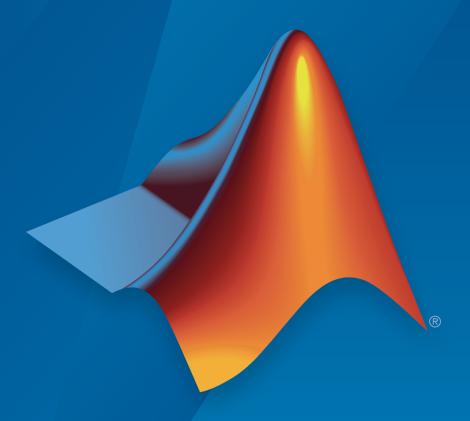
## MATLAB® Mathematics



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#### **Creating and Concatenating Matrices**

# In this section... "Overview" on page 1-2 "Constructing a Simple Matrix" on page 1-3 "Specialized Matrix Functions" on page 1-4 "Concatenating Matrices" on page 1-6 "Matrix Concatenation Functions" on page 1-7 "Generating a Numeric Sequence" on page 1-9

#### Overview

The most basic MATLAB® data structure is the *matrix*: a two-dimensional, rectangularly shaped data structure capable of storing multiple elements of data in an easily accessible format. These data elements can be numbers, characters, logical states of true or false, or even other MATLAB structure types. MATLAB uses these two-dimensional matrices to store single numbers and linear series of numbers as well. In these cases, the dimensions are 1-by-1 and 1-by-n respectively, where n is the length of the numeric series. MATLAB also supports data structures that have more than two dimensions. These data structures are referred to as *arrays* in the MATLAB documentation.

MATLAB is a matrix-based computing environment. All of the data that you enter into MATLAB is stored in the form of a matrix or a multidimensional array. Even a single numeric value like 100 is stored as a matrix (in this case, a matrix having dimensions 1-by-1):

```
A = 100;

whos A
Name Size Bytes Class

A 1x1 8 double array
```

Regardless of the class being used, whether it is numeric, character, or logical true or false data, MATLAB stores this data in matrix (or array) form. For example, 'Hello World' is a 1-by-11 matrix of individual character elements in MATLAB. You can also build matrices composed of more complex classes, such as MATLAB structures and cell arrays.

To create a matrix of basic data elements such as numbers or characters, see

- "Constructing a Simple Matrix" on page 1-3
- "Specialized Matrix Functions" on page 1-4

To build a matrix composed of other matrices, see

- "Concatenating Matrices" on page 1-6
- "Matrix Concatenation Functions" on page 1-7

#### Constructing a Simple Matrix

The simplest way to create a matrix in MATLAB is to use the matrix constructor operator, []. Create a row in the matrix by entering elements (shown as E below) within the brackets. Separate each element with a comma or space:

$$row = [E_1, E_2, ..., E_m]$$
  $row = [E_1 E_2 ... E_m]$ 

For example, to create a one row matrix of five elements, type

$$A = [12 62 93 -8 22];$$

To start a new row, terminate the current row with a semicolon:

```
A = [row_1; row_2; ...; row_n]
```

This example constructs a 3 row, 5 column (or 3-by-5) matrix of numbers. Note that all rows must have the same number of elements:

The square brackets operator constructs two-dimensional matrices only, (including 0-by-0, 1-by-1, and 1-by-n matrices). To construct arrays of more than two dimensions, see "Creating Multidimensional Arrays" on page 1-49.

For instructions on how to read or overwrite any matrix element, see "Matrix Indexing" on page 1-11.

#### **Entering Signed Numbers**

When entering signed numbers into a matrix, make sure that the sign immediately precedes the numeric value. Note that while the following two expressions are equivalent,

the next two are *not*:

#### **Specialized Matrix Functions**

MATLAB has a number of functions that create different kinds of matrices. Some create specialized matrices like the Hankel or Vandermonde matrix. The functions shown in the table below create matrices for more general use.

Function	Description			
ones	Create a matrix or array of all ones.			
zeros	Create a matrix or array of all zeros.			
eye	Create a matrix with ones on the diagonal and zeros elsewhere.			
accumarray	Distribute elements of an input matrix to specified locations in an output matrix, also allowing for accumulation.			
diag	Create a diagonal matrix from a vector.			
magic	Create a square matrix with rows, columns, and diagonals that add up to the same number.			
rand	Create a matrix or array of uniformly distributed random numbers.			
randn	Create a matrix or array of normally distributed random numbers and arrays.			
randperm	Create a vector (1-by-n matrix) containing a random permutation of the specified integers.			

Most of these functions return matrices of type double (double-precision floating point). However, you can easily build basic arrays of any numeric type using the ones, zeros, and eye functions.

To do this, specify the MATLAB class name as the last argument:

```
A = zeros(4, 6, 'uint32')
A =
  4×6 uint32 matrix
   0
       0
            0
                         0
   0
       0
            0
                     0
                         0
   0
       0
            0
                0
                     0
                         0
   0
            0
```

#### Examples

Here are some examples of how you can use these functions.

#### Creating a Magic Square Matrix

A magic square is a matrix in which the sum of the elements in each column, or each row, or each main diagonal is the same. To create a 5-by-5 magic square matrix, use the magic function as shown.

```
A = magic(5)
A =
                    1
    17
                           8
                                 15
            24
    23
             5
                   7
                          14
                                 16
     4
             6
                   13
                          20
                                 22
                          21
                                  3
    10
           12
                   19
    11
            18
                   25
                           2
                                  9
```

Note that the elements of each row, each column, and each main diagonal add up to the same value: 65.

#### Creating a Diagonal Matrix

Use diag to create a diagonal matrix from a vector. You can place the vector along the main diagonal of the matrix, or on a diagonal that is above or below the main one, as shown here. The -1 input places the vector one row below the main diagonal:

```
A = [12 62 93 -8 22];
```

```
B = diag(A, -1)
B =
      0
              0
                      0
                              0
                                      0
                                              0
     12
              0
                      0
                              0
                                      0
                                              0
      0
             62
                      0
                              0
                                      0
                                              0
      0
              0
                     93
                              0
                                      0
                                              0
      0
              0
                      0
                             - 8
                                      0
                                              0
      0
              0
                      0
                              0
                                     22
                                              0
```

#### **Concatenating Matrices**

Matrix concatenation is the process of joining one or more matrices to make a new matrix. The brackets [] operator discussed earlier in this section serves not only as a matrix constructor, but also as the MATLAB concatenation operator. The expression C = [A B] horizontally concatenates matrices A and B. The expression C = [A; B] vertically concatenates them.

This example constructs a new matrix C by concatenating matrices A and B in a vertical direction:

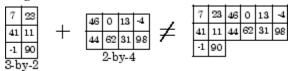
```
A = ones(2, 5) * 6;
                            % 2-by-5 matrix of 6's
B = rand(3, 5);
                            % 3-by-5 matrix of random values
C = [A; B]
                            % Vertically concatenate A and B
C =
    6.0000
               6.0000
                         6.0000
                                    6.0000
                                               6,0000
               6.0000
    6.0000
                         6.0000
                                    6.0000
                                               6.0000
    0.9501
               0.4860
                                    0.4447
                                               0.9218
                         0.4565
    0.2311
               0.8913
                         0.0185
                                    0.6154
                                               0.7382
    0.6068
               0.7621
                         0.8214
                                    0.7919
                                               0.1763
```

#### **Keeping Matrices Rectangular**

You can construct matrices, or even multidimensional arrays, using concatenation as long as the resulting matrix does not have an irregular shape (as in the second illustration shown below). If you are building a matrix horizontally, then each component matrix must have the same number of rows. When building vertically, each component must have the same number of columns.

This diagram shows two matrices of the same height (i.e., same number of rows) being combined horizontally to form a new matrix.

The next diagram illustrates an attempt to horizontally combine two matrices of unequal height. MATLAB does not allow this.



#### **Matrix Concatenation Functions**

The following functions combine existing matrices to form a new matrix.

Function	Description
cat	Concatenate matrices along the specified dimension
horzcat	Horizontally concatenate matrices
vertcat	Vertically concatenate matrices
repmat	Create a new matrix by replicating and tiling existing matrices
blkdiag	Create a block diagonal matrix from existing matrices

#### **Examples**

Here are some examples of how you can use these functions.

#### **Concatenating Matrices and Arrays**

An alternative to using the [] operator for concatenation are the three functions cat, horzcat, and vertcat. With these functions, you can construct matrices (or multidimensional arrays) along a specified dimension. Either of the following commands accomplish the same task as the command C = [A; B] used in the section on "Concatenating Matrices" on page 1-6:

```
C = vertcat(A, B); % Concatenate vertically
```

#### Replicating a Matrix

Use the repmat function to create a matrix composed of copies of an existing matrix. When you enter

```
repmat(M, v, h)
```

MATLAB replicates input matrix M v times vertically and h times horizontally. For example, to replicate existing matrix A into a new matrix B, use

```
A = [8 \ 1 \ 6; \ 3 \ 5 \ 7; \ 4 \ 9 \ 2]
A =
   8
        1
             6
   3
        5
             7
   4
        9
             2
B = repmat(A, 2, 4)
   8
        1
                        1
                            6
                                                           6
   3
        5
             7
                  3
                        5
                            7
                                  3
                                       5
                                            7
                                                 3
                                                      5
                                                           7
        9
             2
                       9
                            2
                                       9
                                            2
                                                      9
                                                           2
   4
                  4
                                  4
                                                4
                                  8
                                            6
   8
        1
             6
                  8
                       1
                            6
                                      1
                                                 8
                                                      1
                                                           6
   3
        5
             7
                  3
                        5
                             7
                                  3
                                       5
                                            7
                                                 3
                                                      5
                                                           7
   4
        9
             2
                   4
                        9
                             2
                                  4
                                            2
                                                      9
                                                           2
```

#### Creating a Block Diagonal Matrix

The blkdiag function combines matrices in a diagonal direction, creating what is called a block diagonal matrix. All other elements of the newly created matrix are set to zero:

```
A = magic(3);
B = [-5 -6 -9; -4 -4 -2];
C = eye(2) * 8;
D = blkdiag(A, B, C)
D =
   8
        1
            6
                 0
                      0
                          0
                               0
                                    0
            7
                 0
   3
        5
                      0
                          0
                               0
                                    0
        9
            2
   4
                 0
                      0
                          0
                               0
                                    0
            0
                - 5
   0
        0
                    -6
                          - 9
                               0
                                    0
   0
        0
            0
                - 4
                     - 4
                          -2
                               0
                                    0
   0
            0
                 0
                      0
                          0
                               8
                                    0
            0
                 0
                      0
                               0
                                    8
        0
                          0
```

#### **Generating a Numeric Sequence**

Because numeric sequences can often be useful in constructing and indexing into matrices and arrays, MATLAB provides a special operator to assist in creating them.

This section covers

- "The Colon Operator" on page 1-9
- "Using the Colon Operator with a Step Value" on page 1-10

#### The Colon Operator

The colon operator (first:last) generates a 1-by-n matrix (or *vector*) of sequential numbers from the first value to the last. The default sequence is made up of incremental values, each 1 greater than the previous one:

```
A = 10:15
A =
10 11 12 13 14 15
```

The numeric sequence does not have to be made up of positive integers. It can include negative numbers and fractional numbers as well:

```
A = -2.5:2.5

A = -2.5000 -1.5000 -0.5000 0.5000 1.5000 2.5000
```

By default, MATLAB always increments by exactly 1 when creating the sequence, even if the ending value is not an integral distance from the start:

```
A = 1:6.3
A =
1 2 3 4 5 6
```

Also, the default series generated by the colon operator always contains increments rather than decrements. The operation shown in this example attempts to increment from 9 to 1 and thus MATLAB returns an empty matrix:

```
A = 9:1
A =
    Empty matrix: 1-by-0
```

The next section explains how to generate a nondefault numeric series.

#### Using the Colon Operator with a Step Value

To generate a series that does not use the default of incrementing by 1, specify an additional value with the colon operator (first:step:last). In between the starting and ending value is a step value that tells MATLAB how much to increment (or decrement, if step is negative) between each number it generates.

To generate a series of numbers from 10 to 50, incrementing by 5, use

You can increment by noninteger values. This example increments by 0.2:

To create a sequence with a decrementing interval, specify a negative step value:

#### **Matrix Indexing**

#### In this section...

"Accessing Single Elements" on page 1-11

"Linear Indexing" on page 1-12

"Functions That Control Indexing Style" on page 1-12

"Assigning to Elements Outside Array Bounds" on page 1-13

"Accessing Multiple Elements" on page 1-13

"Using Logicals in Array Indexing" on page 1-16

"Single-Colon Indexing with Different Array Types" on page 1-19

"Indexing on Assignment" on page 1-20

#### **Accessing Single Elements**

To reference a particular element in a matrix, specify its row and column number using the following syntax, where A is the matrix variable. Always specify the row first and column second:

```
A(row, column)
```

For example, for a 4-by-4 magic square A,

you would access the element at row 4, column 2 with

For arrays with more than two dimensions, specify additional indices following the row and column indices. See the section on "Multidimensional Arrays" on page 1-47.

#### **Linear Indexing**

You can refer to the elements of a MATLAB matrix with a single subscript, A(k). MATLAB stores matrices and arrays not in the shape that they appear when displayed in the MATLAB Command Window, but as a single column of elements. This single column is composed of all of the columns from the matrix, each appended to the last.

So, matrix A

is actually stored in memory as the sequence

The element at row 3, column 2 of matrix A (value = 5) can also be identified as element 6 in the actual storage sequence. To access this element, you have a choice of using the standard A(3,2) syntax, or you can use A(6), which is referred to as *linear indexing*.

If you supply more subscripts, MATLAB calculates an index into the storage column based on the dimensions you assigned to the array. For example, assume a two-dimensional array like A has size [d1 d2], where d1 is the number of rows in the array and d2 is the number of columns. If you supply two subscripts (i, j) representing row-column indices, the offset is

$$(j-1) * d1 + i$$

Given the expression A(3,2), MATLAB calculates the offset into A's storage column as (2-1) \* 3 + 3, or 6. Counting down six elements in the column accesses the value 5.

#### **Functions That Control Indexing Style**

If you have row-column subscripts but want to use linear indexing instead, you can convert to the latter using the sub2ind function. In the 3-by-3 matrix A used in the previous section, sub2ind changes a standard row-column index of (3,2) to a linear index of 6:

```
A = [2 6 9; 4 2 8; 3 5 1];
```

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

To get the row-column equivalent of a linear index, use the ind2sub function:

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

#### **Assigning to Elements Outside Array Bounds**

When you assign to elements outside the bounds of a numeric array, MATLAB expands the array to include those elements and fills the missing values with **0**.

Assign a value to an element outside the bounds of A.

```
A = magic(4);

A(3,5) = 7

A =

16  2  3  13  0

5  11  10  8  0

9  7  6  12  7

4  14  15  1  0
```

When you extend structure and cell arrays, MATLAB fills unaddressed elements with an empty value. MATLAB fills unaddressed elements in categorical arrays with <undefined>. For datetime arrays, MATLAB fills unaddressed elements with NaT (Not-a-Time).

If you try to refer to elements outside an array on the right side of an assignment statement, MATLAB throws an error.

```
test = A(7,7)
```

Index exceeds matrix dimensions.

#### **Accessing Multiple Elements**

For the 4-by-4 matrix A shown below, it is possible to compute the sum of the elements in the fourth column of A by typing

```
A = magic(4);

A(1,4) + A(2,4) + A(3,4) + A(4,4)
```

You can reduce the size of this expression using the colon operator. Subscript expressions involving colons refer to portions of a matrix. The expression

```
A(1:m, n)
```

refers to the elements in rows 1 through m of column n of matrix A. Using this notation, you can compute the sum of the fourth column of A more succinctly:

```
sum(A(1:4, 4))
```

#### **Nonconsecutive Elements**

To refer to nonconsecutive elements in a matrix, use the colon operator with a step value. The m:3:n in this expression means to make the assignment to every third element in the matrix. Note that this example uses linear indexing:

MATLAB supports a type of array indexing that uses one array as the index into another array. You can base this type of indexing on either the values or the positions of elements in the indexing array.

Here is an example of value-based indexing where array B indexes into elements 1, 3, 6, 7, and 10 of array A. In this case, the *numeric values* of array B designate the intended elements of A:

```
A = 5:5:50
A =
            10
                    15
                           20
                                   25
                                          30
                                                  35
                                                         40
                                                                 45
                                                                         50
B = [1 \ 3 \ 6 \ 7 \ 10];
A(B)
ans =
      5
                    30
            15
                           35
                                   50
```

If you index into a vector with another vector, the orientation of the indexed vector is honored for the output:

```
A(B')
ans =

5   15   30   35   50

A1 = A'; A1(B)
ans =

5   15   30   35
50
```

If you index into a vector with a nonvector, the shape of the indices is honored:

```
C = [1 3 6; 7 9 10];
A(C)
ans =
5 15 30
35 45 50
```

#### The end Keyword

MATLAB provides the keyword end to designate the last element in a particular dimension of an array. This keyword can be useful in instances where your program does not know how many rows or columns there are in a matrix. You can replace the expression in the previous example with

```
B(1:3:end) = -10
```

**Note** The keyword end has several meanings in MATLAB. It can be used as explained above, or to terminate a conditional block of code such as if and for blocks, or to terminate a nested function.

#### Specifying All Elements of a Row or Column

The colon by itself refers to *all* the elements in a row or column of a matrix. Using the following syntax, you can compute the sum of all elements in the second column of a 4-by-4 magic square A:

```
sum(A(:, 2))
ans =
34
```

By using the colon with linear indexing, you can refer to all elements in the entire matrix. This example displays all the elements of matrix A, returning them in a columnwise order:

```
A(:)
ans =
16
5
9
4
.
.
.
```

#### **Using Logicals in Array Indexing**

A logical array index designates the elements of an array A based on their *position* in the indexing array, B, not their value. In this *masking* type of operation, every true element in the indexing array is treated as a positional index into the array being accessed.

In the following example, B is a matrix of logical ones and zeros. The position of these elements in B determines which elements of A are designated by the expression A(B):

```
A = [1 \ 2 \ 3; \ 4 \ 5 \ 6; \ 7 \ 8 \ 9]
A =
             2
                     3
      1
                     6
      4
             5
                     9
B = logical([0 1 0; 1 0 1; 0 0 1])
B =
  3×3 logical array
             0
   0
        1
   1
        0
             1
   0
        0
             1
```

```
A(B)
ans =
4
2
6
```

The find function can be useful with logical arrays as it returns the linear indices of nonzero elements in B, and thus helps to interpret A(B):

```
find(B)
ans = 2
4
8
9
```

#### Logical Indexing - Example 1

This example creates logical array B that satisfies the condition A > 0.5, and uses the positions of ones in B to index into A:

```
rng(0, 'twister'); % Reset the random number generator A = rand(5); B = A > 0.5; A(B) = 0 A =
```

0.0975	0.1576	0.1419	0
0.2785	0	0.4218	0.0357
0	0	0	0
0	0.4854	0	0
0	0	0	0
	0.2785	0.2785 0 0 0	0.2785 0 0.4218 0 0 0 0 0.4854 0

A simpler way to express this is

$$A(A > 0.5) = 0$$

#### Logical Indexing - Example 2

The next example highlights the location of the prime numbers in a magic square using logical indexing to set the nonprimes to 0:

```
A = magic(4)
A =
```

```
16
             2
                     3
                           13
      5
            11
                    10
                            8
      9
             7
                    6
                           12
      4
            14
                    15
                            1
B = isprime(A)
B =
  4×4 logical array
   0
        1
             1
                  1
   1
        1
             0
                  0
   0
        1
             0
                  0
   0
        0
             0
                  0
A(\sim B) = 0;
                                        % Logical indexing
             2
      0
                     3
                           13
      5
            11
                     0
                            0
      0
             7
                     0
                            0
      0
             0
                     0
                            0
find(B)
ans =
      2
      5
      6
      7
      9
     13
```

#### Logical Indexing with a Smaller Array

In most cases, the logical indexing array should have the same number of elements as the array being indexed into, but this is not a requirement. The indexing array may have smaller (but not larger) dimensions:

```
B =
    2×3 logical array
    0    1    0
    1    0    1
isequal(numel(A), numel(B))
ans =
    logical
    0
A(B)
ans =
    4
    7
    8
```

MATLAB treats the missing elements of the indexing array as if they were present and set to zero, as in array C below:

```
% Add zeros to indexing array C to give it the same number of
% elements as A.
C = logical([B(:);0;0;0]);
isequal(numel(A), numel(C))
ans =
   logical
   1

A(C)
ans =
   4
   7
   8
```

#### Single-Colon Indexing with Different Array Types

When you index into a standard MATLAB array using a single colon, MATLAB returns a column vector (see variable n, below). When you index into a structure or cell array using

a single colon, you get a comma-separated list (see "Access Data in a Structure Array" and "Access Data in a Cell Array" for more information.)

Create three types of arrays:

```
n = [1 2 3; 4 5 6];
c = {1 2; 3 4};
s = cell2struct(c, {'a', 'b'}, 1); s(:,2)=s(:,1);
```

Use single-colon indexing on each:

#### **Indexing on Assignment**

When assigning values from one matrix to another matrix, you can use any of the styles of indexing covered in this section. Matrix assignment statements also have the following requirement.

