of the example.)

Code Initial Condition

The initial condition function for the heat equation assigns a constant value for u_0 . This function must accept an input for x, even if it is unused.

```
function u0 = heatic(x)
u0 = 0.5;
end
```

Code Boundary Conditions

The standard form for the boundary conditions expected by the pdepe solver is

$$p(x,t,u)+q(x,t)f\Big(x,t,u,\frac{\partial u}{\partial x}\Big)=0\;.$$

Written in this form, the boundary conditions for this problem are

```
u(0,t) + (0 \cdot f) = 0,

(u(L,t) - 1) + (0 \cdot f) = 0.
```

So the values for p and q are

- $\bullet \quad p_L=u_L, \qquad q_L=0 \; .$
- $\bullet \quad p_R=u_R-1, \quad q_R=0.$

The corresponding function is then

```
function [pl,ql,pr,qr] = heatbc(xl,ul,xr,ur,t)
pl = ul;
ql = 0;
pr = ur - 1;
qr = 0;
end
```

Select Solution Mesh

Use a spatial mesh of 20 points and a time mesh of 30 points. Since the solution rapidly reaches a steady state, the time points near t = 0 are more closely spaced together to capture this behavior in the output.

```
L = 1;
x = linspace(0,L,20);
t = [linspace(0,0.05,20), linspace(0.5,5,10)];
```

Solve Equation

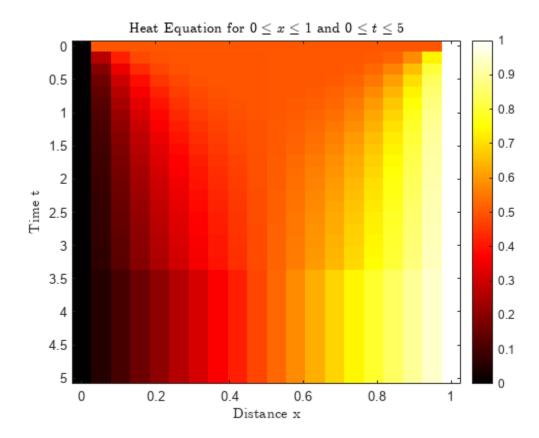
Finally, solve the equation using the symmetry m, the PDE equation, the initial condition, the boundary conditions, and the meshes for x and t.

```
m = 0;
sol = pdepe(m,@heatpde,@heatic,@heatbc,x,t);
```

Plot Solution

Use imagesc to visualize the solution matrix.

```
colormap hot
imagesc(x,t,sol)
colorbar
xlabel('Distance x','interpreter','latex')
ylabel('Time t','interpreter','latex')
title('Heat Equation for $0 \le x \le 1$ and $0 \le t \le 5$','interpreter','latex')
```



Local Functions

```
function [c,f,s] = heatpde(x,t,u,dudx)
c = 1;
f = dudx;
s = 0;
end
function u0 = heatic(x)
u0 = 0.5;
end
function [pl,ql,pr,qr] = heatbc(xl,ul,xr,ur,t)
pl = ul;
ql = 0;
pr = ur - 1;
```

```
qr = 0;
end
```

PDE Examples and Files

Several available example files serve as excellent starting points for most common 1-D PDE problems. To explore and run examples, use the Differential Equations Examples app. To run this app, type

odeexamples

To open an individual file for editing, type

edit exampleFileName.m

To run an example, type

exampleFileName

This table contains a list of the available PDE example files.

Example File	Description	Example Link							
pdex1	Simple PDE that illustrates the formulation, computation, and plotting of the solution.	"Solve Single PDE" on page 13-9							
pdex2	Problem that involves discontinuities.	"Solve PDE with Discontinuity" on page 13-16							
pdex3	Problem that requires computing values of the partial derivative.	"Solve PDE and Compute Partial Derivatives" on page 13-23							
pdex4	System of two PDEs whose solution has boundary layers at both ends of the interval and changes rapidly for small t .	"Solve System of PDEs" on page 13-32							
pdex5	System of PDEs with step functions as initial conditions.	"Solve System of PDEs with Initial Condition Step Functions" on page 13-39							

References

[1] Skeel, R. D. and M. Berzins, "A Method for the Spatial Discretization of Parabolic Equations in One Space Variable," SIAM Journal on Scientific and Statistical Computing, Vol. 11, 1990, pp. 1-32.

See Also

bvp4c | ode45 | pdepe | odeset | pdeval

More About

- "Solve Single PDE" on page 13-9
- "Solve System of PDEs" on page 13-32

Solve Single PDE

This example shows how to formulate, compute, and plot the solution to a single PDE.

Consider the partial differential equation

$$\pi^2 \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}.$$

The equation is defined on the interval $0 \le x \le 1$ for times $t \ge 0$. At t = 0, the solution satisfies the initial condition

$$u(x,0) = \sin(\pi x).$$

Also, at x = 0 and x = 1, the solution satisfies the boundary conditions

$$u(0,t)=0,$$

$$\pi e^{-t} + \frac{\partial u}{\partial x}(1,t) = 0.$$

To solve this equation in MATLAB®, you need to code the equation, the initial conditions, and the boundary conditions, then select a suitable solution mesh before calling the solver pdepe. You either can include the required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Code Equation

Before you can code the equation, you need to rewrite it in a form that the pdepe solver expects. The standard form that pdepe expects is

$$c(x,t,u,\frac{\partial u}{\partial x})\frac{\partial u}{\partial t} = x^{-m}\frac{\partial}{\partial x}(x^m f(x,t,u,\frac{\partial u}{\partial x})) + s(x,t,u,\frac{\partial u}{\partial x}).$$

Written in this form, the PDE becomes

$$\pi^2 \frac{\partial u}{\partial t} = x^0 \frac{\partial}{\partial x} \left(x^0 \frac{\partial u}{\partial x} \right) + 0.$$

With the equation in the proper form you can read off the relevant terms:

$$m = 0$$

$$c(x, t, u, \frac{\partial u}{\partial x}) = \pi^2$$

$$f(x, t, u, \frac{\partial u}{\partial x}) = \frac{\partial u}{\partial x}$$

$$s\left(x,t,u,\frac{\partial u}{\partial x}\right)=0$$

Now you can create a function to code the equation. The function should have the signature [c,f,s] = pdex1pde(x,t,u,dudx):

- x is the independent spatial variable.
- t is the independent time variable.
- u is the dependent variable being differentiated with respect to x and t.
- dudx is the partial spatial derivative $\partial u/\partial x$.
- The outputs c, f, and s correspond to coefficients in the standard PDE equation form expected by pdepe. These coefficients are coded in terms of the input variables x, t, u, and dudx.

As a result, the equation in this example can be represented by the function:

```
function [c,f,s] = pdex1pde(x,t,u,dudx)
c = pi^2;
f = dudx;
s = 0;
end
```

(Note: All functions are included as local functions at the end of the example.)

Code Initial Condition

Next, write a function that returns the initial condition. The initial condition is applied at the first time value tspan(1). The function should have the signature u0 = pdexlic(x).

The corresponding function is

```
function u0 = pdexlic(x)
u0 = sin(pi*x);
end
```

Code Boundary Conditions

Now, write a function that evaluates the boundary conditions. For problems posed on the interval $a \le x \le b$, the boundary conditions apply for all t and either x = a or x = b. The standard form for the boundary conditions expected by the solver is

$$p(x, t, u) + q(x, t)f(x, t, u, \frac{\partial u}{\partial x}) = 0.$$

Rewrite the boundary conditions in this standard form and read off the coefficient values.

For x = 0, the equation is

$$u(0,t) = 0 \rightarrow u + 0 \cdot \frac{\partial u}{\partial x} = 0$$
.

The coefficients are:

- p(0, t, u) = u
- q(0,t) = 0

For x = 1, the equation is

$$\pi e^{-t} + \frac{\partial u}{\partial x}(1,t) = 0 \rightarrow \pi e^{-t} + 1 \cdot \frac{\partial u}{\partial x}(1,t) = 0.$$

The coefficients are:

```
• p(1,t,u)=\pi e^{-t}
```

• q(1,t) = 1

Since the boundary condition function is expressed in terms of $f(x, t, u, \frac{\partial u}{\partial x})$, and this term is already defined in the main PDE function, you do not need to specify this piece of the equation in the boundary condition function. You need only specify the values of p(x, t, u) and q(x, t) at each boundary.

The boundary function should use the function signature [pl,ql,pr,qr] = pdex1bc(xl,ul,xr,ur,t):

- The inputs x1 and u1 correspond to *u* and *x* for the left boundary.
- The inputs xr and ur correspond to *u* and *x* for the right boundary.
- t is the independent time variable.
- The outputs pl and ql correspond to p(x, t, u) and q(x, t) for the left boundary (x = 0 for this problem).
- The outputs pr and qr correspond to p(x, t, u) and q(x, t) for the right boundary (x = 1 for this problem).

The boundary conditions in this example are represented by the function:

```
function [pl,ql,pr,qr] = pdex1bc(xl,ul,xr,ur,t)
pl = ul;
ql = 0;
pr = pi * exp(-t);
qr = 1;
end
```

Select Solution Mesh

Before solving the equation you need to specify the mesh points (t, x) at which you want pdepe to evaluate the solution. Specify the points as vectors t and x. The vectors t and x play different roles in the solver. In particular, the cost and accuracy of the solution depend strongly on the length of the vector x. However, the computation is much less sensitive to the values in the vector t.

For this problem, use a mesh with 20 equally spaced points in the spatial interval [0,1] and five values of t from the time interval [0,2].

```
x = linspace(0,1,20);
t = linspace(0,2,5);
```

Solve Equation

Finally, solve the equation using the symmetry m, the PDE equation, the initial conditions, the boundary conditions, and the meshes for x and t.

```
m = 0;
sol = pdepe(m,@pdex1pde,@pdex1ic,@pdex1bc,x,t);
```

pdepe returns the solution in a 3-D array sol, where sol(i,j,k) approximates the kth component of the solution u_k evaluated at t(i) and x(j). The size of sol is length(t)-by-length(x)-by-length(u0), since u0 specifies an initial condition for each solution component. For this problem, u has only one component, so sol is a 5-by-20 matrix, but in general you can extract the kth solution component with the command u = sol(:,:,k).

Extract the first solution component from sol.

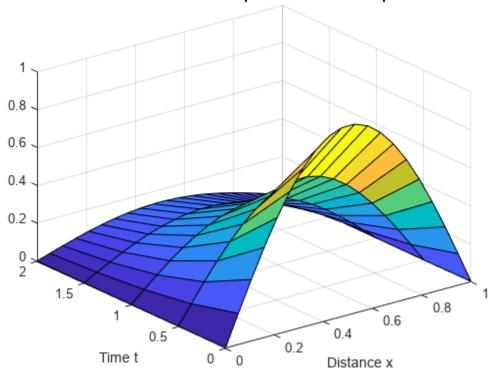
```
u = sol(:,:,1);
```

Plot Solution

Create a surface plot of the solution.

```
surf(x,t,u)
title('Numerical solution computed with 20 mesh points')
xlabel('Distance x')
ylabel('Time t')
```

Numerical solution computed with 20 mesh points

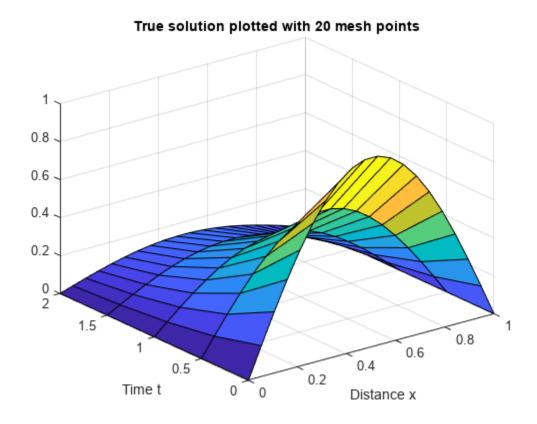


The initial condition and boundary conditions of this problem were chosen so that there would be an analytical solution, given by

$$u(x,t) = e^{-t} \sin(\pi x).$$

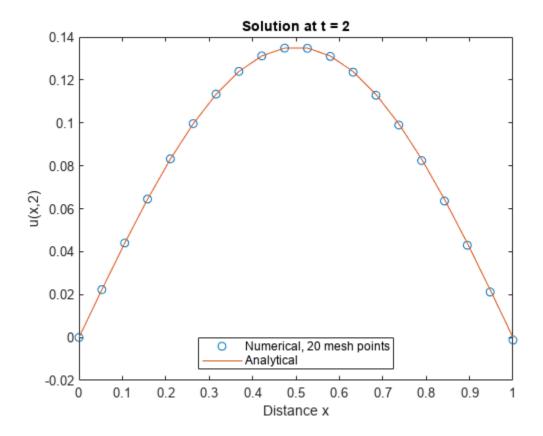
Plot the analytical solution with the same mesh points.

```
surf(x,t,exp(-t)'*sin(pi*x))
title('True solution plotted with 20 mesh points')
xlabel('Distance x')
ylabel('Time t')
```



Now, compare the numerical and analytical solutions at t_f , the final value of t. In this example $t_f = 2$.

```
plot(x,u(end,:),'o',x,exp(-t(end))*sin(pi*x))
title('Solution at t = 2')
legend('Numerical, 20 mesh points','Analytical','Location','South')
xlabel('Distance x')
ylabel('u(x,2)')
```



Local Functions

Listed here are the local helper functions that the PDE solver pdepe calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

See Also

pdepe

More About

- "Solving Partial Differential Equations" on page 13-2
- "Solve PDE with Discontinuity" on page 13-16

Solve PDE with Discontinuity

This example shows how to solve a PDE that interfaces with a material. The material interface creates a discontinuity in the problem at x = 0.5, and the initial condition has a discontinuity at the right boundary x = 1.

Consider the piecewise PDE

$$\begin{cases} \frac{\partial u}{\partial t} = x^{-2} \frac{\partial}{\partial x} \left(x^2 \, 5 \frac{\partial u}{\partial x} \right) - 1000 e^u & (0 \le x \le 0.5) \\ \frac{\partial u}{\partial t} = x^{-2} \frac{\partial}{\partial x} \left(x^2 \, \frac{\partial u}{\partial x} \right) - e^u & (0.5 \le x \le 1) \end{cases}$$

The initial conditions are

$$u(x, 0) = 0 \ (0 \le x < 1),$$

 $u(1, 0) = 1 \ (x = 1).$

The boundary conditions are

$$\frac{\partial u}{\partial x} = 0 \ (x = 0),$$

$$u(1, t) = 1 \ (x = 1).$$

To solve this equation in MATLAB®, you need to code the equation, the initial conditions, and the boundary conditions, then select a suitable solution mesh before calling the solver pdepe. You either can include the required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Code Equation

Before you can code the equation, you need to make sure that it is in a form that the pdepe solver expects. The standard form that pdepe expects is

$$c(x, t, u, \frac{\partial u}{\partial x}) \frac{\partial u}{\partial t} = x^{-m} \frac{\partial}{\partial x} (x^m f(x, t, u, \frac{\partial u}{\partial x})) + s(x, t, u, \frac{\partial u}{\partial x}).$$

In this case, the PDE is in the proper form, so you can read off the values of the coefficients.

$$\begin{cases} \frac{\partial u}{\partial t} = x^{-2} \frac{\partial}{\partial x} \left(x^2 \, 5 \frac{\partial u}{\partial x} \right) - 1000 e^u & (0 \le x \le 0.5) \\ \frac{\partial u}{\partial t} = x^{-2} \frac{\partial}{\partial x} \left(x^2 \, \frac{\partial u}{\partial x} \right) - e^u & (0.5 \le x \le 1) \end{cases}$$

The values for the flux term $f(x, t, u, \frac{\partial u}{\partial x})$ and source term $s(x, t, u, \frac{\partial u}{\partial x})$ change depending on the value of x. The coefficients are:

$$m = 2$$

$$c(x, t, u, \frac{\partial u}{\partial x}) = 1$$

$$\begin{cases} f\left(x,t,u,\frac{\partial u}{\partial x}\right) = 5\frac{\partial u}{\partial x} \ (0 \le x \le 0.5) \\ f\left(x,t,u,\frac{\partial u}{\partial x}\right) = \frac{\partial u}{\partial x} \ (0.5 \le x \le 1) \\ \end{cases}$$

$$\begin{cases} s\left(x,t,u,\frac{\partial u}{\partial x}\right) = -1000e^{u} \ (0 \le x \le 0.5) \\ s\left(x,t,u,\frac{\partial u}{\partial x}\right) = -e^{u} \ (0.5 \le x \le 1) \end{cases}$$

Now you can create a function to code the equation. The function should have the signature [c,f,s] = pdex2pde(x,t,u,dudx):

- x is the independent spatial variable.
- t is the independent time variable.
- u is the dependent variable being differentiated with respect to x and t.
- dudx is the partial spatial derivative $\partial u/\partial x$.
- The outputs c, f, and s correspond to coefficients in the standard PDE equation form expected by pdepe. These coefficients are coded in terms of the input variables x, t, u, and dudx.

As a result, the equation in this example can be represented by the function:

```
function [c,f,s] = pdex2pde(x,t,u,dudx)
c = 1;
if x <= 0.5
    f = 5*dudx;
    s = -1000*exp(u);
else
    f = dudx;
    s = -exp(u);
end
end</pre>
```

(Note: All functions are included as local functions at the end of the example.)

Code Initial Conditions

Next, write a function that returns the initial conditions. The initial condition is applied at the first time value and provides the value of $u(x, t_0)$ for any value of x. Use the function signature $u\theta = pdex2ic(x)$ to write the function.

The initial conditions are

```
u(x, 0) = 0  (0 \le x < 1),

u(1, 0) = 1  (x = 1).
```

The corresponding function is

```
function u0 = pdex2ic(x)
if x < 1
    u0 = 0;
else
    u0 = 1;
end
end</pre>
```

Code Boundary Conditions

Now, write a function that evaluates the boundary conditions. For problems posed on the interval $a \le x \le b$, the boundary conditions apply for all t and either x = a or x = b. The standard form for the boundary conditions expected by the solver is

$$p(x, t, u) + q(x, t)f\left(x, t, u, \frac{\partial u}{\partial x}\right) = 0.$$

Since this example has spherical symmetry (m=2), the pdepe solver automatically enforces the left boundary condition to bound the solution at the origin, and ignores any conditions specified for the left boundary in the boundary function. So for the left boundary condition, you can specify $p_L=q_L=0$. For the right boundary condition, you can rewrite the boundary condition in the standard form and read off the coefficient values for p_R and q_R .

For x = 1, the equation is $u(1, t) = 1 \rightarrow (u - 1) + 0 \cdot \frac{\partial u}{\partial x} = 0$. The coefficients are:

- $p_R(1, t, u) = u 1$
- $q_R(1,t) = 0$

The boundary function should use the function signature [pl,ql,pr,qr] = pdex2bc(xl,ul,xr,ur,t):

- The inputs xl and ul correspond to *u* and *x* for the left boundary.
- The inputs xr and ur correspond to *u* and *x* for the right boundary.
- t is the independent time variable.
- The outputs pl and ql correspond to $p_L(x, t, u)$ and $q_L(x, t)$ for the left boundary (x = 0 for this problem).
- The outputs pr and qr correspond to $p_R(x, t, u)$ and $q_R(x, t)$ for the right boundary (x = 1 for this problem).

The boundary conditions in this example are represented by the function:

```
function [pl,ql,pr,qr] = pdex2bc(xl,ul,xr,ur,t)
pl = 0;
ql = 0;
pr = ur - 1;
qr = 0;
end
```

Select Solution Mesh

The spatial mesh should include several values near x=0.5 to account for the discontinuous interface, as well as points near x=1 because of the inconsistent initial value (u(1,0)=1) and boundary value (u(1,t)=0) at that point. The solution changes rapidly for small t, so use a time step that can resolve this sharp change.

```
x = [0 \ 0.1 \ 0.2 \ 0.3 \ 0.4 \ 0.45 \ 0.475 \ 0.5 \ 0.525 \ 0.55 \ 0.6 \ 0.7 \ 0.8 \ 0.9 \ 0.95 \ 0.975 \ 0.99 \ 1];
t = [0 \ 0.001 \ 0.005 \ 0.01 \ 0.05 \ 0.1 \ 0.5 \ 1];
```

Solve Equation

Finally, solve the equation using the symmetry m, the PDE equation, the initial conditions, the boundary conditions, and the meshes for x and t.

```
m = 2;
sol = pdepe(m,@pdex2pde,@pdex2ic,@pdex2bc,x,t);
```

pdepe returns the solution in a 3-D array sol, where sol(i,j,k) approximates the kth component of the solution u_k evaluated at t(i) and x(j). The size of sol is length(t)-by-length(x)-by-length(u0), since u0 specifies an initial condition for each solution component. For this problem, u has only one component, so sol is a 8-by-18 matrix, but in general you can extract the kth solution component with the command u = sol(:,:,k).

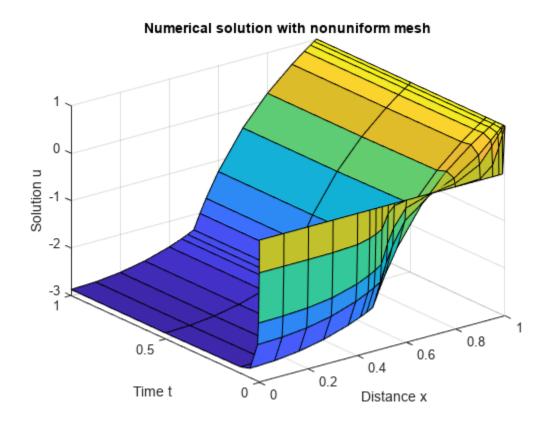
Extract the first solution component from sol.

```
u = sol(:,:,1);
```

Plot Solution

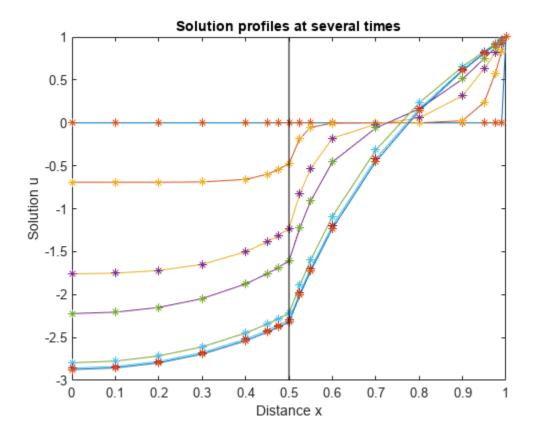
Create a surface plot of the solution u plotted at the selected mesh points for x and t. Since m=2 the problem is posed in a spherical geometry with spherical symmetry, so the solution only changes in the radial x direction.

```
surf(x,t,u)
title('Numerical solution with nonuniform mesh')
xlabel('Distance x')
ylabel('Time t')
zlabel('Solution u')
```



Now, plot just x and u to get a side view of the contours in the surface plot. Add a line at x = 0.5 to highlight the effect of the material interface.

```
plot(x,u,x,u,'*')
line([0.5 0.5], [-3 1], 'Color', 'k')
xlabel('Distance x')
ylabel('Solution u')
title('Solution profiles at several times')
```



Local Functions

Listed here are the local helper functions that the PDE solver pdepe calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

```
function [c,f,s] = pdex2pde(x,t,u,dudx) % Equation to solve
c = 1;
if x <= 0.5
    f = 5*dudx;
    s = -1000*exp(u);
else
    f = dudx;
    s = -exp(u);
end
function u0 = pdex2ic(x) %Initial conditions
if x < 1
    u\theta = \theta;
else
    u0 = 1;
end
function [pl,ql,pr,qr] = pdex2bc(xl,ul,xr,ur,t) % Boundary conditions
pl = 0;
ql = 0;
```

```
pr = ur - 1;
qr = 0;
end
```

See Also

pdepe

More About

- "Solving Partial Differential Equations" on page 13-2
- "Solve PDE and Compute Partial Derivatives" on page 13-23

Solve PDE and Compute Partial Derivatives

This example shows how to solve a transistor partial differential equation (PDE) and use the results to obtain partial derivatives that are part of solving a larger problem.

Consider the PDE

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} - \frac{D\eta}{L} \frac{\partial u}{\partial x}.$$

This equation arises in transistor theory [1], and u(x,t) is a function describing the concentration of excess charge carriers (or *holes*) in the base of a PNP transistor. D and η are physical constants. The equation holds on the interval $0 \le x \le L$ for times $t \ge 0$.

The initial condition includes a constant K and is given by

$$u(x,0) = \frac{KL}{D} \left(\frac{1 - e^{-\eta(1 - x/L)}}{\eta} \right).$$

The problem has boundary conditions given by

$$u(0,t) = u(L,t) = 0$$
.

For fixed x, the solution to the equation u(x,t) describes the collapse of excess charge as $t \to \infty$. This collapse produces a current, called the *emitter discharge current*, which has another constant I_p :

$$I(t) = \left[\frac{I_p D}{K} \frac{\partial}{\partial x} u(x, t)\right]_{x = 0}.$$

The equation is valid for t > 0 due to the inconsistency in the boundary values at x = 0 for t = 0 and t > 0. Since the PDE has a closed-form series solution for u(x, t), you can calculate the emitter discharge current analytically as well as numerically, and compare the results.

To solve this problem in MATLAB®, you need to code the PDE equation, initial conditions, and boundary conditions, then select a suitable solution mesh before calling the solver pdepe. You either can include the required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Define Physical Constants

To keep track of the physical constants, create a structure array with fields for each one. When you later define functions for the equations, the initial condition, and the boundary conditions, you can pass in this structure as an extra argument so that the functions have access to the constants.

```
C.L = 1;
C.D = 0.1;
C.eta = 10;
C.K = 1;
C.Ip = 1;
```

Code Equation

Before you can code the equation, you need to make sure that it is in the form that the pdepe solver expects:

$$c\left(x,t,u,\frac{\partial u}{\partial x}\right)\frac{\partial u}{\partial t} = x^{-m}\frac{\partial}{\partial x}\left(x^{m}f\left(x,t,u,\frac{\partial u}{\partial x}\right)\right) + s\left(x,t,u,\frac{\partial u}{\partial x}\right).$$

In this form, the PDE is

$$\frac{\partial u}{\partial t} = x^0 \frac{\partial}{\partial x} \left(x^0 D \frac{\partial u}{\partial x} \right) - \frac{D\eta}{L} \frac{\partial u}{\partial x}.$$

So the values of the coefficients in the equation are

- m = 0 (Cartesian coordinates with no angular symmetry)
- $c(x, t, u, \frac{\partial u}{\partial x}) = 1$
- $f(x, t, u, \frac{\partial u}{\partial x}) = D \frac{\partial u}{\partial x}$
- $s(x, t, u, \frac{\partial u}{\partial x}) = -\frac{D\eta}{L} \frac{\partial u}{\partial x}$

Now you can create a function to code the equation. The function should have the signature [c,f,s] = transistorPDE(x,t,u,dudx,C):

- x is the independent spatial variable.
- t is the independent time variable.
- u is the dependent variable being differentiated with respect to x and t.
- dudx is the partial spatial derivative $\partial u/\partial x$.
- C is an extra input containing the physical constants.
- The outputs c, f, and s correspond to coefficients in the standard PDE equation form expected by pdepe.

As a result, the equation in this example can be represented by the function:

```
function [c,f,s] = transistorPDE(x,t,u,dudx,C)
D = C.D;
eta = C.eta;
L = C.L;

c = 1;
f = D*dudx;
s = -(D*eta/L)*dudx;
end
```

(Note: All functions are included as local functions at the end of the example.)

Code Initial Condition

Next, write a function that returns the initial condition. The initial condition is applied at the first time value, and provides the value of $u(x, t_0)$ for any value of x. Use the function signature $u\theta = transistorIC(x,C)$ to write the function.

The initial condition is

$$u(x,0) = \frac{KL}{D} \left(\frac{1 - e^{-\eta(1 - x/L)}}{\eta} \right).$$

The corresponding function is

```
function u0 = transistorIC(x,C)
K = C.K;
L = C.L;
D = C.D;
eta = C.eta;

u0 = (K*L/D)*(1 - exp(-eta*(1 - x/L)))/eta;
end
```

Code Boundary Conditions

Now, write a function that evaluates the boundary conditions u(0,t) = u(1,t) = 0. For problems posed on the interval $a \le x \le b$, the boundary conditions apply for all t and either x = a or x = b. The standard form for the boundary conditions expected by the solver is

$$p(x, t, u) + q(x, t)f(x, t, u, \frac{\partial u}{\partial x}) = 0$$
.

Written in this form, the boundary conditions for this problem are

- For x = 0, the equation is $u + 0 \cdot d\frac{\partial u}{\partial x} = 0$. The coefficients are:
- $p_L(x, t, u) = u$,
- $q_I(x,t) = 0$.
- Likewise for x=1, the equation is $u+0\cdot d\frac{\partial u}{\partial x}=0$. The coefficients are:
- $p_R(x, t, u) = u$,
- $q_R(x,t)=0$.