In the assignment A(J,K,...) = B(M,N,...), subscripts J,K,M,N, etc. may be scalar, vector, or array, provided that all of the following are true:

- The number of subscripts specified for B, not including trailing subscripts equal to 1, does not exceed ndims(B).
- The number of nonscalar subscripts specified for A equals the number of nonscalar subscripts specified for B. For example, A(5, 1:4, 1, 2) = B(5:8) is valid because both sides of the equation use one nonscalar subscript.
- The order and length of all nonscalar subscripts specified for A matches the order and length of nonscalar subscripts specified for B. For example, A(1:4, 3, 3:9)
  B(5:8, 1:7) is valid because both sides of the equation (ignoring the one scalar subscript 3) use a 4-element subscript followed by a 7-element subscript.

#### **Related Examples**

"Access Data Using Categorical Arrays"

- "Access Data in a Table"
- "Access Data in a Structure Array"
- "Access Data in a Cell Array"

# **Getting Information About a Matrix**

I	In this section
6	"Dimensions of the Matrix" on page 1-22
١	"Classes Used in the Matrix" on page 1-23
6	"Data Structures Used in the Matrix" on page 1-24

## **Dimensions of the Matrix**

These functions return information about the shape and size of a matrix.

Function	Description	
length	Return the length of the longest dimension. (The length of a matrix or array with any zero dimension is zero.)	
ndims	Return the number of dimensions.	
numel	Return the number of elements.	
size	Return the length of each dimension.	

The following examples show some simple ways to use these functions. Both use the 3-by-5 matrix A shown here:

```
A = 10*gallery('uniformdata',[5],0);
A(4:5, :) = []
A =
    9.5013
              7.6210
                         6.1543
                                    4.0571
                                              0.5789
    2.3114
              4.5647
                         7.9194
                                    9.3547
                                              3.5287
    6.0684
              0.1850
                         9.2181
                                    9.1690
                                              8.1317
```

## **Example Using numel**

Using the numel function, find the average of all values in matrix A:

```
sum(A(:))/numel(A)
ans =
    5.8909
```

## Example Using ndims, numel, and size

Using ndims and size, go through the matrix and find those values that are between 5 and 7, inclusive:

## Classes Used in the Matrix

These functions test elements of a matrix for a specific data type.

Function	Description	
isa	Detect if input is of a given data type.	
iscell	Determine if input is a cell array.	
iscellstr	Determine if input is a cell array of strings.	
ischar	Determine if input is a character array.	
isfloat	Determine if input is a floating-point array.	
isinteger	Determine if input is an integer array.	
islogical	Determine if input is a logical array.	
isnumeric	Determine if input is a numeric array.	
isreal	Determine if input is an array of real numbers.	
isstruct	Determine if input is a MATLAB structure array.	

## Example Using isnumeric and isreal

Pick out the real numeric elements from this vector:

```
A = [5+7i 8/7 4.23 39j pi 9-2i];
for m = 1:numel(A)
   if isnumeric(A(m)) && isreal(A(m))
        disp(A(m))
   end
end
The values returned are
   1.1429
   4.2300
   3.1416
```

## **Data Structures Used in the Matrix**

These functions test elements of a matrix for a specific data structure.

Function	Description	
isempty	Determine if input has any dimension with size zero.	
isscalar	Determine if input is a 1-by-1 matrix.	
issparse	Determine if input is a sparse matrix.	
isvector	Determine if input is a 1-by-n or n-by-1 matrix.	

# **Resizing and Reshaping Matrices**

#### In this section...

"Expanding the Size of a Matrix" on page 1-25

"Delete Matrix Rows and Columns" on page 1-29

"Reshaping a Matrix" on page 1-30

"Preallocating Memory" on page 1-32

# **Expanding the Size of a Matrix**

You can expand the size of any existing matrix as long as doing so does not give the resulting matrix an irregular shape. (See "Keeping Matrices Rectangular" on page 1-6). For example, you can vertically combine a 4-by-3 matrix and 7-by-3 matrix because all rows of the resulting matrix have the same number of columns (3).

Two ways of expanding the size of an existing matrix are

- · Concatenating new elements onto the matrix
- Storing to a location outside the bounds of the matrix

**Note** If you intend to expand the size of a matrix repeatedly over time as it requires more room (usually done in a programming loop), it is advisable to preallocate space for the matrix when you initially create it. See "Preallocating Memory" on page 1-32.

## **Concatenating Onto the Matrix**

Concatenation is most useful when you want to expand a matrix by adding new elements or blocks that are compatible in size with the original matrix. This means that the size of all matrices being joined along a specific dimension must be equal along that dimension. See "Concatenating Matrices" on page 1-6.

This example runs a user-defined function compareResults on the data in matrices stats04 and stats03. Each time through the loop, it concatenates the results of this function onto the end of the data stored in comp04:

```
col = 10;
comp04 = [];
```

```
for k = 1:50
   t = compareResults(stats04(k,1:col), stats03(k,1:col));
   comp04 = [comp04; t];
end
```

### Concatenating to a Structure or Cell Array

You can add on to arrays of structures or cells in the same way as you do with ordinary matrices. This example creates a 3-by-8 matrix of structures S, each having 3 fields: x, y, and z, and then concatenates a second structure matrix S2 onto the original:

Create a 3-by-8 structure array S:

```
for k = 1:24
   S(k) = struct('x', 10*k, 'y', 10*k+1, 'z', 10*k+2);
end
S = reshape(S, 3, 8);
```

Create a second array that is 3-by-2 and uses the same field names:

```
for k = 25:30
   S2(k-24) = struct('x', 10*k, 'y', 10*k+1, 'z', 10*k+2);
end
S2= reshape(S2, 3, 2);
```

Concatenate S2 onto S along the horizontal dimension:

```
S = [S S2]
S =
3x10 struct array with fields:
    Х
    У
```

## Adding Smaller Blocks to a Matrix

To add one or more elements to a matrix where the sizes are not compatible, you can often just store the new elements outside the boundaries of the original matrix. The MATLAB software automatically pads the matrix with zeros to keep it rectangular.

Construct a 3-by-5 matrix, and attempt to add a new element to it using concatenation. The operation fails because you are attempting to join a one-column matrix with one that has five columns:

```
A = [ 10  20  30  40  50; ...
      60  70  80  90  100; ...
      110  120  130  140  150];

A = [A; 160]
Error using vertcat
CAT arguments dimensions are not consistent.
```

Try this again, but this time do it in such a way that enables MATLAB to make adjustments to the size of the matrix. Store the new element in row 4, a row that does not yet exist in this matrix. MATLAB expands matrix A by an entire new row by padding columns 2 through 5 with zeros:

**Note** Attempting to read from nonexistent matrix locations generates an error. You can only write to these locations.

You can also expand the matrix by adding a matrix instead of just a single element:

You do not have to add new elements sequentially. Wherever you store the new elements, MATLAB pads with zeros to make the resulting matrix rectangular in shape:

```
0 0 0 0 0 0 300
```

### **Expanding a Structure or Cell Array**

You can expand a structure or cell array in the same way that you can a matrix. This example adds an additional cell to a cell array by storing it beyond the bounds of the original array. MATLAB pads the data structure with empty cells ([]) to keep it rectangular.

```
The original array is 2-by-3:
```

C = {'Madison', 'G', [5 28 1967]; ... 46, '325 Maple Dr', 3015.28}

'325 Maple Dr'

### **Expanding a Character Array**

[1×1 struct]

'Madison'

You can expand character arrays in the same manner as other MATLAB arrays, but it is generally not recommended. MATLAB expands any array by padding uninitialized elements with zeros. Because zero is interpreted by MATLAB and some other programming languages as the end of a character array, you may find that some functions treat the expanded character array as if it were less than its full length.

[]

[1×3 double]

[3.0153e+03]

[]

Expand a 1-by-5 character vector to twelve characters. The result appears at first to be a typical character vector:

```
greeting = 'Hello'; greeting(1,8:12) = 'World'
greeting =
```

```
Hello World
```

Closer inspection however reveals zeros at the point of expansion:

```
uint8(greeting)
ans =
  1×12 uint8 row vector
  72  101  108  108  111   0   0  87  111  114  108  100
```

This causes some functions, like strcmp, to return what might be considered an unexpected result:

```
strcmp(greeting, 'Hello World')
ans =
  logical
  0
```

## **Delete Matrix Rows and Columns**

You can delete rows and columns from a matrix by assigning the empty array [] to those rows or columns. Start with

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

Then, delete the second column of A using

$$A(:,2) = []$$

This changes matrix A to

If you delete a single element from a matrix, the result is not a matrix anymore. So expressions like

$$A(1,2) = []$$

result in an error. However, you can use linear indexing to delete a single element, or a sequence of elements. This reshapes the remaining elements into a row vector:

# Reshaping a Matrix

The following functions change the shape of a matrix.

Function	Description	
reshape	Modify the shape of a matrix.	
rot90	Rotate the matrix by 90 degrees.	
fliplr	Flip the matrix about a vertical axis.	
flipud	Flip the matrix about a horizontal axis.	
flip	Flip the matrix along the specified direction.	
transpose	Flip a matrix about its main diagonal, turning row vectors into column vectors and vice versa.	
ctranspose	Transpose a matrix and replace each element with its complex conjugate.	

## **Examples**

Here are a few examples to illustrate some of the ways you can reshape matrices.

## Reshaping a Matrix

Reshape 3-by-4 matrix A to have dimensions 2-by-6:

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

#### Transposing a Matrix

Transpose A so that the row elements become columns. You can use either the transpose function or the transpose operator (.') to do this:

There is a separate function called ctranspose that performs a complex conjugate transpose of a matrix. The equivalent operator for ctranpose on a matrix A is A':

```
A = [1+9i \ 2-8i \ 3+7i; \ 4-6i \ 5+5i \ 6-4i]
A =
   1.0000 + 9.0000i
                       2.0000 - 8.0000i
                                           3.0000 + 7.0000i
   4.0000 - 6.0000i
                       5.0000 + 5.0000i
                                           6.0000 - 4.0000i
B = A'
B =
   1.0000 - 9.0000i
                       4.0000 + 6.0000i
   2.0000 + 8.0000i
                       5.0000 - 5.0000i
   3.0000 - 7.0000i
                       6.0000 + 4.0000i
```

### Rotating a Matrix

Rotate the matrix by 90 degrees:

```
B = rot90(A)
B = 10 11 12
7 8 9
4 5 6
1 2 3
```

### Flipping a Matrix

Flip A in a left-to-right direction:

```
B = fliplr(A)
B = 10 7 4 1
11 8 5 2
12 9 6 3
```

# **Preallocating Memory**

Repeatedly expanding the size of an array over time, (for example, adding more elements to it each time through a programming loop), can adversely affect the performance of your program. This is because

- MATLAB has to spend time allocating more memory each time you increase the size
  of the array.
- This newly allocated memory is likely to be noncontiguous, thus slowing down any
  operations that MATLAB needs to perform on the array.

The preferred method for sizing an array that is expected to grow over time is to estimate the maximum possible size for the array, and preallocate this amount of memory for it at the time the array is created. In this way, your program performs one memory allocation that reserves one contiguous block.

The following command preallocates enough space for a 25,000 by 10,000 matrix, and initializes each element to zero:

```
A = zeros(25000, 10000);
```

## **Building a Preallocated Array**

Once memory has been preallocated for the maximum estimated size of the array, you can store your data in the array as you need it, each time appending to the existing data. This example preallocates a large array, and then reads blocks of data from a file into the array until it gets to the end of the file:

```
blocksize = 5000;
maxrows = 2500000; cols = 20;
rp = 1; % row pointer
```

```
% Preallocate A to its maximum possible size
A = zeros(maxrows, cols);
% Open the data file, saving the file pointer.
fid = fopen('statfile.dat', 'r');
while true
   % Read from file into a cell array. Stop at EOF.
  block = textscan(fid, '%n', blocksize*cols);
   if isempty(block{1})
                         break,
   % Convert cell array to matrix, reshape, place into A.
   A(rp:rp+blocksize-1, 1:cols) = ...
      reshape(cell2mat(block), blocksize, cols);
   % Process the data in A.
                                    % User-defined function
   evaluate stats(A);
   % Update row pointer
   rp = rp + blocksize;
end
```

**Note** If you eventually need more room in a matrix than you had preallocated, you can preallocate additional storage in the same manner, and concatenate this additional storage onto the original array.

# **Shifting and Sorting Matrices**

#### In this section...

"Shift and Sort Functions" on page 1-34

"Shifting the Location of Matrix Elements" on page 1-34

"Sorting the Data in Each Column" on page 1-35

"Sorting the Data in Each Row" on page 1-36

"Sorting Row Vectors" on page 1-37

## **Shift and Sort Functions**

Use these functions to shift or sort the elements of a matrix.

Function	Description	
circshift	Circularly shift matrix contents.	
sort	Sort array elements in ascending or descending order.	
sortrows	Sort rows in ascending order.	
issorted Determine if matrix elements are in sorted order.		

You can sort matrices, multidimensional arrays, and cell arrays of character vectors along any dimension and in ascending or descending order of the elements. The sort functions also return an optional array of indices showing the order in which elements were rearranged during the sorting operation.

# **Shifting the Location of Matrix Elements**

The circshift function shifts the elements of a matrix in a circular manner along one or more dimensions. Rows or columns that are shifted out of the matrix circulate back into the opposite end. For example, shifting a 4-by-7 matrix one place to the left moves the elements in columns 2 through 7 to columns 1 through 6, and moves column 1 to column 7.

Create a 5-by-8 matrix named A and shift it to the right along the second (horizontal) dimension by three places (you would use [0,-3] to shift to the left by three places):

```
A = [1:8; 11:18; 21:28; 31:38; 41:48]
A =
```

```
2
                                                         8
     1
                    3
                           4
                                   5
                                          6
                                                 7
     11
            12
                   13
                           14
                                  15
                                         16
                                                17
                                                        18
    21
            22
                   23
                          24
                                  25
                                         26
                                                27
                                                        28
    31
            32
                   33
                          34
                                  35
                                         36
                                                37
                                                        38
            42
    41
                   43
                          44
                                  45
                                         46
                                                47
                                                        48
B = circshift(A, [0, 3])
B =
      6
             7
                    8
                            1
                                   2
                                          3
                                                 4
                                                         5
            17
     16
                   18
                          11
                                  12
                                         13
                                                14
                                                        15
    26
            27
                   28
                          21
                                  22
                                         23
                                                24
                                                        25
    36
            37
                   38
                          31
                                  32
                                         33
                                                34
                                                        35
    46
            47
                   48
                          41
                                  42
                                         43
                                                44
                                                        45
```

Now take A and shift it along both dimensions: three columns to the right and two rows up:

```
A = [1:8; 11:18; 21:28; 31:38; 41:48];
B = circshift(A, [-2, 3])
B =
    26
                  28
                         21
                                22
                                      23
                                             24
                                                    25
           27
    36
           37
                  38
                         31
                                32
                                      33
                                                    35
                                             34
                                42
    46
           47
                  48
                         41
                                      43
                                             44
                                                    45
     6
            7
                   8
                          1
                                 2
                                        3
                                                     5
    16
           17
                  18
                         11
                                12
                                       13
                                             14
                                                    15
```

Since circshift circulates shifted rows and columns around to the other end of a matrix, shifting by the exact size of A returns all rows and columns to their original location:

# Sorting the Data in Each Column

The sort function sorts matrix elements along a specified dimension. The syntax for the function is

```
sort(matrix, dimension)
```

To sort the columns of a matrix, specify 1 as the dimension argument. To sort along rows, specify dimension as 2.

This example makes a 6-by-7 arbitrary test matrix:

```
A = floor(gallery('uniformdata',[6 7],0)*100)
A =
    95
           45
                   92
                          41
                                 13
                                         1
                                               84
    23
                   73
                          89
                                 20
                                               52
             1
                                        74
    60
           82
                   17
                           5
                                 19
                                        44
                                               20
    48
           44
                   40
                          35
                                 60
                                        93
                                               67
    89
            61
                   93
                                 27
                                        46
                          81
                                               83
           79
                   91
                                 19
    76
                           0
                                        41
```

Sort each column of A in ascending order:

```
c = sort(A, 1)
c =
    23
             1
                   17
                           0
                                 13
                                         1
                                                1
    48
           44
                   40
                           5
                                 19
                                        41
                                               20
    60
           45
                   73
                          35
                                 19
                                        44
                                               52
    76
           61
                   91
                          41
                                 20
                                        46
                                               67
    89
           79
                   92
                          81
                                 27
                                        74
                                               83
    95
           82
                   93
                          89
                                 60
                                        93
                                               84
issorted(c(:, 1))
ans =
  logical
   1
```

## Sorting the Data in Each Row

Use issorted to sort data in each row. Using the example above, if you sort each row of A in descending order, issorted tests for an ascending sequence. You can flip the vector to test for a sorted descending sequence:

```
A = floor(gallery('uniformdata',[6 7],0)*100);
r = sort(A, 2, 'descend')
r =
    95    92    84    45    41    13    1
```

```
89
                  73
           74
                         52
                                23
                                       20
                                               1
                                               5
    82
           60
                  44
                         20
                                19
                                       17
    93
                  60
                         48
                                44
                                       40
                                              35
           67
    93
           89
                  83
                         81
                                61
                                       46
                                              27
    91
           79
                  76
                         41
                                19
                                        1
                                               0
issorted(fliplr(r(1, :)))
ans =
  logical
   1
```

When you specify a second output, **sort** returns the indices of the original matrix A positioned in the order they appear in the output matrix.

```
[r,index] = sort(A, 2, 'descend');
index
index =
      1
             3
                    7
                                   4
                                          5
                                                 6
                    3
                           7
                                          5
      4
             6
                                                 2
                                   1
                           7
      2
             1
                    6
                                   5
                                          3
                                                 4
      6
             7
                    5
                           1
                                   2
                                          3
                                                 4
      3
             1
                    7
                           4
                                   2
                                          6
                                                 5
      3
             2
                    1
                           6
                                          7
                                                 4
```

The second row of index contains the sequence, 4 6 3 7 1 5 2, which means that the second row of matrix r is comprised of A(2,4), A(2,6), A(2,3), A(2,7), A(2,1), A(2,5), and A(2,2).

## **Sorting Row Vectors**

The sortrows function sorts the entire row of a matrix according to the elements in a specified column, maintaining the order of elements in each row.

For example, create a random matrix A:

```
A = floor(gallery('uniformdata',[6 7],0)*100);
A =
    95
           45
                  92
                         41
                                13
                                        1
                                              84
    23
            1
                  73
                         89
                                20
                                       74
                                              52
    60
           82
                          5
                                19
                                       44
                                              20
                  17
    48
           44
                  40
                         35
                                60
                                       93
                                              67
    89
           61
                  93
                         81
                                27
                                       46
                                              83
    76
                  91
           79
                          0
                                19
                                       41
                                               1
```

Use the sortrows function to sort the rows of A in ascending order according to the values in the first column:

```
r = sortrows(A, 1)
r =
    23
             1
                   73
                          89
                                  20
                                         74
                                                52
    48
                                         93
                                                67
            44
                   40
                          35
                                  60
            82
    60
                   17
                           5
                                  19
                                         44
                                                20
    76
            79
                   91
                           0
                                  19
                                         41
                                                 1
    89
            61
                   93
                                  27
                                         46
                          81
                                                83
    95
            45
                   92
                          41
                                  13
                                          1
                                                84
```

Now sort the rows of A in ascending order according to the values in the fourth column:

```
r = sortrows(A, 4)
r =
    76
           79
                   91
                           0
                                 19
                                        41
                                                1
    60
           82
                   17
                           5
                                        44
                                               20
                                 19
    48
           44
                   40
                          35
                                 60
                                        93
                                               67
    95
           45
                  92
                          41
                                 13
                                         1
                                               84
    89
           61
                   93
                          81
                                 27
                                        46
                                               83
                                        74
    23
             1
                   73
                          89
                                 20
                                               52
```

# **Operating on Diagonal Matrices**

### In this section...

"Diagonal Matrix Functions" on page 1-39

"Constructing a Matrix from a Diagonal Vector" on page 1-39

"Returning a Triangular Portion of a Matrix" on page 1-40

"Concatenating Matrices Diagonally" on page 1-40

## **Diagonal Matrix Functions**

There are several MATLAB functions that work specifically on diagonal matrices.

Function	Description	
blkdiag	Construct a block diagonal matrix from input arguments.	
Return a diagonal matrix or the diagonals of a matrix.		
trace	Compute the sum of the elements on the main diagonal.	
tril	Return the lower triangular part of a matrix.	
triu	Return the upper triangular part of a matrix.	

# Constructing a Matrix from a Diagonal Vector

The diag function has two operations that it can perform. You can use it to generate a diagonal matrix:

You can also use the diag function to scan an existing matrix and return the values found along one of the diagonals:

```
A = magic(5)
```

```
A =
    17
           24
                   1
                          8
                                15
    23
            5
                   7
                         14
                                16
     4
            6
                  13
                         20
                                22
                                3
    10
           12
                  19
                         21
                          2
                                9
    11
           18
                  25
diag(A, 2)
                   % Return contents of second diagonal of A
ans =
     1
    14
    22
```

# Returning a Triangular Portion of a Matrix

The tril and triu functions return a triangular portion of a matrix, the former returning the piece from the lower left and the latter from the upper right. By default, the main diagonal of the matrix divides these two segments. You can use an alternate diagonal by specifying an offset from the main diagonal as a second input argument:

```
A = magic(6);
B = tril(A, -1)
B =
             0
                    0
                                  0
                                          0
      0
      3
             0
                    0
                           0
                                          0
     31
             9
                    0
                           0
                                  0
                                          0
      8
            28
                   33
                           0
                                          0
    30
             5
                   34
                          12
                                  0
                                          0
            36
                   29
                          13
                                 18
                                          0
```

# **Concatenating Matrices Diagonally**

You can diagonally concatenate matrices to form a composite matrix using the blkdiag function. See "Creating a Block Diagonal Matrix" on page 1-8 for more information on how this works.

# **Empty Matrices, Scalars, and Vectors**

#### In this section...

"Overview" on page 1-41

"The Empty Matrix" on page 1-42

"Scalars" on page 1-44

"Vectors" on page 1-45

### Overview

Although matrices are two dimensional, they do not always appear to have a rectangular shape. A 1-by-8 matrix, for example, has two dimensions yet is linear. These matrices are described in the following sections:

• "The Empty Matrix" on page 1-42

An *empty matrix* has one or more dimensions that are equal to zero. A two-dimensional matrix with both dimensions equal to zero appears in the MATLAB application as []. The expression A = [] assigns a 0-by-0 empty matrix to A.

• "Scalars" on page 1-44

A *scalar* is 1-by-1 and appears in MATLAB as a single real or complex number (e.g., 7, 583.62, -3.51, 5.46097e-14, 83+4i).

"Vectors" on page 1-45

A *vector* is 1-by-n or n-by-1, and appears in MATLAB as a row or column of real or complex numbers:

Column Vector	Row Vector		
53.2	53.2 87.39 4-12i 43.9		
87.39			
4-12i			
43.9			

# The Empty Matrix

A matrix having at least one dimension equal to zero is called an empty matrix. The simplest empty matrix is 0-by-0 in size. Examples of more complex matrices are those of dimension 0-by-5 or 10-by-0.

To create a 0-by-0 matrix, use the square bracket operators with no value specified:

```
A = [];
whos A
Name Size Bytes Class Attributes
A 0x0 0 double
```

You can create empty matrices (and arrays) of other sizes using the zeros, ones, rand, or eye functions. To create a 0-by-5 matrix, for example, use

```
A = zeros(0,5)
A =
    0×5 empty double matrix
```

## Operating on an Empty Matrix

The basic model for empty matrices is that any operation that is defined for m-by-n matrices, and that produces a result whose dimension is some function of m and n, should still be allowed when m or n is zero. The size of the result of this operation is consistent with the size of the result generated when working with nonempty values, but instead is evaluated at zero.

For example, horizontal concatenation

$$C = [A B]$$

requires that A and B have the same number of rows. So if A is m-by-n and B is m-by-p, then C is m-by-(n+p). This is still true if m, n, or p is zero.

As with all matrices in MATLAB, you must follow the rules concerning compatible dimensions. In the following example, an attempt to add a 1-by-3 matrix to a 0-by-3 empty matrix results in an error:

```
[1 2 3] + ones(0,3)
Error using +
```

Matrix dimensions must agree.

#### **Common Operations**

The following operations return zero on an empty array:

```
A = [];
size(A), length(A), numel(A), any(A), sum(A)
These operations return a nonzero value on an empty array:
A = [];
ndims(A), isnumeric(A), isreal(A), isfloat(A), isempty(A), ...
```

### **Using Empty Matrices in Relational Operations**

You can use empty matrices in relational operations such as "equal to" (==) or "greater than" (>) as long as both operands have the same dimensions, or the nonempty operand is scalar. The result of any relational operation involving an empty matrix is the empty matrix. Even comparing an empty matrix for equality to itself does not return true, but instead yields an empty matrix:

```
x = ones(0,3);
y = x;

y == x
ans =
    0×3 empty logical array
```

all(A), prod(A)

## **Using Empty Matrices in Logical Operations**

MATLAB has two distinct types of logical operators:

- Short-circuit (&&, ||) Used in testing multiple logical conditions (e.g., x >= 50 && x < 100) where each condition evaluates to a scalar true or false.</li>
- Element-wise (&, |) Performs a logical AND, OR, or NOT on each element of a matrix or array.

### **Short-circuit Operations**

The rule for operands used in short-circuit operations is that each operand must be convertible to a logical scalar value. Because of this rule, empty matrices cannot be used in short-circuit logical operations. Such operations return an error.

The only exception is in the case where MATLAB can determine the result of a logical statement without having to evaluate the entire expression. This is true for the following two statements because the result of the entire statements are known by considering just the first term:

```
true || []
ans =
  logical
  1
false && []
ans =
  logical
  0
```

#### **Element-wise Operations**

Unlike the short-circuit operators, all element-wise operations on empty matrices are considered valid as long as the dimensions of the operands agree, or the nonempty operand is scalar. Element-wise operations on empty matrices always return an empty matrix:

```
true | []
ans =

0×0 empty logical array
```

**Note** This behavior is consistent with the way MATLAB does scalar expansion with binary operators, wherein the nonscalar operand determines the size of the result.

## **Scalars**

Any individual real or complex number is represented in MATLAB as a 1-by-1 matrix called a scalar value:

```
A = 5;
ndims(A) % Check number of dimensions in A
```

Use the isscalar function to tell if a variable holds a scalar value:

```
isscalar(A)
ans =
  logical
1
```

### **Vectors**

Matrices with one dimension equal to one and the other greater than one are called vectors. Here is an example of a numeric vector:

You can construct a vector out of other vectors, as long as the critical dimensions agree. All components of a row vector must be scalars or other row vectors. Similarly, all components of a column vector must be scalars or other column vectors:

```
A = [29 43 77 9 21];
B = [0 46 11];
C = [A 5 ones(1,3) B]
C = 29 43 77 9 21 5 1 1 0 46 11
```

Concatenating an empty matrix to a vector has no effect on the resulting vector. The empty matrix is ignored in this case:

```
A = [5.36; 7.01; []; 9.44]
A = 5.3600
```

```
7.0100
9.4400
```

Use the isvector function to tell if a variable holds a vector:

```
isvector(A)
ans =
  logical
1
```

# **Multidimensional Arrays**

### In this section...

"Overview" on page 1-47

"Creating Multidimensional Arrays" on page 1-49

"Accessing Multidimensional Array Properties" on page 1-52

"Indexing Multidimensional Arrays" on page 1-52

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"Permuting Array Dimensions" on page 1-58

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"Organizing Data in Multidimensional Arrays" on page 1-62

"Multidimensional Cell Arrays" on page 1-63

"Multidimensional Structure Arrays" on page 1-64

### Overview

An array having more than two dimensions is called a multidimensional array in the MATLAB application. Multidimensional arrays in MATLAB are an extension of the normal two-dimensional matrix. Matrices have two dimensions: the row dimension and the column dimension.

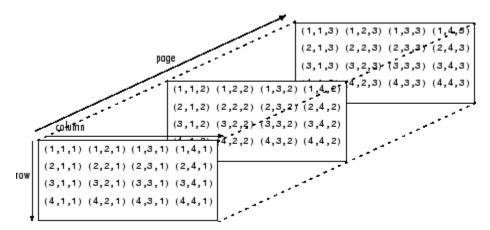
	column			
	(1,1)	(1,2)	(1,3)	(1,4)
row	(2,1)	(2,2)	(2,3)	(2,4)
	(3,1)	(3,2)	(3,3)	(3,4)
ļ	(4,1)	(4,2)	(4,3)	(4,4)

You can access a two-dimensional matrix element with two subscripts: the first representing the row index, and the second representing the column index.

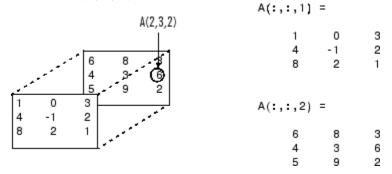
Multidimensional arrays use additional subscripts for indexing. A three-dimensional array, for example, uses three subscripts:

· The first references array dimension 1, the row.

- The second references dimension 2, the column.
- The third references dimension 3. This illustration uses the concept of a *page* to represent dimensions 3 and higher.



To access the element in the second row, third column of page 2, for example, you use the subscripts (2,3,2).



As you add dimensions to an array, you also add subscripts. A four-dimensional array, for example, has four subscripts. The first two reference a row-column pair; the second two access the third and fourth dimensions of data.

Most of the operations that you can perform on matrices (i.e., two-dimensional arrays) can also be done on multidimensional arrays.

**Note** The general multidimensional array functions reside in the datatypes directory.

# **Creating Multidimensional Arrays**

You can use the same techniques to create multidimensional arrays that you use for twodimensional matrices. In addition, MATLAB provides a special concatenation function that is useful for building multidimensional arrays.

This section discusses

- "Creating and Extending Multidimensional Arrays Using Indexed Assignment" on page 1-49
- "Generating Arrays Using MATLAB Functions" on page 1-50
- "Building Multidimensional Arrays with the cat Function" on page 1-51

### Creating and Extending Multidimensional Arrays Using Indexed Assignment

You can create a multidimensional array by creating a 2-D array and extending it. Create a 2-D array A and extend A to a 3-D array using indexed assignment:

You can extend an array by assigning a single value to the new elements. MATLAB expands the scalar value to match the dimensions of the addressed elements. This expansion is called scalar expansion.

Extend A by a third page using scalar expansion.

$$A(:,:,3) = 5$$
 $A(:,:,1) = 5$ 
 $5$ 
 $0$ 
 $1$ 
 $9$ 
 $4$ 
 $3$ 
 $6$ 

To extend the rows, columns, or pages of an array, use similar assignment statements. The dimensions of arrays on the right side and the left side of the assignment must be the same.

Extend A into a 3-by-3-by-2, four-dimensional array. In the first assignment, MATLAB pads A to fill the unassigned elements in the extended dimension with zeros. The second and third assignments replace the zeros with the specified values.

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

A(:,:,2,2) = [9 \ 8 \ 7; \ 6 \ 5 \ 4; \ 3 \ 2 \ 1];

A(:,:,3,2) = [1 \ 0 \ 1; \ 1 \ 1 \ 0; \ 0 \ 1 \ 1];
```

### **Generating Arrays Using MATLAB Functions**

You can use MATLAB functions such as randn, ones, and zeros to generate multidimensional arrays in the same way you use them for two-dimensional arrays. Each argument you supply represents the size of the corresponding dimension in the resulting array. For example, to create a 4-by-3-by-2 array of normally distributed random numbers:

$$B = randn(4,3,2)$$

To generate an array filled with a single constant value, use the repmat function. repmat replicates an array (in this case, a 1-by-1 array) through a vector of array dimensions.

```
B = repmat(5, [3 \ 4 \ 2])
B(:,:,1) = 5 5 5 5 5
5 5 5 5 5 5
B(:,:,2) = 5 5 5 5
```

**Note** Any dimension of an array can have size zero, making it a form of empty array. For example, 10-by-0-by-20 is a valid size for a multidimensional array.

### **Building Multidimensional Arrays with the cat Function**

The cat function is a simple way to build multidimensional arrays; it concatenates a list of arrays along a specified dimension:

$$B = cat(dim, A1, A2...)$$

where A1, A2, and so on are the arrays to concatenate, and dim is the dimension along which to concatenate the arrays.

For example, to create a new array with cat:

The cat function accepts any combination of existing and new data. In addition, you can nest calls to cat. The lines below, for example, create a four-dimensional array.

```
A = cat(3, [9 2; 6 5], [7 1; 8 4])
B = cat(3, [3 5; 0 1], [5 6; 2 1])
D = cat(4, A, B, cat(3, [1 2; 3 4], [4 3;2 1]))
```

cat automatically adds subscripts of 1 between dimensions, if necessary. For example, to create a 2-by-2-by-1-by-2 array, enter

```
C = cat(4, [1 2; 4 5], [7 8; 3 2])
```

In the previous case, cat inserts as many singleton dimensions as needed to create a four-dimensional array whose last dimension is not a singleton dimension. If the dim

argument had been 5, the previous statement would have produced a 2-by-2-by-1-by-2 array. This adds additional 1s to indexing expressions for the array. To access the value 8 in the four-dimensional case, use

```
C(1,2,1,2)
Singleton dimension index
```

# **Accessing Multidimensional Array Properties**

You can use the following MATLAB functions to get information about multidimensional arrays you have created.

size — Returns the size of each array dimension.

• ndims — Returns the number of dimensions in the array.

```
ndims(C)
ans =
4
```

· whos — Provides information on the format and storage of the array.

	Size Bytes Cl	ass
B 2x2x2 64 double arr C 4-D 64 double arr	2x2x2 64 do 4-D 64 do	,

Grand total is 48 elements using 384 bytes

## **Indexing Multidimensional Arrays**

Many of the concepts that apply to two-dimensional matrices extend to multidimensional arrays as well.

To access a single element of a multidimensional array, use integer subscripts. Each subscript indexes a dimension—the first indexes the row dimension, the second indexes the column dimension, the third indexes the first page dimension, and so on.

Consider a 10-by-5-by-3 array nddata of random integers:

```
nddata = fix(8 * randn(10,5,3));
```

To access element (3,2) on page 2 of nddata, for example, use nddata(3,2,2).

You can use vectors as array subscripts. In this case, each vector element must be a valid subscript, that is, within the bounds defined by the dimensions of the array. To access elements (2,1), (2,3), and (2,4) on page 3 of nddata, use

```
nddata(2,[1 3 4],3);
```

### The Colon and Multidimensional Array Indexing

The MATLAB colon indexing extends to multidimensional arrays. For example, to access the entire third column on page 2 of nddata, use nddata(:,3,2).

The colon operator is also useful for accessing other subsets of data. For example, nddata(2:3,2:3,1) results in a 2-by-2 array, a subset of the data on page 1 of nddata. This matrix consists of the data in rows 2 and 3, columns 2 and 3, on the first page of the array.

The colon operator can appear as an array subscript on both sides of an assignment statement. For example, to create a 4-by-4 array of zeros:

```
C = zeros(4, 4)
```

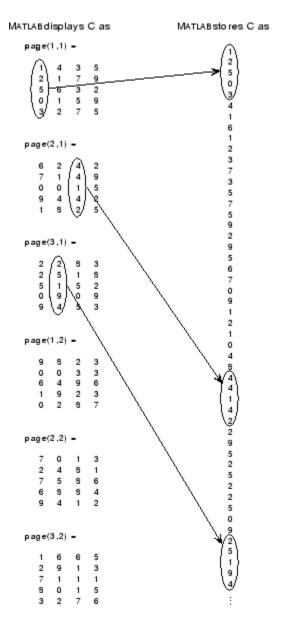
Now assign a 2-by-2 subset of array nddata to the four elements in the center of C.

```
C(2:3,2:3) = nddata(2:3,1:2,2)
```

## **Linear Indexing with Multidimensional Arrays**

MATLAB linear indexing also extends to multidimensional arrays. In this case, MATLAB operates on a page-by-page basis to create the storage column, again appending elements columnwise. See "Linear Indexing" on page 1-12 for an introduction to this topic.

For example, consider a 5-by-4-by-3-by-2 array C.



Again, a single subscript indexes directly into this column. For example, C(4) produces the result

If you specify two subscripts (i,j) indicating row-column indices, MATLAB calculates the offset as described above. Two subscripts always access the first page of a multidimensional array, provided they are within the range of the original array dimensions.

If more than one subscript is present, all subscripts must conform to the original array dimensions. For example, C(6,2) is invalid because all pages of C have only five rows.

If you specify more than two subscripts, MATLAB extends its indexing scheme accordingly. For example, consider four subscripts (i,j,k,l) into a four-dimensional array with size [d1 d2 d3 d4]. MATLAB calculates the offset into the storage column by

$$(1-1)(d3)(d2)(d1)+(k-1)(d2)(d1)+(j-1)(d1)+i$$

For example, if you index the array C using subscripts (3, 4, 2, 1), MATLAB returns the value 5 (index 38 in the storage column).

In general, the offset formula for an array with dimensions  $[d_1 \ d_2 \ d_3 \ \dots \ d_n]$  using any subscripts  $(S_1 \ S_2 \ S_3 \ \dots \ S_n)$  is

$$(s_{n}-1)(d_{n-1})(d_{n-2})\dots(d_{1})+(s_{n-1}-1)(d_{n-2})\dots(d_{1})+\dots+(s_{2}-1)(d_{1})+s_{1}$$

Because of this scheme, you can index an array using any number of subscripts. You can append any number of 1s to the subscript list because these terms become zero. For example,

is equivalent to

C(3,2)

## Avoiding Ambiguity in Multidimensional Indexing

Some assignment statements, such as

$$A(:,:,2) = 1:10$$

are ambiguous because they do not provide enough information about the shape of the dimension to receive the data. In the case above, the statement tries to assign a one-dimensional vector to a two-dimensional destination. MATLAB produces an error for

such cases. To resolve the ambiguity, be sure you provide enough information about the destination for the assigned data, and that both data and destination have the same shape. For example:

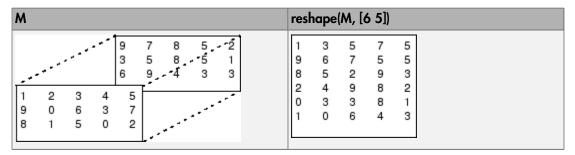
$$A(1,:,2) = 1:10;$$

# **Reshaping Multidimensional Arrays**

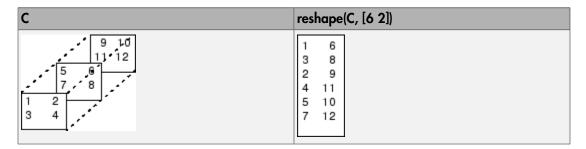
Unless you change its shape or size, a MATLAB array retains the dimensions specified at its creation. You change array size by adding or deleting elements. You change array shape by re-specifying the array's row, column, or page dimensions while retaining the same elements. The reshape function performs the latter operation. For multidimensional arrays, its form is

$$B = reshape(A,[s1 s2 s3 ...])$$

**\$1, \$2**, and so on represent the desired size for each dimension of the reshaped matrix. Note that a reshaped array must have the same number of elements as the original array (that is, the product of the dimension sizes is constant).



The reshape function operates in a columnwise manner. It creates the reshaped matrix by taking consecutive elements down each column of the original data construct.



Here are several new arrays from reshaping nddata:

```
B = reshape(nddata, [6 25])
C = reshape(nddata, [5 3 10])
D = reshape(nddata, [5 3 2 5])
```

#### **Removing Singleton Dimensions**

MATLAB automatically removes trailing singleton dimensions (dimensions whose sizes are equal to 1) from all multidimensional arrays. For example, if you attempt to create an array of size 3-by-2-by-1-by-1, perhaps with the command rand(3,2,1,1), then MATLAB strips away the singleton dimensions at the end of the array and creates a 3-by-2 matrix. This is because every array technically has an *infinite* number of trailing singleton dimensions. A 3-by-2 array is the same as an array with size 3-by-2-by-1-by-1-by-1-by-...

For example, consider the following 2-by-2 matrix, A.

```
A = eye(2)
A =

1 0
0 1
```

A is a 2-by-2 identity matrix.

Find the size of the fourth dimension of A.

Although A is a 2-by-2 matrix, the size of the fourth dimension in A is 1. In fact, the size of each dimension beyond the second is 1.

The first two dimensions of an array are never stripped away, since they are always relevant.