The boundary function should use the function signature [pl,ql,pr,qr] = transistorBC(xl,ul,xr,ur,t):

- The inputs xl and ul correspond to x and u for the left boundary.
- The inputs xr and ur correspond to x and u for the right boundary.
- t is the independent time variable.
- The outputs pl and ql correspond to $p_L(x, t, u)$ and $q_L(x, t)$ for the left boundary (x = 0 for this problem).
- The outputs pr and qr correspond to $p_R(x, t, u)$ and $q_R(x, t)$ for the right boundary (x = 1 for this problem).

The boundary conditions in this example are represented by the function:

```
function [pl,ql,pr,qr] = transistorBC(xl,ul,xr,ur,t)
pl = ul;
```

```
ql = 0;
pr = ur;
qr = 0;
end
```

Select Solution Mesh

The solution mesh defines the values of x and t where the solution is evaluated by the solver. Since the solution to this problem changes rapidly, use a relatively fine mesh of 50 spatial points in the interval $0 \le x \le L$ and 50 time points in the interval $0 \le t \le 1$.

```
x = linspace(0,C.L,50);
t = linspace(0,1,50);
```

Solve Equation

Finally, solve the equation using the symmetry m, the PDE equation, the initial condition, the boundary conditions, and the meshes for x and t. Since pdepe expects the PDE function to use four inputs and the initial condition function to use one input, create function handles that pass in the structure of physical constants as an extra input.

```
m = 0;
eqn = @(x,t,u,dudx) transistorPDE(x,t,u,dudx,C);
ic = @(x) transistorIC(x,C);
sol = pdepe(m,eqn,ic,@transistorBC,x,t);
```

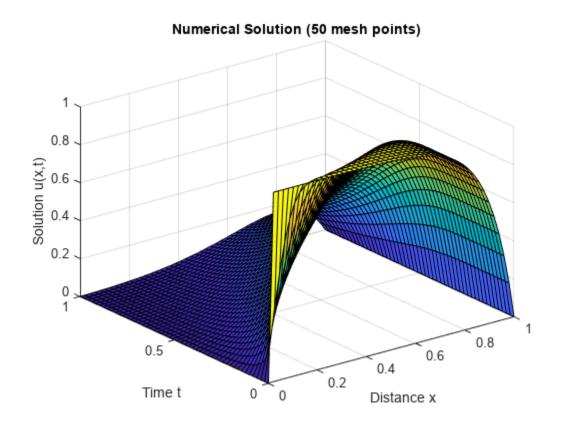
pdepe returns the solution in a 3-D array sol, where sol(i,j,k) approximates the kth component of the solution u_k evaluated at t(i) and x(j). For this problem u has only one component, but in general you can extract the kth solution component with the command u = sol(:,:,k).

```
u = sol(:,:,1);
```

Plot Solution

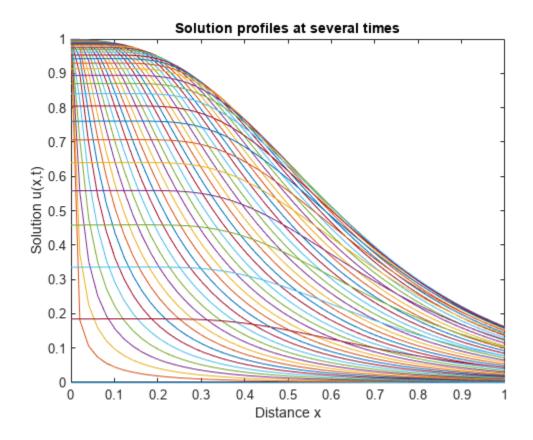
Create a surface plot of the solution u plotted at the selected mesh points for x and t.

```
surf(x,t,u)
title('Numerical Solution (50 mesh points)')
xlabel('Distance x')
ylabel('Time t')
zlabel('Solution u(x,t)')
```



Now, plot just x and u to get a side view of the contours in the surface plot.

```
plot(x,u)
xlabel('Distance x')
ylabel('Solution u(x,t)')
title('Solution profiles at several times')
```



Compute Emitter Discharge Current

Using a series solution for u(x, t), the emitter discharge current can be expressed as the infinite series [1]:

$$I(t) = 2\pi^2 I_p \bigg(\frac{1-e^{-\eta}}{\eta}\bigg) \sum_{n=1}^{\infty} \frac{n^2}{n^2 \pi^2 + \eta^2/4} e^{-\frac{dt}{L^2} \left(n^2 \pi^2 + \eta^2/4\right)}.$$

Write a function to calculate the analytic solution for I(t) using 40 terms in the series. The only variable is time, but specify a second input to the function for the structure of constants.

```
function It = serex3(t,C) % Approximate I(t) by series expansion.
Ip = C.Ip;
eta = C.eta;
D = C.D;
L = C.L;

It = 0;
for n = 1:40 % Use 40 terms
    m = (n*pi)^2 + 0.25*eta^2;
    It = It + ((n*pi)^2 / m)* exp(-(D/L^2)*m*t);
end
It = 2*Ip*((1 - exp(-eta))/eta)*It;
end
```

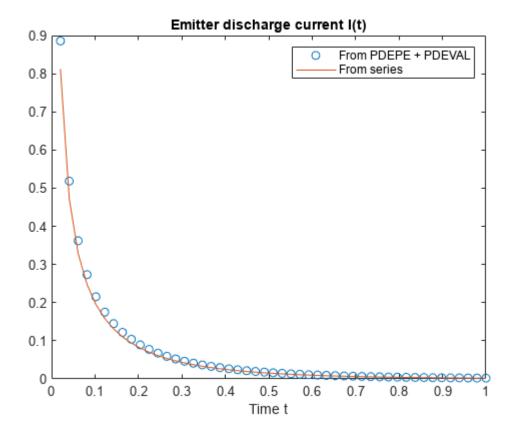
Using the numeric solution for u(x, t) as computed by pdepe, you can also calculate the numeric approximation for I(t) at x = 0 with

$$I(t) = \left[\frac{I_p D}{K} \frac{\partial}{\partial x} u(x, t)\right]_{x = 0}.$$

Calculate the analytic and numeric solutions for I(t) and plot the results. Use pdeval to compute the value of $\partial u/\partial x$ at x=0.

```
nt = length(t);
I = zeros(1,nt);
seriesI = zeros(1,nt);
iok = 2:nt;
for j = iok
    % At time t(j), compute du/dx at x = 0.
    [~,I(j)] = pdeval(m,x,u(j,:),0);
    seriesI(j) = serex3(t(j),C);
end
% Numeric solution has form I(t) = (I_p*D/K)*du(0,t)/dx
I = (C.Ip*C.D/C.K)*I;

plot(t(iok),I(iok),'o',t(iok),seriesI(iok))
legend('From PDEPE + PDEVAL','From series')
title('Emitter discharge current I(t)')
xlabel('Time t')
```



The results match reasonably well. You can further improve the numeric result from pdepe by using a finer solution mesh.

Local Functions

Listed here are the local helper functions that the PDE solver pdepe calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

```
function [c,f,s] = transistorPDE(x,t,u,dudx,C) % Equation to solve
D = C.D;
eta = C.eta;
L = C.L;
c = 1;
f = D*dudx;
s = -(D*eta/L)*dudx;
end
function u0 = transistorIC(x,C) % Initial condition
K = C.K:
L = C.L;
D = C.D;
eta = C.eta;
u0 = (K*L/D)*(1 - exp(-eta*(1 - x/L)))/eta;
end
% -----
function [pl,ql,pr,qr] = transistorBC(xl,ul,xr,ur,t) % Boundary conditions
pl = ul;
ql = 0;
pr = ur;
qr = 0;
end
function It = serex3(t,C) % Approximate I(t) by series expansion.
Ip = C.Ip;
eta = C.eta;
D = C.D;
L = C.L;
It = 0;
for n = 1:40 % Use 40 terms
 m = (n*pi)^2 + 0.25*eta^2;
 It = It + ((n*pi)^2 / m)* exp(-(D/L^2)*m*t);
It = 2*Ip*((1 - exp(-eta))/eta)*It;
```

References

[1] Zachmanoglou, E.C. and D.L. Thoe. *Introduction to Partial Differential Equations with Applications*. Dover, New York, 1986.

See Also

pdepe

More About

- "Solving Partial Differential Equations" on page 13-2
- "Solve System of PDEs" on page 13-32

Solve System of PDEs

This example shows how to formulate, compute, and plot the solution to a system of two partial differential equations.

Consider the system of PDEs

$$\frac{\partial u_1}{\partial t} = 0.024 \frac{\partial^2 u_1}{\partial x^2} - F(u_1 - u_2),$$

$$\frac{\partial u_2}{\partial t} = 0.170 \frac{\partial^2 u_2}{\partial x^2} + F(u_1 - u_2).$$

(The function $F(y) = e^{5.73y} - e^{-11.46y}$ is used as a shorthand.)

The equation holds on the interval $0 \le x \le 1$ for times $t \ge 0$. The initial conditions are

$$u_1(x,0)=1,$$

$$u_2(x,0) = 0$$
.

The boundary conditions are

$$\frac{\partial}{\partial x}u_1(0,t)=0,$$

$$u_2(0,t)=0,$$

$$\frac{\partial}{\partial x}u_2(1,t)=0,$$

$$u_1(1,t) = 1$$
.

To solve this equation in MATLAB®, you need to code the equation, the initial conditions, and the boundary conditions, then select a suitable solution mesh before calling the solver pdepe. You either can include the required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Code Equation

Before you can code the equation, you need to make sure that it is in the form that the pdepe solver expects:

$$c\left(x,t,u,\frac{\partial u}{\partial x}\right)\frac{\partial u}{\partial t} = x^{-m}\frac{\partial}{\partial x}\left(x^{m}f\left(x,t,u,\frac{\partial u}{\partial x}\right)\right) + s\left(x,t,u,\frac{\partial u}{\partial x}\right).$$

In this form, the PDE coefficients are matrix-valued and the equation becomes

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \frac{\partial}{\partial t} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \frac{\partial}{\partial x} \begin{bmatrix} 0 \cdot 024 \frac{\partial u_1}{\partial x} \\ 0 \cdot 170 \frac{\partial u_2}{\partial x} \end{bmatrix} + \begin{bmatrix} -F(u_1 - u_2) \\ F(u_1 - u_2) \end{bmatrix}.$$

So the values of the coefficients in the equation are

$$m = 0$$

$$c(x, t, u, \frac{\partial u}{\partial x}) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$
 (diagonal values only)

$$f\left(x, t, u, \frac{\partial u}{\partial x}\right) = \begin{bmatrix} 0.024 \frac{\partial u_1}{\partial x} \\ 0.170 \frac{\partial u_2}{\partial x} \end{bmatrix}$$

$$s(x, t, u, \frac{\partial u}{\partial x}) = \begin{bmatrix} -F(u_1 - u_2) \\ F(u_1 - u_2) \end{bmatrix}$$

Now you can create a function to code the equation. The function should have the signature [c,f,s] = pdefun(x,t,u,dudx):

- x is the independent spatial variable.
- t is the independent time variable.
- u is the dependent variable being differentiated with respect to x and t. It is a two-element vector where u(1) is $u_1(x,t)$ and u(2) is $u_2(x,t)$.
- dudx is the partial spatial derivative $\partial u/\partial x$. It is a two-element vector where dudx(1) is $\partial u_1/\partial x$ and dudx(2) is $\partial u_2/\partial x$.
- The outputs c, f, and s correspond to coefficients in the standard PDE equation form expected by pdepe.

As a result, the equations in this example can be represented by the function:

```
function [c,f,s] = pdefun(x,t,u,dudx)
c = [1; 1];
f = [0.024; 0.17] .* dudx;
y = u(1) - u(2);
F = exp(5.73*y)-exp(-11.47*y);
s = [-F; F];
end
```

(Note: All functions are included as local functions at the end of the example.)

Code Initial Conditions

Next, write a function that returns the initial condition. The initial condition is applied at the first time value and provides the value of $u(x, t_0)$ for any value of x. The number of initial conditions must equal the number of equations, so for this problem there are two initial conditions. Use the function signature u0 = pdeic(x) to write the function.

The initial conditions are

$$u_1(x,0) = 1$$
,

$$u_2(x,0) = 0$$
.

The corresponding function is

```
function u0 = pdeic(x)
u0 = [1; 0];
end
```

Code Boundary Conditions

Now, write a function that evaluates the boundary conditions

$$\frac{\partial}{\partial x}u_1(0,t) = 0,$$

$$u_2(0,t) = 0,$$

$$\frac{\partial}{\partial x}u_2(1,t) = 0,$$

$$u_1(1,t) = 1.$$

For problems posed on the interval $a \le x \le b$, the boundary conditions apply for all t and either x = a or x = b. The standard form for the boundary conditions expected by the solver is

$$p(x, t, u) + q(x, t)f(x, t, u, \frac{\partial u}{\partial x}) = 0.$$

Written in this form, the boundary conditions for the partial derivatives of u need to be expressed in terms of the flux $f(x, t, u, \frac{\partial u}{\partial x})$. So the boundary conditions for this problem are

For x = 0, the equation is

$$\begin{bmatrix} 0 \\ u_2 \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 0.024 \frac{\partial u_1}{\partial x} \\ 0.170 \frac{\partial u_2}{\partial x} \end{bmatrix} = 0.$$

The coefficients are:

$$p_L(x, t, u) = \begin{bmatrix} 0 \\ u_2 \end{bmatrix},$$

$$q_L(x, t) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

Likewise, for x = 1 the equation is

$$\begin{bmatrix} u_1 - 1 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} \cdot \begin{bmatrix} 0.024 \frac{\partial u_1}{\partial x} \\ 0.170 \frac{\partial u_2}{\partial x} \end{bmatrix} = 0.$$

The coefficients are:

$$p_R(x, t, u) = \begin{bmatrix} u_1 - 1 \\ 0 \end{bmatrix},$$

$$q_R(x, t) = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

The boundary function should use the function signature [pl,ql,pr,qr] = pdebc(xl,ul,xr,ur,t):

- The inputs xl and ul correspond to *u* and *x* for the left boundary.
- The inputs xr and ur correspond to *u* and *x* for the right boundary.
- t is the independent time variable.
- The outputs pl and ql correspond to $p_L(x, t, u)$ and $q_L(x, t)$ for the left boundary (x = 0 for this problem).
- The outputs pr and qr correspond to $p_R(x, t, u)$ and $q_R(x, t)$ for the right boundary (x = 1 for this problem).

The boundary conditions in this example are represented by the function:

```
function [pl,ql,pr,qr] = pdebc(xl,ul,xr,ur,t)
pl = [0; ul(2)];
ql = [1; 0];
pr = [ur(1)-1; 0];
qr = [0; 1];
end
```

Select Solution Mesh

The solution to this problem changes rapidly when t is small. Although pdepe selects a time step that is appropriate to resolve the sharp changes, to see the behavior in the output plots you need to select appropriate output times. For the spatial mesh, there are boundary layers in the solution at both ends of $0 \le x \le 1$, so you need to specify mesh points there to resolve the sharp changes.

```
x = [0 \ 0.005 \ 0.01 \ 0.05 \ 0.1 \ 0.2 \ 0.5 \ 0.7 \ 0.9 \ 0.95 \ 0.99 \ 0.995 \ 1];
t = [0 \ 0.005 \ 0.01 \ 0.05 \ 0.1 \ 0.5 \ 1 \ 1.5 \ 2];
```

Solve Equation

Finally, solve the equation using the symmetry m, the PDE equation, the initial conditions, the boundary conditions, and the meshes for x and t.

```
m = 0;
sol = pdepe(m,@pdefun,@pdeic,@pdebc,x,t);
```

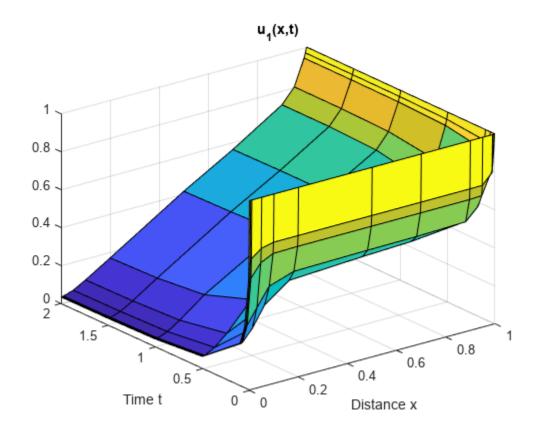
pdepe returns the solution in a 3-D array sol, where sol(i,j,k) approximates the kth component of the solution u_k evaluated at t(i) and x(j). Extract each solution component into a separate variable.

```
u1 = sol(:,:,1);
u2 = sol(:,:,2);
```

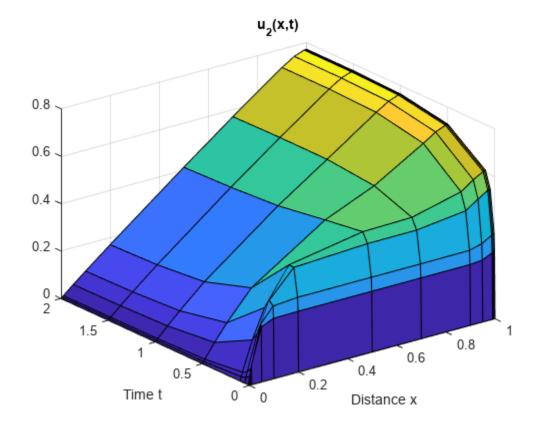
Plot Solution

Create surface plots of the solutions for u_1 and u_2 plotted at the selected mesh points for x and t.

```
surf(x,t,u1)
title('u_1(x,t)')
xlabel('Distance x')
ylabel('Time t')
```



```
surf(x,t,u2)
title('u_2(x,t)')
xlabel('Distance x')
ylabel('Time t')
```



Local Functions

Listed here are the local helper functions that the PDE solver pdepe calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

See Also

pdepe

More About

- "Solving Partial Differential Equations" on page 13-2
- "Solve Single PDE" on page 13-9
- "Solve System of PDEs with Initial Condition Step Functions" on page 13-39

Solve System of PDEs with Initial Condition Step Functions

This example shows how to solve a system of partial differential equations that uses step functions in the initial conditions.

Consider the PDEs

$$\frac{\partial n}{\partial t} = \frac{\partial}{\partial x} \left[d \frac{\partial n}{\partial x} - a \, n \frac{\partial c}{\partial x} \right] + S \, r \, n(N - n),$$

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} + S \left(\frac{n}{n+1} - c \right).$$

The equations involve the constant parameters d, a, S, r, and N, and are defined for $0 \le x \le 1$ and $t \ge 0$. These equations arise in a mathematical model of the first steps of tumor-related angiogenesis [1]. n(x,t) represents the cell density of endothelial cells, and c(x,t) the concentration of a protein they release in response to the tumor.

This problem has a constant, steady state when

$$\begin{bmatrix} n_0 \\ c_0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0.5 \end{bmatrix}.$$

However, a stability analysis predicts evolution of the system to an inhomogeneous solution [1]. So step functions are used as the initial conditions to perturb the steady state and stimulate evolution of the system.

The boundary conditions require that both solution components have zero flux at x = 0 and x = 1.

$$\frac{\partial}{\partial x}n(0,t) = \frac{\partial}{\partial x}n(1,t) = 0,$$
$$\frac{\partial}{\partial x}c(0,t) = \frac{\partial}{\partial x}c(1,t) = 0.$$

To solve this system of equations in MATLAB®, you need to code the equations, initial conditions, and boundary conditions, then select a suitable solution mesh before calling the solver pdepe. You either can include the required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Code Equation

Before you can code the equation, you need to make sure that it is in the form that the pdepe solver expects:

$$c\left(x,t,u,\frac{\partial u}{\partial x}\right)\frac{\partial u}{\partial t} = x^{-m}\frac{\partial}{\partial x}\left(x^m f\left(x,t,u,\frac{\partial u}{\partial x}\right)\right) + s\left(x,t,u,\frac{\partial u}{\partial x}\right).$$

Since there are two equations in the system of PDEs, the system of PDEs can be rewritten as

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \frac{\partial}{\partial t} \begin{bmatrix} n \\ c \end{bmatrix} = \frac{\partial}{\partial x} \begin{bmatrix} d \frac{\partial n}{\partial x} - a \, n \frac{\partial c}{\partial x} \\ \frac{\partial c}{\partial x} \end{bmatrix} + \begin{bmatrix} S \, r \, n (N - n) \\ S \Big(\frac{n}{n+1} - c \Big) \end{bmatrix}.$$

The values of the coefficients in the equation are then

$$m = 0$$

$$c(x, t, u, \frac{\partial u}{\partial x}) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$
 (diagonal values only)

$$f(x, t, u, \frac{\partial u}{\partial x}) = \begin{bmatrix} d\frac{\partial n}{\partial x} - a n \frac{\partial c}{\partial x} \\ \frac{\partial c}{\partial x} \end{bmatrix}$$

$$s\left(x,t,u,\frac{\partial u}{\partial x}\right) = \begin{bmatrix} S \, r \, n(N-n) \\ S\left(\frac{n}{n+1}-c\right) \end{bmatrix}$$

Now you can create a function to code the equation. The function should have the signature [c,f,s] = angiopde(x,t,u,dudx):

- x is the independent spatial variable.
- t is the independent time variable.
- u is the dependent variable being differentiated with respect to x and t. It is a two-element vector where u(1) is n(x,t) and u(2) is c(x,t).
- dudx is the partial spatial derivative $\partial u/\partial x$. It is a two-element vector where dudx(1) is $\partial n/\partial x$ and dudx(2) is $\partial c/\partial x$.
- The outputs c, f, and s correspond to coefficients in the standard PDE equation form expected by pdepe.

As a result, the equations in this example can be represented by the function:

(Note: All functions are included as local functions at the end of the example.)

Code Initial Conditions

Next, write a function that returns the initial condition. The initial condition is applied at the first time value and provides the value of $n(x, t_0)$ and $c(x, t_0)$ for any value of x. Use the function signature u0 = angioic(x) to write the function.

This problem has a constant, steady state when

However, a stability analysis predicts evolution of the system to an inhomogenous solution [1]. So, step functions are used as the initial conditions to perturb the steady state and stimulate evolution of the system.

$$u(x,0) = \begin{bmatrix} n_0 \\ c_0 \end{bmatrix},$$

$$u(x,0) = \begin{cases} 1.05u_1 & 0.3 \le x \le 0.6 \\ 1.0005u_2 & 0.3 \le x \le 0.6 \end{cases}$$

The corresponding function is

```
function u0 = angioic(x)
u0 = [1; 0.5];
if x >= 0.3 && x <= 0.6
   u0(1) = 1.05 * u0(1);
   u0(2) = 1.0005 * u0(2);
end
end</pre>
```

Code Boundary Conditions

Now, write a function that evaluates the boundary conditions

$$\frac{\partial}{\partial x}n(0,t) = \frac{\partial}{\partial x}n(1,t) = 0,$$

$$\frac{\partial}{\partial x}c(0,t) = \frac{\partial}{\partial x}c(1,t) = 0.$$

For problems posed on the interval $a \le x \le b$, the boundary conditions apply for all t and either x = a or x = b. The standard form for the boundary conditions expected by the solver is

$$p(x, t, u) + q(x, t)f\left(x, t, u, \frac{\partial u}{\partial x}\right) = 0$$
.

For x = 0, the boundary condition equation is

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 1 \\ 1 \end{bmatrix} \cdot \begin{bmatrix} d \frac{\partial n}{\partial x} - a \, n \frac{\partial c}{\partial x} \\ \frac{\partial c}{\partial x} \end{bmatrix} = 0 \, .$$

So the coefficients are:

•
$$p_L(x, t, u) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

•
$$q_L(x,t) = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$
.

For x=1 the boundary conditions are the same, so $p_R(x,t,u)=\begin{bmatrix} 0 \\ 0 \end{bmatrix}$ and $q_R(x,t)=\begin{bmatrix} 1 \\ 1 \end{bmatrix}$.

The boundary function should use the function signature [pl,ql,pr,qr] = angiobc(xl,ul,xr,ur,t), where:

- The inputs xl and ul correspond to *u* and *x* for the left boundary.
- The inputs xr and ur correspond to *u* and *x* for the right boundary.
- t is the independent time variable.
- The outputs pl and ql correspond to $p_L(x, t, u)$ and $q_L(x, t)$ for the left boundary (x = 0 for this problem).
- The outputs pr and qr correspond to $p_R(x, t, u)$ and $q_R(x, t)$ for the right boundary (x = 1 for this problem).

The boundary conditions in this example are represented by the function:

```
function [pl,ql,pr,qr] = angiobc(xl,ul,xr,ur,t)
pl = [0; 0];
ql = [1; 1];
pr = pl;
qr = ql;
end
```

Select Solution Mesh

A long time interval is required to see the limiting behavior of the equations, so use 10 points in the interval $0 \le t \le 200$. Also, the limit distribution of c(x, t) varies by only about 0.1% over the interval $0 \le x \le 1$, so a relatively fine spatial mesh with 50 points is appropriate.

```
x = linspace(0,1,50);
t = linspace(0,200,10);
```

Solve Equation

Finally, solve the equation using the symmetry m, the PDE equation, the initial condition, the boundary conditions, and the meshes for x and t.

```
m = 0;
sol = pdepe(m,@angiopde,@angioic,@angiobc,x,t);
```

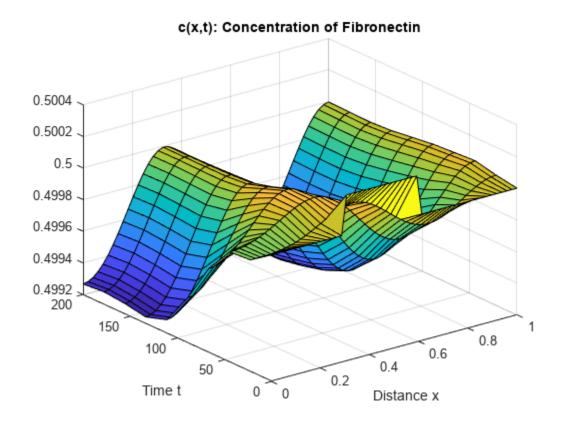
pdepe returns the solution in a 3-D array sol, where sol(i,j,k) approximates the kth component of the solution u_k evaluated at t(i) and x(j). Extract the solution components into separate variables.

```
n = sol(:,:,1);
c = sol(:,:,2);
```

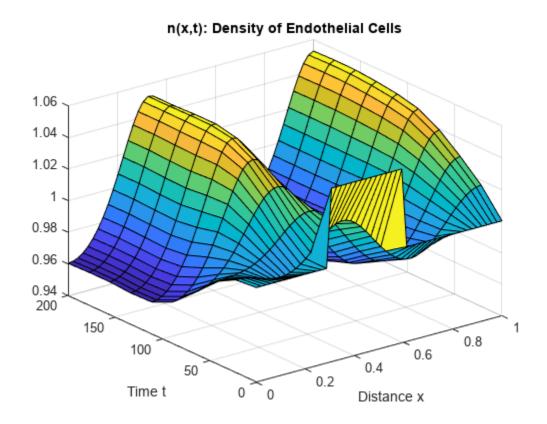
Plot Solution

Create a surface plot of the solution components n and c plotted at the selected mesh points for x and t.

```
surf(x,t,c)
title('c(x,t): Concentration of Fibronectin')
xlabel('Distance x')
ylabel('Time t')
```

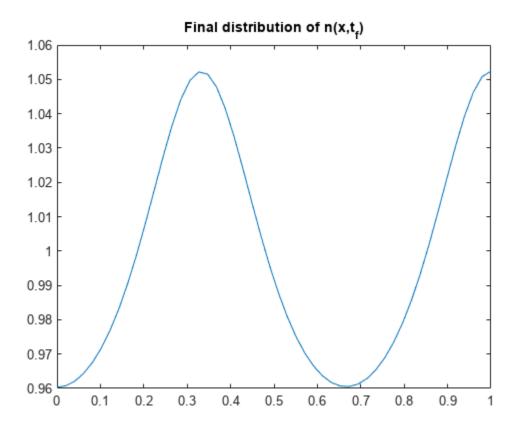


```
surf(x,t,n)
title('n(x,t): Density of Endothelial Cells')
xlabel('Distance x')
ylabel('Time t')
```

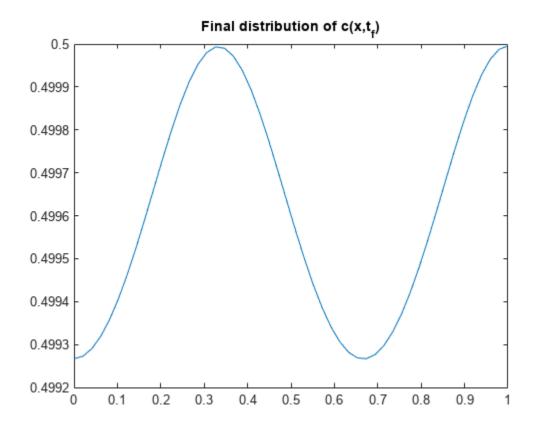


Now plot just the final distributions of the solutions at $t_f = 200$. These plots correspond to Figures 3 and 4 in [1].

```
plot(x,n(end,:))
title('Final distribution of n(x,t_f)')
```



plot(x,c(end,:))
title('Final distribution of c(x,t_f)')



References

[1] Humphreys, M.E. and M.A.J. Chaplain. "A mathematical model of the first steps of tumour-related angiogenesis: Capillary sprout formation and secondary branching." *IMA Journal of Mathematics Applied in Medicine & Biology*, 13 (1996), pp. 73-98.