```
size(3)
```

```
ans =
```

Even a scalar in MATLAB is a 1-by-1 matrix.

MATLAB creates singleton dimensions if you explicitly specify them when you create or reshape an array, or if you perform a calculation that results in an array dimension of one:

```
B = repmat(5, [2 3 1 4]);

size(B)

ans =

2 3 1 4
```

The squeeze function removes singleton dimensions from an array:

The squeeze function does not affect two-dimensional arrays; row vectors remain rows.

## **Permuting Array Dimensions**

The permute function reorders the dimensions of an array:

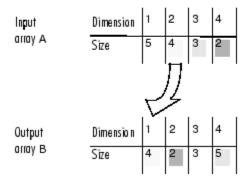
```
B = permute(A, dims);
```

dims is a vector specifying the new order for the dimensions of A, where 1 corresponds to the first dimension (rows), 2 corresponds to the second dimension (columns), 3 corresponds to pages, and so on.

A			B = perm	ute(A,	[21	3])	C = perm	ute(A,	[3 2	1])
A(:,:,1) =			B(:,:,1) =			C(:,:,1) =				
1	2	3	1	4	7	Row and column	1	2	3	Row and page
4	5	6	2	5	8	subscripts are	0	5	4	subscripts are
7	8	9	3	6	9	reversed				reversed.
						(page-by-page	C(:,:,2)	=		icicisca.
A(:,:,2) =		B(:,:,2)	=							
,			, , , ,			transposition).	4	5	6	
0	5	4	0	2	9		2	7	6	
2	7	6	5	7	3					
9	3	1	4	6	1		C(:,:,3)	=		
							7	8	9	
							9	3	1	

For a more detailed look at the permute function, consider a four-dimensional array A of size 5-by-4-by-3-by-2. Rearrange the dimensions, placing the column dimension first, followed by the second page dimension, the first page dimension, then the row dimension. The result is a 4-by-2-by-3-by-5 array.

Move dimension 2 of A to first subscript position of B, dimension 4 to second subscript position, and so on.



The order of dimensions in permute's argument list determines the size and shape of the output array. In this example, the second dimension moves to the first position. Because the second dimension of the original array had size 4, the output array's first dimension also has size 4.

You can think of permute's operation as an extension of the transpose function, which switches the row and column dimensions of a matrix. For permute, the order of the

input dimension list determines the reordering of the subscripts. In the example above, element (4,2,1,2) of A becomes element (2,2,1,4) of B, element (5,4,3,2) of A becomes element (4,2,3,5) of B, and so on.

#### **Inverse Permutation**

The ipermute function is the inverse of permute. Given an input array A and a vector of dimensions v, ipermute produces an array B such that permute(B,v) returns A.

For example, these statements create an array E that is equal to the input array C:

```
D = ipermute(C, [1 4 2 3]);
E = permute(D, [1 4 2 3])
```

You can obtain the original array after permuting it by calling ipermute with the same vector of dimensions.

## **Computing with Multidimensional Arrays**

Many of the MATLAB computational and mathematical functions accept multidimensional arrays as arguments. These functions operate on specific dimensions of multidimensional arrays; that is, they operate on individual elements, on vectors, or on matrices.

#### **Operating on Vectors**

Functions that operate on vectors, like sum, mean, and so on, by default typically work on the first nonsingleton dimension of a multidimensional array. Most of these functions optionally let you specify a particular dimension on which to operate. There are exceptions, however. For example, the cross function, which finds the cross product of two vectors, works on the first nonsingleton dimension having length 3.

**Note** In many cases, these functions have other restrictions on the input arguments — for example, some functions that accept multiple arrays require that the arrays be the same size. Refer to the online help for details on function arguments.

#### **Operating Element-by-Element**

MATLAB functions that operate element-by-element on two-dimensional arrays, like the trigonometric and exponential functions in the elfun directory, work in exactly the same way for multidimensional cases. For example, the sin function returns an array the same size as the function's input argument. Each element of the output array is the sine of the corresponding element of the input array.

Similarly, the arithmetic, logical, and relational operators all work with corresponding elements of multidimensional arrays that are the same size in every dimension. If one operand is a scalar and one an array, the operator applies the scalar to each element of the array.

#### **Operating on Planes and Matrices**

Functions that operate on planes or matrices, such as the linear algebra and matrix functions in the matfun directory, do not accept multidimensional arrays as arguments. That is, you cannot use the functions in the matfun directory, or the array operators \*, ^, \, or /, with multidimensional arguments. Supplying multidimensional arguments or operands in these cases results in an error.

You can use indexing to apply a matrix function or operator to matrices within a multidimensional array. For example, create a three-dimensional array A:

```
A = cat(3, [1 2 3; 9 8 7; 4 6 5], [0 3 2; 8 8 4; 5 3 5], ... [6 4 7; 6 8 5; 5 4 3]);
```

Applying the eig function to the entire multidimensional array results in an error:

```
eig(A)
??? Undefined function or method 'eig' for input
arguments of type 'double' and attributes 'full 3d real'.
```

You can, however, apply eig to planes within the array. For example, use colon notation to index just one page (in this case, the second) of the array:

```
eig(A(:,:,2))
ans =
12.9129
-2.6260
2.7131
```

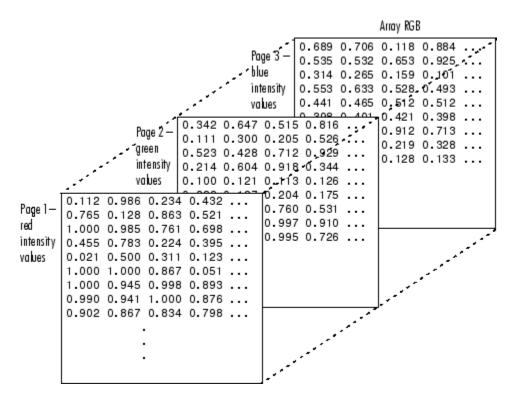
**Note** In the first case, subscripts are not colons; you must use squeeze to avoid an error. For example, eig(A(2,:,:)) results in an error because the size of the input is [1 3 3]. The expression eig(squeeze(A(2,:,:))), however, passes a valid two-dimensional matrix to eig.

## **Organizing Data in Multidimensional Arrays**

You can use multidimensional arrays to represent data in two ways:

- As planes or pages of two-dimensional data. You can then treat these pages as matrices.
- As multivariate or multidimensional data. For example, you might have a fourdimensional array where each element corresponds to either a temperature or air pressure measurement taken at one of a set of equally spaced points in a room.

For example, consider an RGB image. For a single image, a multidimensional array is probably the easiest way to store and access data.



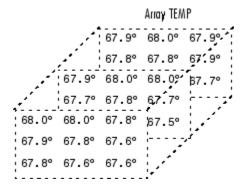
To access an entire plane of the image, use

```
redPlane = RGB(:,:,1);
```

To access a subimage, use

```
subimage = RGB(20:40,50:85,:);
```

The RGB image is a good example of data that needs to be accessed in planes for operations like display or filtering. In other instances, however, the data itself might be multidimensional. For example, consider a set of temperature measurements taken at equally spaced points in a room. Here the location of each value is an integral part of the data set—the physical placement in three-space of each element is an aspect of the information. Such data also lends itself to representation as a multidimensional array.



Now to find the average of all the measurements, use

```
mean(mean(TEMP)));
```

To obtain a vector of the "middle" values (element (2,2)) in the room on each page, use

```
B = TEMP(2,2,:);
```

## **Multidimensional Cell Arrays**

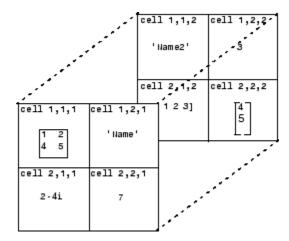
Like numeric arrays, the framework for multidimensional cell arrays in MATLAB is an extension of the two-dimensional cell array model. You can use the cat function to build multidimensional cell arrays, just as you use it for numeric arrays.

For example, create a simple three-dimensional cell array C:

```
A{1,1} = [1 2;4 5];
A{1,2} = 'Name';
A{2,1} = 2-4i;
```

```
A{2,2} = 7;
B{1,1} = 'Name2';
B{1,2} = 3;
B{2,1} = 0:1:3;
B{2,2} = [4 5]';
C = cat(3, A, B);
```

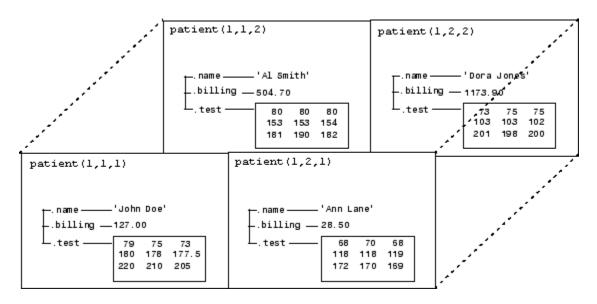
The subscripts for the cells of C look like



## **Multidimensional Structure Arrays**

Multidimensional structure arrays are extensions of rectangular structure arrays. Like other types of multidimensional arrays, you can build them using direct assignment or the cat function:

```
patient(1,1,1).name = 'John Doe';
patient(1,1,1).billing = 127.00;
patient(1,1,1).test = [79 75 73; 180 178 177.5; 220 210 205];
patient(1,2,1).name = 'Ann Lane';
patient(1,2,1).billing = 28.50;
patient(1,2,1).test = [68 70 68; 118 118 119; 172 170 169];
patient(1,1,2).name = 'Al Smith';
patient(1,1,2).billing = 504.70;
patient(1,1,2).test = [80 80 80; 153 153 154; 181 190 182];
patient(1,2,2).name = 'Dora Jones';
patient(1,2,2).billing = 1173.90;
patient(1,2,2).test = [73 73 75; 103 103 102; 201 198 200];
```



#### **Applying Functions to Multidimensional Structure Arrays**

To apply functions to multidimensional structure arrays, operate on fields and field elements using indexing. For example, find the sum of the columns of the test array in patient(1,1,2):

```
sum((patient(1,1,2).test));
```

Similarly, add all the billing fields in the patient array:

```
total = sum([patient.billing]);
```

# **Summary of Matrix and Array Functions**

This section summarizes the principal functions used in creating and handling matrices. Most of these functions work on multidimensional arrays as well.

#### **Functions to Create a Matrix**

Function	Description			
[a,b] or [a;b]	Create a matrix from specified elements, or concatenate matrices together.			
accumarray	Construct a matrix using accumulation.			
blkdiag	Construct a block diagonal matrix.			
cat	Concatenate matrices along the specified dimension.			
diag	Create a diagonal matrix from a vector.			
horzcat	Concatenate matrices horizontally.			
magic	Create a square matrix with rows, columns, and diagonals that add up to the same number.			
ones	Create a matrix of all ones.			
rand	Create a matrix of uniformly distributed random numbers.			
repmat	Create a new matrix by replicating or tiling another.			
vertcat	Concatenate two or more matrices vertically.			
zeros	Create a matrix of all zeros.			

#### Functions to Modify the Shape of a Matrix

Function	Description
ctranspose	Flip a matrix about the main diagonal and replace each element with its complex conjugate.
flip	Flip a matrix along the specified dimension.
fliplr	Flip a matrix about a vertical axis.
flipud	Flip a matrix about a horizontal axis.
reshape	Change the dimensions of a matrix.
rot90	Rotate a matrix by 90 degrees.

Function	Description
transpose	Flip a matrix about the main diagonal.

## Functions to Find the Structure or Shape of a Matrix

Function	Description
isempty	Return true for 0-by-0 or 0-by-n matrices.
isscalar	Return true for 1-by-1 matrices.
issparse	Return true for sparse matrices.
isvector	Return true for 1-by-n matrices.
length	Return the length of a vector.
ndims	Return the number of dimensions in a matrix.
numel	Return the number of elements in a matrix.
size	Return the size of each dimension.

#### **Functions to Determine Class**

Function	Description
iscell	Return true if the matrix is a cell array.
ischar	Return true if matrix elements are character arrays.
isfloat	Determine if input is a floating point array.
isinteger	Determine if input is an integer array.
islogical	Return true if matrix elements are logicals.
isnumeric	Return true if matrix elements are numeric.
isreal	Return true if matrix elements are real numbers.
isstruct	Return true if matrix elements are MATLAB structures.

#### **Functions to Sort and Shift Matrix Elements**

Function	Description
circshift	Circularly shift matrix contents.
issorted	Return true if the matrix elements are sorted.
sort	Sort elements in ascending or descending order.

Function	Description
sortrows	Sort rows in ascending order.

## Functions That Work on Diagonals of a Matrix

Function	Description
blkdiag	Construct a block diagonal matrix.
diag	Return the diagonals of a matrix.
trace	Compute the sum of the elements on the main diagonal.
tril	Return the lower triangular part of a matrix.
triu	Return the upper triangular part of a matrix.

#### Functions to Change the Indexing Style

Function	Description
ind2sub	Convert a linear index to a row-column index.
sub2ind	Convert a row-column index to a linear index.

#### **Functions for Working with Multidimensional Arrays**

Function	Description
cat	Concatenate arrays.
circshift	Shift array circularly.
ipermute	Inverse permute array dimensions.
ndgrid Generate arrays for n-dimensional functions and inter	
ndims	Return the number of array dimensions.
permute	Permute array dimensions.
shiftdim	Shift array dimensions.
squeeze	Remove singleton dimensions.

# Linear Algebra

- "Matrices in the MATLAB Environment" on page 2-2
- "Systems of Linear Equations" on page 2-11
- "Inverses and Determinants" on page 2-23
- "Factorizations" on page 2-27
- "Powers and Exponentials" on page 2-35
- "Eigenvalues" on page 2-39
- "Singular Values" on page 2-43

## Matrices in the MATLAB Environment

#### In this section...

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## **Creating Matrices**

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.

Symbolic Math Toolbox $^{\text{TM}}$  software extends the capabilities of MATLAB software to matrices of mathematical expressions.

MATLAB has dozens of functions that create different kinds of matrices. There are two functions you can use to create a pair of 3-by-3 example matrices for use throughout this chapter. The first example is symmetric:

The second example is not symmetric:

```
B = magic(3)
```

Another example is a 3-by-2 rectangular matrix of random integers:

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. The statements

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

produce a column vector, a row vector, and a scalar:

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

## **Adding and Subtracting Matrices**

Addition and subtraction of matrices is defined just as it is for arrays, element by element. Adding A to B, and then subtracting A from the result recovers B:

```
A = pascal(3);
```

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

Addition and subtraction require both matrices to have the same dimension, or one of them be a scalar. If the dimensions are incompatible, an error results:

```
C = fix(10*rand(3,2))
X = A + C
Error using +
Matrix dimensions must agree.
```

## **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, the *inner* product, or a matrix, the *outer product*:

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

v = [2 0 -1];

x = v*u

x = 2

X = u*v

X = 6 0 -3

2 0 -1

8 0 -4
```

For real matrices, the *transpose* operation interchanges  $a_{ij}$  and  $a_{ji}$ . MATLAB uses the apostrophe operator (') to perform a complex conjugate transpose, and uses 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 is *symmetric*, so A' is equal to A. But, B is not symmetric:

```
B = magic(3);
X = B'

X =

    8     3     4
    1     5     9
    6     7     2
```

Transposition turns a row vector into a column vector:

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

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

are the same scalar. This quantity is used so frequently, it has three different names: *inner* product, *scalar* product, or *dot* product.

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. So if

```
z = [1+2i 7-3i 3+4i; 6-2i 9i 4+7i]
z =
1.0000 + 2.0000i 7.0000 - 3.0000i 3.0000 + 4.0000i
6.0000 - 2.0000i 0 + 9.0000i 4.0000 + 7.0000i
then
```

z'

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

```
z.'
ans =
1.0000 + 2.0000i 6.0000 - 2.0000i
7.0000 - 3.0000i 0 + 9.0000i
3.0000 + 4.0000i 4.0000 + 7.0000i
```

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 a single asterisk to denote matrix multiplication. The next two examples illustrate the fact that matrix multiplication is not commutative; AB is usually not equal to BA:

```
X = A*B
X =
15 15 15
```

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

Rectangular matrix multiplications must satisfy the dimension compatibility conditions:

Anything can be multiplied by a scalar:

```
s = 7;
```

```
w = s*v
w =
14 0 -7
```

## **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.

#### **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 in the following order:

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

kron(	I,X)			
are				
	1 0 3 0	0 1 0 3	2 0 4 0	0 2 0 4
and				
	1 3 0 0	2 4 0 0	0 0 1 3	0 0 2 4

#### **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 is defined by any value of p > 1, but the most common values of p are 1, 2, and  $\infty$ . The default value is p = 2, which corresponds to *Euclidean length*:

The p-norm of a matrix A,

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

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

```
C = fix(10*rand(3,2));
[norm(C,1) norm(C) norm(C,inf)]
```

```
ans = 19.0000 14.8015 13.0000
```

## **Using Multithreaded Computation with Linear Algebra Functions**

MATLAB software 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.

#### **Acknowledgments**

LAPACK is a library of routines that provides fast, robust algorithms for numerical linear algebra and matrix computations. Since the year 2000, 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.

## **Systems of Linear Equations**

#### In this section...

"Computational Considerations" on page 2-11

"General Solution" on page 2-12

"Square Systems" on page 2-13

"Overdetermined Systems" on page 2-15

"Underdetermined Systems" on page 2-18

"Using Multithreaded Computation with Systems of Linear Equations" on page 2-20

"Iterative Methods for Solving Systems of Linear Equations" on page 2-21

"Acknowledgments" on page 2-22

## **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; the MATLAB software 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, slash, /, and backslash, \, correspond to the two MATLAB functions mrdivide and mldivide. mrdivide and mldivide 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 $xA = b$ .
$x = A \setminus b$	Denotes the solution to the matrix equation $Ax = b$ .

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 is *m*-by-*n*, there are three cases:

m = n	Square system. Seek an exact solution.
$m \ge n$	Overdetermined system. Find a least-squares solution.
$m \le n$	Underdetermined system. 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 A and a single right side column vector b.

#### **Nonsingular Coefficient Matrix**

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

```
A = pascal(3);

u = [3; 1; 4];

x = A\u

x = 10

-12

5
```

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:

```
b = magic(3);
X = A \setminus b
X = \begin{bmatrix} 19 & -3 & -1 \\ -17 & 4 & 13 \\ 6 & 0 & -6 \end{bmatrix}
```

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 and raises an error condition 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

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

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

For example:

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.

**Note:** For information about using pinv to solve systems with rectangular coefficient matrices, see "Pseudoinverses" on page 2-24.

#### **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.

```
t = [0 .3 .8 1.1 1.6 2.3]';
y = [.82.72.63.60.55.50]';
B = table(t,y)
B =
     t
            У
      0
           0.82
    0.3
           0.72
    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 <code>exp(-t)</code>. The unknown coefficients, <code>c1</code> and <code>c2</code>, 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.

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

```
c = E\y
c =

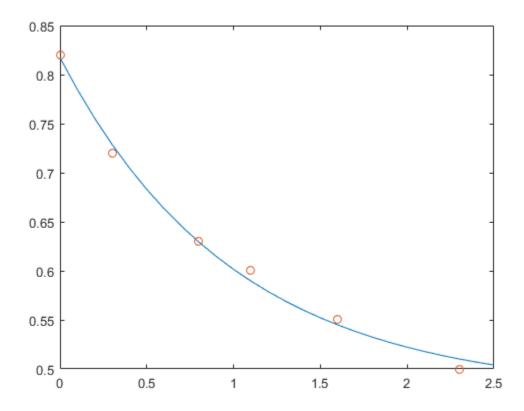
0.4760
0.3413
```

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, the least-squares solution to AX = B is not unique. The backslash operator, A\B, issues a warning if A is rank deficient and produces a least-squares solution if the system has no solution and a basic solution if the system has infinitely many 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 solution, which has at most m nonzero components for an m-by-n coefficient matrix.

Here is a small, random example:

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 =
```

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:

$$Z * q = (\bar{x}_1 \quad \bar{x}_2) \begin{pmatrix} u \\ w \end{pmatrix} = u\bar{x}_1 + w\bar{x}_2.$$

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
```

## **Using Multithreaded Computation with Systems of Linear Equations**

MATLAB software 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.

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.

## Iterative Methods for Solving Systems of Linear Equations

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.

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

lsgr

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
```

## **Acknowledgments**

LAPACK is a library of routines that provides fast, robust algorithms for numerical linear algebra and matrix computations. Since the year 2000, 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.

#### Inverses and Determinants

#### In this section...

"Introduction" on page 2-23

"Pseudoinverses" on page 2-24

"Acknowledgments" on page 2-26

#### Introduction

If A is square and nonsingular, the equations AX = I and XA = I have the same solution, X. This solution is called the inverse of A, is denoted by  $A^{-1}$ , and is computed by the function inv.

The *determinant* of a matrix is useful in theoretical considerations and some types of symbolic computation, but its scaling and round-off error properties make it far less satisfactory for numeric computation. Nevertheless, the function det computes the determinant of a square matrix:

Again, because A is symmetric, has integer elements, and has determinant equal to one, so does its inverse. However,

```
B = magic(3)
```

```
B =
        8
                     6
              1
        3
              5
                     7
              9
                     2
d = det(B)
X = inv(B)
d =
     -360
X =
      0.1472
                 -0.1444
                             0.0639
     -0.0611
                  0.0222
                             0.1056
     -0.0194
                  0.1889
                            -0.1028
```

Closer examination of the elements of X, or use of format rat, would reveal that they are integers divided by 360.

If A is square and nonsingular, then, without round-off error, X = inv(A)\*B is theoretically the same as  $X = A \setminus B$  and Y = B\*inv(A) is theoretically the same as Y = B/A. But the computations involving the backslash and slash operators are preferable because they require less computer time, less memory, and have better error-detection properties.

#### **Pseudoinverses**

Rectangular matrices do not have inverses or determinants. At least one of the equations AX = I and XA = I does not have a solution. A partial replacement for the inverse is provided by the *Moore-Penrose pseudoinverse*, which is computed by the pinv function:

```
1.0000 0.0000
0.0000 1.0000
```

is the 2-by-2 identity, but the matrix

```
P = C*X

P = 0.8293 -0.1958 0.3213

-0.1958 0.7754 0.3685

0.3213 0.3685 0.3952
```

is not the 3-by-3 identity. However, P acts like an identity on a portion of the space in the sense that P is symmetric, P\*C is equal to C, and X\*P is equal to X.

#### Solving a Rank-Deficient System

If A is m-by-n with m > n and full rank n, each of the three statements

```
x = A\b
x = pinv(A)*b
x = inv(A'*A)*A'*b
```

theoretically computes the same least-squares solution x, although the backslash operator does it faster.

However, if A does not have full rank, the solution to the least-squares problem is not unique. There are many vectors X that minimize

```
norm(A*x -b)
```

The solution computed by  $x = A \setminus b$  is a basic solution; it has at most r nonzero components, where r is the rank of A. The solution computed by x = pinv(A) \*b is the minimal norm solution because it minimizes norm(x). An attempt to compute a solution with x = inv(A'\*A) \*A'\*b fails because A'\*A is singular.

Here is an example that illustrates the various solutions:

```
A = [ 1 2 3
4 5 6
7 8 9
10 11 12 ];
```

does not have full rank. Its second column is the average of the first and third columns. If

```
b = A(:,2)
is the second column, then an obvious solution to A^*x = b is x = [0 \ 1 \ 0]'. But none
of the approaches computes that x. The backslash operator gives
x = A \setminus b
Warning: Rank deficient, rank = 2, tol = 1.4594e-014.
      0.5000
      0
      0.5000
This solution has two nonzero components. The pseudoinverse approach gives
y = pinv(A)*b
y =
      0.3333
      0.3333
      0.3333
There is no warning about rank deficiency. But norm(y) = 0.5774 is less than
norm(x) = 0.7071. Finally,
z = inv(A'*A)*A'*b
fails completely:
Warning: Matrix is close to singular or badly scaled.
          Results may be inaccurate. RCOND = 9.868649e-018.
7 =
   -0.8594
    1.3438
```

#### **Acknowledgments**

-0.6875

LAPACK is a library of routines that provides fast, robust algorithms for numerical linear algebra and matrix computations. Since the year 2000, 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.

## **Factorizations**

#### In this section...

"Introduction" on page 2-27

"Cholesky Factorization" on page 2-27

"LU Factorization" on page 2-28

"QR Factorization" on page 2-30

"Using Multithreaded Computation for Factorization" on page 2-33

"Acknowledgments" on page 2-34

#### 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)
A =
                              1
                                             1
        1
               2
                      3
                                     5
                              4
                                            6
        1
               3
                      6
                                    15
                                           21
                             10
               4
                      10
                             20
                                    35
                                           56
                             35
                      15
                                    70
                                          126
```

1 6 21 56 126 252

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

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  $\varepsilon$  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:

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'Q = 1.

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)
Q =
    0.6191
               0.1406
                         -0.1899
                                    -0.5058
                                               0.5522
    0.1506
               0.4084
                          0.5034
                                    0.5974
                                               0.4475
    0.3954
                                    -0.1478
                                               -0.2008
              -0.5564
                          0.6869
                                    -0.1729
    0.3167
               0.6676
                          0.1351
                                               -0.6370
    0.5808
              -0.2410
                         -0.4695
                                    0.5792
                                               -0.2207
R =
               1.0663
    1.5346
                          1.2010
                                     1.4036
               0.7245
                          0.3474
                                    -0.0126
         0
         0
                          0.9320
                    0
                                    0.6596
         0
                    0
                                    0.6648
                               0
         0
                    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:

```
[Q,R] = qr(C,0)
Q =
    0.6191
               0.1406
                         -0.1899
                                    -0.5058
    0.1506
               0.4084
                          0.5034
                                     0.5974
                          0.6869
                                    -0.1478
    0.3954
              -0.5564
    0.3167
               0.6676
                          0.1351
                                    -0.1729
    0.5808
              -0.2410
                         -0.4695
                                     0.5792
R =
    1.5346
               1.0663
                          1.2010
                                     1.4036
         0
               0.7245
                          0.3474
                                    -0.0126
```

0	0	0.9320	0.6596
0	0	0	0.6648

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  $\mathbf C$  has a larger norm than the first, so the two columns are exchanged:

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

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

p =

2 1

The QR factorization transforms an overdetermined linear system into an equivalent triangular system. The expression

```
norm(A*x - b)
equals
norm(Q*R*x - b)
Multiplication by orthogonal matrices preserves the Euclidean norm, so this expression is also equal 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 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.

1u and qr show significant increase in speed on large double-precision arrays (on order of 10,000 elements).

#### **Acknowledgments**

LAPACK is a library of routines that provides fast, robust algorithms for numerical linear algebra and matrix computations. Since the year 2000, 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.

# **Powers and Exponentials**

#### In this section...

"Positive Integer Powers" on page 2-35

"Inverse and Fractional Powers" on page 2-35

"Element-by-Element Powers" on page 2-36

"Exponentials" on page 2-36

#### **Positive Integer Powers**

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

```
A = [1 \ 1 \ 1; 1 \ 2 \ 3; 1 \ 3 \ 6]
A =
      1
                      1
      1
              2
                      3
      1
              3
                      6
X = A^2
χ =
      3
              6
                     10
      6
             14
                     25
     10
             25
                     46
```

## **Inverse and Fractional Powers**

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

```
Y = A^(-3)

Y =

145.0000 -207.0000 81.0000

-207.0000 298.0000 -117.0000
```

```
81.0000 -117.0000 46.0000
```

Fractional powers, like A^(2/3), are also permitted; the results depend upon the distribution of the eigenvalues of the matrix.

#### **Element-by-Element Powers**

The . ^ operator produces element-by-element powers. For example:

## **Exponentials**

The function

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.

A system of linear, constant coefficient, ordinary differential equations can be written

$$dx/dt = Ax$$

where x = x(t) is a vector of functions of t and A is a matrix independent of t. The solution can be expressed in terms of the matrix exponential

$$x(t) = e^{tA}x(0)$$

The function

computes the matrix exponential. An example is provided by the 3-by-3 coefficient matrix,

```
A = [0 -6 -1; 6 2 -16; -5 20 -10]

A =

0 -6 -1
6 2 -16
-5 20 -10
```

and the initial condition, x(0).

```
x0 = [1 1 1]'
x0 =

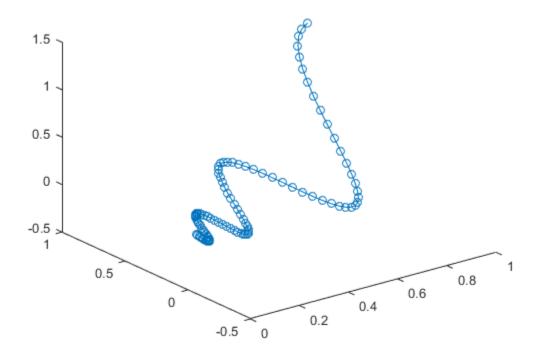
1
1
1
```

The matrix exponential is used to compute the solution, x(t), to the differential equation at 101 points on the interval  $0 \le t \le 1$ .

```
X = [];
for t = 0:.01:1
   X = [X expm(t*A)*x0];
end
```

A three-dimensional phase plane plot shows the solution spiraling in towards the origin. This behavior is related to the eigenvalues of the coefficient matrix.

```
plot3(X(1,:),X(2,:),X(3,:),'-0')
```



# **Eigenvalues**

#### In this section...

"Eigenvalue Decomposition" on page 2-39

"Multiple Eigenvalues" on page 2-40

"Schur Decomposition" on page 2-41

"Acknowledgments" on page 2-42

#### **Eigenvalue Decomposition**

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

 $Av = \lambda v$ .

With the eigenvalues on the diagonal of a diagonal matrix  $\Lambda$  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 provided by the coefficient matrix of the ordinary differential equation in the previous section:

The statement

lambda = eig(A)

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

```
lambda =
-3.0710
-2.4645+17.6008i
-2.4645-17.6008i
```

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)
V =
  -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
        0
                     -2.4645+17.6008i
                                              0
        0
                                        -2.4645-17.6008i
```

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:

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**

The MATLAB 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 a basis with much better numerical properties than a set of eigenvectors. The Schur decomposition of this defective example is

```
[U,S] = schur(A)
U =
   -0.4741
               0.6648
                          0.5774
    0.8127
               0.0782
                          0.5774
   -0.3386
              -0.7430
                          0.5774
S =
   -1.0000
              20.7846
                          -44.6948
          0
               1,0000
                          -0.6096
          0
                     0
                           1.0000
```

The double eigenvalue is contained in the lower 2-by-2 block of S.

**Note:** If A is complex, schur returns the complex Schur form, which is upper triangular with the eigenvalues of A on the diagonal.

## **Acknowledgments**

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# **Singular Values**

A *singular value* and corresponding *singular vectors* of a rectangular matrix A are, respectively, a scalar  $\sigma$  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 u are singular vectors of u as well.

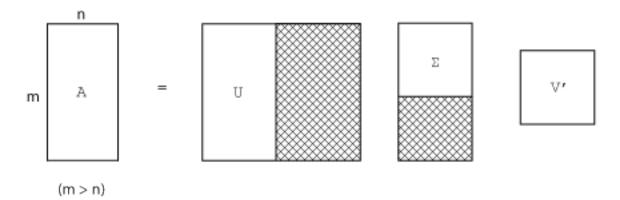
The singular values  $\sigma$  are always real and nonnegative, even if A is complex. With the singular values on the diagonal of a diagonal matrix  $\Sigma$  and the corresponding singular vectors forming the columns of two orthogonal matrices U and V, you obtain the equations

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

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 an m-by-m U, an m-by-n  $\Sigma$ , and an n-by-n V. In other words, U and V are both square, and  $\Sigma$  is the same size as A. If A has many more rows than columns, the resulting U can be quite large, but most of its columns are multiplied by zeros in  $\Sigma$ . In this situation, the economy-sized decomposition saves both time and storage by producing an m-by-n U, an n-by-n  $\Sigma$  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

the full singular value decomposition is

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.

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

If the matrix A is large and sparse, then using svd to calculate *all* of the singular values and 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 a lot of extra work. In cases where only a subset of the singular values and vectors are required, the svds function is preferred over svd.

```
For 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. However, for truly large and sparse matrices, using svds becomes necessary.

## **Acknowledgments**

LAPACK is a library of routines that provides fast, robust algorithms for numerical linear algebra and matrix computations. Since the year 2000, 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.

## **See Also**

gsvd | svd | svds

# **Random Numbers**

- "Random Numbers in MATLAB" on page 3-2
- "Why Do Random Numbers Repeat After Startup?" on page 3-3
- "Create Arrays of Random Numbers" on page 3-4
- "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  $3\mbox{-}15$
- "Managing the Global Stream" on page 3-17
- "Creating and Controlling a Random Number Stream" on page 3-23
- "Multiple Streams" on page 3-31
- "Replace Discouraged Syntaxes of rand and randn" on page 3-34

## Random Numbers in MATLAB

When you create random numbers using software, the results are not random in a strict, mathematical sense. However, software applications, such as MATLAB, use algorithms that make your results appear to be random and independent. The results also pass various statistical tests of randomness and independence. These apparently random and independent numbers are often described as *pseudorandom* and *pseudoindependent*. You can use these numbers as if they are truly random and independent. One benefit of using pseudorandom, pseudoindependent numbers is that you can repeat a random number calculation at any time. This approach can be useful in testing or diagnostic situations.

Although repeatability can be useful, it is possible to repeat your results accidentally when you really want different results. There are several ways to avoid this problem. The documentation contains several examples that show how to ensure that your results are different when that is your intention.

**Note:** You can assume any reference to random numbers in the MATLAB documentation is actually referring to pseudorandom numbers, unless otherwise stated.

#### **Related Examples**

- "Generate Random Numbers That Are Repeatable" on page 3-11
- "Generate Random Numbers That Are Different" on page 3-15

# 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,

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

#### See Also

rng

# **Create Arrays of Random Numbers**

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

```
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 1,2,...,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 arrays of random integer values that have no repeated values. For example,

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

r4 is a 1-by-5 array containing randomly selected integer values on the closed interval, [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.

#### See Also

```
rand | randi | randn | randperm
```

# **Related Examples**

- "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

#### More About

• "Random Numbers in MATLAB" on page 3-2

# 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.

# **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.

# 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  $\mu_x$  and variance is  $\sigma_x^2$ , 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 = [mean(y) std(y) var(y)]

stats = 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.

# 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,  $(0, 2\pi)$ .

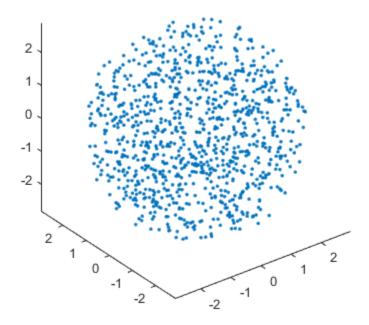
```
azimuth = 2*pi*rand(1000,1);
```

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.

# 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.

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  ${\bf 1}$  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.

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

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

Save the generator settings in a structure S.

```
s = rng;
```

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

Repeat the same command.

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

Now, return the generator to the original state stored in  ${\bf s}$  and reproduce the first array  ${\bf A}$ .

Unlike reseeding, which reinitializes the generator, this approach allows you to save and restore the generator settings at any point.

# **See Also**

rng

# **Related Examples**

• "Generate Random Numbers That Are Different" on page 3-15

# **More About**

• "Random Numbers in MATLAB" on page 3-2

# 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 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.

Alternatively, specify different seeds explicitly. For example,

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

**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.

### See Also

rng

## **Related Examples**

• "Generate Random Numbers That Are Repeatable" on page 3-11

### More About

- "Random Numbers in MATLAB" on page 3-2
- "Startup Options in MATLAB Startup File"

# Managing the Global Stream

rand, randn, and randi draw random numbers from an underlying random number stream, called the global stream. The rng function provides a simple way to control the global stream. For more comprehensive control, the RandStream class allows you to get a handle to the global stream and control random number generation.

Get a handle to the global stream as follows:

Return the properties of the stream with the get method:

Now, use the rand function to generate uniform random values from the global stream.

```
rand(1,5);
```

Use the randn and randi functions to generate normal random values and integer random values from the global stream.

```
A = randi(100,1,5);
A = randn(1,5);
```

The State property is the internal state of the generator. You can save the State of globalStream.

```
myState = globalStream.State;
```

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

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

rand, randi, and randn 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;
randi(100);
B = rand(1,100);
isequal(A,B)
ans =
0
```

The global stream is a handle object of the RandStream class.

RandStream.getGlobalStream returns a handle. The properties of the global stream can be viewed or modified from any handle to the stream.

```
stream1=RandStream.getGlobalStream;
stream2=RandStream.getGlobalStream;
stream1.NormalTransform='Polar';
stream2.NormalTransform
ans =
Polar
```

The following table shows the methods available for the RandStream class. Static methods are indicated with the syntax RandStream.methodName.

Method	Description	
RandStream	Create a random number stream	
RandStream.create	Create multiple independent random number streams	
get	Get the properties of a random stream	
RandStream.list	List available random number generator algorithms	
RandStream.getGlobalStream	Get the global random number stream	
RandStream.setGlobalStream	Set the global random number stream	
set	Set a property of a random stream	
reset	Reset a stream to its initial internal state	
rand	Generate pseudorandom numbers from a uniform distribution	
randn	Generate pseudorandom numbers from a standard normal distribution	
randi	Generate pseudorandom integers from a uniform discrete distribution	
randperm	Random permutation of a set of values	

The properties of a random stream are given the following table.

Property	Description
Туре	(Read-only) Generator algorithm used by the stream. RandStream.list specifies the possible generators.
Seed	(Read-only) Seed value used to create the stream.
NumStreams	(Read-only) Number of streams in the group in which the current stream was created.
StreamIndex	(Read-only) Index of the current stream from among the group of streams with which the current stream was created.

Property	Description
State	Internal state of the generator. Do not depend on the format of this property. The value you assign to S.State must be a value previously read from S.State.
Substream	Index of the substream to which the stream is currently set. The default is 1. Multiple substreams are not supported by all generator types; the multiplicative lagged Fibonacci generator (mlfg6331_64) and combined multiple recursive generator (mrg32k3a) support substreams.
NormalTransform	Transformation algorithm used by randn(s,) to generate normal pseudorandom values. Possible values are 'Ziggurat', 'Polar', or 'Inversion'.
Antithetic	Logical value indicating whether S generates antithetic pseudorandom values. For uniform values, these are the usual values subtracted from 1. The default is false.
FullPrecision	Logical value indicating whether S generates values using its full precision. Some generators can create pseudorandom values faster, but with fewer random bits, if FullPrecision is false. The default is true.

Suppose you want to repeat a simulation. The RandStream class gives you several ways to replicate output. As shown in the previous example, you can save the state of the global stream.

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

1

You can also reset a stream to its initial settings with the method reset.

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

# **Random Number Data Types**

rand and randn generate values in double precision by default.

```
GlobalStream=RandStream.getGlobalStream;
myState=GlobalStream.State;
A=rand(1,5);
class(A)

ans =
double

To specify the class as double explicitly:
GlobalStream.State=myState;
B=rand(1,5,'double');
class(B)

ans =
double
isequal(A,B)
ans =

1
```

rand and randn will also generate values in single precision.

```
GlobalStream.State=myState;
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 =
    0.8235
               0.6948
                          0.3171
                                     0.9502
                                               0.0344
B =
    0.8235
               0.6948
                          0.3171
                                     0.9502
                                               0.0344
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
```

# Creating and Controlling a Random Number Stream

```
In this section...

"Substreams" on page 3-24

"Choosing a Random Number Generator" on page 3-25
```

The RandStream class allows you to create a random number stream. This is useful for several reasons. For example, you might want to generate random values without affecting the state of the global stream. You might want separate sources of randomness in a simulation. Or you may need to use a different generator algorithm than the one MATLAB software uses at startup. With the RandStream constructor, you can create your own stream, set the writable properties, and use it 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 constructor.

```
myStream=RandStream('mlfg6331_64');
rand(myStream,1,5)
ans =
     0.6530     0.8147     0.7167     0.8615     0.0764
```

The random stream myStream acts separately from the global stream. The functions rand, randn, and randi will continue to draw from the global stream, and will not affect the results of the RandStream methods rand, randn and randi applied to myStream.

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

```
ans =
```

### **Substreams**

You may want to return to a previous part of a simulation. A random stream can be controlled by having it jump to fixed checkpoints, called substreams. The Substream property allows you to jump back and forth among multiple substreams. To use the Substream property, create a stream using a generator that supports substreams. (See "Choosing a Random Number Generator" on page 3-25 for a list of generator algorithms and their properties.)

```
stream=RandStream('mlfg6331_64');
RandStream.setGlobalStream(stream)
The initial value of Substream is 1.
stream.Substream
ans =
    1
```

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, they can be used in loops.

```
for i=1:5
    stream.Substream=i;
    rand(1,i)
end

ans =
    0.6530

ans =
    0.3364    0.8265

ans =
    0.9539    0.6446    0.4913
ans =
```

```
0.0244 0.5134 0.6305 0.6534

ans =

0.3323 0.9296 0.5767 0.1233 0.6934
```

Each of these substreams can reproduce its loop iteration. For example, you can return to the 5th substream. The result will return the same values as the 5th output above.

```
stream.Substream=5;
rand(1,5)
ans =
    0.3323    0.9296    0.5767    0.1233    0.6934
```

# **Choosing a Random Number Generator**

MATLAB software offers six generator algorithms. The following 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.

### Generator algorithms

Keyword	Generator	Multiple Stream and Substream Support	Approximate Period In Full Precision
mt19937ar	Mersenne twister (default)	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 <sup>124</sup>
mrg32k3a	Combined multiple recursive generator	Yes	2 <sup>191</sup>
shr3cong	Shift-register generator summed	No	$2^{64}$

Keyword	Generator	Multiple Stream and Substream Support	Approximate Period In Full Precision
	with linear congruential generator		
swb2712	Modified subtract with borrow generator	No	2 <sup>1492</sup>

Some of the generators (mcg16807, shr3cong, swb2712) provide for backwards compatibility with earlier versions of MATLAB. Two generators (mrg32k3a, mlfg6331\_64) provide explicit support for parallel random number generation. The remaining generators (mt19937ar, dsfmt19937) are designed primarily for sequential applications. Depending on the application, some generators may be faster or return values with more precision.

Another reason for the choice of generators has to do with applications. All pseudorandom number generators are based on deterministic algorithms, and all will fail 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 MATLAB software's choice of generators provide you with the means to do that. Although it is unlikely that your results will differ by more than 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**

### 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). The randn algorithm used by default for mcg16807 streams 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).

mlfg6331\_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  $2^{-53}$  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. It has a period of  $2^{191}$  and supports up to  $2^{63}$  parallel streams via 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.

#### 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.

#### 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 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.

### References

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- [13] Moler, C.B. *Numerical Computing with MATLAB*. SIAM, 2004. Available online at http://www.mathworks.com/moler
- [14] Park, S.K., and K.W. Miller. "Random Number Generators: Good Ones Are Hard to Find." *Communications of the ACM*, 31(10):1192–1201. 1998.

# **Multiple Streams**

MATLAB software includes generator algorithms that allow you to create multiple independent random number streams. The RandStream.create factory method allows you to create three 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 =
    1.0000
             -0.0017
                        -0.0010
   -0.0017
              1.0000
                        -0.0050
```

```
-0.0010 -0.0050 1.0000
```

By using different seeds, you can create streams that return different values and act separately from one another.

```
s1=RandStream('mt19937ar','seed',1);
s2=RandStream('mt19937ar','seed',2);
s3=RandStream('mt19937ar','seed',3);
```

Seed values must be integers between 0 and  $2^{32}-1$ . With different seeds, streams typically return values that are uncorrelated.

For generator types that do not explicitly support independent streams, different seeds provide a method to create multiple streams. However, using a generator specifically designed for multiple independent streams is a better option, as the statistical properties across streams are better understood.

Depending on the application, it might be useful to create only some of the streams in a set of independent streams. The StreamIndex property returns the index of a specified stream from a set of factory-generated streams.