Local Functions

Listed here are the local helper functions that the PDE solver pdepe calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

```
if x >= 0.3 && x <= 0.6
    u0(1) = 1.05 * u0(1);
    u0(2) = 1.0005 * u0(2);
end
end
%
function [pl,ql,pr,qr] = angiobc(xl,ul,xr,ur,t) % Boundary Conditions
pl = [0; 0];
ql = [1; 1];
pr = pl;
qr = ql;
end
%</pre>
```

See Also

pdepe

More About

- "Solving Partial Differential Equations" on page 13-2
- "Solve Single PDE" on page 13-9
- "Solve System of PDEs" on page 13-32

Delay Differential Equations (DDEs)

- "Solving Delay Differential Equations" on page 14-2
- "DDE with Constant Delays" on page 14-6
- "DDE with State-Dependent Delays" on page 14-10
- "Cardiovascular Model DDE with Discontinuities" on page 14-14
- "DDE of Neutral Type" on page 14-19
- "Initial Value DDE of Neutral Type" on page 14-23

Solving Delay Differential Equations

Delay differential equations (DDEs) are ordinary differential equations that relate the solution at the current time to the solution at past times. This delay can be constant, time-dependent, statedependent, or derivative-dependent. In order for the integration to begin, you generally must provide a solution history so that the solution is accessible to the solver for times before the initial integration point.

Constant Delay DDEs

A system of differential equations with constant delays has the form:

$$y'(t) = f(t, y(t), y(t - \tau_1), ..., y(t - \tau_k)).$$

Here, t is the independent variable, y is a column vector of dependent variables, and y' represents the first derivative of y with respect to t. The delays, $\tau_1, ..., \tau_k$, are positive constants.

The dde23 function solves DDEs with constant delays with history y(t) = S(t) for $t < t_0$.

The solutions of DDEs are generally continuous, but they have discontinuities in their derivatives. The dde23 function tracks discontinuities in low-order derivatives. It integrates the differential equations with the same explicit Runge-Kutta (2,3) pair and interpolant used by ode23. The Runge-Kutta formulas are implicit for step sizes bigger than the delays. When y(t) is smooth enough to justify steps this big, the implicit formulas are evaluated by a predictor-corrector iteration.

Time-Dependent and State-Dependent DDEs

Constant time delays are a special case of the more general DDE form:

$$y'(t) = f(t, y(t), y(dy_1), ..., y(dy_p)).$$

Time-dependent and state-dependent DDEs involve delays $dy_1,...,dy_k$ that can depend on both time t and state y. The delays $dy_i(t, y)$ must satisfy $dy_i(t, y) \le t$ on the interval $[t_0, t_f]$ with $t_0 < t_f$.

The ddesd function finds the solution, y(t), for time-dependent and state-dependent DDEs with history y(t) = S(t) for $t < t_0$. The ddesd function integrates with the classic four-stage, fourth-order explicit Runge-Kutta method, and it controls the size of the residual of a natural interpolant. It uses iteration to take steps that are longer than the delays.

DDEs of Neutral Type

Delay differential equations of neutral type involve delays in y' as well as y:

$$y'(t) = f(t, y(t), y(dy_1), ..., y(dy_p), y'(dyp_1), ..., y'(dyp_q)).$$

The delays in the solution must satisfy $dy_i(t,y) \le t$. The delays in the first derivative must satisfy $dyp_i(t,y) < t$ so that y' does not appear on both sides of the equation.

The ddensd function solves DDEs of neutral type by approximating them with DDEs of the form given for time-dependent and state-dependent delays:

$$y'(t) = f(t, y(t), y(dy_1), ..., y(dy_p)).$$

For more information, see Shampine [1].

Evaluating the Solution at Specific Points

Use the deval function and the output from any of the DDE solvers to evaluate the solution at specific points in the interval of integration. For example, y = deval(sol, 0.5*(sol.x(1) + sol.x(end))) evaluates the solution at the midpoint of the interval of integration.

History and Initial Values

When you solve a DDE, you approximate the solution on an interval $[t_0,t_f]$ with $t_0 < t_f$. The DDEs show how y'(t) depends on values of the solution (and possibly its derivative) at times prior to t. For example, with constant delays $y'(t_0)$ depends on $y(t_0 - \tau_1),...,y(t_0 - \tau_k)$ for positive constants τ_j . Because of this, a solution on $[t_0,t_k]$ depends on values it has at $t \le t_0$. You must define these values with a history function, y(t) = S(t) for $t < t_0$.

Discontinuities in DDEs

If your problem has discontinuities, it is best to communicate them to the solver using an options structure. To do this, use the ddeset function to create an options structure containing the discontinuities in your problem.

There are three properties in the options structure that you can use to specify discontinuities; InitialY, Jumps, and Events. The property you choose depends on the location and nature of the discontinuities.

Nature of Discontinuity	Property	Comments
At the initial value $t = t_0$	InitialY	Generally the initial value $y(t_0)$ is the value $S(t_0)$ returned by the history function, meaning the solution is continuous at the initial point. If this is not the case, supply a different initial value using the InitialY property.
In the history, i.e., the solution at $t < t_0$, or in the equation coefficients for $t > t_0$	Jumps	Provide the known locations t of the discontinuities in a vector as the value of the Jumps property. Applies only to dde23.

Nature of Discontinuity	Property	Comments
State-dependent	Events	dde23, ddesd, and ddensd use the events function you supply to locate these discontinuities. When the solver finds such a discontinuity, restart the integration to continue. Specify the solution structure for the current integration as the history for the new integration. The solver extends each element of the solution structure after each restart so that the final structure provides the solution for the whole interval of integration. If the new problem involves a change in the solution, use the InitialY property to specify the initial value for the new integration.

Propagation of Discontinuities

Generally, the first derivative of the solution has a jump at the initial point. This is because the first derivative of the history function, S(t), generally does not satisfy the DDE at this point. A discontinuity in any derivative of y(t) propagates into the future at spacings of τ_1, \ldots, τ_k when the delays are constant. If the delays are not constant, the propagation of discontinuities is more complicated. For neutral DDEs of the forms in "Constant Delay DDEs" on page 14-2 and "Time-Dependent and State-Dependent DDEs" on page 14-2, the discontinuity appears in the next higher order derivative each time it is propagated. In this sense, the solution gets smoother as the integration proceeds. Solutions of neutral DDEs of the form given in "DDEs of Neutral Type" on page 14-2 are qualitatively different. The discontinuity in the solution does not propagate to a derivative of higher order. In particular, the typical jump in y'(t) at t_0 propagates as jumps in y'(t) throughout $[t_0,$ $t_{\rm f}$].

DDE Examples and Files

Several available example files serve as excellent starting points for most common DDE problems. To easily explore and run examples, simply use the **Differential Equations Examples** app. To run this app, type

odeexamples

To open an individual example file for editing, type

edit exampleFileName.m

To run an example, type

exampleFileName

This table contains a list of the available DDE example files, as well as the solvers and the options they use.

Example File	Solver Used	Options Specified	Description	Example Link
ddex1	dde23	_	DDE with constant history	"DDE with Constant Delays" on page 14-6
ddex2	dde23	• 'Jumps'	DDE with a discontinuity	"Cardiovascular Model DDE with Discontinuities" on page 14-14
ddex3	ddesd	_	DDE with state-dependent delays	"DDE with State- Dependent Delays" on page 14-10
ddex4	ddensd	_	Neutral DDE with two delays	"DDE of Neutral Type" on page 14- 19
ddex5	ddensd	_	Neutral DDE with initial value	"Initial Value DDE of Neutral Type" on page 14-23

References

[1] Shampine, L.F. "Dissipative Approximations to Neutral DDEs." Applied Mathematics & Computation, Vol. 203, 2008, pp. 641–648.

See Also

dde23 | ddesd | ddensd | ddeset

More About

- "DDE with Constant Delays" on page 14-6
- "DDE with State-Dependent Delays" on page 14-10

DDE with Constant Delays

This example shows how to use dde23 to solve a system of DDEs (delay differential equations) with constant delays.

The system of equations is

```
y_1'(t) = y_1(t-1)
y_2'(t) = y_1(t-1) + y_2(t-0.2)
y_3'(t) = y_2(t).
```

The history function for $t \le 0$ is constant, $y_1(t) = y_2(t) = y_3(t) = 1$.

The time delays in the equations are only present in y terms, and the delays themselves are constants, so the equations form a system of *constant delay* equations.

To solve this system of equations in MATLAB®, you need to code the equations, delays, and history before calling the delay differential equation solver dde23, which is meant for systems with constant delays. You either can include the required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Code Delays

First, create a vector to define the delays in the system of equations. This system has two different delays:

- A delay of 1 in the first component $y_1(t-1)$.
- A delay of 0.2 in the second component $y_2(t-0.2)$.

dde23 accepts a vector argument for the delays, where each element is the constant delay for one component.

```
lags = [1 \ 0.2];
```

Code Equation

Now, create a function to code the equations. This function should have the signature dydt = ddefun(t,y,Z), where:

- t is time (independent variable).
- y is the solution (dependent variable).
- Z(:,j) approximates the delay $y(t-\tau_i)$, where the constant delay τ_i is given by lags(j).

These inputs are automatically passed to the function by the solver, but the variable names determine how you code the equations. In this case:

```
• Z(:,1) \rightarrow y_1(t-1)
• Z(:,2) \rightarrow y_2(t-0.2)
function dydt = ddefun(t,y,Z)
  ylag1 = Z(:,1);
```

Note: All functions are included as local functions at the end of the example.

Code Solution History

Next, create a function to define the solution history. The solution history is the solution for times $t \le t_0$.

```
function s = history(t)
  s = ones(3,1);
end
```

Solve Equation

Finally, define the interval of integration $[t_0 \ t_f]$ and solve the DDE using the dde23 solver.

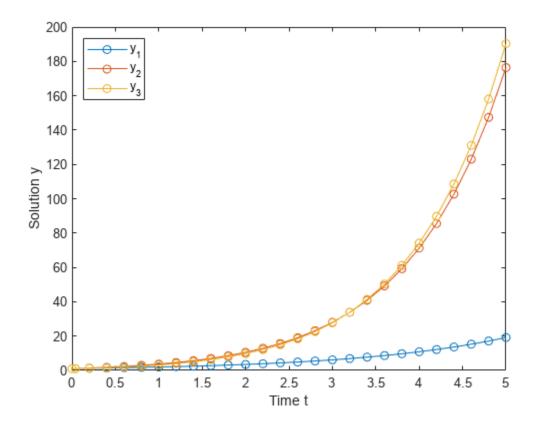
```
tspan = [0 5];
sol = dde23(@ddefun, lags, @history, tspan);
```

Plot Solution

The solution structure sol has the fields sol.x and sol.y that contain the internal time steps taken by the solver and corresponding solutions at those times. (If you need the solution at specific points, you can use deval to evaluate the solution at the specific points.)

Plot the three solution components against time.

```
plot(sol.x,sol.y,'-o')
xlabel('Time t');
ylabel('Solution y');
legend('y_1','y_2','y_3','Location','NorthWest');
```



Local Functions

Listed here are the local helper functions that the DDE solver dde23 calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

```
function dydt = ddefun(t,y,Z) % equation being solved
 ylag1 = Z(:,1);
 ylag2 = Z(:,2);
  dydt = [ylag1(1);
          ylag1(1)+ylag2(2);
end
function s = history(t) % history function for t <= 0</pre>
 s = ones(3,1);
end
```

See Also

dde23 | ddesd | ddensd | deval

More About

"Solving Delay Differential Equations" on page 14-2

• "DDE with State-Dependent Delays" on page 14-10

DDE with State-Dependent Delays

This example shows how to use ddesd to solve a system of DDEs (delay differential equations) with state-dependent delays. This system of DDEs was used as a test problem by Enright and Hayashi [1].

The system of equations is

$$y_1'(t) = y_2(t),$$

 $y_2'(t) = -y_2(e^{1-y_2(t)}) \cdot y_2(t)^2 \cdot e^{1-y_2(t)}.$

The history functions for $t \le 0$. 1 are the analytical solutions

$$y_1(t) = \log(t),$$

$$y_2(t) = \frac{1}{t}.$$

The time delays in the equations are only present in y terms. The delays depend only on the state of the second component $y_2(t)$, so the equations form a system of state-dependent delay equations.

To solve this system of equations in MATLAB®, you need to code the equations, delays, and history before calling the delay differential equation solver ddesd, which is meant for systems with statedependent delays. You either can include the required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Code Delays

First, write a function to define the time delays in the system. The only delay present in this system of equations is in the term- $y_2(e^{1-y_2(t)})$.

```
function d = dely(t,y)
d = \exp(1 - y(2));
```

Note: All functions are included as local functions at the end of the example.

Code Equation

Now, create a function to code the equations. This function should have the signature dydt = ddefun(t,y,Z), where:

- t is time (independent variable).
- y is the solution (dependent variable).
- Z(n,j) approximates the delays $y_n(d(j))$, where the delay d(j) is given by component j of dely(t,y).

These inputs are automatically passed to the function by the solver, but the variable names determine how you code the equations. In this case:

•
$$Z(2,1) \rightarrow y_2(e^{1-y_2(t)})$$

Code Solution History

Next, create a function to define the solution history. The solution history is the solution for times $t \le t_0$.

```
function v = history(t) % history function for t < t0
v = [log(t);
        1./t];
end</pre>
```

Solve Equation

Finally, define the interval of integration $[t_0 \ t_f]$ and solve the DDE using the ddesd solver.

```
tspan = [0.1 5];
sol = ddesd(@ddefun, @dely, @history, tspan);
```

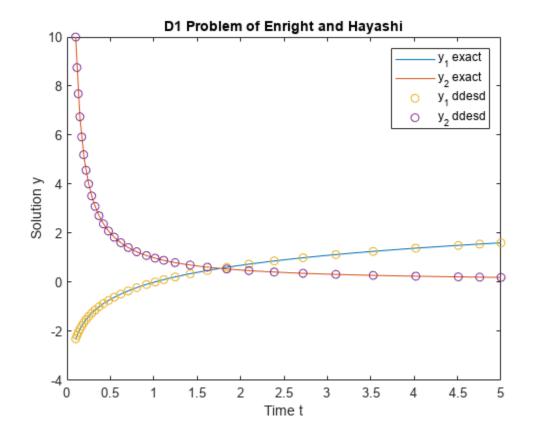
Plot Solution

The solution structure sol has the fields sol.x and sol.y that contain the internal time steps taken by the solver and corresponding solutions at those times. (If you need the solution at specific points, you can use deval to evaluate the solution at the specific points.)

Plot the two solution components against time using the history function to calculate the analytical solution within the integration interval for comparison.

```
ta = linspace(0.1,5);
ya = history(ta);

plot(ta,ya,sol.x,sol.y,'o')
legend('y_1 exact','y_2 exact','y_1 ddesd','y_2 ddesd')
xlabel('Time t')
ylabel('Solution y')
title('D1 Problem of Enright and Hayashi')
```



Local Functions

Listed here are the local helper functions that the DDE solver ddesd calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

```
function dydt = ddefun(t,y,Z) % equation being solved
dydt = [y(2);
       -Z(2,1).*y(2)^2.*exp(1 - y(2))];
end
function d = dely(t,y) % delay for y
d = \exp(1 - y(2));
function v = history(t) % history function for t < t0</pre>
v = [log(t);
     1./t];
end
```

References

[1] Enright, W.H. and H. Hayashi. "The Evaluation of Numerical Software for Delay Differential Equations." In Proceedings of the IFIP TC2/WG2.5 working conference on Quality of numerical $software: assessment \ and \ enhancement.$ (R.F. Boisvert, ed.). London, UK: Chapman & Hall, Ltd., pp. 179-193.

See Also

ddensd | ddesd | dde23 | deval

- "Solving Delay Differential Equations" on page 14-2
- "Cardiovascular Model DDE with Discontinuities" on page 14-14

Cardiovascular Model DDE with Discontinuities

This example shows how to use dde23 to solve a cardiovascular model that has a discontinuous derivative. The example was originally presented by Ottesen [1].

The system of equations is

$$\dot{P}_a(t) = -\frac{1}{c_a R} P_a(t) + \frac{1}{c_a R} P_{\nu}(t) + \frac{1}{c_a} V_{\text{Str}} \left(P_a^{\tau}(t) \right) H(t)$$

$$\dot{P}_{\nu}(t) = \frac{1}{c_{\nu} R} P_a(t) - \left(\frac{1}{c_{\nu} R} + \frac{1}{c_{\nu} r} \right) P_{\nu}(t)$$

$$\dot{H}(t) = \frac{\alpha_H T_S}{1 + \gamma_H T_p} - \beta_H T_p.$$

The terms for T_s and T_p are variations of the same equation with and without time delay. P_a^{τ} and P_a represent the mean arterial pressure with and without time delay, respectively.

$$T_S = \frac{1}{1 + \left(\frac{P_d^{\mathsf{T}}}{\alpha_S}\right)^{\beta_S}}$$

$$T_p = \frac{1}{1 + \left(\frac{P_a}{\alpha_p}\right)^{-\beta_p}}.$$

This problem has a number of physical parameters:

- Arterial compliance $c_a = 1.55 \text{ ml/mmHg}$
- Venous compliance $c_v = 519 \text{ ml/mmHg}$
- Peripheral resistance R = 1.05(0.84)mmHg s/ml
- Venous outflow resistance $r = 0.068 \, \text{mmHg s/ml}$
- Stroke volume $V_{\text{str}} = 67.9(77.9) \,\text{ml}$
- Typical mean arterial pressure $P_0 = 93 \text{ mmHg}$
- $\alpha_0 = \alpha_s = \alpha_p = 93(121) \,\text{mmHg}$
- $\alpha_H = 0.84 \, \text{sec}^{-2}$
- $\beta_0 = \beta_S = \beta_D = 7$
- $\beta_H = 1.17$
- $y_H = 0$

The system is heavily influenced by peripheral pressure, which decreases exponentially from R = 1.05 to R = 0.84 beginning at t = 600. As a result, the system has a discontinuity in a low-order derivative at t = 600.

The constant solution history is defined in terms of the physical parameters

$$P_a = P_0, \qquad P_v(t) = \frac{1}{1 + \frac{R}{r}} P_0, \qquad H(t) = \frac{1}{\text{RV}_{\text{str}}} \frac{1}{1 + \frac{r}{R}} P_0.$$

To solve this system of equations in MATLAB®, you need to code the equations, parameters, delays, and history before calling the delay differential equation solver dde23, which is meant for systems with constant time delays. You either can include the required functions as local functions at the end of a file (as done here), or save them as separate, named files in a directory on the MATLAB path.

Define Physical Parameters

First, define the physical parameters of the problem as fields in a structure.

```
= 1.55:
p.ca
        = 519;
p.cv
p.R
        = 1.05;
        = 0.068;
p.r
p.Vstr = 67.9;
p.alpha0 = 93;
p.alphas = 93;
p.alphap = 93;
p.alphaH = 0.84;
p.beta0 = 7;
p.betas = 7;
p.betap = 7;
p.betaH = 1.17;
p.gammaH = 0;
```

Code Delay

Next, create a variable tau to represent the constant time delay τ in the equations for the terms $P_{\sigma}^{\tau}(t) = P_{\sigma}(t - \tau)$.

```
tau = 4;
```

Code Equations

Now, create a function to code the equations. This function should have the signature dydt = ddefun(t,y,Z,p), where:

- t is time (independent variable).
- y is the solution (dependent variable).
- Z(n,j) approximates the delays $y_n(d(j))$, where the delay d(j) is given by component j of dely(t,y).
- p is an optional fourth input used to pass in the values of the parameters.

The first three inputs are automatically passed to the function by the solver, and the variable names determine how you code the equations. The structure of parameters p is passed to the function when you call the solver. In this case the delays are represented with:

```
• Z(:,1) \rightarrow P_a(t-\tau)

function dydt = ddefun(t,y,Z,p)

if t <= 600

p.R = 1.05;

else
```

```
p.R = 0.21 * exp(600-t) + 0.84;
   end
   ylag = Z(:,1);
   Patau = ylag(1);
   Paoft = y(1);
   Pvoft = y(2);
   Hoft = y(3);
   dPadt = - (1 / (p.ca * p.R)) * Paoft ...
            + (1/(p.ca * p.R)) * Pvoft ...
           + (1/p.ca) * p.Vstr * Hoft;
   dPvdt = (1 / (p.cv * p.R)) * Paoft...
            - ( 1 / (p.cv * p.R)...
            + 1 / (p.cv * p.r) ) * Pvoft;
   Ts = 1 / (1 + (Patau / p.alphas)^p.betas);
   Tp = 1 / (1 + (p.alphap / Paoft)^p.betap );
   dHdt = (p.alphaH * Ts) / (1 + p.gammaH * Tp) ...
           p.betaH * Tp;
    dydt = [dPadt; dPvdt; dHdt];
end
```

Note: All functions are included as local functions at the end of the example.

Code Solution History

Next, create a vector to define the constant solution history for the three components P_a , P_{v} , and H. The solution history is the solution for times $t \le t_0$.

```
P0 = 93;
Paval = P0;
Pvval = (1 / (1 + p.R/p.r)) * P0;
Hval = (1 / (p.R * p.Vstr)) * (1 / (1 + p.r/p.R)) * P0;
history = [Paval; Pvval; Hval];
```

Solve Equation

Use ddeset to specify the presence of the discontinuity at t = 600. Finally, define the interval of integration $[t_0, t_f]$ and solve the DDE using the dde23 solver. Specify ddefun using an anonymous function to pass in the structure of parameters, p.

```
options = ddeset('Jumps',600);
tspan = [0 1000];
sol = dde23(@(t,y,Z) ddefun(t,y,Z,p), tau, history, tspan, options);
```

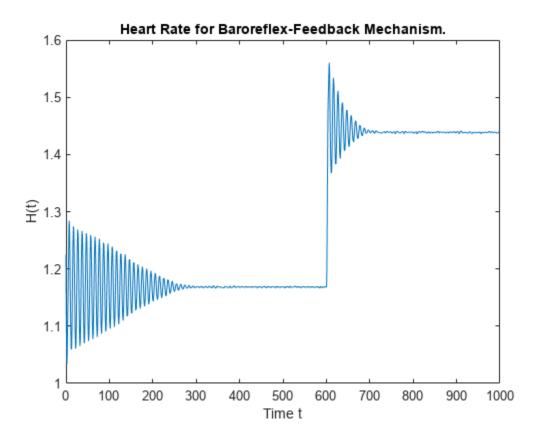
Plot Solution

The solution structure sol has the fields sol.x and sol.y that contain the internal time steps taken by the solver and corresponding solutions at those times. (If you need the solution at specific points, you can use **deval** to evaluate the solution at the specific points.)

Plot the third solution component (heart rate) against time.

```
plot(sol.x,sol.y(3,:))
title('Heart Rate for Baroreflex-Feedback Mechanism.')
```

```
xlabel('Time t')
ylabel('H(t)')
```



Local Functions

Listed here are the local helper functions that the DDE solver dde23 calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

```
function dydt = ddefun(t,y,Z,p) % equation being solved
   if t <= 600
     p.R = 1.05;
   else
     p.R = 0.21 * exp(600-t) + 0.84;
   end
   ylag = Z(:,1);
   Patau = ylag(1);
   Paoft = y(1);
   Pvoft = y(2);
   Hoft = y(3);
   dPadt = - (1 / (p.ca * p.R)) * Paoft ...
            + (1/(p.ca * p.R)) * Pvoft ...
            + (1/p.ca) * p.Vstr * Hoft;
   dPvdt = (1 / (p.cv * p.R)) * Paoft...
            - ( 1 / (p.cv * p.R)...
            + 1 / (p.cv * p.r) ) * Pvoft;
```

```
Ts = 1 / (1 + (Patau / p.alphas)^p.betas);
   Tp = 1 / (1 + (p.alphap / Paoft)^p.betap );
   dHdt = (p.alphaH * Ts) / (1 + p.gammaH * Tp) ...
          p.betaH * Tp;
   dydt = [dPadt; dPvdt; dHdt];
end
```

References

[1] Ottesen, J. T. "Modelling of the Baroreflex-Feedback Mechanism with Time-Delay." J. Math. Biol. Vol. 36, Number 1, 1997, pp. 41-63.

See Also

ddensd | ddesd | dde23 | deval

- "Solving Delay Differential Equations" on page 14-2
- "DDE of Neutral Type" on page 14-19

DDE of Neutral Type

This example shows how to use ddensd to solve a neutral DDE (delay differential equation), where delays appear in derivative terms. The problem was originally presented by Paul [1].

The equation is

$$y'(t) = 1 + y(t) - 2y\left(\frac{t}{2}\right)^2 - y'(t - \pi).$$

The history function isy(t) = cos(t) for $t \le 0$.

Since the equation has time delays in a *y'* term, the equation is called a *neutral DDE*. If the time delays are only present in *y* terms, then the equation would be a constant or state-dependent DDE, depending on what form the time delays have.

To solve this equation in MATLAB®, you need to code the equation, delays, and history before calling the delay differential equation solver ddensd. You either can include these as local functions at the end of a file (as done here), or save them as separate files in a directory on the MATLAB path.

Code Delays

First, write functions to define the delays in the equation. The first term in the equation with a delay is $y(\frac{t}{2})$.

```
function dy = dely(t,y)
    dy = t/2;
end
```

The other term in the equation with a delay is $y'(t - \pi)$.

```
function dyp = delyp(t,y)
    dyp = t-pi;
end
```

In this example, only one delay for y and one delay for y' are present. If there were more delays, then you can add them in these same function files, so that the functions return vectors instead of scalars.

Note: All functions are included as local functions at the end of the example.

Code Equation

Now, create a function to code the equation. This function should have the signature yp = ddefun(t,y,ydel,ypdel), where:

- t is time (independent variable).
- y is the solution (dependent variable).
- ydel contains the delays for y.
- ypdel contains the delays for $y' = \frac{dy}{dt}$.

These inputs are automatically passed to the function by the solver, but the variable names determine how you code the equation. In this case:

```
• ydel \rightarrow y(\frac{t}{2})
• ypdel \rightarrow y'(t - \pi)
function yp = ddefun(t,y,ydel,ypdel)
     yp = 1 + y - 2*ydel^2 - ypdel;
```

Code Solution History

Next, create a function to define the solution history. The solution history is the solution for times $t \leq t_0$.

```
function y = history(t)
    y = cos(t);
```

Solve Equation

Finally, define the interval of integration $[t_0 \ t_f]$ and solve the DDE using the ddensd solver.

```
tspan = [0 pi];
sol = ddensd(@ddefun, @dely, @delyp, @history, [0,pi]);
```

Plot Solution

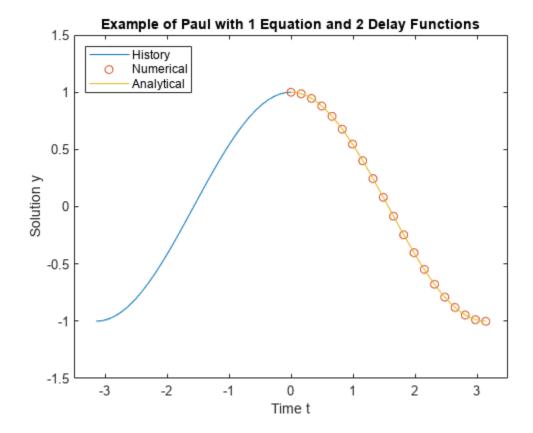
The solution structure sol has the fields sol.x and sol.y that contain the internal time steps taken by the solver and corresponding solutions at those times. However, you can use deval to evaluate the solution at the specific points.

Evaluate the solution at 20 equally spaced points between 0 and pi.

```
tn = linspace(0,pi,20);
yn = deval(sol,tn);
```

Plot the calculated solution and history against the analytical solution.

```
th = linspace(-pi,0);
yh = history(th);
ta = linspace(0,pi);
ya = cos(ta);
plot(th,yh,tn,yn,'o',ta,ya)
legend('History','Numerical','Analytical','Location','NorthWest')
xlabel('Time t')
ylabel('Solution y')
title('Example of Paul with 1 Equation and 2 Delay Functions')
axis([-3.5 3.5 -1.5 1.5])
```



Local Functions

Listed here are the local helper functions that the DDE solver ddensd calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

References

[1] Paul, C.A.H. "A Test Set of Functional Differential Equations." Numerical Analysis Reports. No. 243. Manchester, UK: Math Department, University of Manchester, 1994.

See Also

ddensd | ddesd | dde23 | deval

- "Solving Delay Differential Equations" on page 14-2
- "Initial Value DDE of Neutral Type" on page 14-23

Initial Value DDE of Neutral Type

This example shows how to use ddensd to solve a system of initial value DDEs (delay differential equations) with time-dependent delays. The example was originally presented by Jackiewicz [1].

The equation is

$$y'(t) = 2\cos(2t)y\left(\frac{t}{2}\right)^{2\cos(t)} + \log\left(y'\left(\frac{t}{2}\right)\right) - \log(2\cos(t)) - \sin(t).$$

This equation is an *initial value* DDE because the time delays are zero at t_0 . Therefore, a solution history is unnecessary to calculate a solution, only the initial values are needed:

$$y(0)=1,$$

$$y'(0) = s$$
.

s is the solution of $2 + \log(s) - \log(2) = 0$. The values of s that satisfy this equation are $s_1 = 2$ and $s_2 = 0.4063757399599599$.

Since the time delays in the equations are present in a y' term, this equation is called a *neutral DDE*.

To solve this equation in MATLAB®, you need to code the equation and delays before calling the delay differential equation solver ddensd, which is the solver for neutral equations. You either can include the required functions as local functions at the end of a file (as done here), or save them as separate files in a directory on the MATLAB path.

Code Delays

First, write an anonymous function to define the delays in the equation. Since both y and y' have delays of the form $\frac{t}{2}$, only one function definition is required. This delay function is later passed to the solver twice, once to indicate the delay for y and once for y'.

$$delay = @(t,y) t/2;$$

Code Equation

Now, create a function to code the equation. This function should have the signature yp = ddefun(t,y,ydel,ypdel), where:

- t is time (independent variable).
- y is the solution (dependent variable).
- ydel contains the delays for y.
- ypdel contains the delays for $y' = \frac{dy}{dt}$.

These inputs are automatically passed to the function by the solver, but the variable names determine how you code the equation. In this case:

- ydel $\rightarrow y(\frac{t}{2})$
- ypdel $\rightarrow y'\left(\frac{t}{2}\right)$

```
function yp = ddefun(t,y,ydel,ypdel)
   yp = 2*cos(2*t)*ydel^(2*cos(t)) + log(ypdel) - log(2*cos(t)) - sin(t);
end
```

Note: All functions are included as local functions at the end of the example.

Solve Equation

Finally, define the interval of integration $[t_0, t_f]$ and the initial values, and then solve the DDE using the ddensd solver. Pass the initial values to the solver by specifying them in a cell array in the fourth input argument.

```
tspan = [0 \ 0.1];
y0 = 1;
s1 = 2;
sol1 = ddensd(@ddefun, delay, delay, {y0,s1}, tspan);
```

Solve the equation a second time, this time using the alternate value of s for the initial condition.

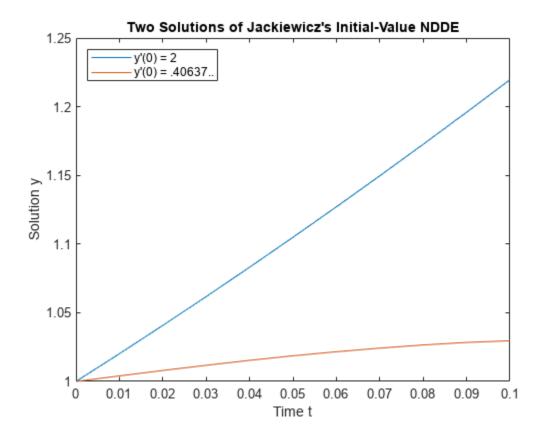
```
s2 = 0.4063757399599599;
sol2 = ddensd(@ddefun, delay, delay, {y0,s2}, tspan);
```

Plot Solution

The solution structures sol1 and sol2 have the fields x and y that contain the internal time steps taken by the solver and corresponding solutions at those times. However, you can use deval to evaluate the solution at the specific points.

Plot the two solutions to compare results.

```
plot(sol1.x,sol1.y,sol2.x,sol2.y);
legend('y''(0) = 2','y''(0) = .40637...','Location','NorthWest');
xlabel('Time t');
ylabel('Solution y');
title('Two Solutions of Jackiewicz''s Initial-Value NDDE');
```



Local Functions

Listed here are the local helper functions that the DDE solver ddensd calls to calculate the solution. Alternatively, you can save these functions as their own files in a directory on the MATLAB path.

```
function yp = ddefun(t,y,ydel,ypdel)
  yp = 2*\cos(2*t)*ydel^(2*\cos(t)) + \log(ypdel) - \log(2*\cos(t)) - \sin(t);
end
```

References

[1] Jackiewicz, Z. "One step Methods of any Order for Neutral Functional Differential Equations." *SIAM Journal on Numerical Analysis*. Vol. 21, Number 3. 1984. pp. 486-511.

See Also

ddensd | ddesd | dde23 | deval

- "Solving Delay Differential Equations" on page 14-2
- "DDE of Neutral Type" on page 14-19

Numerical Integration

- "Integration to Find Arc Length" on page 15-2
- "Complex Line Integrals" on page 15-3
- "Singularity on Interior of Integration Domain" on page 15-5
- "Analytic Solution to Integral of Polynomial" on page 15-7
- "Integration of Numeric Data" on page 15-8
- "Calculate Tangent Plane to Surface" on page 15-12

Integration to Find Arc Length

This example shows how to parametrize a curve and compute the arc length using integral.

Consider the curve parameterized by the equations

$$x(t) = \sin(2t), \ y(t) = \cos(t), \ z(t) = t,$$
 where $t \in [0,3\pi].$

Create a three-dimensional plot of this curve.

```
t = 0:0.1:3*pi;
plot3(sin(2*t),cos(t),t)
```

The arc length formula says the length of the curve is the integral of the norm of the derivatives of the parameterized equations.

$$\int_{0}^{3\pi} \sqrt{4\cos^{2}(2t) + \sin^{2}(t) + 1} dt.$$

Define the integrand as an anonymous function.

Integrate this function with a call to integral.

```
len = integral(f,0,3*pi)
len =
    17.2220
```

The length of this curve is about 17.2.

See Also

integral

- "Create Function Handle"
- "Singularity on Interior of Integration Domain" on page 15-5
- "Integration of Numeric Data" on page 15-8

Complex Line Integrals

This example shows how to calculate complex line integrals using the 'Waypoints' option of the integral function. In MATLAB®, you use the 'Waypoints' option to define a sequence of straight line paths from the first limit of integration to the first waypoint, from the first waypoint to the second, and so forth, and finally from the last waypoint to the second limit of integration.

Define the Integrand with an Anonymous Function

Integrate

$$\oint_C \frac{e^z}{z} dz$$

where C is a closed contour that encloses the simple pole of e^{z}/z at the origin.

Define the integrand with an anonymous function.

```
fun = @(z) exp(z)./z;
```

Integrate Without Using Waypoints

You can evaluate contour integrals of complex-valued functions with a parameterization. In general, a contour is specified, and then differentiated and used to parameterize the original integrand. In this case, specify the contour as the unit circle, but in all cases, the result is independent of the contour chosen.

```
g = @(theta) cos(theta) + 1i*sin(theta);
gprime = @(theta) -sin(theta) + 1i*cos(theta);
q1 = integral(@(t) fun(g(t)).*gprime(t),0,2*pi)
g1 = -0.0000 + 6.2832i
```

This method of parameterizing, although reliable, can be difficult and time consuming since a derivative must be calculated before the integration is performed. Even for simple functions, you need to write several lines of code to obtain the correct result. Since the result is the same with any closed contour that encloses the pole (in this case, the origin), instead you can use the 'Waypoints' option of integral to construct a square or triangular path that encloses the pole.

Integrate Along a Contour That Encloses No Poles

If any limit of integration or element of the waypoints vector is complex, then integral performs the integration over a sequence of straight line paths in the complex plane. The natural direction around a contour is counterclockwise; specifying a clockwise contour is akin to multiplying by -1. Specify the contour in such a way that it encloses a single functional singularity. If you specify a contour that encloses no poles, then Cauchy's integral theorem guarantees that the value of the closed-loop integral is zero.

To see this, integrate fun around a square contour away from the origin. Use equal limits of integration to form a closed contour.

```
C = [2+i 2+2i 1+2i];
q = integral(fun,1+i,1+i,'Waypoints',C)
q = -3.6082e-16 + 6.6613e-16i
```

The result is on the order of eps and effectively zero.

Integrate Along a Contour with a Pole in the Interior

Specify a square contour that completely encloses the pole at the origin, and then integrate.

```
C = [1+i -1+i -1-i 1-i];
q2 = integral(fun,1,1,'Waypoints',C)

q2 = 0.0000 + 6.2832i
```

This result agrees with the q1 calculated above, but uses much simpler code.

The exact answer for this problem is $2\pi i$.

```
2*pi*i
ans = 0.0000 + 6.2832i
```

See Also

integral

- "Create Function Handle"
- "Singularity on Interior of Integration Domain" on page 15-5
- "Integration of Numeric Data" on page 15-8

Singularity on Interior of Integration Domain

This example shows how to split the integration domain to place a singularity on the boundary.

Define the Integrand with an Anonymous Function

The integrand of the complex-valued integral

$$\int_{-1}^{1} \int_{-1}^{1} \frac{1}{\sqrt{x+y}} \, dx \, dy$$

has a singularity when x = y = 0 and is, in general, singular on the line y = -x.

Define this integrand with an anonymous function.

fun =
$$@(x,y) ((x+y).^{(-1/2)});$$

Integrate over a Square

Integrate fun over a square domain specified by $-1 \le x \le 1$ and $-1 \le y \le 1$.

```
format long q = integral2(fun, -1, 1, -1, 1) Warning: Non-finite result. The integration was unsuccessful. Singularity likely. q = \frac{NaN + NaNi}{NaN}
```

If there are singular values in the interior of the integration region, the integration fails to converge and returns a warning.

Split the Integration Domain into Two Triangles

You can redefine the integral by splitting the integration domain into complementary pieces and adding the smaller integrations together. Avoid integration errors and warnings by placing singularities on the boundary of the domain. In this case, you can split the square integration region into two triangles along the singular line y = -x and add the results.

```
q1 = integral2(fun,-1,1,-1,@(x)-x);
q2 = integral2(fun,-1,1,@(x)-x,1);
q = q1 + q2

q =
   3.771236166328258 - 3.771236166328255i
```

The integration succeeds when the singular values are on the boundary.

The exact value of this integral is

$$\frac{8\sqrt{2}}{3}(1-i)$$

$$8/3*sqrt(2)*(1-i)$$

```
ans =
  3.771236166328253 \ - \ 3.771236166328253 i
```

See Also

integral | integral2 | integral3

- "Create Function Handle"
- "Complex Line Integrals" on page 15-3
- "Integration of Numeric Data" on page 15-8

Analytic Solution to Integral of Polynomial

This example shows how to use the polyint function to integrate polynomial expressions analytically. Use this function to evaluate indefinite integral expressions of polynomials.

Define the Problem

Consider the real-valued indefinite integral,

$$\int \left(4x^5 - 2x^3 + x + 4\right) dx$$

The integrand is a polynomial, and the analytic solution is

$$\frac{2}{3}x^6 - \frac{1}{2}x^4 + \frac{1}{2}x^2 + 4x + k$$

where k is the constant of integration. Since the limits of integration are unspecified, the integral function family is not well-suited to solving this problem.

Express the Polynomial with a Vector

Create a vector whose elements represent the coefficients for each descending power of *x*.

$$p = [4 \ 0 \ -2 \ 0 \ 1 \ 4];$$

Integrate the Polynomial Analytically

Integrate the polynomial analytically using the polyint function. Specify the constant of integration with the second input argument.

The output is a vector of coefficients for descending powers of x. This result matches the analytic solution above, but has a constant of integration k = 2.

See Also

polyint | polyval

- "Singularity on Interior of Integration Domain" on page 15-5
- "Integration of Numeric Data" on page 15-8

Integration of Numeric Data

This example shows how to integrate a set of discrete velocity data numerically to approximate the distance traveled. The integral family only accepts function handles as inputs, so those functions cannot be used with discrete data sets. Use trapz or cumtrapz when a functional expression is not available for integration.

View the Velocity Data

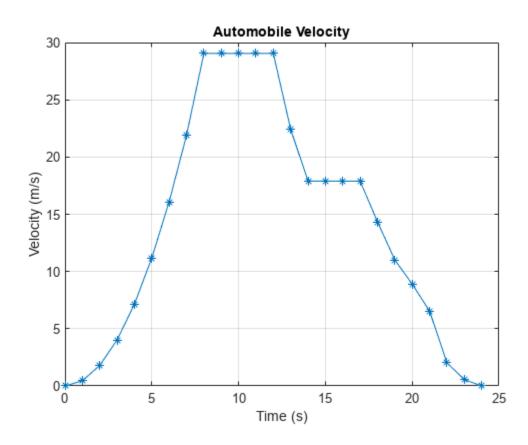
Consider the following velocity data and corresponding time data.

```
vel = [0 .45 1.79 4.02 7.15 11.18 16.09 21.90 29.05 29.05 ...
29.05 29.05 29.05 22.42 17.9 17.9 17.9 17.9 14.34 11.01 ...
8.9 6.54 2.03 0.55 0];
time = 0:24;
```

This data represents the velocity of an automobile (in m/s) taken at 1 s intervals over 24 s.

Plot the velocity data points and connect each point with a straight line.

```
figure
plot(time,vel,'-*')
grid on
title('Automobile Velocity')
xlabel('Time (s)')
ylabel('Velocity (m/s)')
```

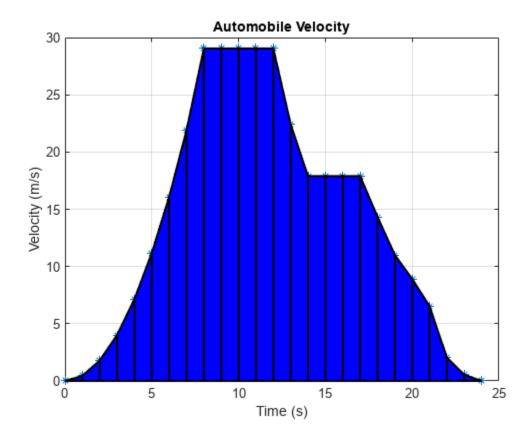


The slope is positive during periods of acceleration, zero during periods of constant velocity, and negative during periods of deceleration. At time t=0, the vehicle is at rest with vel(1)=0 m/s. The vehicle accelerates until reaching a maximum velocity at t=8 s of vel(9)=29.05 m/s and maintains this velocity for 4 s. It then decelerates to vel(14)=17.9 m/s for 3 s and eventually back down to rest. Since this velocity curve has multiple discontinuities, a single continuous function cannot describe it.

Calculate the Total Distance Traveled

trapz performs discrete integration by using the data points to create trapezoids, so it is well suited to handling data sets with discontinuities. This method assumes linear behavior between the data points, and accuracy may be reduced when the behavior between data points is nonlinear. To illustrate, you can draw trapezoids onto the graph using the data points as vertices.

```
xverts = [time(1:end-1); time(1:end-1); time(2:end); time(2:end)];
yverts = [zeros(1,24); vel(1:end-1); vel(2:end); zeros(1,24)];
p = patch(xverts, yverts, 'b', 'LineWidth', 1.5);
```



trapz calculates the area under a set of discrete data by breaking the region into trapezoids. The function then adds the area of each trapezoid to compute the total area.

Calculate the total distance traveled by the automobile (corresponding to the shaded area) by integrating the velocity data numerically using trapz. By default, the spacing between points is assumed to be 1 if you use the syntax trapz(Y). However, you can specify a different uniform or nonuniform spacing X with the syntax trapz(X,Y). In this case, the spacing between readings in the time vector is 1, so it is acceptable to use the default spacing.

```
distance = trapz(vel)
distance = 345.2200
```

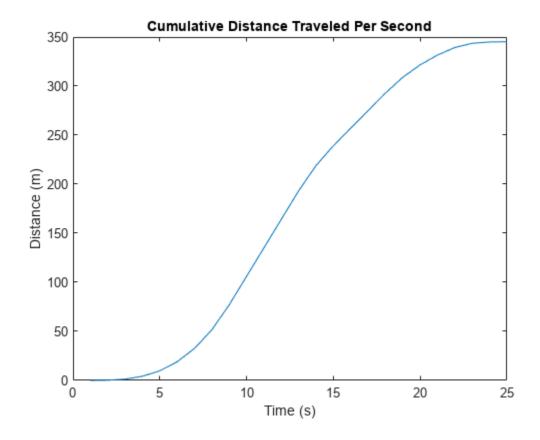
The distance traveled by the automobile in t = 24 s is about 345.22 m.

Plot Cumulative Distance Traveled

The cumtrapz function is closely related to trapz. While trapz returns only the final integration value, cumtrapz also returns intermediate values in a vector.

Calculate the cumulative distance traveled and plot the result.

```
cdistance = cumtrapz(vel);
T = table(time',cdistance','VariableNames',{'Time','CumulativeDistance'})
T=25×2 table
   Time
            CumulativeDistance
      0
                       0
                   0.225
      1
      2
                   1.345
      3
                   4.25
      4
                   9.835
      5
                      19
      6
                  32.635
      7
                  51.63
      8
                  77.105
      9
                  106.15
     10
                  135.2
     11
                  164.25
    12
                  193.31
    13
                  219.04
    14
                   239.2
    15
                   257.1
plot(cdistance)
title('Cumulative Distance Traveled Per Second')
xlabel('Time (s)')
ylabel('Distance (m)')
```



See Also trapz | cumtrapz | integral

- "Singularity on Interior of Integration Domain" on page 15-5
- "Analytic Solution to Integral of Polynomial" on page 15-7

Calculate Tangent Plane to Surface

This example shows how to approximate gradients of a function by finite differences. It then shows how to plot a tangent plane to a point on the surface by using these approximated gradients.

Create the function $f(x, y) = x^2 + y^2$ using a function handle.

```
f = @(x,y) x.^2 + y.^2;
```

Approximate the partial derivatives of f(x, y) with respect to x and y by using the gradient function. Choose a finite difference length that is the same as the mesh size.

```
[xx,yy] = meshgrid(-5:0.25:5);
[fx,fy] = gradient(f(xx,yy),0.25);
```

The tangent plane to a point on the surface, $P = (x_0, y_0, f(x_0, y_0))$, is given by

$$z=f(x_0,y_0)+\frac{\partial f(x_0,y_0)}{\partial x}(x-x_0)+\frac{\partial f(x_0,y_0)}{\partial y}(y-y_0)\,.$$

The fx and fy matrices are approximations to the partial derivatives $\frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial y}$. The point of interest in this example, where the tangent plane meets the functional surface, is (x0,y0) = (1,2). The function value at this point of interest is f(1,2) = 5.

To approximate the tangent plane z you need to find the value of the derivatives at the point of interest. Obtain the index of that point, and find the approximate derivatives there.

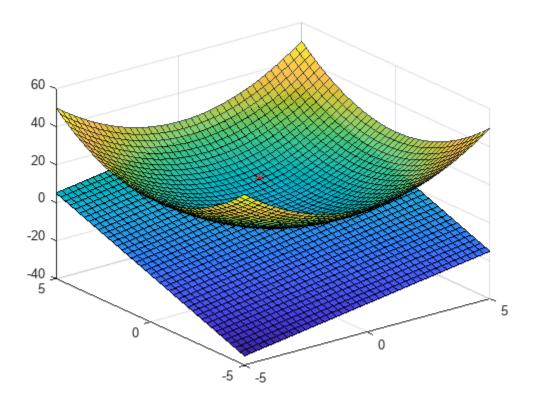
```
x0 = 1;
y0 = 2;
t = (xx == x0) & (yy == y0);
indt = find(t);
fx0 = fx(indt);
fy0 = fy(indt);
```

Create a function handle with the equation of the tangent plane z.

```
z = @(x,y) f(x0,y0) + fx0*(x-x0) + fy0*(y-y0);
```

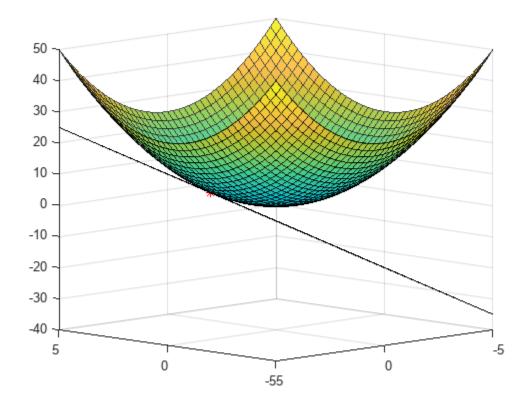
Plot the original function f(x, y), the point P, and a piece of plane z that is tangent to the function at P.

```
surf(xx,yy,f(xx,yy),'EdgeAlpha',0.7,'FaceAlpha',0.9)
hold on
surf(xx,yy,z(xx,yy))
plot3(1,2,f(1,2),'r*')
```



View a side profile.

view(-135,9)



See Also gradient

More About

"Create Function Handle"

Fourier Transforms

- "Fourier Transforms" on page 16-2
- "Basic Spectral Analysis" on page 16-10
- "Polynomial Interpolation Using FFT" on page 16-16
- "2-D Fourier Transforms" on page 16-19
- "Square Wave from Sine Waves" on page 16-23
- "Analyzing Cyclical Data with FFT" on page 16-28

Fourier Transforms

The Fourier transform is a mathematical formula that transforms a signal sampled in time or space to the same signal sampled in temporal or spatial frequency. In signal processing, the Fourier transform can reveal important characteristics of a signal, namely, its frequency components.

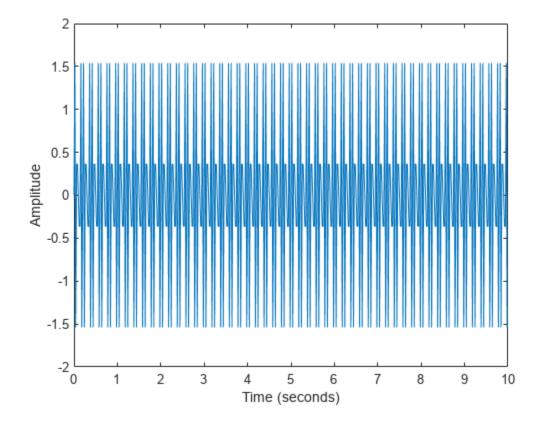
The Fourier transform is defined for a vector *x* with *n* uniformly sampled points by

$$y_{k+1} = \sum_{j=0}^{n-1} \omega^{jk} x_{j+1}.$$

 $\omega = e^{-2\pi i/n}$ is one of the *n* complex roots of unity where *i* is the imaginary unit. For *x* and *y*, the indices *j* and *k* range from 0 to n-1.

The fft function in MATLAB® uses a fast Fourier transform algorithm to compute the Fourier transform of data. Consider a sinusoidal signal x that is a function of time t with frequency components of 15 Hz and 20 Hz. Use a time vector sampled in increments of 1/50 seconds over a period of 10 seconds.

```
Ts = 1/50;
t = 0:Ts:10-Ts;
x = sin(2*pi*15*t) + sin(2*pi*20*t);
plot(t,x)
xlabel('Time (seconds)')
ylabel('Amplitude')
```

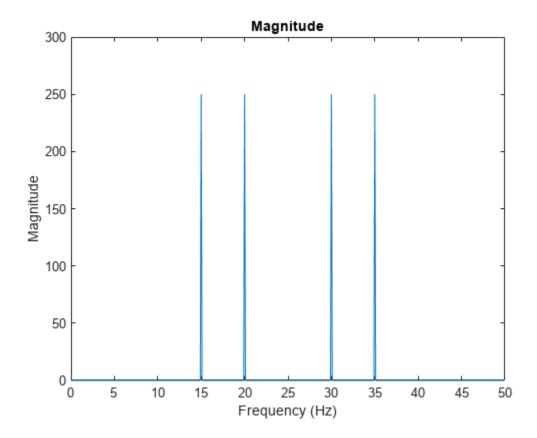


Compute the Fourier transform of the signal, and create the vector **f** that corresponds to the signal's sampling in frequency space.

```
y = fft(x);
fs = 1/Ts;
f = (0:length(y)-1)*fs/length(y);
```

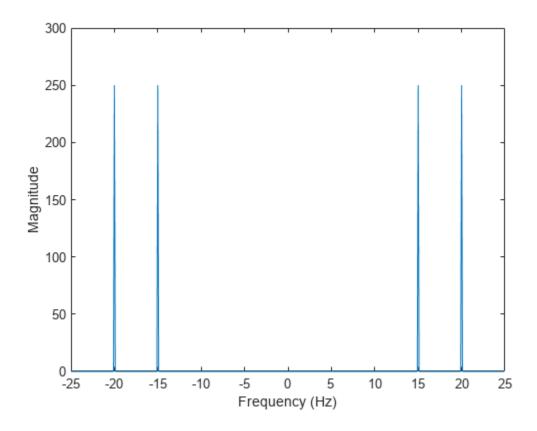
When you plot the magnitude of the signal as a function of frequency, the spikes in magnitude correspond to the signal's frequency components of 15 Hz and 20 Hz.

```
plot(f,abs(y))
xlabel('Frequency (Hz)')
ylabel('Magnitude')
title('Magnitude')
```



The transform also produces a mirror copy of the spikes, which correspond to the signal's negative frequencies. To better visualize this periodicity, you can use the fftshift function, which performs a zero-centered, circular shift on the transform.

```
n = length(x);
fshift = (-n/2:n/2-1)*(fs/n);
yshift = fftshift(y);
plot(fshift,abs(yshift))
xlabel('Frequency (Hz)')
ylabel('Magnitude')
```



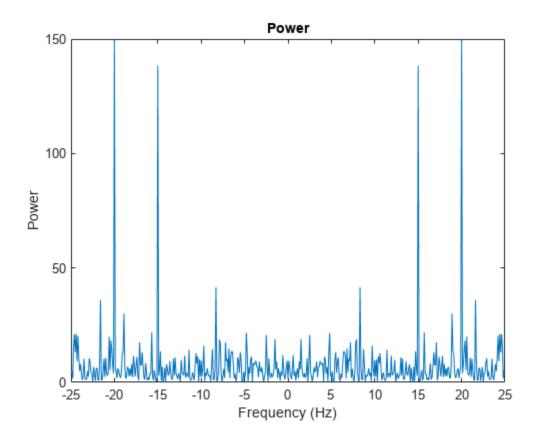
Noisy Signals

In scientific applications, signals are often corrupted with random noise, disguising their frequency components. The Fourier transform can process out random noise and reveal the frequencies. For example, create a new signal, xnoise, by injecting Gaussian noise into the original signal, x.

```
rng('default')
xnoise = x + 2.5*randn(size(t));
```

Signal power as a function of frequency is a common metric used in signal processing. Power is the squared magnitude of a signal's Fourier transform, normalized by the number of frequency samples. Compute and plot the power spectrum of the noisy signal centered at the zero frequency. Despite noise, you can still make out the signal's frequencies due to the spikes in power.

```
ynoise = fft(xnoise);
ynoiseshift = fftshift(ynoise);
power = abs(ynoiseshift).^2/n;
plot(fshift,power)
title('Power')
xlabel('Frequency (Hz)')
ylabel('Power')
```

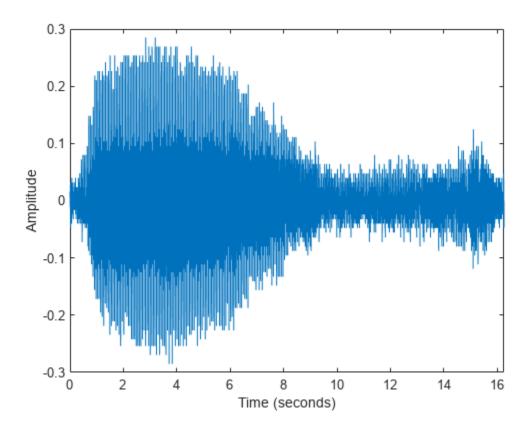


Computational Efficiency

Using the Fourier transform formula directly to compute each of the n elements of y requires on the order of n^2 floating-point operations. The fast Fourier transform algorithm requires only on the order of $n \log n$ operations to compute. This computational efficiency is a big advantage when processing data that has millions of data points. Many specialized implementations of the fast Fourier transform algorithm are even more efficient when n has small prime factors, such as n is a power of n.