```
numLabs=256;
labIndex=4;
s1=RandStream.create('mlfg6331_64',
    'NumStreams',numLabs,'StreamIndices',labIndex)
s1=
mlfg6331_64 random stream
    StreamIndex: 4
    NumStreams: 256
    Seed: 0
    NormalTransform: Ziggurat
```

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.

**Note:** Not all generators algorithms support multiple streams. See the table of generator algorithms in "Choosing a Random Number Generator" on page 3-25 for a summary of generator properties.

# Replace Discouraged Syntaxes of rand and randn

#### In this section...

"Description of the Discouraged Syntaxes" on page 3-34

"Description of Replacement Syntaxes" on page 3-35

"Replacement Syntaxes for Initializing the Generator with an Integer Seed" on page 3-35

"Replacement Syntaxes for Initializing the Generator with a State Vector" on page 3-36

"If You Are Unable to Upgrade from Discouraged Syntax" on page 3-37

# **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) or '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)	riig(su, v4 )		
rand('state',sd)	rng(sd,'v5uniform')	Trig(su)	
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
% Save v5 generator state.	% Get generator settings.
<pre>st = rand('state');</pre>	s = rng;
% Call rand.	% Call rand.
x = rand;	x = rand;
% Restore v5 generator state.	% Restore previous generator
<pre>rand('state',st);</pre>	% settings.
	rng(s);
% Call rand again and hope	
% for the same results.	% Call rand again and
y = rand	% 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:

```
s = rng % Save current settings of the generator.
... % Call code using legacy random number generator syntaxes.
rng(s) % Restore previous settings of the generator.
```

# **Sparse Matrices**

- "Computational Advantages of Sparse Matrices" on page 4-2
- "Constructing Sparse Matrices" on page 4-4
- "Accessing Sparse Matrices" on page 4-9
- "Sparse Matrix Operations" on page 4-16

# **Computational Advantages of Sparse Matrices**

```
In this section...

"Memory Management" on page 4-2

"Computational Efficiency" on page 4-3
```

### **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
                     Size
                                                  Class
                                                              Attributes
                                           Bytes
                                         9680000
  M full
                 1100x1100
                                                  double
                 1100x1100
                                            9608
                                                  double
  M sparse
                                                              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). The resulting efficiencies can lead to dramatic improvements in execution time for programs working with large amounts of sparse data.

For more information, see "Sparse Matrix Operations" on page 4-16.

# **Constructing Sparse Matrices**

```
In this section...

"Creating Sparse Matrices" on page 4-4

"Importing Sparse Matrices" on page 4-8
```

# **Creating Sparse Matrices**

- "Converting Full to Sparse" on page 4-4
- "Creating Sparse Matrices Directly" on page 4-5
- "Creating Sparse Matrices from Their Diagonal Elements" on page 4-7

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.

### produces

```
S =
(3,1) 1
(2,2) 2
(3,2) 3
(4,3) 4
(1,4) 5
```

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 for the resulting matrix, and n is the column dimension.

The matrix S of the previous example can be generated directly with

```
(1,4) 5
```

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'
For n = 5, MATLAB responds with
S =
                 -2
   (1,1)
   (2,1)
                  1
                  1
   (1,2)
   (2,2)
                 -2
                  1
   (3,2)
                  1
   (2,3)
                 -2
   (3,3)
                  1
   (4,3)
                  1
   (3,4)
                 -2
   (4,4)
                  1
   (5,4)
                  1
   (4,5)
                 -2
   (5,5)
```

Now F = full(S) displays the corresponding full matrix.

```
F = full(S)
F =
     -2
             1
                    0
                                    0
            -2
      1
                    1
                            0
                                    0
      0
             1
                    -2
                            1
                                    0
                    1
                           -2
      0
             0
                                    1
      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 B and the vector 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:

(3,3)	33
(6,3)	63
(2,4)	24
(4,4)	44
(7,4)	74

In its full form, A looks like this:

```
full(A)
ans =
     11
             0
                    13
                            0
      0
            22
                     0
                           24
      0
             0
                    33
                            0
     41
             0
                     0
                           44
      0
            52
                     0
                            0
      0
             0
                    63
                            0
      0
             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.

# **Accessing Sparse Matrices**

#### In this section...

"Nonzero Elements" on page 4-9

"Indices and Values" on page 4-11

"Indexing in Sparse Matrix Operations" on page 4-11

"Visualizing Sparse Matrices" on page 4-14

### **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.

load west0479 whos

Name	Size	Bytes	Class	Attributes
M_full M_sparse	1100x1100 1100x1100	9680000 5004	double	sparse
west0479	479x479	24564	double	sparse

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
              -3.6613e-02
  (31,3)
  (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.

```
[i,j,s] = find(S)
[m,n] = size(S)
S = 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
     3
                  42
     2
            2
                   1
     3
            3
                   1
     4
                   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 intmax.

```
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 takes considerably more time than a similar vectorized operation:

```
tic; A(1:n-1,n) = -1; A(n,1:n-1) = -1; toc
```

Elapsed time is 0.001899 seconds.

```
tic; for k = 1:n-1, C(k,n) = -1; C(n,k) = -1; end, toc Elapsed time is 0.286563 seconds.
```

The difference in execution time in this example is over two orders of magnitude. 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 26.281000 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 0.078000 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:

$$\mathbf{C} = \begin{pmatrix} 4 & 0 & 0 & 0 & -1 \\ 0 & 4 & 0 & 0 & -1 \\ 0 & 0 & 4 & 0 & -1 \\ 0 & 0 & 0 & 4 & -1 \\ 1 & 1 & 1 & 1 & 4 \end{pmatrix}$$

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]';
s = [4 1 4 1 4 1 4 1 -1 -1 -1 -1 4]';
C = sparse(i,i,s)
C =
   (1,1)
   (5,1)
   (2,2)
   (5,2)
   (3,3)
   (5,3)
   (4,4)
   (5,4)
   (1,5)
   (2,5)
   (3,5)
                  - 1
   (4,5)
                  - 1
    (5,5)
```

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.

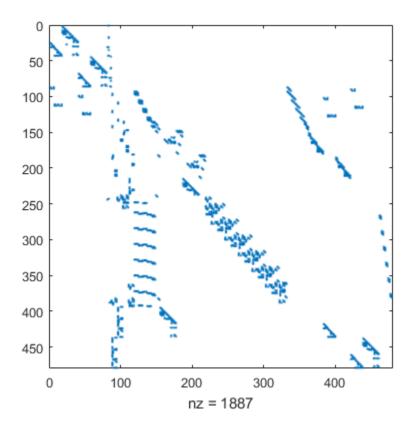
For example:

Load the supplied sparse matrix west0479, one of the Harwell-Boeing collection.

load west0479

View the sparsity structure.

spy(west0479)



# **Sparse Matrix Operations**

#### In this section...

"Efficiency of Operations" on page 4-16

"Permutations and Reordering" on page 4-17

"Factoring Sparse Matrices" on page 4-20

"Systems of Linear Equations" on page 4-28

"Eigenvalues and Singular Values" on page 4-31

"References" on page 4-34

## **Efficiency of Operations**

- · "Computational Complexity" on page 4-16
- "Algorithmic Details" on page 4-16

#### **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**

- · "Reordering for Sparsity" on page 4-19
- "Reordering to Reduce Bandwidth" on page 4-19
- · "Approximate Minimum Degree Ordering" on page 4-19

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, the statements

```
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)
produce:
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	=				
	11	1	0	0	0
	1	22	1	0	0
	0	1	33	1	0
	0	0	1	44	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 produce

ans = 

Similarly, S(:,p) and S\*P' produce

ans = 

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 representations, let I = speye(n) be an identity matrix of the appropriate size. Then,

#### **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 function p = colperm(S) 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 function Symrcm(A) actually operates on the nonzero structure of the symmetric matrix A + A', but the result is also useful for asymmetric 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 the 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.

The following 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" on page 4-21 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].

## **Factoring Sparse Matrices**

- "LU Factorization" on page 4-20
- "Cholesky Factorization" on page 4-24
- "QR Factorization" on page 4-25
- "Incomplete Factorizations" on page 4-26

#### 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.

$$[L,U,P] = lu(S)$$

1u 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

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 1u 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

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.

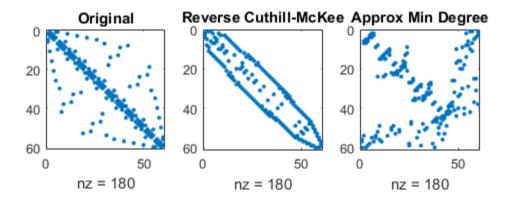
```
r = symrcm(B);
m = symamd(B);
```

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('Approx 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, 1u 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

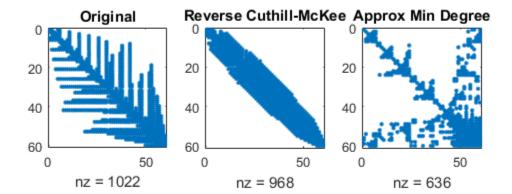
Even though this is a small example, the results are typical. The original numbering scheme leads to the most fill-in. The fill-in for the reverse Cuthill-McKee ordering is concentrated within the band, but it is almost as extensive as the first two orderings. For the approximate minimum degree ordering, 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('Approx 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 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 Q-less QR factorization allows the solution of sparse least squares problems

$$\min \operatorname{minimize} \|Ax - b\|_{2}$$

with two steps

$$[c,R] = qr(A,b)$$
  
x = R\c

If A is sparse, but not square, MATLAB uses these steps for the linear equation solving backslash operator:

```
x = A \setminus 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 "semi-normal 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-017
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-005
opts.type = 'crout';
nnz(L)+nnz(U)-size(A,1)
ans =
       31083
norm(P*A-L*U, 'fro')./norm(A, 'fro')
ans =
  9.7344e-005
```

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:

```
A = delsq(numgrid('S',200));
nnz(A)
ans =
```

ans =

2.3997e-004

195228

```
nnz(chol(A, 'lower'))
ans =
     7762589
shows that A has 195228 nonzeros, and its complete Cholesky factorization without
reordering has 7762589 nonzeros. By contrast:
L = ichol(A);
nnz(L)
ans =
      117216
norm(A-(L*L').*spones(A),'fro')./norm(A,'fro')
  3.5805e-017
opts.type = 'ict';
opts.droptol = 1e-4;
L = ichol(A, opts);
nnz(L)
ans =
     1166754
norm(A-L*L','fro')./norm(A,'fro')
```

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.

## Systems of Linear Equations

There are two different classes of methods for solving systems of simultaneous linear equations:

• Direct methods are usually variants of Gaussian elimination. These methods involve the individual matrix elements directly, through matrix operations such as LU or Cholesky factorization. MATLAB implements direct methods through the matrix division operators / and \, which you can use to solve linear systems.

Iterative methods produce only an approximate solution after a finite number of steps.
These methods involve the coefficient matrix only indirectly, through a matrix-vector
product or an abstract linear operator. Iterative methods are usually applied only to
sparse matrices.

#### **Direct Methods**

Direct methods are usually faster and more generally applicable than indirect methods, if there is enough storage available to carry them out. Iterative methods are usually applicable to restricted cases of equations and depend on properties like diagonal dominance or the existence of an underlying differential operator. Direct methods are implemented in the core of the MATLAB software and are made as efficient as possible for general classes of matrices. Iterative methods are usually implemented in MATLAB-language files and can use the direct solution of subproblems or preconditioners.

#### Using a Different Preordering

If A is not diagonal, banded, triangular, or a permutation of a triangular matrix, backslash (\) reorders the indices of A to reduce the amount of fill-in—that is, the number of nonzero entries that are added to the sparse factorization matrices. The new ordering, called a *preordering*, is performed before the factorization of A. In some cases, you might be able to provide a better preordering than the one used by the backslash algorithm.

To use a different preordering, first turn off both of the automatic preorderings that backslash might perform by default, using the function **spparms** as follows:

```
currentParms = spparms;
spparms('autoamd',0);
spparms('autommd',0);
```

Now, assuming you have created a permutation vector  $\mathbf{p}$  that specifies a preordering of the indices of A, apply backslash to the matrix A(:,p), whose columns are the columns of A, permuted according to the vector  $\mathbf{p}$ .

```
x = A (:,p) \ b;
x(p) = x;
spparms(currentParms);
```

The command spparms (defaultParms) restores the controls to their prior state, in case you use A\b later without specifying an appropriate preordering.

#### **Iterative Methods**

Eleven functions are available that implement iterative methods for sparse systems of simultaneous linear systems.

#### **Functions for Iterative Methods for Sparse Systems**

Function	Method
bicg	Biconjugate gradient
bicgstab	Biconjugate gradient stabilized
bicgstabl	Biconjugate gradient stabilized (l)
cgs	Conjugate gradient squared
gmres	Generalized minimum residual
lsqr	Least squares
minres	Minimum residual
pcg	Preconditioned conjugate gradient
qmr	Quasiminimal residual
symmlq	Symmetric LQ
tfqmr	Transpose-free quasiminimal residual

These methods are designed to solve Ax = b or minimize the norm of b - Ax. For the Preconditioned Conjugate Gradient method, pcg, A must be a symmetric, positive definite matrix. minres and symmlq can be used on symmetric indefinite matrices. For lsqr, the matrix need not be square. The other seven can handle nonsymmetric, square matrices and each method has a distinct benefit.

All eleven methods can make use of preconditioners. The linear system

$$Ax = b$$

is replaced by the equivalent system

$$M^{-1}Ax = M^{-1}b$$

The preconditioner M is chosen to accelerate convergence of the iterative method. In many cases, the preconditioners occur naturally in the mathematical model. A partial

differential equation with variable coefficients can be approximated by one with constant coefficients, for example. Incomplete matrix factorizations can be used in the absence of natural preconditioners.

The five-point finite difference approximation to Laplace's equation on a square, two-dimensional domain provides an example. The following statements use the preconditioned conjugate gradient method preconditioner  $M = L^*L'$ , where L is the zero-fill incomplete Cholesky factor of A.

```
A = delsq(numgrid('S',50));
b = ones(size(A,1),1);
tol = 1e-3;
maxit = 100;
L = ichol(A);
[x,flag,err,iter,res] = pcg(A,b,tol,maxit,L,L');
```

Twenty-one iterations are required to achieve the prescribed accuracy. On the other hand, using a different preconditioner may yield better results. For example, using ichol to construct a modified incomplete Cholesky, the prescribed accuracy is met after only 15 iterations:

```
L = ichol(A,struct('type','nofill','michol','on'));
[x,flag,err,iter,res] = pcg(A,b,tol,maxit,L,L');
```

Background information on these iterative methods and incomplete factorizations is available in [2] and [6].

## **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 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:  $A\nu = \lambda B\nu$ .

The statement

```
[U,S,V] = svds(A,k)
```

finds the k largest singular values of A and

$$[U,S,V] = svds(A,k,0)$$

finds the k smallest singular values.

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)
nnz(A)

ans =

2945

2945

ans =
```

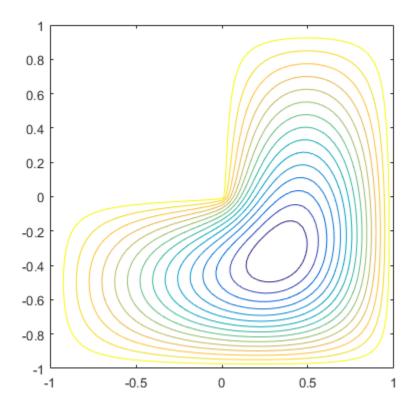
A is a matrix of order 2945 with 14,473 nonzero elements.

Compute the smallest eigenvalue and eigenvector.

```
[v,d] = eigs(A,1,0);
```

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
```



The numerical techniques used in eigs and svds are described in [6].

### 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.

# **Graph and Network Algorithms**

- "Directed and Undirected Graphs" on page 5-2
- "Modify Nodes and Edges of Existing Graph" on page 5-11
- "Add Graph Node Names, Edge Weights, and Other Attributes" on page 5-15
- "Graph Plotting and Customization" on page 5-20
- "Visualize Breadth-First and Depth-First Search" on page 5-34
- "Partition Graph with Laplacian Matrix" on page 5-38
- "Add Node Properties to Graph Plot Data Cursor" on page 5-43

# **Directed and Undirected Graphs**

#### In this section...

"What Is a Graph?" on page 5-2

"Creating Graphs" on page 5-4

"Graph Node IDs" on page 5-9

"Modify an Existing Graph" on page 5-10

## What Is a Graph?

A graph is a collection of *nodes* and *edges* that represents relationships:

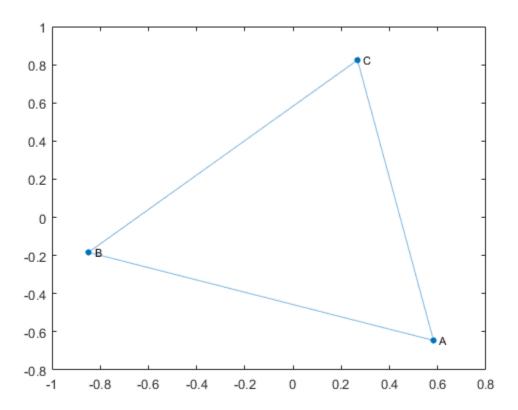
- **Nodes** are vertices that correspond to objects.
- Edges are the connections between objects.
- The graph edges sometimes have **Weights**, which indicate the strength (or some other attribute) of each connection between the nodes.

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:

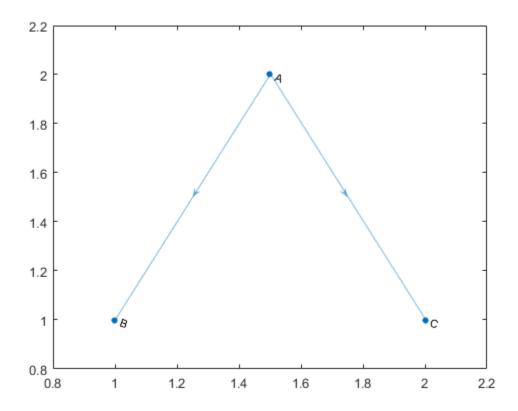
- The Internet The graph nodes are computers, and the edges are network connections between computers.
- A brain The graph nodes are neurons, and the edges represent neuron connections.
- Web page linking The graph nodes are web pages, and the edges represent links between pages.
- Airports The graph 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. The figure below 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. The figure below 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.

Graphs created using graph and digraph can have self-loops (an edge connecting a node to itself). However, graphs cannot have multiple edges with the same source and target nodes.

## **Creating Graphs**

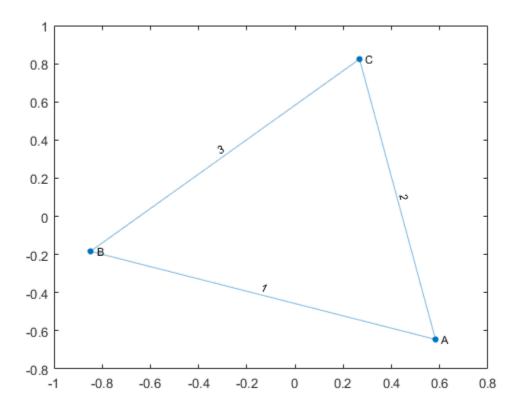
The primary ways to create a graph are to use an adjacency matrix or an edge list.

#### **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.

- The adjacency matrix for undirected graphs created by graph must be symmetric. Although, in practice the matrices are frequently triangular to avoid repetition. Use graph(A, 'upper') or graph(A, 'lower') to construct an undirected graph using only the upper or lower triangle of the adjacency matrix.
- The adjacency matrix for a directed graph created by digraph does not need to be symmetric.
- For large graphs, the adjacency matrix contains many zeros and is typically a sparse 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:

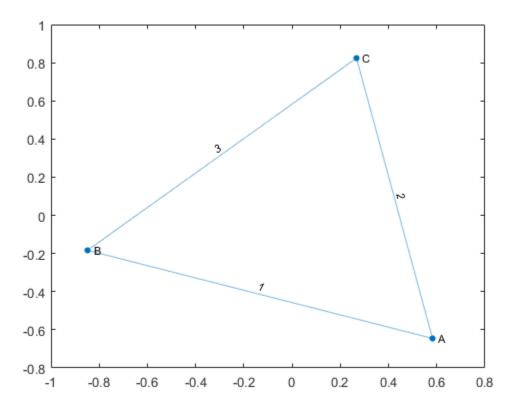
```
A = [0 1 2; 1 0 3; 2 3 0];
node_names = {'A','B','C'};
G = graph(A,node names)
```

You can use adjacency matrices to create a graph using the graph or digraph functions, or you can use the adjacency function to find the unweighted sparse adjacency matrix of a pre-existing graph.

#### **Edge List**

Another way to represent the information in a graph is by listing all of the edges. For connected graphs, the graph nodes are implied by the list of the graph edges. However, some graphs have disconnected nodes that need to be listed separately.

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.