Consider audio data collected from underwater microphones off the coast of California. This data can be found in a library maintained by the Cornell University Bioacoustics Research Program. Load and format a subset of the data in bluewhale.au, which contains a Pacific blue whale vocalization. Because blue whale calls are low-frequency sounds, they are barely audible to humans. The time scale in the data is compressed by a factor of 10 to raise the pitch and make the call more clearly audible. You can use the command sound(x,fs) to listen to the entire audio file.

```
whaleFile = 'bluewhale.au';
[x,fs] = audioread(whaleFile);
whaleMoan = x(2.45e4:3.10e4);
t = 10*(0:1/fs:(length(whaleMoan)-1)/fs);
plot(t,whaleMoan)
xlabel('Time (seconds)')
ylabel('Amplitude')
xlim([0 t(end)])
```

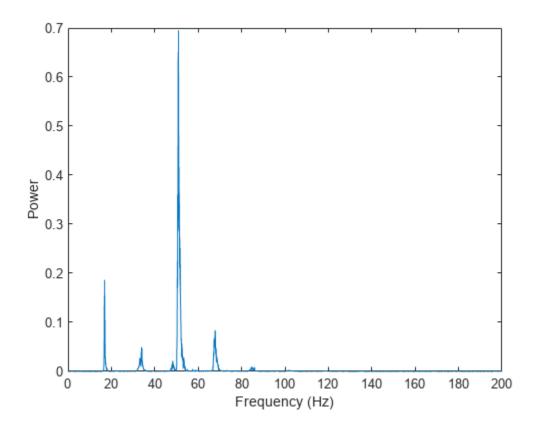


Specify a new signal length that is the next power of 2 greater than the original length. Then, use fft to compute the Fourier transform using the new signal length. fft automatically pads the data with zeros to increase the sample size. This padding can make the transform computation significantly faster, particularly for sample sizes with large prime factors.

```
m = length(whaleMoan);
n = pow2(nextpow2(m));
y = fft(whaleMoan,n);
```

Plot the power spectrum of the signal. The plot indicates that the moan consists of a fundamental frequency around 17 Hz and a sequence of harmonics, where the second harmonic is emphasized.

```
f = (0:n-1)*(fs/n)/10; % frequency vector
power = abs(y).^2/n; % power spectrum
plot(f(1:floor(n/2)),power(1:floor(n/2)))
xlabel('Frequency (Hz)')
ylabel('Power')
```



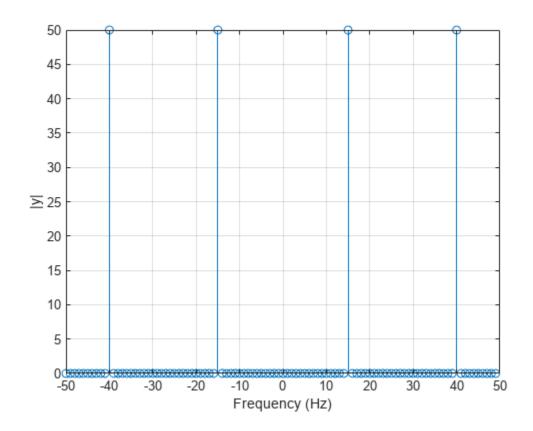
Phase of Sinusoids

Using the Fourier transform, you can also extract the phase spectrum of the original signal. For example, create a signal that consists of two sinusoids of frequencies 15 Hz and 40 Hz. The first sinusoid is a cosine wave with phase $-\pi/4$, and the second is a cosine wave with phase $\pi/2$. Sample the signal at 100 Hz for 1 second.

```
fs = 100;
t = 0:1/fs:1-1/fs;
x = cos(2*pi*15*t - pi/4) - sin(2*pi*40*t);
```

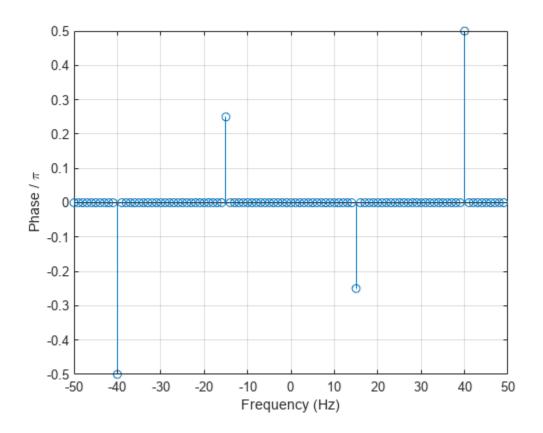
Compute the Fourier transform of the signal. Plot the magnitude of the transform as a function of frequency.

```
y = fft(x);
z = fftshift(y);
ly = length(y);
f = (-ly/2:ly/2-1)/ly*fs;
stem(f,abs(z))
xlabel("Frequency (Hz)")
ylabel("|y|")
grid
```



Compute the phase of the transform, removing small-magnitude transform values. Plot the phase as a function of frequency.

```
tol = 1e-6;
z(abs(z) < tol) = 0;
theta = angle(z);
stem(f,theta/pi)
xlabel("Frequency (Hz)")
ylabel("Phase / \pi")
grid
```



See Also

fft|fftshift|nextpow2|ifft|fft2|fftn|fftw

Related Examples

• "2-D Fourier Transforms" on page 16-19

External Websites

• Fourier Analysis (MathWorks Teaching Resources)

Basic Spectral Analysis

The Fourier transform is a tool for performing frequency and power spectrum analysis of time-domain signals.

Spectral Analysis Quantities

Spectral analysis studies the frequency spectrum contained in discrete, uniformly sampled data. The Fourier transform is a tool that reveals frequency components of a time- or space-based signal by representing it in frequency space. The following table lists common quantities used to characterize and interpret signal properties. To learn more about the Fourier transform, see "Fourier Transforms" on page 16-2.

Quantity	Description
х	Sampled data
n = length(x)	Number of samples
fs	Sample frequency (samples per unit time or space)
dt = 1/fs	Time or space increment per sample
t = (0:n-1)/fs	Time or space range for data
y = fft(x)	Discrete Fourier transform of data (DFT)
abs(y)	Amplitude of the DFT
(abs(y).^2)/n	Power of the DFT
fs/n	Frequency increment
f = (0:n-1)*(fs/n)	Frequency range
fs/2	Nyquist frequency (midpoint of frequency range)

Noisy Signal

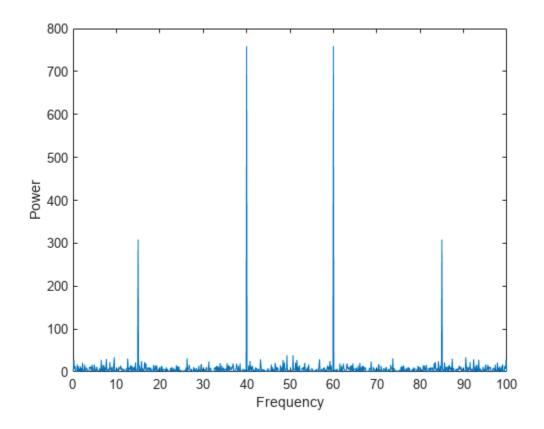
The Fourier transform can compute the frequency components of a signal that is corrupted by random noise.

Create a signal with component frequencies at 15 Hz and 40 Hz, and inject random Gaussian noise.

The Fourier transform of the signal identifies its frequency components. In MATLAB®, the fft function computes the Fourier transform using a fast Fourier transform algorithm. Use fft to compute the discrete Fourier transform of the signal.

```
y = fft(x);
```

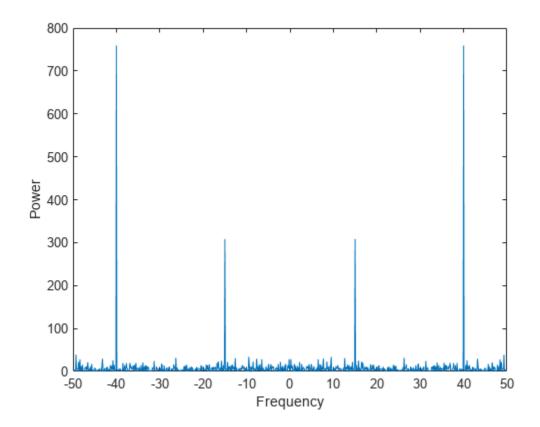
Plot the power spectrum as a function of frequency. While noise disguises a signal's frequency components in time-based space, the Fourier transform reveals them as spikes in power.



In many applications, it is more convenient to view the power spectrum centered at 0 frequency because it better represents the signal's periodicity. Use the fftshift function to perform a circular shift on y, and plot the 0-centered power.

```
y0 = fftshift(y); % shift y values
f0 = (-n/2:n/2-1)*(fs/n); % 0-centered frequency range
power0 = abs(y0).^2/n; % 0-centered power

plot(f0,power0)
xlabel('Frequency')
ylabel('Power')
```



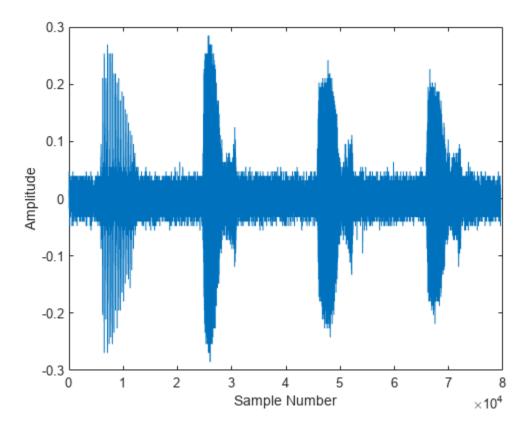
Audio Signal

You can use the Fourier transform to analyze the frequency spectrum of audio data.

The file bluewhale.au contains audio data from a Pacific blue whale vocalization recorded by underwater microphones off the coast of California. The file is from the library of animal vocalizations maintained by the Cornell University Bioacoustics Research Program.

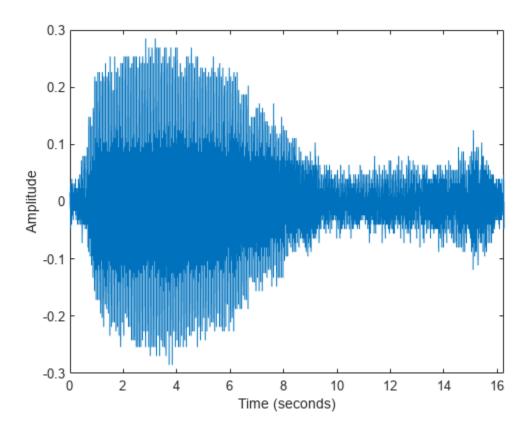
Because blue whale calls are so low, they are barely audible to humans. The time scale in the data is compressed by a factor of 10 to raise the pitch and make the call more clearly audible. Read and plot the audio data. You can use the command sound(x, fs) to listen to the audio.

```
whaleFile = 'bluewhale.au';
[x,fs] = audioread(whaleFile);
plot(x)
xlabel('Sample Number')
ylabel('Amplitude')
```



The first sound is a "trill" followed by three "moans". This example analyzes a single moan. Specify new data that approximately consists of the first moan, and correct the time data to account for the factor-of-10 speed-up. Plot the truncated signal as a function of time.

```
moan = x(2.45e4:3.10e4);
t = 10*(0:1/fs:(length(moan)-1)/fs);
plot(t,moan)
xlabel('Time (seconds)')
ylabel('Amplitude')
xlim([0 t(end)])
```



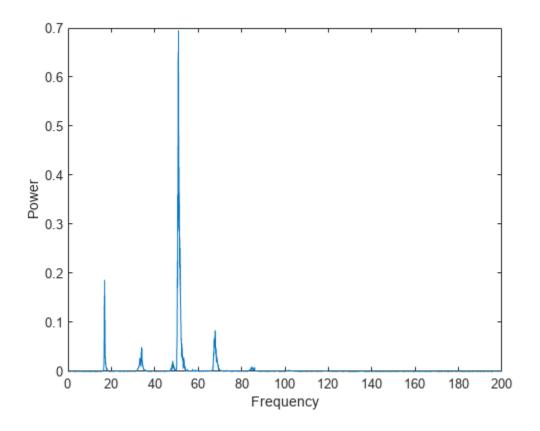
The Fourier transform of the data identifies frequency components of the audio signal. In some applications that process large amounts of data with fft, it is common to resize the input so that the number of samples is a power of 2. This can make the transform computation significantly faster, particularly for sample sizes with large prime factors. Specify a new signal length n that is a power of 2, and use the fft function to compute the discrete Fourier transform of the signal. fft automatically pads the original data with zeros to increase the sample size.

```
m = length(moan); % original sample length
n = pow2(nextpow2(m)); % transform length
y = fft(moan,n); % DFT of signal
```

Adjust the frequency range due to the speed-up factor, and compute and plot the power spectrum of the signal. The plot indicates that the moan consists of a fundamental frequency around 17 Hz and a sequence of harmonics, where the second harmonic is emphasized.

```
f = (0:n-1)*(fs/n)/10;
power = abs(y).^2/n;

plot(f(1:floor(n/2)),power(1:floor(n/2)))
xlabel('Frequency')
ylabel('Power')
```



See Also fft | fftshift | nextpow2 | ifft | fft2 | fftn

Related Examples

- "Fourier Transforms" on page 16-2
- "2-D Fourier Transforms" on page 16-19

Polynomial Interpolation Using FFT

Use the fast Fourier transform (FFT) to estimate the coefficients of a trigonometric polynomial that interpolates a set of data.

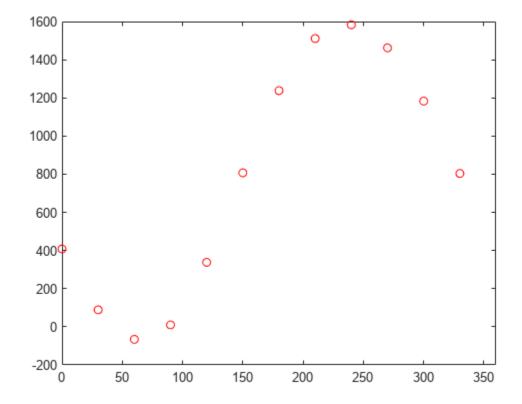
FFT in Mathematics

The FFT algorithm is associated with applications in signal processing, but it can also be used more generally as a fast computational tool in mathematics. For example, coefficients c_i of an nth degree polynomial $c_1x^n + c_2x^{n-1} + ... + c_nx + c_{n+1}$ that interpolates a set of data are commonly computed by solving a straightforward system of linear equations. While studying asteroid orbits in the early 19th century, Carl Friedrich Gauss discovered a mathematical shortcut for computing the coefficients of a polynomial interpolant by splitting the problem up into smaller subproblems and combining the results. His method was equivalent to estimating the discrete Fourier transform of his data.

Interpolate Asteroid Data

In a paper by Gauss, he describes an approach to estimating the orbit of the Pallas asteroid. He starts with the following twelve 2-D positional data points x and y.

```
x = 0:30:330;
y = [408 89 -66 10 338 807 1238 1511 1583 1462 1183 804];
plot(x,y,'ro')
xlim([0 360])
```



Gauss models the asteroid's orbit with a trigonometric polynomial of the following form.

```
y = a_0 + a_1 \cos(2\pi(x/360)) + b_1 \sin(2\pi(x/360))
a_2 \cos(2\pi(2x/360)) + b_2 \sin(2\pi(2x/360))
...
a_5 \cos(2\pi(5x/360)) + b_5 \sin(2\pi(5x/360))
a_6 \cos(2\pi(6x/360))
```

Use fft to compute the coefficients of the polynomial.

```
m = length(y);
n = floor((m+1)/2);
z = fft(y)/m;
a0 = z(1);
an = 2*real(z(2:n));
a6 = z(n+1);
bn = -2*imag(z(2:n));
```

Plot the interpolating polynomial over the original data points.

```
hold on

px = 0:0.01:360;

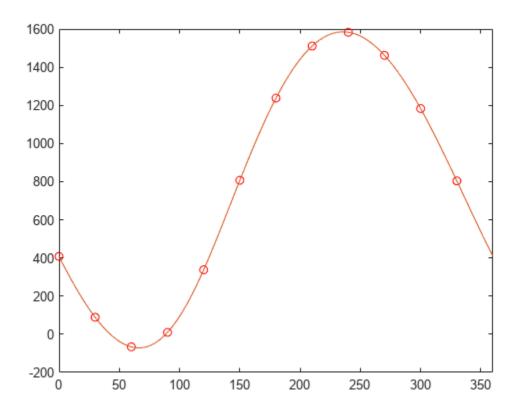
k = 1:length(an);

py = a0 + an*cos(2*pi*k'*px/360) ...

+ bn*sin(2*pi*k'*px/360) ...

+ a6*cos(2*pi*6*px/360);

plot(px,py)
```



References

- [1] Briggs, W. and V.E. Henson. *The DFT: An Owner's Manual for the Discrete Fourier Transform*. Philadelphia: SIAM, 1995.
- [2] Gauss, C. F. "Theoria interpolationis methodo nova tractata." *Carl Friedrich Gauss Werke*. Band 3. Göttingen: Königlichen Gesellschaft der Wissenschaften, 1866.
- [3] Heideman M., D. Johnson, and C. Burrus. "Gauss and the History of the Fast Fourier Transform." *Arch. Hist. Exact Sciences*. Vol. 34. 1985, pp. 265–277.
- [4] Goldstine, H. H. A History of Numerical Analysis from the 16th through the 19th Century. Berlin: Springer-Verlag, 1977.

See Also

fft

Related Examples

• "Fourier Transforms" on page 16-2

2-D Fourier Transforms

The fft2 function transforms 2-D data into frequency space. For example, you can transform a 2-D optical mask to reveal its diffraction pattern.

Two-Dimensional Fourier Transform

The following formula defines the discrete Fourier transform Y of an m-by-n matrix X.

$$Y_{p+1,q+1} = \sum_{j=0}^{m-1} \sum_{k=0}^{n-1} \omega_m^{jp} \omega_n^{kq} X_{j+1,k+1}$$

 ω_m and ω_n are complex roots of unity defined by the following equations.

$$\omega_m = e^{-2\pi i/m}$$
$$\omega_n = e^{-2\pi i/n}$$

i is the imaginary unit, p and j are indices that run from 0 to m-1, and q and k are indices that run from 0 to m-1. The indices for X and Y are shifted by 1 in this formula to reflect matrix indices in MATLAB.

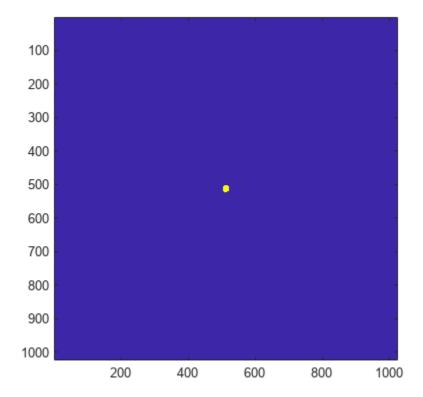
Computing the 2-D Fourier transform of X is equivalent to first computing the 1-D transform of each column of X, and then taking the 1-D transform of each row of the result. In other words, the command fft2(X) is equivalent to Y = fft(fft(X).').'.

2-D Diffraction Pattern

In optics, the Fourier transform can be used to describe the diffraction pattern produced by a plane wave incident on an optical mask with a small aperture [1]. This example uses the fft2 function on an optical mask to compute its diffraction pattern.

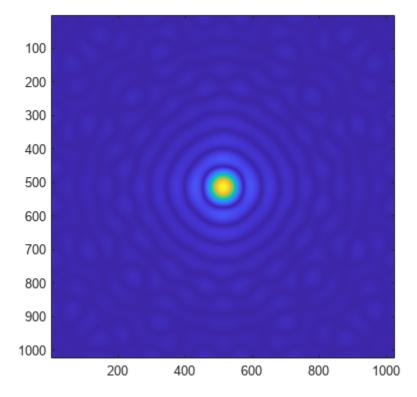
Create a logical array that defines an optical mask with a small, circular aperture.

```
n = 2^10;
                          % size of mask
M = zeros(n);
I = 1:n;
x = I - n/2;
                          % mask x-coordinates
y = n/2-I;
                          % mask y-coordinates
[X,Y] = meshgrid(x,y); % create 2-D mask grid
                         % aperture radius
R = 10;
A = (X.^2 + Y.^2 \le R^2); % circular aperture of radius R
M(A) = 1;
                          % set mask elements inside aperture to 1
imagesc(M)
                          % plot mask
axis image
```



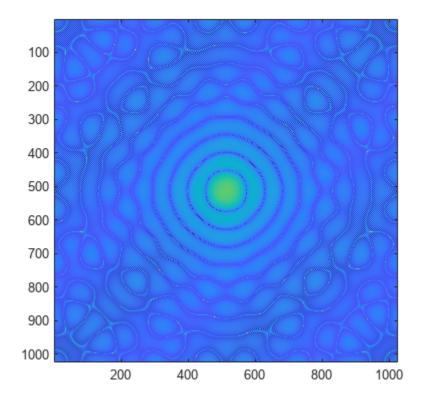
Use fft2 to compute the 2-D Fourier transform of the mask, and use the fftshift function to rearrange the output so that the zero-frequency component is at the center. Plot the resulting diffraction pattern frequencies. Blue indicates small amplitudes and yellow indicates large amplitudes.

```
DP = fftshift(fft2(M));
imagesc(abs(DP))
axis image
```



To enhance the details of regions with small amplitudes, plot the 2-D logarithm of the diffraction pattern. Very small amplitudes are affected by numerical round-off error, and the rectangular grid causes radial asymmetry.

imagesc(abs(log2(DP)))
axis image



References

[1] Fowles, G. R. Introduction to Modern Optics. New York: Dover, 1989.

See Also

fft2|fftshift|fftn|ifft2|fft

Related Examples

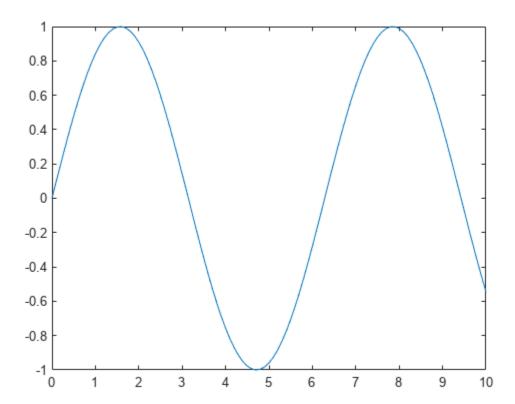
"Fourier Transforms" on page 16-2

Square Wave from Sine Waves

This example shows how the Fourier series expansion for a square wave is made up of a sum of odd harmonics.

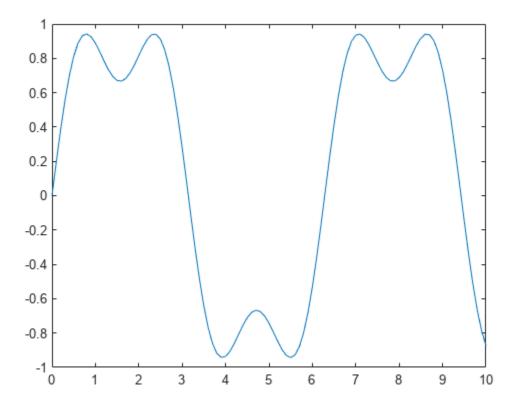
Start by forming a time vector running from 0 to 10 in steps of 0.1, and take the sine of all the points. Plot this fundamental frequency.

```
t = 0:.1:10;
y = sin(t);
plot(t,y);
```



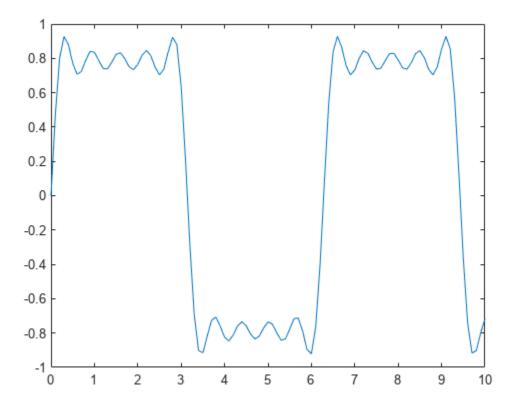
Next add the third harmonic to the fundamental, and plot it.

```
y = \sin(t) + \sin(3*t)/3;
plot(t,y);
```



Now use the first, third, fifth, seventh, and ninth harmonics.

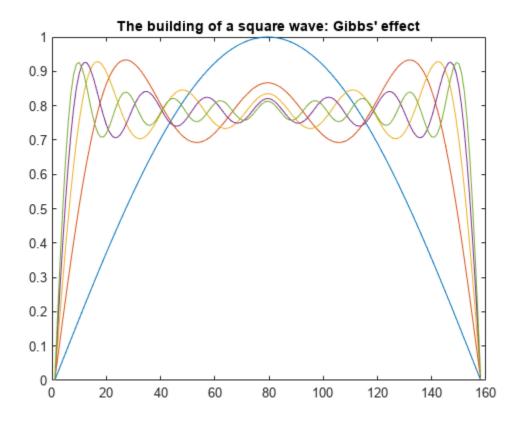
```
y = \sin(t) + \sin(3*t)/3 + \sin(5*t)/5 + \sin(7*t)/7 + \sin(9*t)/9; plot(t,y);
```



For a finale, go from the fundamental all the way to the 19th harmonic, creating vectors of successively more harmonics, and saving all intermediate steps as the rows of a matrix.

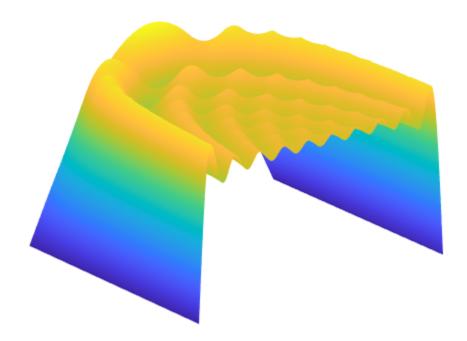
Plot the vectors on the same figure to show the evolution of the square wave. Note that the Gibbs effect says it will never quite get there.

```
t = 0:.02:3.14;
y = zeros(10,length(t));
x = zeros(size(t));
for k = 1:2:19
    x = x + sin(k*t)/k;
    y((k+1)/2,:) = x;
end
plot(y(1:2:9,:)')
title('The building of a square wave: Gibbs'' effect')
```



Here is a 3-D surface representing the gradual transformation of a sine wave into a square wave.

```
surf(y);
shading interp
axis off ij
```

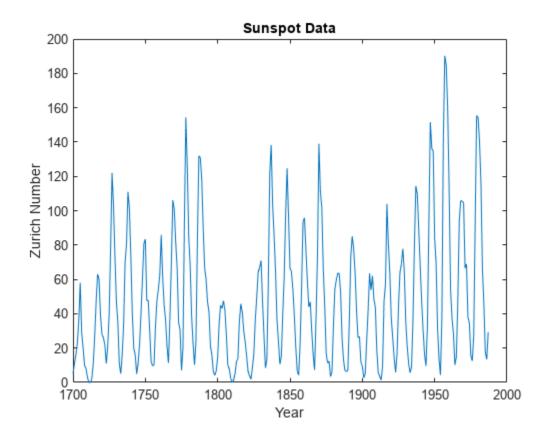


Analyzing Cyclical Data with FFT

You can use the Fourier transform to analyze variations in data, such as an event in nature over a period time.