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)
```

Another way to construct a graph from the edge list is by creating a table with the appropriate variables. When using this method, the first variable in the table must be a two column matrix or cell array of character vectors named EndNodes. To construct this graph using a table, input:

Both graph and digraph permit construction of a graph from the edge list. After constructing a graph, G, you can look at the edges (and any properties they might have) with G.Edges. The order of the edges in G.Edges is sorted by source node (first column) and secondarily by target node (second column).

Since the underlying implementation of graph and digraph depends on sparse matrices, many of the same indexing costs apply. Ultimately, it is quickest to construct a graph all at once from the triplet pairs (source, target, weight) using one of the aforementioned methods, instead of creating an empty graph and iteratively adding more nodes and edges. Performance is best when you 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. Thus, it's always an option to refer to the nodes in a graph 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 of a node refers to both the node index and the node name.

For convenience, MATLAB remembers which type of node ID you use in calling 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.

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).

```
p1 = shortestpath(G, 'a', 'd')
p1 =
    '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 an Existing Graph

After you construct a graph or digraph object, you can use a variety of functions to modify the graph structure. The table lists the available graph manipulation functions, which modify the nodes and edges of either graph or digraph objects.

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	
numedges	Find the number of edges in a graph	
numnodes	Find the number of nodes in a graph	
reordernodes	Permute the order of the nodes in a graph	
subgraph	Extract subgraph	

See "Modify Nodes and Edges of Existing Graph" on page 5-11 for some common graph modification examples.

## **See Also**

digraph | graph

## More About

- graph
- digraph
- "Modify Nodes and Edges of Existing Graph" on page 5-11
- "Add Graph Node Names, Edge Weights, and Other Attributes" on page 5-15
- "Graph Plotting and Customization" on page 5-20

# 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: [4×1 table]
    Nodes: [4×0 table]
```

View the edge list of the graph.

#### G.Edges

```
ans =

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: [4×1 table]
  Nodes: [9×0 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: [2×1 table]
  Nodes: [6×0 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: [4×1 table]
  Nodes: [6×0 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: [3×1 table]
  Nodes: [6×0 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: [1×1 table]
  Nodes: [2×1 table]
```

View the edge list of the subgraph.

#### H.Edges

```
ans =

EndNodes

'a' 'b'
```

#### 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

addedge | addnode | digraph | findedge | findnode | graph | rmedge | rmnode | subgraph

# **More About**

- "Directed and Undirected Graphs" on page 5-2
- graph
- · digraph

# 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: [5×1 table]
        Nodes: [4×0 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 an N-by-1 cell array of character vectors, 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.

```
'First'
'Second'
'Third'
'Fourth'
```

Use table indexing to view the names of nodes 1 and 4.

```
ans =

2×1 cell array

'First'

'Fourth'
```

G.Nodes.Name([1 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 =

EndNodes		Weight	
'First'	'Second'	10	
'First'	'Fourth'	20	
'Second'	'Third'	30	
'Second'	'Fourth'	40	
'Third'	'Fourth'	50	

Use table indexing to view the first and third rows of G.Edges.

#### G.Edges([1 3],:)

ans =

EndNodes		Weight	
'First' 'Second'	'Second' 'Third'	10 30	

#### 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 =

EndNodes		Weight	Power	
'First'	'Second'	10	'on'	
'First'	'Fourth'	20	'on'	
'Second'	'Third'	30	'on'	
'Second'	'Fourth'	40	'off'	
'Third'	'Fourth'	50	'off'	

Add a variable named Size to G.Nodes to indicate the physical size of each node.

```
G.Nodes.Size = [10 20 10 30]';
G.Nodes
```

#### **Modify Tables with Variables Editor**

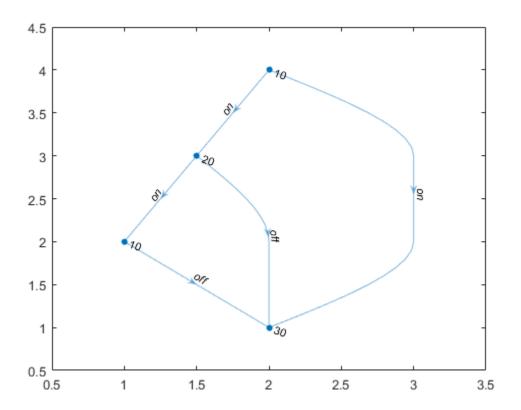
Since Nodes and Edges are both tables, you can use the Variables editor to interactively view or edit the tables. For more information, see "Create and Edit Variables".

#### 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)
p =
 GraphPlot with properties:
     NodeColor: [0 0.4470 0.7410]
   MarkerSize: 4
        Marker: 'o'
     EdgeColor: [0 0.4470 0.7410]
     LineWidth: 0.5000
     LineStvle: '-'
     NodeLabel: {'10'
                       '20' '10'
                                    '30'}
     EdgeLabel: { 'on' 'on' 'off' 'off'}
         XData: [2 1.5000 1 2]
        YData: [4 3 2 1]
         ZData: [0 0 0 0]
 Use GET to show all properties
```



# **See Also**

digraph | graph

# **More About**

- "Directed and Undirected Graphs" on page 5-2
- "Modify Nodes and Edges of Existing Graph" on page 5-11
- graph
- digraph

# **Graph Plotting and Customization**

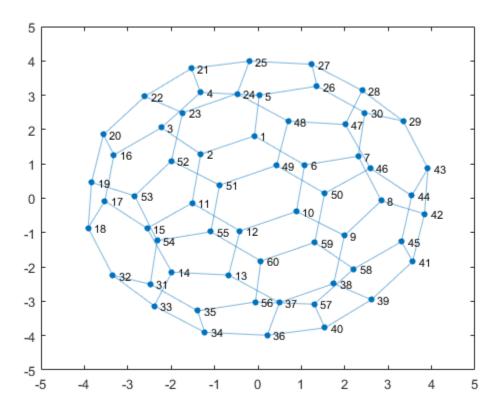
This example shows how to plot graphs, and then customize the display to add labels or highlighting to the graph nodes and edges.

#### **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 and adds node labels to 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.

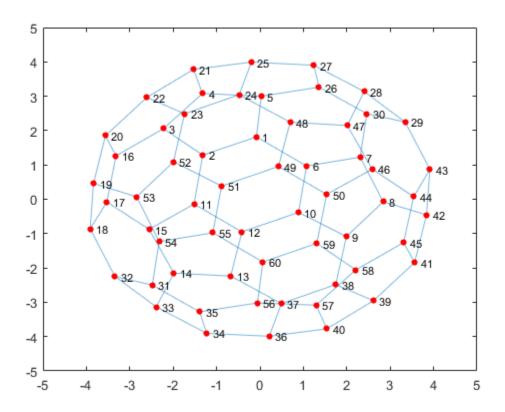
```
G = graph(bucky);
p = plot(G)
p =
  GraphPlot with properties:
     NodeColor: [0 0.4470 0.7410]
    MarkerSize: 4
        Marker: 'o'
     EdgeColor: [0 0.4470 0.7410]
     LineWidth: 0.5000
     LineStyle: '-'
     NodeLabel: {1×60 cell}
     EdgeLabel: {}
         XData: [1×60 double]
         YData: [1×60 double]
         ZData: [1×60 double]
  Use GET to show all properties
```



After you have a handle to the <code>GraphPlot</code> object, use dot indexing to access or change the property values. For a complete list of the properties that you can adjust, see <code>GraphPlot</code>.

Change the value of NodeColor to 'red'.

```
p.NodeColor = 'red';
```



Determine the line width of the edges.

## p.LineWidth

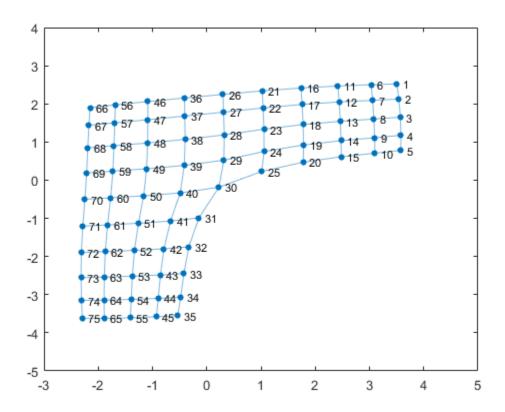
ans =

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: [130×2 table]
    Nodes: [75×0 table]
p = plot(G)
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: {1×75 cell}
     EdgeLabel: {}
         XData: [1×75 double]
         YData: [1×75 double]
         ZData: [1×75 double]
  Use GET to show all properties
```

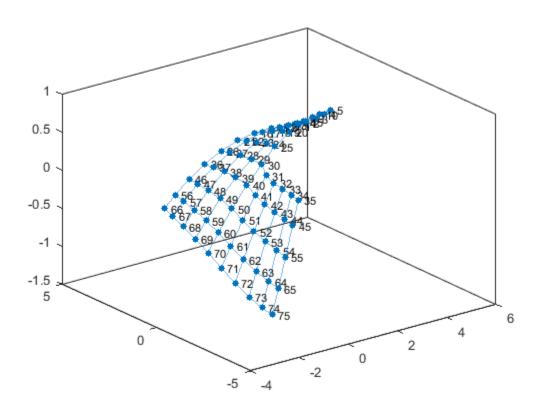


## **Change Graph Node Layout**

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.

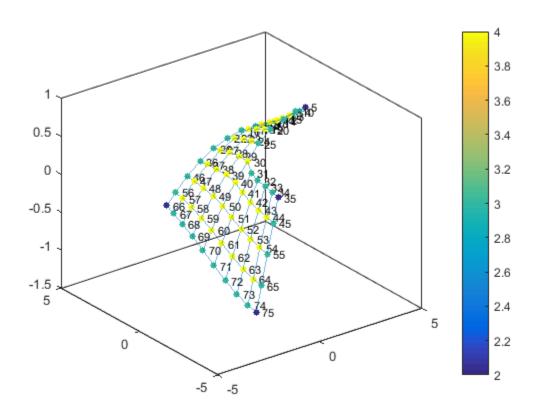
```
layout(p,'force3')
view(3)
```



#### **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.

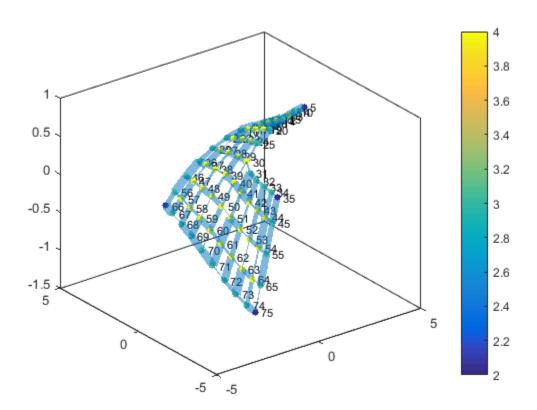
```
G.Nodes.NodeColors = degree(G);
p.NodeCData = G.Nodes.NodeColors;
colorbar
```



# 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.

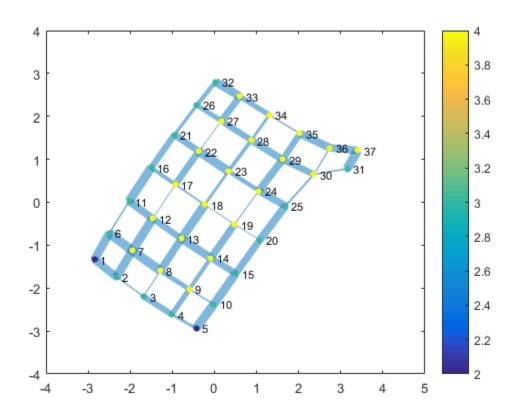
```
G.Edges.Weight = randi([10 250],130,1);
G.Edges.LWidths = 7*G.Edges.Weight/max(G.Edges.Weight);
p.LineWidth = G.Edges.LWidths;
```



# **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.

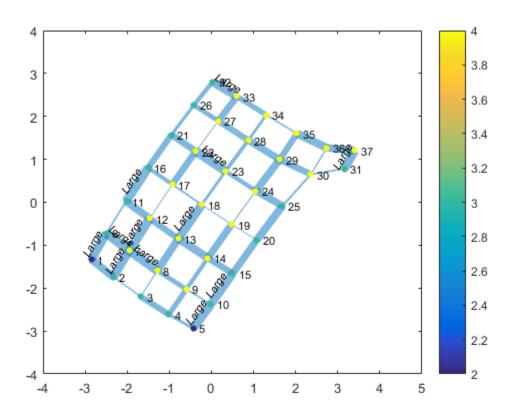
```
H = subgraph(G,[1:31 36:41]);
p1 = plot(H,'NodeCData',H.Nodes.NodeColors,'LineWidth',H.Edges.LWidths);
colorbar
```



## **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**

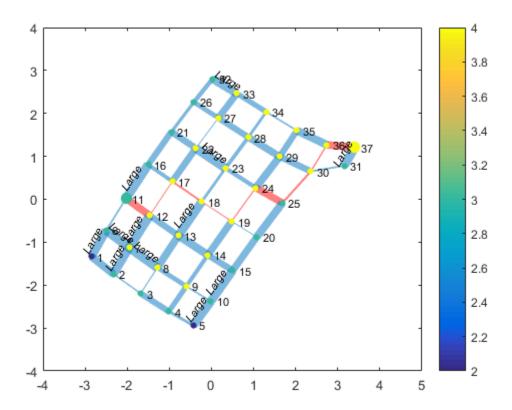
Find the shortest path between node 11 and node 37 in the subgraph, H. Highlight the edges along this path in red, and increase the size of the end nodes on the path.

```
path = shortestpath(H,11,37)

path =
    11    12    17    18    19    24    25    30    36    37

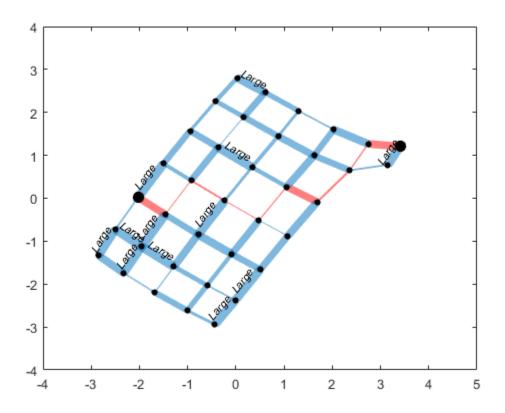
highlight(p1,[11 37])
```





Remove the node labels and colorbar, and make all of the nodes black.

```
p1.NodeLabel = {};
colorbar off
p1.NodeColor = 'black';
```

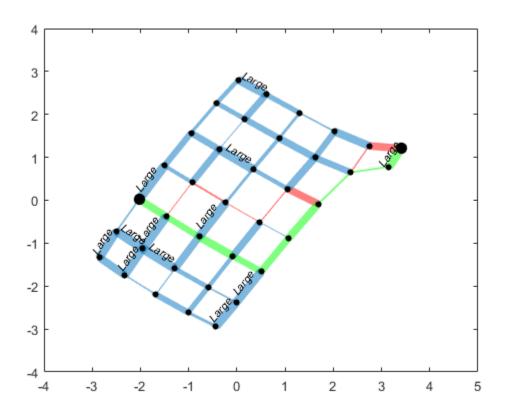


Find a different shortest path that ignores the edge weights. Highlight this path in green.

```
path2 = shortestpath(H,11,37,'Method','unweighted')

path2 =
    11    12    13    14    15    20    25    30    31    37

highlight(p1,path2,'EdgeColor','g')
```



#### **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

digraph | graph | plot

# **More About**

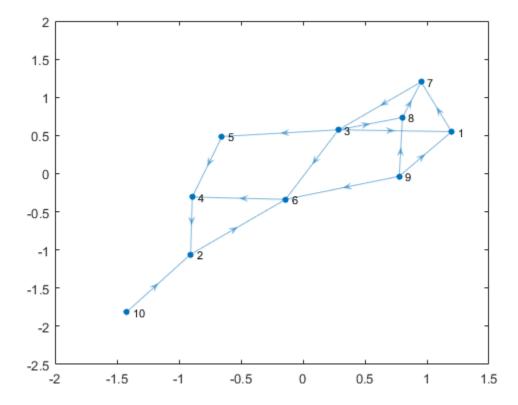
- "Directed and Undirected Graphs" on page 5-2
- graph
- digraph
- GraphPlot
- GraphPlot Properties
- "Add Node Properties to Graph Plot Data Cursor" on page 5-43

# 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.

T = dfsearch(G, 1, 'allevents', 'Restart', true)

T =

Event	Node	Edge	
startnode	1	NaN	NaN
discovernode	1	NaN	NaN
edgetonew	NaN	1	7
discovernode	7	NaN	NaN
edgetonew	NaN	7	3
discovernode	3	NaN	NaN
edgetodiscovered	NaN	3	1
edgetonew	NaN	3	5
discovernode	5	NaN	NaN
edgetonew	NaN	5	4
discovernode	4	NaN	NaN
edgetonew	NaN	4	2
discovernode	2	NaN	NaN
edgetonew	NaN	2	6
discovernode	6	NaN	NaN
edgetodiscovered	NaN	6	4
finishnode	6	NaN	NaN
finishnode	2	NaN	NaN
finishnode	4	NaN	NaN
finishnode	5	NaN	NaN
edgetofinished	NaN	3	6
edgetonew	NaN	3	8
discovernode	8	NaN	NaN
edgetodiscovered	NaN	8	7
finishnode	8	NaN	NaN
finishnode	3	NaN	NaN
finishnode	7	NaN	NaN
finishnode	1	NaN	NaN
startnode	9	NaN	NaN
discovernode	9	NaN	NaN
edgetofinished	NaN	9	1
edgetofinished	NaN	9	6

edgetofinished	NaN	9	8
finishnode	9	NaN	NaN
startnode	10	NaN	NaN
discovernode	10	NaN	NaN
edgetofinished	NaN	10	2
finishnode	10	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 1984-2015 The MathWorks, Inc.
if isa(G, 'graph')
    % Replace graph with corresponding digraph, because we need separate
    % edges for both directions
    G = digraph(adjacency(G));
end
h = plot(G, 'NodeColor', [0.5 0.5 0.5], 'EdgeColor', [0.5 0.5 0.5]);
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');
        case 'edgetonew'
```

```
highlight(h,t.Edge(ii,1),t.Edge(ii,2),'EdgeColor','b');
    case 'edgetodiscovered'
        highlight(h,t.Edge(ii,1),t.Edge(ii,2),'EdgeColor',[0.8 0 0.8]);
    case 'edgetofinished'
        highlight(h,t.Edge(ii,1),t.Edge(ii,2),'EdgeColor',[0 0.8 0]);
    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.
- <code>'edgetodiscovered'</code> <code>Edges</code> that lead to discovered nodes turn  $\it magenta.$
- 'edgetofinished' Edges that lead to finished nodes turn green.

## See Also

bfsearch | dfsearch | digraph | graph

# More About

- "Directed and Undirected Graphs" on page 5-2
- · graph
- digraph

# 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

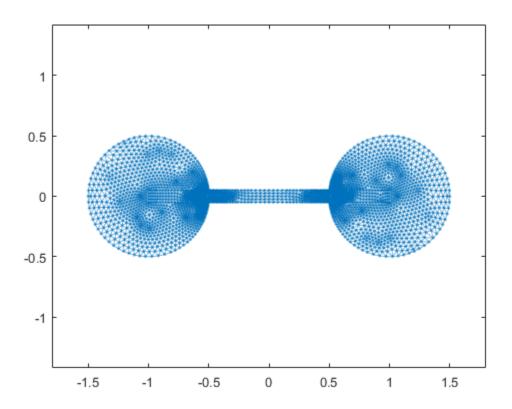
Load the data set barbellgraph.mat, which contains the sparse adjacency matrix and node coordinates of a barbell graph.

```
load(fullfile(matlabroot, 'examples', 'matlab', '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','.','MarkerSize',4.5);
axis equal
```



## Calculate Laplacian Matrix and Fiedler Vector

Calculate the Laplacian matrix of the graph. Then, calculate the two smallest eigenvalues and corresponding eigenvectors using eigs.

```
L = laplacian(G);
[V,D] = eigs(L,2,'sm');
```

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 first column in V corresponds to the second smallest eigenvalue D(1,1).

D

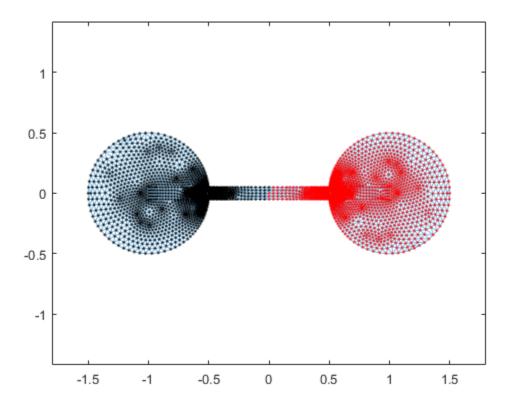
Finding the Fiedler vector using eigs is scalable to larger graphs, since only a subset of the eigenvalues and eigenvectors are computed, but for smaller graphs it is equally feasible to convert the Laplacian matrix to full storage and use eig(full(L)).

#### **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.