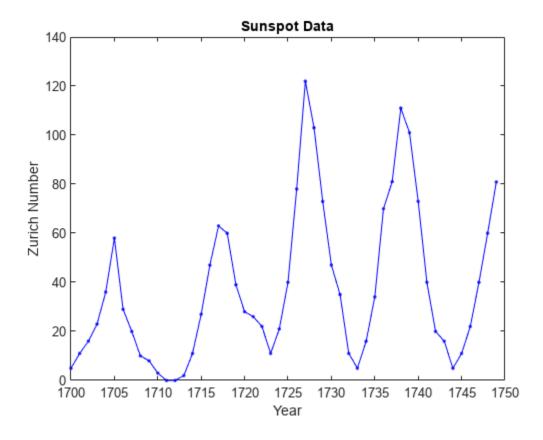
For almost 300 years, astronomers have tabulated the number and size of sunspots using the Zurich sunspot relative number. Plot the Zurich number over approximately the years 1700 to 2000.

```
load sunspot.dat
year = sunspot(:,1);
relNums = sunspot(:,2);
plot(year,relNums)
xlabel('Year')
ylabel('Zurich Number')
title('Sunspot Data')
```



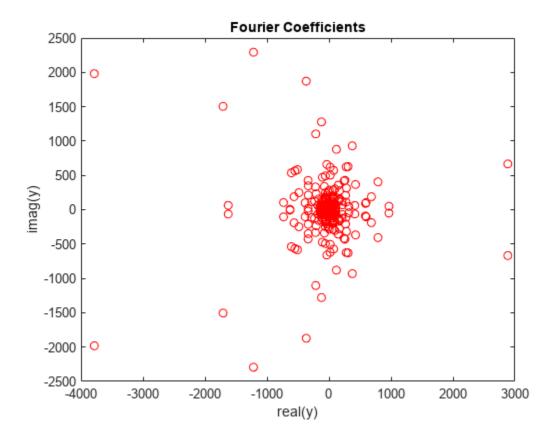
To take a closer look at the cyclical nature of sunspot activity, plot the first 50 years of data.

```
plot(year(1:50), relNums(1:50), 'b.-');
xlabel('Year')
ylabel('Zurich Number')
title('Sunspot Data')
```



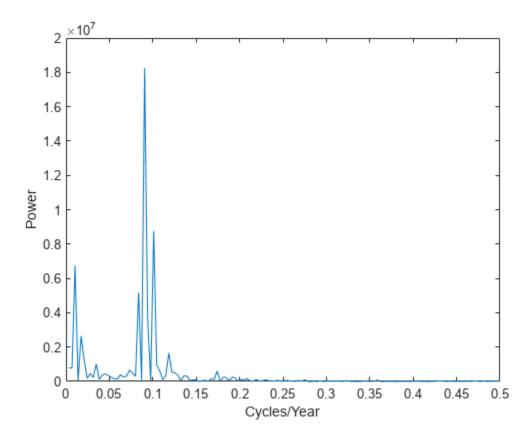
The Fourier transform is a fundamental tool in signal processing that identifies frequency components in data. Using the fft function, take the Fourier transform of the Zurich data. Remove the first element of the output, which stores the sum of the data. Plot the remainder of the output, which contains a mirror image of complex Fourier coefficients about the real axis.

```
y = fft(relNums);
y(1) = [];
plot(y,'ro')
xlabel('real(y)')
ylabel('imag(y)')
title('Fourier Coefficients')
```



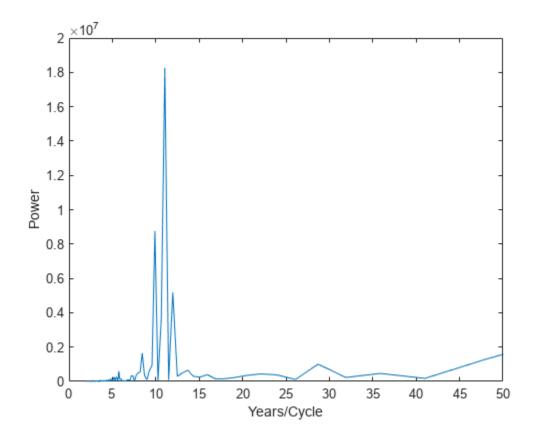
Fourier coefficients on their own are difficult to interpret. A more meaningful measure of the coefficients is their magnitude squared, which is a measure of power. Since half of the coefficients are repeated in magnitude, you only need to compute the power on one half of the coefficients. Plot the power spectrum as a function of frequency, measured in cycles per year.

```
n = length(y);
power = abs(y(1:floor(n/2))).^2; % power of first half of transform data
                                 % maximum frequency
maxfreq = 1/2;
freq = (1:n/2)/(n/2)*maxfreq;
                                 % equally spaced frequency grid
plot(freq,power)
xlabel('Cycles/Year')
ylabel('Power')
```



Maximum sunspot activity happens less frequently than once per year. For a view of the cyclical activity that is easier to interpret, plot power as a function of period, measured in years per cycle. The plot reveals that sunspot activity peaks about once every 11 years.

```
period = 1./freq;
plot(period,power);
xlim([0 50]); %zoom in on max power
xlabel('Years/Cycle')
ylabel('Power')
```



See Also fft | fft2 | fftw

Related Examples

- "Fourier Transforms" on page 16-2
- "2-D Fourier Transforms" on page 16-19

Gate-Based Quantum Algorithms

- "Introduction to Quantum Computing" on page 17-2
- "Types of Quantum Gates" on page 17-18
- "Local Quantum State Simulation" on page 17-25
- "Run Quantum Circuit on Hardware Using AWS" on page 17-29
- "Graph Coloring with Grover's Algorithm" on page 17-34
- "Ground-State Protein Folding Using Variational Quantum Eigensolver (VQE)" on page 17-45

Introduction to Quantum Computing

Note Installation Required: This functionality requires MATLAB Support Package for Quantum Computing. Install the support package from **Add-On Explorer** using the instructions in "Get and Manage Add-Ons".

Quantum computing is an emerging technology that uses the laws of quantum physics to perform computations. Quantum computations use phenomena in quantum physics, such as superposition and entanglement to perform computations. In contrast to classical computing where information is stored as binary bits, which can only be in either the 0 or 1 state, quantum computing uses quantum bits, or *qubits*, which can be in the 0 and 1 states at the same time. Because of this fundamental difference, quantum computers have the potential to outperform classical computers when solving certain types of problems, such as optimization or simulation.

This topic describes three building blocks of quantum computing: qubits, quantum gates, and quantum circuits. This topic also shows how to perform measurements of a quantum circuit, either by simulating the circuit locally with random sampling or by running the circuit remotely on a quantum device.

Qubit

The qubit is the basic building block of quantum computing. Qubits store information and can be physically realized by two-state quantum devices. A qubit can be in a linear combination of the $|0\rangle$ and $|1\rangle$ states with complex coefficients, referred to as a *superposition*. If the complex coefficients are normalized, then they represent the probability amplitudes of measuring the qubit in the $|0\rangle$ or $|1\rangle$ state. For example, a qubit can be in the $\frac{i|0\rangle-\sqrt{2}|1\rangle}{\sqrt{3}}$ state. You can determine the probability of measuring the qubit in the $|0\rangle$ state by taking the magnitude squared of the probability amplitude of the $|0\rangle$ state, which is 1/3. Similarly, the probability of measuring the qubit in the $|1\rangle$ state is 2/3.

Visualize State of Single Qubit in Bloch Sphere

A practical way to visualize the quantum state of a single qubit is using the Bloch sphere. In general, the state of a qubit can be written as

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + \exp(i\phi)\sin\frac{\theta}{2}|1\rangle$$
.

The Bloch sphere represents the parameters θ and ϕ in spherical coordinates, respectively, as the colatitude with respect to the z-axis and the longitude with respect to the x-axis of the unit sphere. The state is plotted as a point \mathbf{u} on the unit sphere with coordinates

$$\mathbf{u} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta).$$

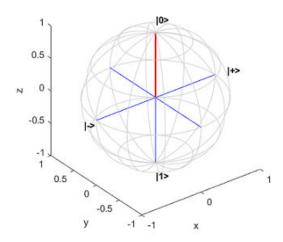
By convention, the north pole is the $|0\rangle$ state, the south pole is the $|1\rangle$ state, and the equator is a linear combination of these two states with equal probability of measuring $|0\rangle$ or $|1\rangle$.

To plot any quantum state of a qubit on the Bloch sphere, use the plotBlochSphere function (provided in the "Helper Functions" on page 17-16 section). This function takes a complex vector with two elements that represent the probability amplitudes of the $|0\rangle$ and $|1\rangle$ states.

For example, plot the $|0\rangle$ state on the Bloch sphere.

```
plotBlochSphere([1; 0])
title("|0> state on Bloch sphere")
```

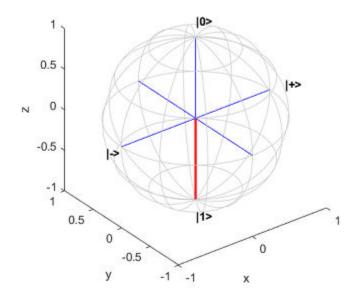
|0> state on Bloch sphere



Plot the |1> state on the Bloch sphere.

```
plotBlochSphere([0; 1])
title("|1> state on Bloch sphere")
```

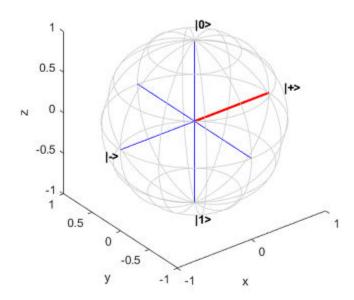
|1> state on Bloch sphere



Plot the $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$ state on the Bloch sphere. This state is represented by a point on the equator. Its opposite point on the other side of the sphere represents the $|-\rangle$ state.

```
plotBlochSphere([1; 1]/sqrt(2))
title("|+> state on Bloch sphere")
```

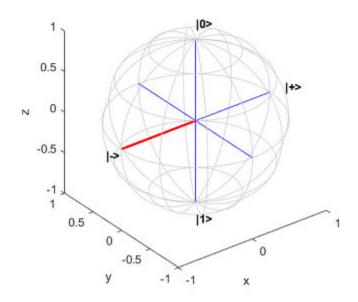
|+> state on Bloch sphere



Plot the $|-\rangle = (|0\rangle - |1\rangle)/\sqrt{2}$ state on the Bloch sphere.

plotBlochSphere([1; -1]/sqrt(2))
title("|-> state on Bloch sphere")

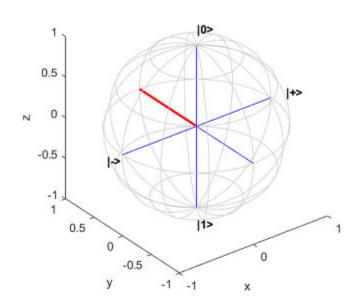
|-> state on Bloch sphere



Plot the $|R\rangle = (|0\rangle + i|1\rangle)/\sqrt{2}$ state on the Bloch sphere.

plotBlochSphere([1; 1i]/sqrt(2))
title("|R> state on Bloch sphere")

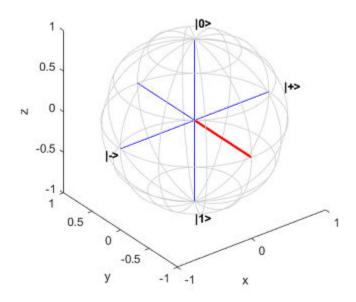
|R> state on Bloch sphere



```
Plot the |L\rangle = (|0\rangle - i|1\rangle)/\sqrt{2} state on the Bloch sphere.
```

```
plotBlochSphere([1; -1i]/sqrt(2))
title("|L> state on Bloch sphere")
```

L> state on Bloch sphere



Find Probabilities of Measuring Possible States

The quantum state of a single qubit is expressed as a normalized two-element complex vector, where the first element gives the amplitude of the $|0\rangle$ state and the second element gives the amplitude of the $|1\rangle$ state. A measurement of this qubit yields a classical $|0\rangle$ or $|1\rangle$ state, with the probability of measuring each state given by the magnitude squared of its respective amplitude.

You can use the quantum.gate.QuantumState constructor to create a quantum state, and then use the querystates function to find the possible states to measure and their probabilities. For example, create a quantum state that represents the |1> state.

```
state = quantum.gate.QuantumState([0 1]);
state.Amplitudes
ans =
    0
    1
```

The querystates function returns all possible states to measure and the probability of measuring each one. Here, only the $|1\rangle$ state is possible.

```
[states,probabilities] = querystates(state)
states =
   "1"
```

```
probabilities =
    1
```

As another example, create a quantum state where the two elements of the vector have different amplitudes with the same absolute value.

```
state = quantum.gate.QuantumState([1 li]/sqrt(2));
state.Amplitudes
ans =
    0.7071 + 0.0000i
    0.0000 + 0.7071i
```

The querystates function returns the "0" and "1" states as the possible states to measure and a 0.5 probability of measuring each state.

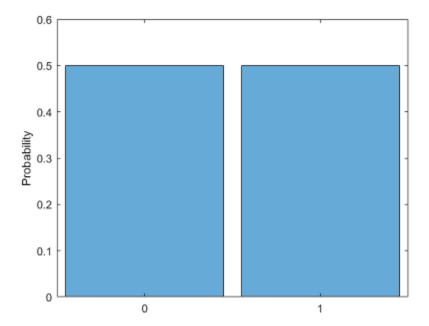
```
[states,probabilities] = querystates(state)
```

```
states =
  2×1 string array
    "0"
    "1"

probabilities =
    0.5000
    0.5000
```

You can plot a histogram that shows the probabilities of measuring all possible states by using histogram.

histogram(state)



As another example, create a quantum state where the two elements of the vector have different amplitudes and different absolute values. If you call quantum.gate.QuantumState with a general complex vector, then the constructor creates a quantum state that is normalized. For example, create a quantum state and find its measurement probabilities.

```
state = quantum.gate.QuantumState([3 -4i]);
state.Amplitudes

ans =
     0.6000 + 0.0000i
     0.0000 - 0.8000i

[states,probabilities] = querystates(state)

states =
     2×1 string array
     "0"
     "1"

probabilities =
     0.3600
     0.6400
```

Only properties of a quantum state that translate into probabilities are measurable. For example, multiplying every amplitude of a quantum state by -1 or $\exp(i\theta)$ has no measurable impact. This type of transformation is called applying a *global phase*. However, multiplying one of the amplitudes by -1 or $\exp(i\theta)$ (applying a *relative phase*) has a measurable impact. If you measure the state directly after

applying the relative phase, you do not see a difference in the probabilities. But if you apply additional gate operations on the qubits, you can detect the difference due to the relative phase.

Quantum Gate

The quantum gate is the next building block of quantum computing. Quantum gates represent reversible operations that transform the quantum state according to unitary matrices. While all gate operations are deterministic, measuring in quantum computing is probabilistic, with the probabilities of various measurements depending on the states of the qubits. For a complete list of quantum gates available in MATLAB, see "Types of Quantum Gates" on page 17-18.

Pauli X Gate

An example of a quantum gate is the Pauli X gate. This gate multiplies the state vector by the Pauli X matrix $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, which flips the $|0\rangle$ state of a qubit to the $|1\rangle$ state and flips the $|1\rangle$ state to the $|0\rangle$ state.

For example, create the initial quantum state of a single qubit.

```
coeffs = [0.7; 0.5i];
inState = quantum.gate.QuantumState(coeffs);
inAmps = inState.Amplitudes

inAmps =

0.8137 + 0.0000i
0.0000 + 0.5812i
```

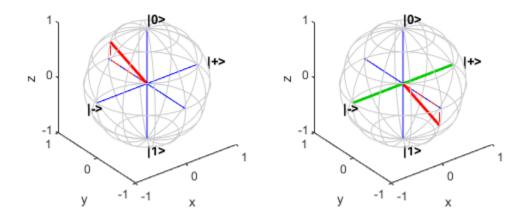
Create a quantum circuit that applies the Pauli X gate (xGate) to the qubit by using quantumCircuit. Simulate this circuit to get the final state of the qubit by using simulate.

```
c = quantumCircuit(xGate(1));
outState = simulate(c,inState);
outAmps = outState.Amplitudes

outAmps =
    0.0000 + 0.5812i
    0.8137 + 0.0000i
```

To illustrate the operation performed by the Pauli X gate, plot the initial state and the final state of the circuit on a Bloch sphere. In the Bloch sphere representation, the Pauli X gate rotates the state around the x-axis (the axis of the $|+\rangle$ and $|-\rangle$ states) by an angle of π .

```
figure
tiledlayout(1,2);
nexttile
plotBlochSphere(inAmps)
nexttile
plotBlochSphere(outAmps)
hold on
plot3([-1 1],[0 0],[0 0],LineWidth=2,Color=[0 0.8 0])
hold off
```



For the choice of basis states of a qubit, the $|0\rangle$ and $|1\rangle$ states are the eigenstates of the Pauli Z gate. Applying the Pauli Z gate (zGate) has no effect on the $|0\rangle$ state and maps the $|1\rangle$ state to $-|1\rangle$. The Pauli Z gate is also known as a phase-flip gate. Similarly, the $|+\rangle$ and $|-\rangle$ states are the eigenstates of the Pauli X gate. The eigenstates of the Pauli Y gate (yGate) are the other two orthogonal directions in the plot, which are the $|R\rangle = (|0\rangle + i|1\rangle)/\sqrt{2}$ state and the $|L\rangle = (|0\rangle - i|1\rangle)/\sqrt{2}$ states. Although each of these pairs would work as basis states, the $|0\rangle$ and $|1\rangle$ basis states are the standard basis states in which measurements are made. To rotate around the x-, y-, or z-axis with an arbitrary angle, you can use the rotation gates rxGate, ryGate, or rzGate.

Hadamard Gate

Another example of a quantum gate is the Hadamard gate, which transforms the Z basis to the X basis. That is, the gate transforms the $|0\rangle$ and $|1\rangle$ states to the $|+\rangle$ and $|-\rangle$ states, respectively. For example, consider the same initial quantum state that was previously created.

```
inAmps = inState.Amplitudes
inAmps =
    0.8137 + 0.0000i
    0.0000 + 0.5812i
```

Create a quantum circuit that applies the Hadamard gate (hGate) to the qubit. Simulate this circuit to get the final state of the qubit.

```
c = quantumCircuit(hGate(1));
outState = simulate(c,inState);
outAmps = outState.Amplitudes

outAmps =
    0.5754 + 0.4110i
    0.5754 - 0.4110i
```

The operation by the Hadamard gate is not apparent from the probability amplitudes of the states. To better understand this operation, transform the complex amplitudes of the states into coordinates on the Bloch sphere by using the mapToBlochSphere function (provided in the "Helper Functions" on page 17-16 section). Show the coordinates of the initial state and final state on the Bloch sphere.

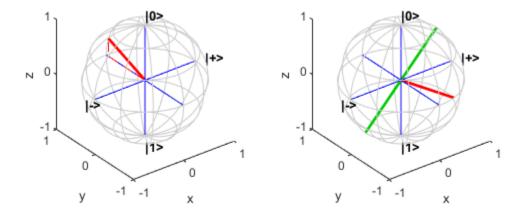
```
inCoords = mapToBlochSphere(inAmps)
```

```
inCoords =
    0.0000    0.9459    0.3243

outCoords = mapToBlochSphere(outAmps)
outCoords =
    0.3243    -0.9459    0.0000
```

In the Bloch sphere representation, the Hadamard gate rotates the state around the [1,0,1] axis by an angle of π .

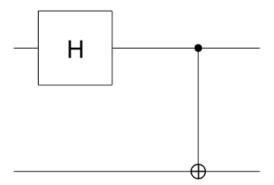
```
figure
tiledlayout(1,2);
nexttile
plotBlochSphere(inAmps)
nexttile
plotBlochSphere(outAmps)
hold on
plot3([-1 1]/sqrt(2),[0 0],[-1 1]/sqrt(2),LineWidth=2,Color=[0,0.8,0])
hold off
```



Quantum devices typically provide measurements only in the Z basis, which is a choice of basis that is not intrinsically special given the various transformations available using quantum gates. For example, to measure a qubit in the X basis instead, you can apply a Hadamard gate to the qubit before performing the measurement.

Quantum Circuit

The quantum circuit is the next building block of quantum computing. Quantum circuits consist of quantum gates that act on qubits. A quantum circuit diagram is commonly used as a visual model for a sequence of quantum gates applied to qubits. This example of quantum circuit diagram includes a Hadamard gate and a controlled X gate acting on two qubits.



- In a quantum circuit diagram, each solid horizontal line represents a qubit, or more generally, a qubit register. In MATLAB, the top line is a qubit with index 1 and the remaining lines from top to bottom are labeled sequentially. In this example, the circuit consists of two qubits with indices 1 and 2.
- Quantum gates perform operations on the qubits. A gate acting on qubits is denoted as a specific gate symbol. In this example, the symbol represents a Hadamard gate acting on qubit 1. The next symbol represents a controlled X gate with qubit 1 as the control and qubit 2 as the target.
- In a circuit diagram, time flows from left to right. Quantum gates are ordered in chronological order with the leftmost gate as the gate first applied to the qubits. The solid horizontal lines hold the overall quantum state of the circuit that is passed through each of the gates in the diagram from left to right.
- For a quantum circuit with n qubits, the overall 2^n basis states are constructed from the Kronecker product of the n qubit bases with ordering from left to right for qubits with the lowest index to the highest index. In other words, if the basis of a single qubit with index k is labeled as $|q_k\rangle$ (which can be $|0\rangle$ or $|1\rangle$), then the basis states of the circuit with n qubits are represented by $|q_1\rangle\otimes ...\otimes |q_k\rangle\otimes ...\otimes |q_n\rangle$. For example, for a circuit with two qubits, all possible basis states expressed as a column vector are $|q_1q_2\rangle = [|00\rangle, |01\rangle, |10\rangle, |11\rangle]^T$. This definition follows most textbooks.
- A gate operation can be represented as a transformation matrix for these basis states. For example, consider the controlled X gate that operates on a target qubit (with index 2) based on the state of a control qubit (with index 1). If the control qubit is in the |0> state, this gate does nothing. If the control qubit is in the |1> state, this gate applies the Pauli X gate to the target qubit. The matrix representation of the controlled X gate is

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

• The quantum state of a circuit with n qubits can then be represented by the linear combinations of the 2^n basis states, which can be a separable or an entangled state. A *separable* state is a quantum state that can be factored into individual states belonging to separate subspaces of the qubits. An *entangled* state is a quantum state that is not separable. For example, for a circuit with two qubits, the quantum state can be a separable state, such as

$$\frac{i}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle) = \frac{(|0\rangle + |1\rangle)}{\sqrt{2}} \frac{i(|0\rangle + |1\rangle)}{\sqrt{2}}$$

where qubit 1 is in the $|+\rangle=(|0\rangle+|1\rangle)/\sqrt{2}$ state and qubit 2 is in the $i(|0\rangle+|1\rangle)/\sqrt{2}$ state. The quantum state of the two qubits can also be an entangled state, such as $1/\sqrt{2}$ ($|00\rangle+|11\rangle$), which cannot be written as the product of each qubit state. For this entangled state, the two qubits are an inseparable whole. If one of these qubits is measured in the $|0\rangle$ state, then the other qubit will also be measured in the $|1\rangle$ state, then the other qubit will also be measured in the $|1\rangle$ state.

• By default, the initial state of each qubit in a quantum circuit is the $|0\rangle$ state. For example, the initial state of the quantum circuit in the diagram is $|00\rangle$. After the operations by the Hadamard and controlled X gates, the final state of the circuit is an entangled state, $1/\sqrt{2}$ ($|00\rangle + |11\rangle$).

Build and Simulate Quantum Circuit

You can build a quantum circuit by using the quantumCircuit function. Create an empty quantum circuit with two qubits. Simulate the quantum state returned by this circuit. Show the quantum state of this circuit as a string formula by using formula.

```
c = quantumCircuit(2);
s = simulate(c);
str = formula(s)
str =
   "1 * |00>"
```

By default, all qubits are set to 0. Next, pass a different initial quantum state, $\frac{1}{2}(|00\rangle - |01\rangle) + \frac{1i}{2}(|10\rangle - |11\rangle)$, to the simulate function, where the quantum state is a linear combination of all basis states of the qubits.

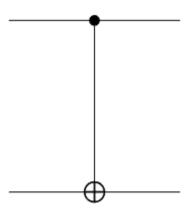
```
inState = quantum.gate.QuantumState([1/2; -1/2; 1i/2; -1i/2]);
s = simulate(c,inState);
str = formula(s,Basis="Z")

str =

"(0.5+0i) * |00> +
    (-0.5+0i) * |01> +
    (0+0.5i) * |10> +
    (0-0.5i) * |10> +
```

You can add quantum gates to the circuit. For this example, add a controlled X (or CNOT) gate to the circuit. Then plot the circuit.

```
c.Gates = cxGate(1,2);
figure
plot(c)
```



Find the final state of this circuit after passing the initial state $\frac{1}{2}(|00\rangle - |01\rangle) + \frac{1i}{2}(|10\rangle - |11\rangle)$ to the controlled X gate.

```
outState = simulate(c,inState);
str = formula(outState,Basis="Z")
str =

"(0.5+0i) * |00> +
    (-0.5+0i) * |01> +
    (0-0.5i) * |10> +
    (0+0.5i) * |11>"
```

You can also pass the initial state as $|+0\rangle$ to this circuit. Find the final state of this circuit for this initial state.

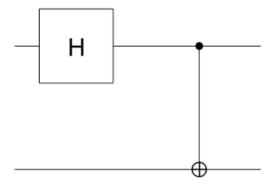
```
outState = simulate(c,"+0");
str = formula(outState,Basis="Z")
str =
    "0.70711 * |00> +
    0.70711 * |11>"
```

Run Circuit and Make Measurement

You can run a circuit built in MATLAB on a remote quantum device and retrieve the measurement result.

Build a quantum circuit that entangles two qubits by using a Hadamard gate and a controlled X gate. Then plot the circuit.

```
gates = [hGate(1); cxGate(1,2)];
c = quantumCircuit(gates);
plot(c)
```



The default initial state of this circuit is $|00\rangle$. Simulate the circuit to get its final state.

```
outState = simulate(c);
str = formula(outState)
str =
   "0.70711 * |00> +
   0.70711 * |11>"
```

To investigate the behavior of this circuit, you can first perform a local simulated measurement of the circuit. Use randsample to randomly sample the quantum state of the circuit with 100 shots.

```
m = randsample(outState,100)
m =
   QuantumMeasurement with properties:
    MeasuredStates: [2×1 string]
        Counts: [2×1 double]
        NumQubits: 2
```

Show the measured states and their counts.

table(m.Counts,m.MeasuredStates,VariableNames=["Counts","States"])
ans =

```
2×2 table

Counts States

54 "00"
46 "11"
```

In theory, because the quantum state is entangled and it is a superposition only of the $|00\rangle$ and $|11\rangle$ states, the probability of measuring the $|01\rangle$ and $|10\rangle$ states is 0. In practice, however, due to the noise in physical quantum devices to date, the $|01\rangle$ and $|10\rangle$ states can appear as measurements.

To run the circuit on a remote quantum device that is available through Amazon® Web Services (AWS®), first connect to a specific quantum device using quantum.backend.QuantumDeviceAWS.

```
dev = quantum.backend.QuantumDeviceAWS("Aspen-M-3");
```

Run the circuit on the device with the default 100 shots using the run function.

```
task = run(c,dev)

task =
QuantumTaskAWS with properties:
    Status: "queued"
    TaskARN: "arn:aws:braket:us-west-1:123456789012:quantum-task/1234abcd-ef56-7890-abc2-34de56f678ab"
```

Wait for the task to finish. Retrieve the measurement result of running the circuit on the device by using fetchOutput.

Show the measurement result. Due to the noise in the quantum device, the $|01\rangle$ and $|10\rangle$ states appear as measurements.

```
table(m.Counts, m.MeasuredStates, VariableNames=["Counts", "States"])
```

Helper Functions

This section provides the complete code of the plotBlochSphere and mapToBlochSphere functions.

```
function plotBlochSphere(u)
% Plot Bloch sphere representation from 2-D complex amplitudes
% Copyright 2021-2023 The MathWorks, Inc.
arguments
    u {mustBeNumeric,mustBeVector}
end
% Compute Bloch sphere representation (3-D real) from a 2-D complex vector
P = mapToBlochSphere(u);
% Grid view of the sphere
alpha = linspace(0,2,101)';
alpha(end+1) = NaN;
beta = linspace(0,1,7);
beta(end) = [];
gamma = linspace(-0.5,0.5,7);
```

```
% Meridian lines
% Latitude circles
latitudeCoordinates = cat(3, cospi(gamma).*cospi(alpha), ...
    cospi(gamma).*sinpi(alpha), repmat(sinpi(gamma), length(alpha), 1));
xyz = [reshape(meridianCoordinates,[],3); reshape(latitudeCoordinates,[],3)];
% Plot the grid and coordinate system
\verb"plot3(xyz(:,1), xyz(:,2), xyz(:,3), "k-", Color=0.8*[1\ 1\ 1])
hold on
plot3([1 0 0; -1 0 0], [0 1 0; 0 -1 0], [0 0 1; 0 0 -1], "b")
% Label qubit basis vectors for X basis and Z basis
Text([0 0 1.2 -1.2], [0 0 0 0], [1.2 -1.2 0 0], ["|0>" "|1>" "|+>" "|->"], ...

FontWeight="bold")
% Configure axis view
xlabel("x")
ylabel("y")
zlabel("z")
axis equal
% Plot the vector
plot3([0 P(1)], [0 P(2)], [0 P(3)], "r-", LineWidth=2) plot3([0 P(1) P(1)], [0 P(2) P(2)], [0 0 P(3)], "r--")
hold off
function P = mapToBlochSphere(u)
% Compute Bloch sphere representation (3-D real) from a 2-D complex vector
theta = 2*atan2(abs(u(2)),abs(u(1)));
phi = angle(u(2)*conj(u(1)));
P = [sin(theta)*cos(phi) sin(theta)*sin(phi) cos(theta)];
end
```

See Also

quantum.gate.SimpleGate | quantum.gate.CompositeGate | quantumCircuit |
quantum.gate.QuantumState | quantum.gate.QuantumMeasurement |
quantum.backend.QuantumDeviceAWS | quantum.backend.QuantumTaskAWS

Related Examples

- "Types of Quantum Gates" on page 17-18
- "Local Quantum State Simulation" on page 17-25
- "Run Quantum Circuit on Hardware Using AWS" on page 17-29

Types of Quantum Gates

Note Installation Required: This functionality requires MATLAB Support Package for Quantum Computing. Install the support package from **Add-On Explorer** using the instructions in "Get and Manage Add-Ons".

This topic provides a list functions that you can use to create quantum gates in MATLAB. Quantum gates are reversible and have unitary matrix representations.

Creation Functions for SimpleGate Objects

Gates on One Target Qubit

Creation Function	Gate Name	No. of Qubit s	Matrix Representation	Properties
- н	Hadamard gate	1	$\begin{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \end{bmatrix}$	Traceless Involutory
hGate			V2[1 -1]	• Involutory
l l l	Identity gate	1	[1 0]	Identity
idGate			[0 1]	• Involutory
	Pauli X gate	1	[0 1]	• Traceless
xGate			[1 0]	• Involutory
				Pauli group
	Pauli Y gate	1	$\begin{bmatrix} 0 & -i \end{bmatrix}$	• Traceless
yGate			[[i 0]	• Involutory
,				Pauli group
	Pauli Z gate	1	[1 0]	Traceless
z zGate			[0 -1]	• Involutory
				Pauli group

Rotation Gates

Creation Function	Gate Name	No. of Qubit s	Matrix Representation	Properties
− RX rxGate	x-axis rotation gate	1	$\begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & -i\sin\left(\frac{\theta}{2}\right) \\ -i\sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{bmatrix}$	• Special unitary (determinant is 1) • Continuous parameter θ with period 4π

Creation Function	Gate Name	No. of Qubit s	Matrix Representation	Properties
RY ryGate	y-axis rotation gate	1	$\begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & -\sin\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{bmatrix}$	• Special unitary (determinant is 1) • Continuous parameter θ with period 4π
RZ rzGate	z-axis rotation gate	1	$\begin{bmatrix} \exp\left(-i\frac{\theta}{2}\right) & 0\\ 0 & \exp\left(i\frac{\theta}{2}\right) \end{bmatrix}$	 Special unitary (determinant is 1) Continuous parameter θ with period 4π
R1 r1Gate	z-axis rotation gate with global phase	1	$\begin{bmatrix} 1 & 0 \\ 0 & \exp(i\theta) \end{bmatrix}$	• Continuous parameter θ with period 2π
sGate	S gate	1	$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$	
- si-siGate	Inverse S gate	1	$\begin{bmatrix} 1 & 0 \\ 0 & -i \end{bmatrix}$	
T tGate	T gate	1	$\begin{bmatrix} 1 & 0 \\ 0 & \frac{1+i}{\sqrt{2}} \end{bmatrix}$	
TI tiGate	Inverse T gate	1	$\begin{bmatrix} 1 & 0 \\ 0 & \frac{1-i}{\sqrt{2}} \end{bmatrix}$	

Gates with One Control Qubit and One Target Qubit

Creation Function	Gate Name	No. of Qubit s	Matrix Representation	Properties
chGate	Controlled Hadamard gate	2	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$	Involutory
cxGate or cnotGate	Controlled X or CNOT gate	2	$ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} $	• Involutory

Creation Function	Gate Name	No. of Qubit s	Matrix Representation	Properties
cyGate	Controlled Y gate	2	$ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{bmatrix} $	Involutory
czGate	Controlled Z gate	2	$ \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} $	 Involutory Swapping control and target qubits does not change gate operation

Gate That Swap States of Two Qubits

Creation Function	Gate Name	No. of Qubit s	Matrix Representation	Properties
-X-swapGate	Swap gate	2	[1 0 0 0] [0 0 1 0] [0 1 0 0] [0 0 0 1]	 Involutory Swapping the two target qubits does not change gate operation

Controlled Rotation Gates

Creation Function	Gate Name	No. of Qubit s	Matrix Representation	Properties
RX crxGate	Controlled <i>x</i> -axis rotation gate	2	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos(\frac{\theta}{2}) & -i\sin(\frac{\theta}{2}) \\ 0 & 0 & -i\sin(\frac{\theta}{2}) & \cos(\frac{\theta}{2}) \end{bmatrix}$	• Continuous parameter θ with period 4π
RY e	Controlled y-axis rotation gate	2	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos(\frac{\theta}{2}) & -\sin(\frac{\theta}{2}) \\ 0 & 0 & \sin(\frac{\theta}{2}) & \cos(\frac{\theta}{2}) \end{bmatrix}$	• Continuous parameter θ with period 4π

Creation Function	Gate Name	No. of Qubit s	Matrix Representation	Properties
RZ crzGate	Controlled z-axis rotation gate	2	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \exp(-i\frac{\theta}{2}) & 0 \\ 0 & 0 & \exp(i\frac{\theta}{2}) \end{bmatrix}$	• Continuous parameter θ with period 4π
R1 e	Controlled z-axis rotation gate with global phase	2	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \exp(i\theta) \end{bmatrix}$	 Continuous parameter θ with period 2π Swapping control and target qubits does not change gate operation

Controlled Controlled X Gate

Creation Function	Gate Name	No. of Qubit s	Matrix Representation	Properties
ccxGate	Controlled controlled X gate (CCNOT or Toffoli gate)	3	$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$	Involutory Swapping the two control qubits does not change gate operation

Ising Coupling Gates

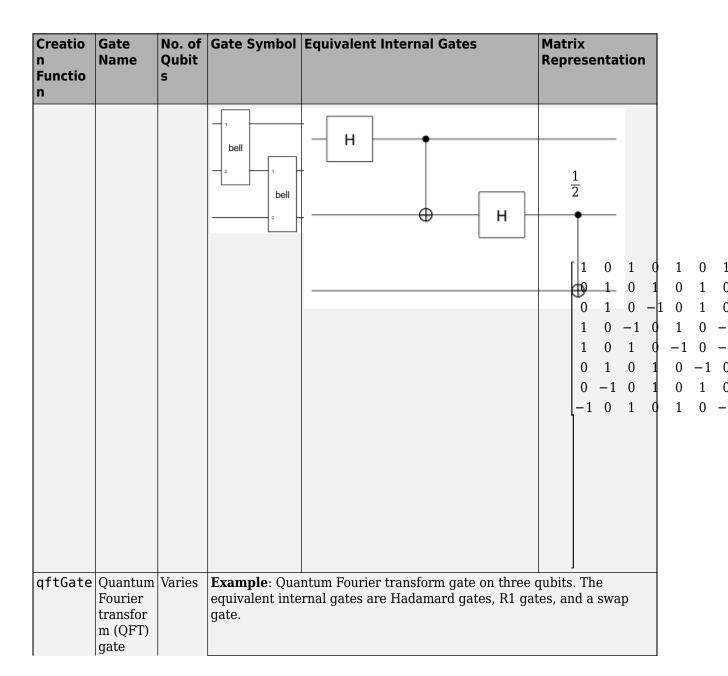
Creation Function	Gate Name	No. of Qubits	Matrix Representation	Properties
RXX e 2 rxxGate	Ising XX coupling gate	2	$\begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & 0 & 0 & -i\sin\left(\frac{\theta}{2}\right) \\ 0 & \cos\left(\frac{\theta}{2}\right) & -i\sin\left(\frac{\theta}{2}\right) & 0 \\ 0 & -i\sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) & 0 \\ -i\sin\left(\frac{\theta}{2}\right) & 0 & 0 & \cos\left(\frac{\theta}{2}\right) \end{bmatrix}$	 Special unitary (determinant is 1) Continuous parameter θ with period 4π Swapping the two target qubits does not change gate operation

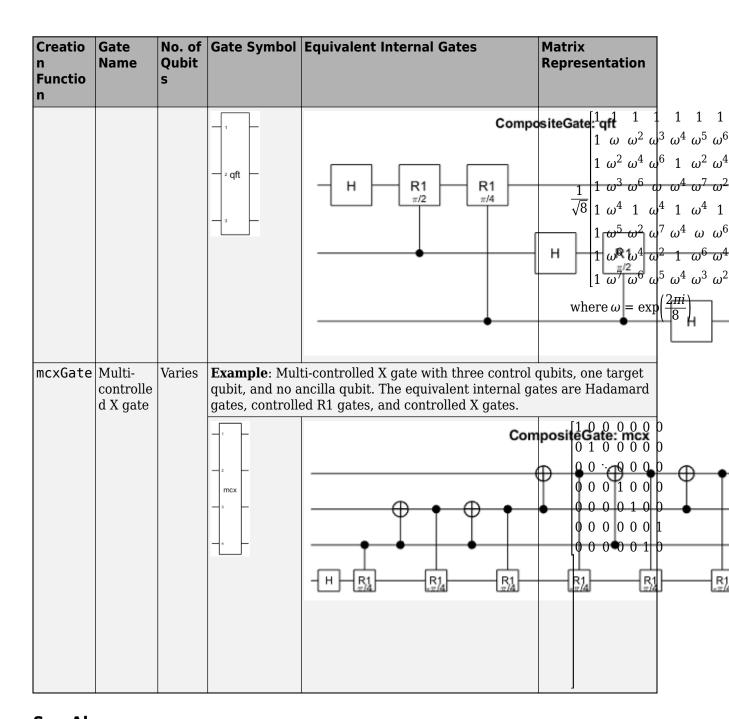
Creation Function	Gate Name	No. of Qubits	Matrix Representation	Properties
RYY e	Ising YY coupling gate	2	$\begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & 0 & 0 & i\sin\left(\frac{\theta}{2}\right) \\ 0 & \cos\left(\frac{\theta}{2}\right) & -i\sin\left(\frac{\theta}{2}\right) & 0 \\ 0 & -i\sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) & 0 \\ i\sin\left(\frac{\theta}{2}\right) & 0 & 0 & \cos\left(\frac{\theta}{2}\right) \end{bmatrix}$	 Special unitary (determinant is 1) Continuous parameter θ with period 4π Swapping the two target qubits does not change gate operation
RZZ e 2 rzzGate	Ising ZZ coupling gate	2	$\begin{bmatrix} \exp\left(-i\frac{\theta}{2}\right) & 0 & 0 & 0 \\ 0 & \exp\left(i\frac{\theta}{2}\right) & 0 & 0 \\ 0 & 0 & \exp\left(i\frac{\theta}{2}\right) & 0 \\ 0 & 0 & 0 & \exp\left(-i\frac{\theta}{2}\right) \end{bmatrix}$	 Special unitary (determinant is 1) Continuous parameter θ with period 4π Swapping the two target qubits does not change gate operation

Creation Functions for CompositeGate Objects

Composite and Specialized Gates

Creatio n Functio n	Gate Name	No. of Qubit s	Gate Symbol	Equivalent Internal Gates	Matrix Representation	
composi teGate	Composi te gate	Varies	Example : Quantum circuit with two composite gates named "bell". The equivalent internal gates of each composite gate are a Hadamard gate and a controlled X gate.			





See Also

quantum.gate.SimpleGate | quantum.gate.CompositeGate

Related Examples

• "Introduction to Quantum Computing" on page 17-2

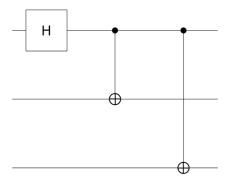
Local Quantum State Simulation

Note Installation Required: This functionality requires MATLAB Support Package for Quantum Computing. Install the support package from **Add-On Explorer** using the instructions in "Get and Manage Add-Ons".

This topic describes how to simulate a quantum circuit locally and analyze the simulation results. Building quantum circuits requires iteration on circuit design to refine circuit gates and confirm behavior. Also, because measurements on quantum hardware are probabilistic, it is useful to examine the probabilities of final states to determine the most likely outcome of a measurement. Use the simulate method of quantumCircuit to simulate circuits on your local computer. Once you simulate a circuit, use the methods of quantum.qate.QuantumState to inspect the results.

Create Circuit

Create a quantum circuit with three qubits and three gates. Apply a Hadamard gate to the first qubit, and apply CNOT gates to the second and third qubits, using the first qubit as the control. Plot the circuit to view its qubits and gates.



Each horizontal line in the plot represents one of the qubits, and the gates are arranged from left to right in the order that they are applied.

Simulate Circuit

Simulate the quantum circuit by using the simulate method. All qubits start in the $|0\rangle$ state by default, but you can use a second input argument to specify a different starting state for the qubits. Specify that each qubit has an initial state of $|1\rangle$.

```
S = simulate(C,"111")
S =
  QuantumState with properties:
```

```
BasisStates: [8×1 string]
Amplitudes: [8×1 double]
NumOubits: 3
```

Display the basis states and corresponding amplitudes by inspecting the properties of the resulting quantum.gate.QuantumState object.

S.BasisStates

```
ans =

8×1 string array

"000"
"001"
"010"
"110"
"110"
"111"
```

S.Amplitudes

```
ans =

0
0
0
0.7071
-0.7071
0
0
```

Display State Formula

Display a formula representation of the simulated quantum state by using the formula method. The formula combines the information in the BasisStates and Amplitudes properties of S. By default, the formula uses the Z basis.

```
f = formula(S)
f =
   "0.70711 * |011> +
    -0.70711 * |100>"
```

Specify the Basis name-value argument to display the formula using the X basis. The formula now shows linear combinations of $|+\rangle$ and $|-\rangle$ states.

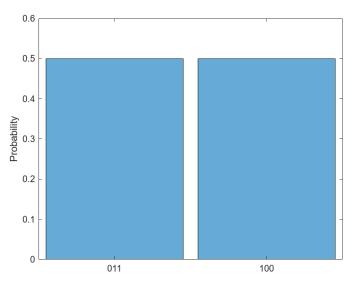
```
f2 = formula(S,Basis="X")
f2 =
   "-0.5 * |++-> +
   -0.5 * |+-+> +
```

```
0.5 * | -++> +
0.5 * | --->"
```

Plot Possible States

Use histogram to plot the possible states and their probabilities. The probability of each state is equal to its amplitude squared. This circuit has only two possible states, and each state has a 50% chance of being measured.





Query Possible States

You can query the possible states and their probabilities using the querystates method. This method returns the same information that the histogram shows, but at the command line.

```
[states,P] = querystates(S)
states =
    2×1 string array
    "011"
    "100"

P =
    0.5000
    0.5000
```

Query Qubit State Probabilities

You can query the probability that specific qubits will be measured in specific states by using the probability method. For example, determine the probability that the second qubit will be measured in the |1> state.

```
p = probability(S,2,"1")
p =
    0.5000
```

Simulate Quantum State Measurement

Quantum measurements are probabilistic, so the results can differ between trials. The randsample method is useful for simulating the aggregated results of many such measurements. You can specify the number of shots, or trials, and each shot returns a single state.

For example, simulate 50 quantum measurements of the circuit.

See Also

29

quantumCircuit | quantum.gate.SimpleGate | quantum.gate.CompositeGate |
quantum.gate.QuantumState

Related Examples

- "Introduction to Quantum Computing" on page 17-2
- "Types of Quantum Gates" on page 17-18

"100"

• "Run Quantum Circuit on Hardware Using AWS" on page 17-29

Run Quantum Circuit on Hardware Using AWS

Note Installation Required: This functionality requires MATLAB Support Package for Quantum Computing. Install the support package from **Add-On Explorer** using the instructions in "Get and Manage Add-Ons".

This topic describes how to connect directly from MATLAB to Amazon Web Services (AWS) to enable running gate-based quantum circuits on remote quantum devices and simulators. Quantum hardware has limited availability as well as associated costs for each task that is run. A best practice is to finalize your circuit design as much as possible by simulating the circuit locally on your computer before running the circuit on a quantum device. See "Local Quantum State Simulation" on page 17-25 for instructions on how to inspect simulated circuit results on your local computer.

Requirements

To run quantum circuits on an AWS device from within MATLAB, you need:

- The MATLAB Support Package for Quantum Computing
- · An AWS account with access to Amazon Braket
- An AWS Access Key and AWS Secret Access Key
- An Amazon S3[™] bucket to store results

Costs for the use of Amazon Braket devices are charged to your AWS account. See Amazon Braket Pricing for details.

Set Up Access to AWS

Follow these steps to enable communication between MATLAB and AWS.

Set up AWS account and retrieve credentials. Go to Setting up your local development environment in Amazon Braket and complete steps 1–3. If you have an existing account, then you can skip the first step and check your account settings in steps 2 and 3.

The account credentials (AWS Access Key and AWS Secret Access Key) are only available to download just after they are created. If your AWS account is managed through your organization, then you might need to contact your administrator for the recommended way to retrieve credentials.

At the end of this step, you should have:

- · Configured or checked permissions for your AWS account
- Received account credentials (AWS Access Key and AWS Secret Access Key)
- Enabled Amazon Braket service for your account
- **Set environment variables**. Specify these environment variables using your AWS Access Key and AWS Secret Access Key. Specify the environment variables using a command prompt for your operating system.
 - Windows[®]

```
set AWS_ACCESS_KEY_ID=YOUR_AWS_ACCESS_KEY_ID
set AWS_SECRET_ACCESS_KEY=YOUR_AWS_SECRET_ACCESS_KEY
```

• Linux[®], macOS, or UNIX[®] with Bourne-based shell

```
export AWS_ACCESS_KEY_ID=YOUR_AWS_ACCESS_KEY_ID export AWS_SECRET_ACCESS_KEY=YOUR_AWS_SECRET_ACCESS_KEY
```

If you are using a C-based shell, replace export with setenv in the commands.

Optional: Two optional environment variables that you can also specify are:

- AWS SESSION TOKEN: A token for one AWS session that expires after a given time period.
- AWS_DEFAULT_REGION: Restricts the region in which the server storing results must reside. When AWS_DEFAULT_REGION is set, you can still use QPUs that are located in any region.
- **3 Create Amazon S3 bucket to store results**. See Create your first S3 bucket for more information about creating a bucket.
 - The bucket you create must have a unique name. A suggested prefix for the name is amazon-braket-mathworks-.
 - If you specified AWS_DEFAULT_REGION in the previous step, then the bucket must reside in the same region.

Device Availability

To see a list of available quantum devices:

- **1** Go to https://aws.amazon.com/.
- **2** Log in to your AWS account.
- 3 Navigate to Amazon Braket using the **Services** menu or the search bar.
- **4** Select **Devices** from the navigation menu.

The device list contains information on device providers, names, availability, and descriptions. Each device has different associated costs, and you can click on a device to see more details. If a device is offline, it does not accept tasks and creating a quantum.backend.QuantumDeviceAWS object for the device returns an error. However, devices that are not currently available might still accept tasks into their queue to be run later. Check the device details to determine the current status before submitting tasks.

The MATLAB Support Package for Quantum Computing works with gate-model QPU devices as well as simulators:

- **QPU Devices:** These devices are quantum computers used to perform probabilistic measurements of circuits. Not all QPU devices are supported. To find out if a device is supported, try connecting to the device using quantum.backend.QuantumDeviceAWS. Availability and number of qubits supported can also vary, so check the device details before sending circuits for measurement.
- **Simulator Devices:** Because memory usage scales exponentially with the number of qubits, larger circuits with many qubits might stretch the limits of memory available on your local computer. To address that issue, AWS also provides cloud-scale simulators. The functionality is similar to using randsample on your local system, but the simulators can support up to 34 qubits with cloud-scale performance.

Connect to Quantum Device

Connect to a quantum device using quantum.backend.QuantumDeviceAWS. Specify the name of the device as well as its region and the path of the Amazon S3 bucket to store results. The SV1 device is a state vector simulator that is preferred for prototyping circuits.

```
reg = "us-west-1";
bucketPath = "s3://amazon-braket-mathworks/doc-example";
device = quantum.backend.QuantumDeviceAWS("SV1",Region=reg,S3Path=bucketPath)

device =

QuantumDeviceAWS with properties:

    Name: "SV1"

DeviceARN: "arn:aws:braket:::device/quantum-simulator/amazon/sv1"
    Region: "us-west-1"
    S3Path: "s3://amazon-braket-mathworks/doc-example"
```

Note If you receive an error or warning while connecting to a device in this step, then your connection to AWS might not be set up properly. See "Set Up Access to AWS" on page 17-29 for more information.

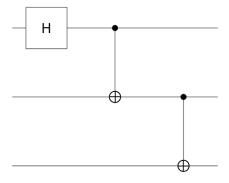
Use fetchDetails to get additional information about the device.

fetchDetails(device)

```
ans =
    struct with fields:
        deviceArn: "arn:aws:braket:::device/quantum-simulator/amazon/sv1"
    deviceCapabilities: "{"service": {"braketSchemaHeader": {"name": "braket.device_schema.device_service_properties",..."
        deviceName: "SV1"
        deviceStatus: "ONLINE"
        deviceType: "SIMULATOR"
        providerName: "Amazon Braket"
```

Create Task to Run Circuit

Create a quantum circuit with three qubits and three gates, and then plot the circuit.



When a circuit is measured on quantum hardware, the superposition of states for the qubits collapses into a single state, and that result is probabilistic. That is, the result of a measurement can change between runs, but the probability of each result follows the state probabilities produced by the gates in the circuit. So, it is common to run several shots, or trials, of a circuit to reveal the underlying probability distribution of results. By default, the run method uses 100 shots.

Create a task to run the circuit on the device.

```
task = run(C,device)

task =
   QuantumTaskAWS with properties:
    Status: "queued"
   TaskARN: "arn:aws:braket:us-west-1:123456789012:quantum-task/1234abcd-ef56-7890-abc2-34de56f678ab"
```

Quantum devices have limited availability, so tasks are often queued for execution. Once a task is finished, the Status property of the task object has a value of "finished". Check the status of a task by querying the Status property periodically, or use the wait method to internally check the status until the task is finished.

```
wait(task)
```

You can use cancel to cancel the task when needed. Canceling has no effect unless the status of the task is "queued".

Fetch Measurement Output

Once the task is finished, retrieve the result of running the circuit by using fetchOutput.

Examine the measured states and their counts in a table. The counts can change slightly from run to run, but will tend to be evenly divided between the two possible states.

See Also

quantumCircuit | quantum.backend.QuantumDeviceAWS |
quantum.backend.QuantumTaskAWS | quantum.gate.QuantumMeasurement

Related Examples

- "Introduction to Quantum Computing" on page 17-2
- "Local Quantum State Simulation" on page 17-25
- "Graph Coloring with Grover's Algorithm" on page 17-34

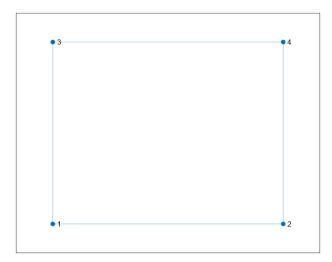
Graph Coloring with Grover's Algorithm

Note Installation Required: This functionality requires MATLAB Support Package for Quantum Computing. Install the support package from **Add-On Explorer** using the instructions in "Get and Manage Add-Ons".

This example shows how to use Grover's algorithm to solve graph coloring problems. Grover's algorithm works generically for any problem where a bit string of a given length is classified as valid or invalid, and the goal is to retrieve one of the valid bit strings. The algorithm uses a state oracle to determine whether a bit string is valid. Although this application of Grover's algorithm is not the most efficient method to solve the graph coloring problem in practice, it illustrates how a quantum algorithm can be applied to a well-known problem.

Create State Oracle for Graph Coloring Problem

Create a graph with four nodes and four edges connecting them.



Because the graph has only four nodes and four edges, there are a limited number of ways to color the nodes in the graph. If each node can be one of two different colors, then there are $2^4 = 16$ ways to color the graph nodes.

A solution of the graph coloring problem is a color assignment such that adjacent nodes are not the same color. Therefore, the quantum state oracle must check that for each edge in a given graph, the nodes it connects have different colors. The oracle accomplishes this check by accepting a bit string of length 4 (represented by 4 qubits), each of which represents the color of one node, and determining whether the colors produce a valid graph coloring.

Create Oracle

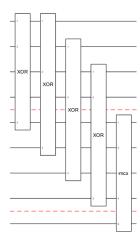
As a first step to creating the oracle, create a helper circuit called xorGate. This circuit reads qubits 1 and 2, and flips qubit 3 from $|0\rangle$ to $|1\rangle$ if qubits 1 and 2 have different values.

Next, loop through all edges in the graph and write the value of xorGate applied to the startNode and endNode qubits into a new helper qubit representing the edge. This increases the number of qubits from 4 to 8 because there are four edges. The first four qubits represent the bit string to evaluate, while the other qubits begin in state $|0\rangle$ before xorGate is applied.

Next, the oracle must verify that the helper qubits representing the edges are in state $|1\rangle$, since xorGate returns $|1\rangle$ when the two nodes connected by the edge have different states. This verification requires the addition of a ninth qubit that has a state of $|1\rangle$ when the coloring is valid, and $|0\rangle$ otherwise. Use the mcxGate function to determine the value of this final qubit, and create a circuit for the oracle.

Plot the circuit representing the oracle to view all of the qubits and gates. Use the QubitBlocks option to draw red lines between the different groups of qubits: the first four qubits at the top of the circuit diagram represent the node colors being checked, the next four qubits are the helper qubits to check the nodes connected by each edge, and the final qubit at the bottom determines whether the graph coloring is valid.

```
plot(oracle,QubitBlocks=[4 4 1])
```



Check Initial Oracle Behavior

Construct two input configurations, one valid (1001) and one invalid (1111), and apply the oracle circuit to each of them to check its behavior. The input configuration is encoded in the left-most four characters of each bit string, and the value of interest is the last qubit (the right-most character) in the output bit string.

Start with the invalid coloring 1111, where all nodes are the same color.

```
invalidColors = "111100000";
inputState1 = quantum.gate.QuantumState(invalidColors);
formula(inputState1)

ans =
    "1 * |111100000>"

outputState1 = simulate(oracle,inputState1);
formula(outputState1)

ans =
    "1 * |111100000>"
```

The last qubit of the simulated state is 0, so the oracle correctly determines that not all of the nodes can be the same color. Next, check the coloring 1001.

```
validColors = "1001000000";
inputState2 = quantum.gate.QuantumState(validColors);
formula(inputState2)

ans =
    "1 * |100100000>"

outputState2 = simulate(oracle, inputState2);
formula(outputState2)

ans =
    "1 * |100111111>"
```

In this case, the last qubit is 1, so 1001 is a valid graph coloring, where each edge connects nodes of different colors. This check confirms that the behavior of the oracle is correct for these two cases.

Refine Oracle into State Oracle

The oracle currently works correctly, but it alters the input bits during execution. A requirement of Grover's algorithm is that the oracle must be a state oracle. That is, after the oracle is applied to a standard state, the bit values must be the same as the input state with only the phase changing. A valid bit string (indicating a valid coloring of the graph) should have a phase of -1 after the oracle operates, while an invalid bit string should have an unchanged phase of 1 after the oracle operates. Achieving this behavior requires additional modifications to the oracle.

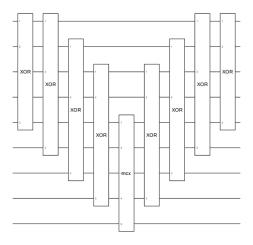
Start by adding gates that revert all the helper qubits for the edges to $|0\rangle$ by flipping any values that were previously flipped.

Next, note how state $|-\rangle = (|0\rangle - |1\rangle)/\sqrt{2}$ interacts with the X gate. Applying the X gate, which flips between the states $|0\rangle$ and $|1\rangle$, flips the phase of the $|-\rangle$ state:

 $X|-\rangle = X(|0\rangle - |1\rangle)/\sqrt{2} = (|1\rangle - |0\rangle)/\sqrt{2} = -|-\rangle$. This behavior is ideal for the last qubit in the oracle. So, passing that qubit into the oracle in state $|-\rangle$ ensures that the output bit string is the same as the input, while indicating valid graph colorings with an altered phase of -1.

Plot the final circuit for the state oracle.

plot(oracle)



Check Final State Oracle Behavior

To check the behavior of the state oracle, use the same two input bit strings as before. Start with the invalid graph coloring 1111, where all nodes are the same color.

```
invalidColors = "11110000-";
inputState1 = quantum.gate.QuantumState(invalidColors);
formula(inputState1)
ans =
    "1 * |11110000->"
```

```
outputState1 = simulate(oracle,inputState1);
formula(outputState1)
ans =
   "1 * |11110000->"
```

The oracle correctly determines that the graph coloring is not valid. The phase of the output bits is unchanged. Next, check the coloring 1001.

```
validColors = "10010000-";
inputState2 = quantum.gate.QuantumState(validColors);
formula(inputState2)

ans =
    "1 * |10010000->"

outputState2 = simulate(oracle,inputState2);
formula(outputState2)

ans =
    "(-1-3.8858e-16i) * |10010000->"
```

In this case, the state oracle correctly flips the phase to -1 because the graph coloring is valid. The small nonzero imaginary part is due to floating-point round-off error.

State Oracle Code

This function creates a state oracle circuit for a specified input graph.

```
function oracle = oracleGraphColoring(g)
xorInnerGates = [cxGate(1,3);
                  cxGate(2,3)];
xorGate = quantumCircuit(xorInnerGates,Name="XOR");
[startNodes,endNodes] = findedge(g);
N = numnodes(g);
E = numedges(g);
gates = [];
for k = 1:E
  gates = [gates;
           compositeGate(xorGate,[startNodes(k),endNodes(k),N+k])];
lastQubit = N+E+1;
gates = [gates; mcxGate(N+(1:E),lastQubit,[])];
oracle = quantumCircuit(gates,lastQubit);
oracle.Name = "Oracle
oracle.Gates = [oracle.Gates;
                 flip(oracle.Gates(1:end-1))];
```

Create Diffuser Circuit

Grover's algorithm combines a state oracle with a diffuser. The combined action of these two composite gates is a reflection in the plane spanned by $|e\rangle$ (a vector of all equal values representing a superposition of all states) and $|t\rangle$ (the target state). The diffuser applies the reflection $I_N-2|e\rangle\langle e|$.

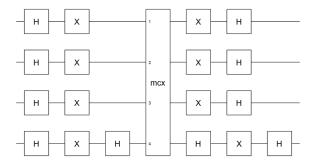
Diffuser Code

This function creates a diffuser circuit with a specified number of nodes. Save this function in a file on the MATLAB path.

Check Diffuser Behavior

Create a diffuser circuit for the four-node graph coloring problem and plot the circuit.

```
diffuserG = diffuser(N);
plot(diffuserG)
```



Verify that the diffuser applies a reflection of $I_N - 2|e\rangle\langle e|$ by comparing the circuit matrix of diffuserG with a manually constructed reflection matrix.

```
e = ones(2^N,1);
e = e/norm(e);
M = eye(2^N) - 2*(e*e');
norm(getMatrix(diffuserG) - M)
ans =
    1.2243e-15
```

The result is zero (up to round-off error), which confirms that the diffuser circuit applies the expected reflection.

Apply Grover's Algorithm to Graph Coloring Oracle

First, create a quantum circuit with the number of qubits required by the oracle. Bring the qubits representing node colors into superposition by applying hGate. Bringing these qubits into superposition represents all combinations of states equally, which is a common step at the beginning of quantum algorithms. Then, set the last qubit into state |-> by applying xGate followed by hGate.

-0.17678 * |010000001> + 0.17678 * |010100000> +

0.17678 * |100000000> + -0.17678 * |100000001> + 0.17678 * |100100000> + -0.17678 * |100100001> + 0.17678 * |101000000> + -0.17678 * |101000001> + 0.17678 * |101100000> + -0.17678 * |101100001> + 0.17678 * |110000000> + -0.17678 * |110000001> + 0.17678 * |110100000> + -0.17678 * |110100001> + 0.17678 * |111000000> + -0.17678 * |111000001> + 0.17678 * | 1111100000> + -0.17678 * |111100001>"

|010100001> +

|011000000> +

|011000001> +

|011100000> +

|011100001> +

-0.17678 *

0.17678 *

-0.17678 *

0.17678 *

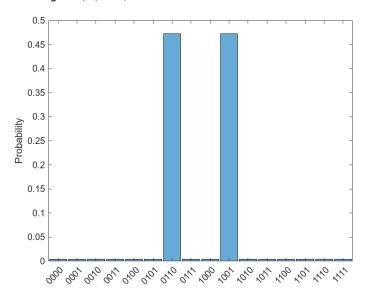
-0.17678 *

```
gates = [hGate(1:N);
         xGate(oracle.NumQubits);
         hGate(oracle.NumQubits)];
c = quantumCircuit(gates);
Check the circuit setup to make sure it produces the expected state.
s = simulate(c);
formula(s)
ans =
    "1 * |++++0000->"
Express the formula in the Z basis to confirm that all combinations of states are represented equally.
formula(s, Basis="Z")
ans =
    "0.17678 * |000000000> +
     -0.17678 * |000000001> +
     0.17678 * |000100000> +
     -0.17678 * |000100001> +
     0.17678 * |001000000> +
     -0.17678 * |001000001> +
     0.17678 * |001100000> +
     -0.17678 * |001100001> +
     0.17678 * |010000000> +
```

Next, apply the oracle and diffuser composite gates two times in the circuit and then plot the resulting circuit. (The number of times that the oracle and diffuser need to be applied depends on the angle of rotation for a given problem, which can be determined based on what percentage of the possible inputs are valid. You can try applying the oracle and diffuser different numbers of times to view the effect on the outputs.)

Simulate the circuit to see which node colorings are most likely to be measured. Plot a histogram of the results for the first four qubits.

s = simulate(c); histogram(s,1:4)



Use querystates to view the same information as a table.

```
[outputBits,probabilities] = querystates(s,1:4);
T = table(outputBits,probabilities);
T = sortrows(T,"probabilities","descend")
T =
```

16×2 table	
outputBits	probabilities
"1001"	0.47266
"0110"	0.47266
"1000"	0.0039063
"0001"	0.0039063
"0111"	0.0039063
"1110"	0.0039063
"1101"	0.0039063
"0100"	0.0039063
"0101"	0.0039063
"1011"	0.0039063
"1100"	0.0039063
"0010"	0.0039063
"0011"	0.0039063
"1010"	0.0039063
"0000"	0.0039062
"1111"	0.0039062

The simulation results show that the two states most likely to be measured are 0110 and 1001, which are the two possible valid graph colorings.

Run Circuit on AWS

Simulating a circuit locally can give an indication of the most probable results on a quantum machine, but running actual calculations on a quantum machine still has probabilistic results. Therefore, it is common to run the same circuit several times on a quantum machine to get a good estimate of the probability of each output. The number of trials is referred to as the number of shots.

To run circuits on AWS, you need an AWS account with access to AWS Braket. See "Run Quantum Circuit on Hardware Using AWS" on page 17-29 for more information on how to set up access and see available devices.

First, connect to a quantum device using quantum.backend.QuantumDeviceAWS. Specify the name of the device as well as its region and the path of the bucket to store results.

```
reg = "us-east-1";
bucketPath = "s3://amazon-braket-mathworks/doc-examples";
device = quantum.backend.QuantumDeviceAWS("5V1",Region=reg,S3Path=bucketPath)

device =

QuantumDeviceAWS with properties:

    Name: "SV1"

DeviceARN: "arn:aws:braket:::device/quantum-simulator/amazon/sv1"
    Region: "us-east-1"
    S3Path: "s3://amazon-braket-mathworks/doc-examples"
```

Create a task to run the circuit on the device. By default, run uses 100 shots.

```
task = run(c,device)
task =
  QuantumTaskAWS with properties:
```

```
Status: "queued"
TaskARN: "arn:aws:braket:us-east-1:123456789012:quantum-task/1234abcd-ef56-7890-abc2-34de56f678ab"
```

Quantum devices have limited availability, so tasks are often queued for execution. Once the task is finished, the Status property of the task object has a value of "finished". Check the status of the task by querying the Status property periodically, or use the wait method to internally check the status until the task is finished.

```
wait(task)
```

Once the task is finished, retrieve the result of running the circuit by using fetchOutput.

Display the measurement results for the circuit.

```
T = table(R.Counts, R.MeasuredStates, VariableNames=["Counts", "States"])
```

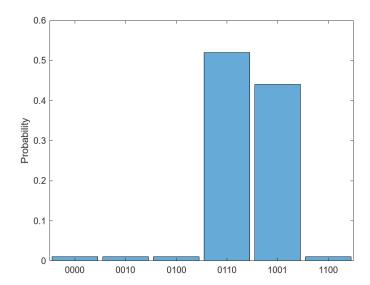
T =

8×2 table

Counts	States
1	"000000001"
1	"001000001"
1	"010000001"
28	"011000000"
24	"011000001"
22	"100100000"
22	"100100001"
1	"110000001"

Plot a histogram of the results for the first four qubits, which correspond to the node colors.

```
histogram(R,1:4)
```



The results agree with the local simulation, showing 0110 and 1001 as valid graph colorings. The results solve the graph coloring problem by indicating that nodes 2 and 3 in the graph can be the same color and that nodes 1 and 4 can be the same color.

See Also

 $\verb"quantumCircuit" | \verb"quantum.gate.QuantumState" | \verb"quantum.gate.QuantumMeasurement" | \verb"quantum.gate.QuantumMeasurement" | \verb"quantum.gate.Quantu$

Related Examples

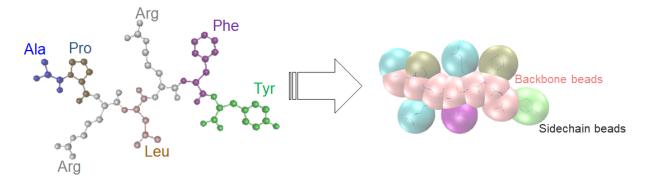
- "Introduction to Quantum Computing" on page 17-2
- "Types of Quantum Gates" on page 17-18

Ground-State Protein Folding Using Variational Quantum Eigensolver (VQE)

Note Installation Required: This functionality requires MATLAB Support Package for Quantum Computing. Install the support package from **Add-On Explorer** using the instructions in "Get and Manage Add-Ons".

This example shows an efficient method for using qubits to encode a protein fold on a 3-D tetrahedral lattice [1],[2]. The ground-state is found through a simulated variational quantum eigensolver (VQE) routine. The final circuit from the simulation is run on a real QPU for comparison. Running this example requires Global Optimization Toolbox as well as MATLAB Support Package for Quantum Computing.

The protein is a neuropeptide with seven amino acids, APRLRFY, pictured below. The example assumes a coarse-grained protein model, where "beads" representing amino acids can traverse the lattice and interact with each other. Each bond between amino acids can be in one of four directions, corresponding to corners of a tetrahedron. These four turns can be represented by two qubits.



Model Protein Fold with Qubits

The purpose of the embedding methods of [1] and [2] is to model the physical pairwise interaction energy of the protein beads while also imposing energy penalties on unrealistic configurations (such as overlaps or beads on the same lattice site). Therefore, the example is configurable in that you can modify the amino acid letters to test the effects on folding. However, the example code assumes a protein with seven amino acids, so you cannot change the length of the protein string.

Configuration Qubits

A protein of N beads (here N=7) can make N-1 turns, therefore 2*(N-1)=12 bits are required for the APRLRFY protein bonds. However, without loss of generality, the first two turns can be fixed to 01 and 00. One of the bits in the third turn is fixed due to other symmetry considerations. The turn2qubit mapping depicts the 12 bits, denoting the value of the 5 that are fixed, and the 7 that are variable which will be represented by qubits. For details, see the dense encoding scheme in [2].

```
hyperParams.protein = 'APRLRFY';
hyperParams.turn2qubit = '0100q1qqqqqq';
hyperParams.numQubitsConfig = sum(hyperParams.turn2qubit=='q');
```

Interaction Qubits

The methods of [1] and [2] can consider interactions between an arbitrary number of nearest-neighbors (NN). This example only considers 1-NN interaction terms, which are only possible between some beads due to the structure of the lattice. Beads separated by less than 5 bonds cannot be 1-NN (Eq. 29 of [2]). There are two interaction pairs in the length-7 protein, between beads 1 and 6, and between beads 2 and 7. Two interaction bits are used to specify whether there is any interaction between the beads in each of these pairs.

```
hyperParams.numQubitsInteraction = 2;
```

A matrix of contact energy values is used as a look-up table for pairwise interaction between different amino acids. For this example, the values are chosen at random.

Save the buildMJInteractions function in a separate file on the path.

```
function mat = buildMJInteractions(protein)
% Create the MJ interaction energy matrix for the protein, specified with
% 1-letter codes
N = length(protein);
mat = zeros(N,N);
rng(29507)
MJ = rand(20)*-6;
MJ = triu(MJ) + triu(MJ, 1)';
acids = ["C","M","F","I","L","V","W","Y","A","G","T","S","N","Q","D","E","H","R","K","P"];
acid2idx = dictionary(acids, 1:20);
for i = 1:N
    for i=1:N
        mat(i,j) = MJ(acid2idx(protein(i)), acid2idx(protein(j)));
    end
end
end
```

Call the buildMJInteractions function to find the interaction energies for the protein.

hyperParams.interactionEnergy = buildMJInteractions(hyperParams.protein);

Write Function to Calculate Energy of Folds

The exactHamiltonian function calculates the energy for each possible fold of the protein. Only 1-NN interactions are considered, and energy penalties are imposed for unrealistic configurations.

Save the exactHamiltonian function in a separate file on the path.

```
function energies = exactHamiltonian(bitstrings,hyperParams)
% Compute the Hamiltonian for each bit string (i.e., the energy for each fold).
% See [2] for details. This does not consider the Hch constraint from
% side-chains and the interaction term is only 1-nearest-neighbor (1-NN).
% H = Hgc + Hin_1
lambdaDis = 720;  % Penalty for interaction distance
lambdaLoc = 20;  % Penalty for interaction location
lambdaBack = 50;  % Penalty for unphysical geometry
energies = zeros(size(bitstrings,1),1);
numBeads = length(hyperParams.protein);
```

```
for idx = 1:length(energies)
    bitstring = bitstrings(idx,:);
    config = hyperParams.turn2qubit;
    config(config=='q') = bitstring(1:hyperParams.numQubitsConfig);
    turns = bin2dec(reshape(config,2,numBeads-1)');
   %% Geometric Hamiltonian Hgc
   % Count number of adjacent turns which are equal and impose a penalty for each
    energies(idx) = lambdaBack*sum(turns(1:end-1) == turns(2:end));
    % 1-NN Interaction Hamiltonian Hin
    currInteractionQubit = hyperParams.numQubitsConfig;
    for i=1:(numBeads-4)
       for j=(i+5):2:numBeads
           currInteractionQubit = currInteractionQubit+1;
           if bitstring(currInteractionQubit)=='0'
               continue;
           end
           % Add the interaction energy
           energies(idx) = energies(idx) + hyperParams.interactionEnergy(i,j);
           % Compute distances between interacting beads
           deltaN ij = zeros(1,4);
           deltaN_ir = zeros(1,4);
           deltaN mj = zeros(1,4);
           for k=0:3
               deltaN_{ij}(k+1) = (-1).^{(i:j-1)*}(turns(i:j-1) == k);
               deltaN ir(k+1) = (-1).^{(i:j-2)*}(turns(i:j-2) == k);
               deltaN_mj(k+1) = (-1).^{(i+1:j-1)*}(turns(i+1:j-1) == k);
           end
           d_ij = norm(deltaN_ij)^2;
           d_ir = norm(deltaN_ir)^2;
           d mj = norm(deltaN mj)^2;
           % Add penalty for distance not equal to 1
           energies(idx) = energies(idx) + lambdaDis*(d ij-1);
           % Add penalty for unphysical nearest neighbour collisons
           energies(idx) = energies(idx) + lambdaLoc*(2-d ir);
           energies(idx) = energies(idx) + lambdaLoc*(2-d mj);
           if i-1 >= 1
               for k=0:3
                   deltaN mj(k+1) = (-1).^{(i-1:j-1)*}(turns(i-1:j-1) == k);
               d mj = norm(deltaN mj)^2;
               energies(idx) = energies(idx) + lambdaLoc*(2-d_mj);
           end
           if j+1 <= numBeads</pre>
               for k=0:3
                   deltaN_ir(k+1) = (-1).^(i:j)*(turns(i:j) == k);
               d ir = norm(deltaN ir)^2;
               energies(idx) = energies(idx) + lambdaLoc*(2-d_ir);
```

```
end
end
end
end
```

-4.7973

Compute Minimum Energy for All Folds

Nine qubits are required to fully model a fold (7 configuration qubits and 2 interaction qubits). Use the exactHamiltonian function directly with all possible bit strings (each representing a possible fold), to find the minimum energy fold. You can later compare this value to the result of the quantum-based optimization. This exhaustive search is realistic for small proteins, but is not practical for larger proteins since the number of combinations of folds grows quickly.

```
hyperParams.numQubitsTotal = hyperParams.numQubitsConfig + hyperParams.numQubitsInteraction;
allFolds = dec2bin(0:2^hyperParams.numQubitsTotal-1,hyperParams.numQubitsTotal);
allEnergies = exactHamiltonian(allFolds,hyperParams);
hyperParams.GroundState.Energy = min(allEnergies);
hyperParams.GroundState.Index = find(allEnergies == hyperParams.GroundState.Energy);
allFolds(hyperParams.GroundState.Index,:)
ans =
    '1010000110'
    '101000110'
    '1010001010'
```

There are two lowest-energy folds because the last amino acid can occupy either position in the lattice. Find the energy of each of the identified folds.

```
allEnergies(hyperParams.GroundState.Index)
ans = 2×1
    -4.7973
```

This minimum-energy value matches the interaction energy between beads 1 and 6.

Write CVaR-VQE Objective Function

Next, use a quantum circuit to translate this optimization problem over a set of bit strings into a different optimization problem, this one over a set of angles between -pi and pi. These angles have no connection to the angles between the protein beads. The objective function accepts the set of angles for use inside of the quantum circuit, and the circuit returns various bit strings with different probabilities. Call the exactHamiltonian function on the bit strings returned by the quantum circuit, and use a weighted mean of the smaller energies computed as the value of the objective function.

Specifically, after the energy is computed for each observed fold, the associated probabilities are sorted by energy. The objective function returns an expectation energy computed from the tail end of the probability distribution, cutoff by an alpha parameter. This expectation energy is a conditional value at risk (CVaR). An alpha value of 0.05 was used experimentally in [1], but for a noise-free simulation ProteinVQEObjective uses a smaller cutoff value of 0.025.

Save the ProteinVQEObjective function in a separate file on the path.

```
function [energy, maxProbFold] = ProteinVQEObjective(parameters, hyperParams)
% Construct and simulate the variational circuit
ansatz = ProteinConfigAnsatz(parameters);
qState = simulate(ansatz);
allProbs = (gState.Amplitudes).^2;
% There are 10 qubits in the circuit, but only these 9 are used to define a fold
foldQubits = [1:8 10];
% Get the most probable fold
% Only compute this if second output maxProbFold is requested
if nargout > 1
    [\sim,idx] = max(allProbs);
   maxProbKet = char(qState.BasisStates(idx));
   maxProbFold = maxProbKet(foldQubits);
end
% Sample, and guery/get the states and probabilities of the fold qubits
qMeasurement = randsample(qState, hyperParams.numShots);
[states, probs] = querystates(qMeasurement, foldQubits);
% Sort the probabilities by the energy
[energies,sort idx] = sort(exactHamiltonian(char(states), hyperParams));
probs = probs(sort_idx);
% Compute CVaR over the low energy tail of the energy distribution,
% delimited by a cutoff parameter alpha.
alpha = .025;
cut idx = nnz(cumsum(probs) < alpha);</pre>
cvar probs = probs(1:cut idx);
cvar_probs(end+1) = alpha - sum(cvar_probs);
% Compute expectation energy as the sum of cutoff state energies weighted by their probability
energy = dot(cvar probs, energies(1:cut idx+1))/alpha;
end
Define the number of shots to use in ProteinVQEObjective, and create a function handle that
```

passes in all of the parameter values to ProteinVQEObjective.

```
hyperParams.numShots = 1024;
objFcn = @(theta) ProteinVQEObjective(theta,hyperParams);
```

Create Circuit Ansatz

Create and plot the variational circuit ansatz for this protein with random angles. Qubits 1-7 represent the configuration, and the other three gubits are for the interaction (including a helper qubit that does not get measured). This circuit can be found as Figure 3 in [1].

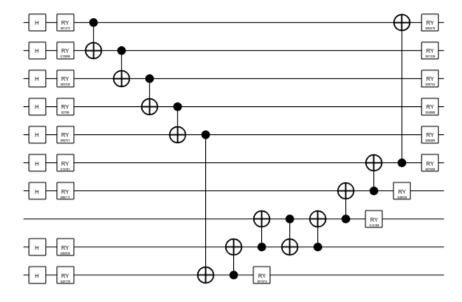
Save the ProteinConfigAnsatz function in a separate file on the path.

```
function ansatz = ProteinConfigAnsatz(parameters)
% Create the circuit ansatz for a 7 amino acid neuropeptide (10 qubit circuit).
parameters = reshape(parameters, [2 9]);
gates = [hGate([1:7 9 10])]
         ryGate([1:7 9 10], parameters(1,:))
         cxGate(1:4, 2:5)
```

```
cxGate(5,10)
    cxGate(10,9)
    cxGate(9,8)
    cxGate(8,9)
    cxGate(9,8)
    cxGate([8 7 6], [7 6 1])
    ryGate([1:8 10], parameters(2,:))
];
ansatz = quantumCircuit(gates);
end
```

Call ProteinConfigAnsatz with random angles to construct the circuit. Plot the circuit to view the qubits and gates.

```
ansatz = ProteinConfigAnsatz(rand(2,9));
plot(ansatz)
```



Simulate Iterations of CVaR-VQE

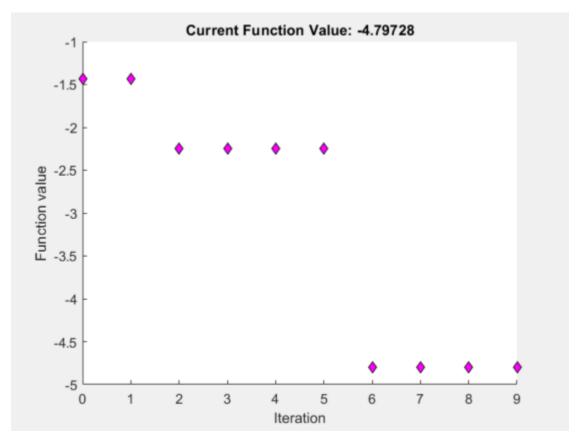
There are two layers of RY rotation gates over the configuration and interaction qubits. These rotation angles are learned parameters in the variational circuit. Use <code>surrogateopt</code> (Global Optimization Toolbox) with the objective function to find the set of RY rotation angles that produce the minimum expectation energy. The original paper [1] uses a genetic algorithm to find the rotation angles. <code>surrogateopt</code> converges to similar values, but because it uses intervals internally, the convergence behavior is comparatively different.

Define the number of angles and set options for the maximum number of function evaluations, plotting function, and initial points. Then call surrogateopt with the objective function, upper and lower bounds for the angles, and options.

```
numAngles = 2*hyperParams.numQubitsTotal;
rng default

options = optimoptions("surrogateopt",...
    "MaxFunctionEvaluations",10, ...
    "PlotFcn", "optimplotfval",...
    "InitialPoints",pi*ones(numAngles,1));

lb = repmat(-pi,numAngles,1);
ub = repmat(pi,numAngles,1);
[angles,minEnergy] = surrogateopt(objFcn,lb,ub,[],[],[],[],[],options);
```



surrogateopt stopped because it exceeded the function evaluation limit set by 'options.MaxFunctionEvaluations'.

Call the objective function using the optimized angles to find the state bit string with highest probability as well as its associated energy.

```
[groundStateEnergy,groundStateFold] = ProteinVQEObjective(angles,hyperParams)
groundStateEnergy = -4.7973
groundStateFold = '1010000110'
```

This ground-state fold is one of the two folds obtained earlier with the minimum energy calculation. ${\tt allFolds(allEnergies==minEnergy,:)}$

```
ans =
```

```
2×9 char array
'101000110'
'101001010'
```

To visualize the ground-state fold, save the plotProtein function in a separate file on the path. This function enables you to plot the protein structure from the qubit values.

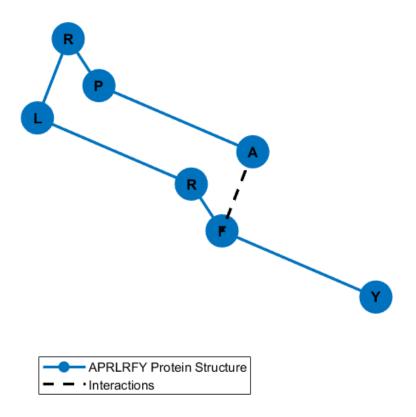
```
function plotProtein(bitstring,hyperParams)
% Plot protein structure from the bitstring
% The input bitstring is expected to be of length 9, with the first 7 bits
% specifying turns in direction in the structure, and the last 2 bits
% specifying interactions between beads.
% Number of beads
N = length(hyperParams.protein);
% Construct 3D coordinates representing the 4 corners of a tetrahedron
% centered in 0. These represent the 4 directions each new bead might
% be added on in a tetrahedral grid.
turn2bead = ones(4,3);
turn2bead(2:4,:) = -1+2*eye(3);
% Construct complete bitstring by inserting input bitstring into
% the complete string mask.
completeBitstring = hyperParams.turn2qubit;
completeBitstring(completeBitstring=='q') = bitstring(1:hyperParams.numQubitsConfig);
% Each pair of bits is converted into a number between 0 and 3
turns = bin2dec(reshape(completeBitstring,2,[])');
% Change direction in which we follow the tetrahedral grid in each bead
% on the line.
signs = (-1).^{(0:N-1)'};
% Compute placements of each bead.
beads = cumsum(signs.*[zeros(1,3);turn2bead(turns+1,:)]);
% Plot the beads connecting by lines, and add a text label to each
plot3(beads(:,1),beads(:,2),beads(:,3),'.-','LineWidth',2,'MarkerSize',80,'SeriesIndex',1)
axis off
viewDir = -[6 \ 4 \ 1];
view(viewDir);
% Plot text, ensuring it is in front of the lines
beadsText = beads + 0.03*viewDir;
text(beadsText(:,1),beadsText(:,2),beadsText(:,3),hyperParams.protein', ...
    'FontWeight', 'bold', 'HorizontalAlignment','center')
% Whether there are interactions between any pair of beads is determined
% by the additional bits in the string.
interactions = [];
currInteractionQubit = hyperParams.numQubitsConfig+1;
for i=1:(N-5)
```

```
for j=(i+5):2:N
    if bitstring(currInteractionQubit) == '1'
        interactions = [interactions; beads(i,:); beads(j,:); nan*ones(1,3)]; %#ok<AGROW>
    end
    currInteractionQubit = currInteractionQubit+1;
end
end

if ~isempty(interactions)
    hold on
    plot3(interactions(:,1),interactions(:,2),interactions(:,3),'k--','LineWidth',2)
    hold off
    legend([hyperParams.protein+" Protein Structure"; "Interactions"], "Location", "southoutside")
else
    legend(hyperParams.protein+" Protein Structure", "Location", "southoutside")
end
end
```

The protein has two possible interactions considered in the 1-NN model. The fold with the lowest energy only has one of these interactions. Use plotProtein to visualize the lowest energy fold.

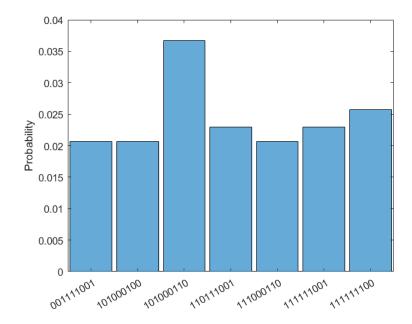
plotProtein(groundStateFold, hyperParams)



Next, construct the quantum circuit using the optimized angles and simulate the circuit to see the expected probability distribution over states. Use a threshold to filter out states with probabilities

less than 2%. The ground-state fold 101000110 appears again as the state with the highest probability.

```
optimized_circuit = ProteinConfigAnsatz(angles);
sv = simulate(optimized_circuit);
histogram(sv,[1:8 10],Threshold=0.02)
```



Run Final Iteration on QPU

Connect to the IonQ device using quantum.backend.QuantumDeviceAWS. Specify the region of the device and path to a bucket to store results.

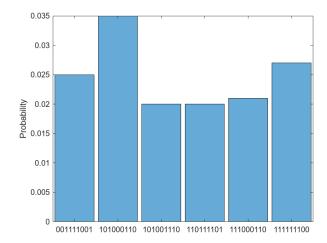
```
reg = "us-east-1";
bucketPath = "s3://amazon-braket-mathworks/doc-examples";
device = quantum.backend.QuantumDeviceAWS("IonQ Device", S3Path=bucketPath, Region=reg)
```

Create a task to run the circuit ansatz with optimized angles on the QPU. Specify the number of shots as 1,000.

```
task = run(optimized_circuit,device,NumShots=1000);
wait(task)
```

Fetch the results and plot a histogram of the states for all but the ninth qubit. Specify a lower threshold of 2% to filter out unlikely states.

```
results = fetchOutput(task);
histogram(results,[1:8 10],Threshold=0.02)
```



The ground-state fold 101000110 appears again as the state with the highest probability, so the QPU results agree with the local simulation of the circuit.

References

- [1] Robert, Anton, Panagiotis Kl. Barkoutsos, Stefan Woerner, and Ivano Tavernelli. "Resource-Efficient Quantum Algorithm for Protein Folding." *Npj Quantum Information* 7, no. 1 (February 17, 2021): 38. https://doi.org/10.1038/s41534-021-00368-4.
- [2] Robert, Anton, Panagiotis Kl. Barkoutsos, Stefan Woerner, and Ivano Tavernelli. "Supplementary Information for 'Resource-Efficient Quantum Algorithm for Protein Folding'" *Npj Quantum Information* 7, no. 1 (February 17, 2021): 38. https://doi.org/10.1038/s41534-021-00368-4.

See Also

quantumCircuit

Related Examples

- "Introduction to Quantum Computing" on page 17-2
- "Run Quantum Circuit on Hardware Using AWS" on page 17-29
- "Graph Coloring with Grover's Algorithm" on page 17-34