```
\label{eq:highlight} $$ highlight(p,find(w>=0),'NodeColor','r') % subgraph A highlight(p,find(w<0),'NodeColor','k') % subgraph B
```



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 \text{ med} = w - \text{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**

digraph | graph | laplacian | subgraph

# More About

- "Directed and Undirected Graphs" on page 5-2
- graph
- digraph

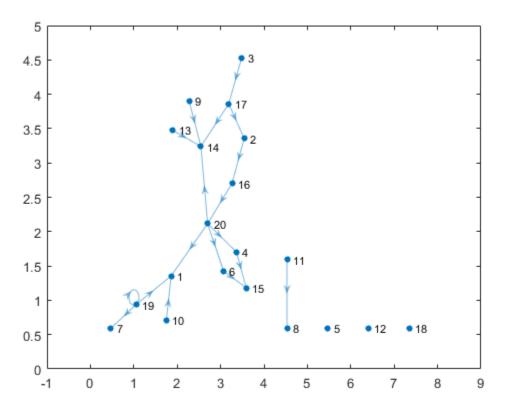
# Add Node Properties to Graph Plot Data Cursor

This example shows how to customize the **GraphPlot** data cursor to display extra node properties of a graph.

#### Create GraphPlot object

Create a GraphPlot graphics object for a random directed graph. Add an extra node property Wifi to the graph.

```
G = digraph(sprandn(20, 20, 0.05));
G.Nodes.wifi = randi([0 1], 20, 1) == 1;
h = plot(G);
```



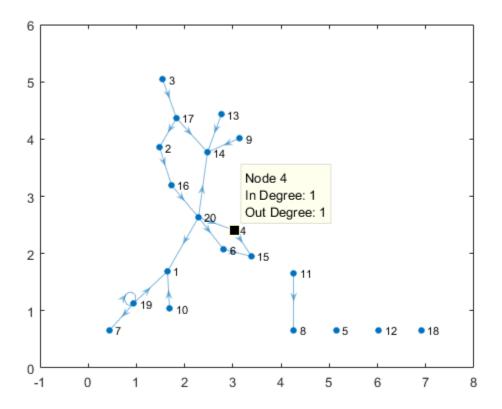
#### **Enable Data Cursor Mode**

Enable data cursor mode by selecting the data cursor icon in the figure toolbar.



Alternatively, you can select the **Data Cursor** item in the **Tools** menu, or type: datacursormode on.

With data cursor mode enabled, click a node in the graph to bring up the cursor display. The data cursor allows you to select nodes in a graph plot and view properties of the nodes. By default, the data cursor for an undirected graph displays the node ID number and degree. For directed graphs, the display includes the node ID number, in-degree, and out-degree.



To display extra node properties, such as wifi, the data cursor callback function needs to be modified. For general information on using and customizing data cursors, see "Display Data Values Interactively".

# Customize Text Displayed by Data Cursor

Customize the text displayed by the data cursor by writing a new data cursor callback function.

1. Save the function  ${\tt GraphCursorCallback.m}$  in your current directory:

```
function output_txt = GraphCursorCallback(obj,event_obj,NodeProperties)
% Display the position of the data cursor
```

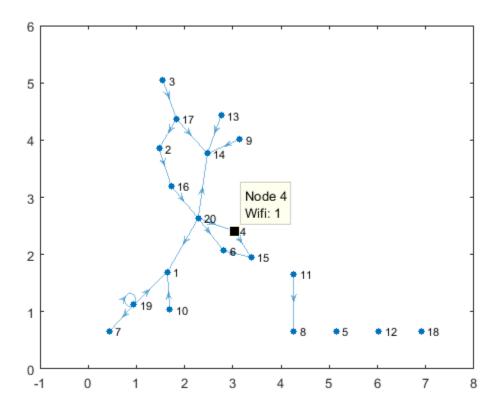
A standard data cursor callback function accepts two input arguments.

GraphCursorCallback accepts an additional input argument, NodeProperties, so that the data cursor gains access to the extra node properties in the graph, such as Wifi.

2. Connect the GraphCursorCallback function to the data cursor by changing the UpdateFcn property of the data cursor manager object. This command uses an anonymous function to pass the G.Nodes table as the third input to GraphCursorCallback. This technique only takes a snapshot of the G.Nodes table, so if the graph properties subsequently change, then you need to change the UpdateFcn property again.

```
hdt = datacursormode;
hdt.UpdateFcn = @(obj,event_obj) GraphCursorCallback(obj,event_obj,G.Nodes);
```

3. Now that GraphCursorCallback is connected to the data cursor, delete any old data tips in the plot, then reenable data cursor mode and select a node. The new display of the data cursor includes the wifi node property as defined in GraphCursorCallback.



# **See Also** datacursormode | digraph | graph

# **More About**

• "Display Data Values Interactively"

# **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 6-10
- "Polynomial Curve Fitting" on page 6-12
- "Roots of Scalar Functions" on page 6-14

# **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,  $\boldsymbol{X}$ , and evaluate  $\boldsymbol{p}$  at  $\boldsymbol{X}$ .

## **See Also**

poly | polyval | polyvalm | roots

## **More About**

- "Roots of Polynomials" on page 6-4
- "Integrate and Differentiate Polynomials" on page 6-10
- "Polynomial Curve Fitting" on page 6-12

# **Roots of Polynomials**

This example shows several different methods to calculate the roots of a polynomial.

```
In this section...

"Numeric Roots" on page 6-4

"Roots Using Substitution" on page 6-5

"Roots in a Specific Interval" on page 6-6

"Symbolic Roots" on page 6-8
```

#### **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.

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  $\theta$  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.

-1.5907 1.2573

To undo the substitution, use  $\theta = \sin^{-1}(x)$ . The asin function calculates the inverse sine.

```
theta = asin(r)

theta =

-1.5708 + 1.0395i

1.5708 - 0.7028i
```

Verify that the elements in theta are the values of  $\theta$  that solve the original equation (within roundoff error).

```
f = @(Z) 3*cos(Z).^2 - sin(Z) + 3;
f(theta)

ans =
    1.0e-14 *
    -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]. 

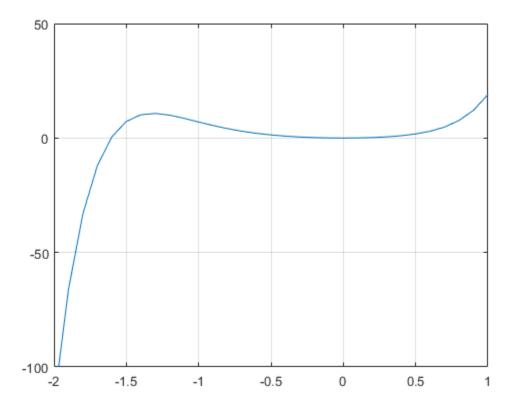
x = -2:0.1:1; 

plot(x,p(x)) 

ylim([-100 50]) 

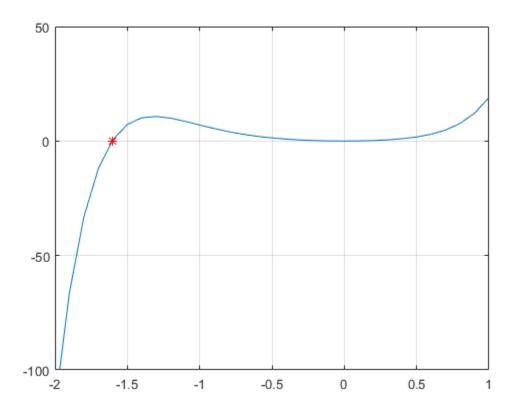
grid on
```

hold on



From the plot, the polynomial has a trivial root at  $\bf 0$  and another near -1.5. Use fzero to calculate and plot the root that is near -1.5.

```
Z = fzero(p, -1.5)
plot(Z,p(Z),'r*')
Z =
    -1.6056
```



# **Symbolic Roots**

If you have Symbolic Math Toolbox, then there are additional options for evaluating polynomials symbolically. One way is to use the solve function.

```
syms x
s = solve(x^2-x-6)
s =
    -2
    3
```

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 Equation" in the Symbolic Math Toolbox documentation for more information.

## **See Also**

eig | poly | roots

## More About

- "Create and Evaluate Polynomials" on page 6-2
- "Roots of Scalar Functions" on page 6-14
- "Integrate and Differentiate Polynomials" on page 6-10

# **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  $q(x)=\frac{d}{dx}p(x)=3x^2-2$ .

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  $b(x)=2x^2+4x+6$ .

```
a = [1 \ 3 \ 5];

b = [2 \ 4 \ 6];
```

Calculate the derivative  $\frac{d}{dx}[a(x)b(x)]$  by calling polyder with a single output argument. c = polyder(a,b)

Calculate the derivative  $\frac{d}{dx} \left[ \frac{a(x)}{b(x)} \right]$  by calling polyder with two output arguments. The resulting polynomial is

$$\frac{d}{dx} \left[ \frac{a(x)}{b(x)} \right] = \frac{-2x^2 - 8x - 2}{4x^4 + 16x^3 + 40x^2 + 48x + 36} = \frac{q(x)}{d(x)}.$$

$$[q,d] = polyder(a,b)$$

## See Also

conv | deconv | polyder | polyint

# **More About**

- "Analytic Solution to Integral of Polynomial" on page 15-8
- "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 using polyfit. Use the polyfit function 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 data to be fitted
- n is the degree of the polynomial to return

Consider the *x*-*y* test data

```
x = [1 \ 2 \ 3 \ 4 \ 5];

y = [5.5 \ 43.1 \ 128 \ 290.7 \ 498.4];
```

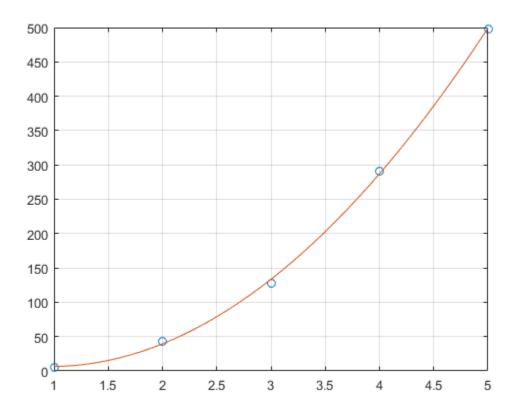
Use polyfit to find a third-degree polynomial that approximately fits the data.

```
p = polyfit(x,y,3)
p =
    -0.1917    31.5821    -60.3262    35.3400
```

After you obtain the polynomial using polyfit, 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.

```
x2 = 1:.1:5;
y2 = polyval(p,x2);
plot(x,y,'o',x2,y2)
grid on
```



# **See Also**

polyfit | polyval

# **More About**

- "Programmatic Fitting"
- "Create and Evaluate Polynomials" on page 6-2

# **Roots of Scalar Functions**

```
In this section...

"Solving a Nonlinear Equation in One Variable" on page 6-14

"Using a Starting Interval" on page 6-16

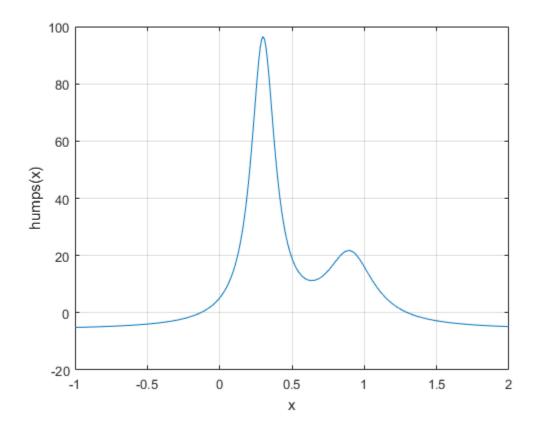
"Using a Starting Point" on page 6-17
```

# 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 Options" on page 9-11, "Using a Starting Interval" on page 6-16, and "Using a Starting Point" on page 6-17.
- Choosing various tolerances that control how fzero determines it is at a root see "Set Options" on page 9-11.
- Choosing a plot function for observing the progress of fzero towards a root see "Plot Functions" on page 9-25.

• Using a custom-programmed output function for observing the progress of fzero towards a root — see "Output Functions" on page 9-17.

# **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.

```
ans =
16
humps(-1)
ans =
-5.1378
```

humps(1)

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
                          f(x)
                                             Procedure
   2
                   - 1
                            -5.13779
                                             initial
   3
           -0.513876
                            -4.02235
                                             interpolation
   4
           -0.513876
                           -4.02235
                                             bisection
           -0.473635
                            -3.83767
                                             interpolation
```

```
6
             -0.115287
                            0.414441
                                             bisection
    7
             -0.115287
                            0.414441
                                             interpolation
    8
             -0.132562
                                             interpolation
                          -0.0226907
    9
             -0.131666
                          -0.0011492
                                             interpolation
   10
             -0.131618
                         1.88371e-07
                                             interpolation
                         -2.7935e-11
                                             interpolation
   11
             -0.131618
   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 a f(a) b f(b) Procedure
```

```
1
                   -0.2
                              -1.35385
                                                  -0.2
                                                             -1.35385
                                                                         initial interval
    3
             -0.194343
                              -1.26077
                                            -0.205657
                                                             -1.44411
                                                                         search
    5
                -0.192
                              -1.22137
                                               -0.208
                                                              -1.4807
                                                                         search
    7
             -0.188686
                              -1.16477
                                            -0.211314
                                                             -1.53167
                                                                         search
    9
                -0.184
                              -1.08293
                                               -0.216
                                                             -1.60224
                                                                         search
   11
             -0.177373
                             -0.963455
                                            -0.222627
                                                             -1.69911
                                                                         search
                                                             -1.83055
   13
                -0.168
                             -0.786636
                                               -0.232
                                                                         search
   15
             -0.154745
                              -0.51962
                                            -0.245255
                                                             -2.00602
                                                                         search
   17
                 -0.136
                                                             -2.23521
                             -0.104165
                                               -0.264
                                                                         search
   18
                                               -0.264
                                                             -2.23521
              -0.10949
                              0.572246
                                                                         search
Search for a zero in the interval [-0.10949, -0.264]:
 Func-count
                            f(x)
                                               Procedure
                Χ
   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
                          8.88178e-16
             -0.131618
                                               interpolation
   25
             -0.131618
                          8.88178e-16
                                               interpolation
Zero found in the interval [-0.10949, -0.264]
a =
   -0.1316
```

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.

**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 the endpoint, -0.10949, but negative at the endpoint, -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.

# **Computational Geometry**

- "Overview" on page 7-2
- "Triangulation Representations" on page 7-3
- "Delaunay Triangulation" on page 7-17
- "Spatial Searching" on page 7-50
- "Voronoi Diagrams" on page 7-59
- "Types of Region Boundaries" on page 7-68
- "Computing the Convex Hull" on page 7-76

## **Overview**

MATLAB provides a variety of tools to solve problems that are geometric in nature. These problems encompass simple geometric queries such as point-in-polygon tests, to more complex problems such as nearest-neighbor queries. Convex hulls, Delaunay triangulations, and Voronoi diagrams are examples of fundamental geometric algorithms that MATLAB provides. These algorithms have many practical uses in the scientific development.

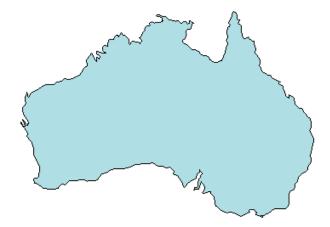
MATLAB provides both function-based and class-based tools for computational geometry. The function-based tools are convenient when the output from the function is sufficiently complete to get you to the solution. The class-based tools are more versatile because they provide complementary methods that are often needed to work with the resulting data. A function typically takes input, performs some computation, and outputs the result in matrix format.

In contrast, a class may take input, perform some computation, cache the result and provide methods that allow you to query and work with the result more efficiently. For example, the delaunay function creates a triangulation from a set of points and returns the triangulation in an array. The delaunay Triangulation class also triangulates a set of points. In addition, it allows you to modify the triangulation and it provides methods for finding nearest neighbors and traversing the triangulation data structure, etc. These methods are very efficient because the class holds the triangulation in memory.

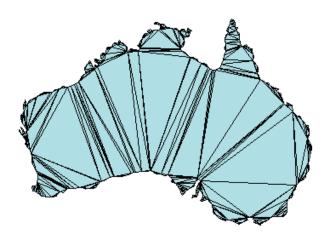
# **Triangulation Representations**

# 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

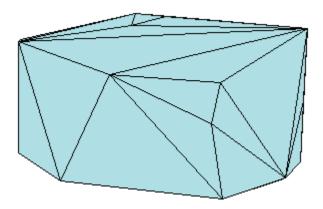


can be represented by the triangulation on the map shown below.



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.

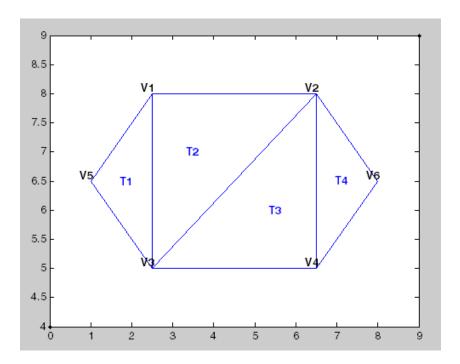


# **Triangulation Matrix Format**

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 tetrahedon.

This figure shows a simple 2-D triangulation.



The following table shows the vertex information.

Vertices						
Vertex ID	x-coordinate	y-coordinate				
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.

/TV1		1 - 4 - 1	1	41. 1. 4. 1.1.
The triangulation	connectivity	aata is s	nown in	tnis table.

Connectivity						
Triangle ID	IDs of Bounding Vertices					
T1	5	3	1			
T2	3	2	1			
Т3	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).

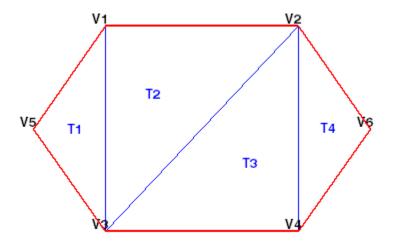
You can represent and query the following types of triangulations using MATLAB:

- · 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.

```
TR = triangulation(T,P)

TR =
    triangulation with properties:
        Points: [6×2 double]
        ConnectivityList: [4×3 double]
```

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 =

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 =

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 = 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
```

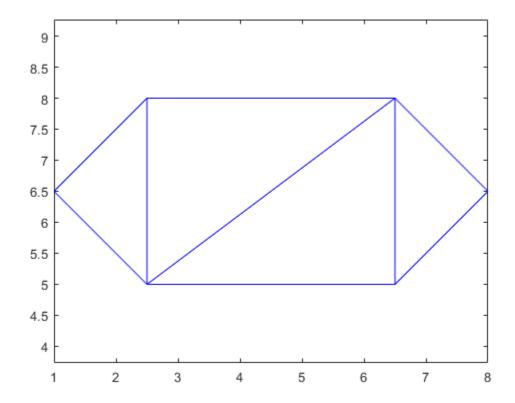
Examine the second vertex of the first triangle.

```
TR(1,2)
ans =
```

Now, examine all the triangles in the triangulation.

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
```

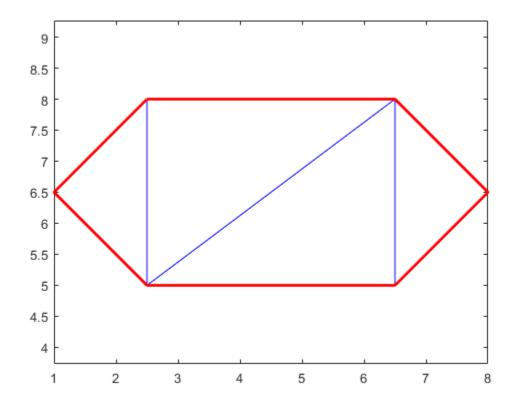


Use the triangulation method, freeBoundary, to query the free boundary and highlight it in a plot. This method returns the edges of the triangulation that are shared by only one triangle. The returned edges are expressed in terms of the vertex IDs.

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  $\mbox{delaunayTriangulation}$  from a set of points.

```
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];
DT = delaunayTriangulation(P)
DT =
  delaunayTriangulation with properties:
              Points: [6×2 double]
    ConnectivityList: [4×3 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,:)

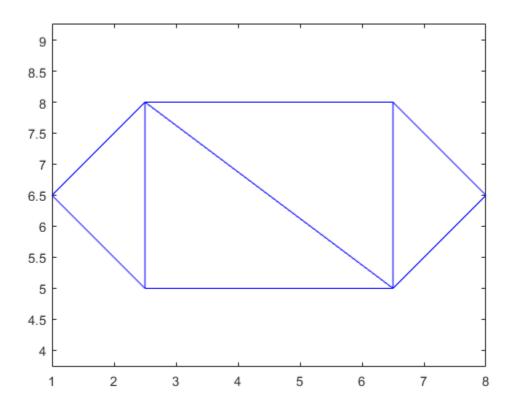
ans =

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 =

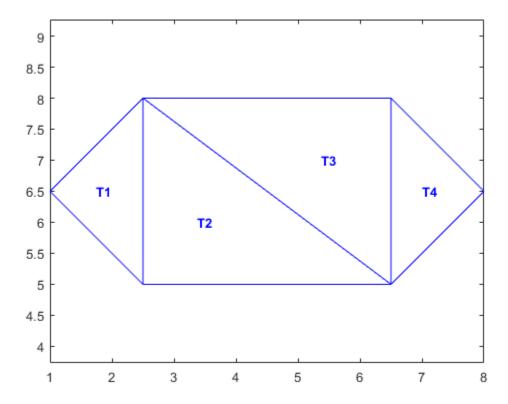
1.8787 6.5000
3.5000 6.0000

```
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,

```
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];

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 | delaunay Triangulation | free Boundary | triangulation | triplot

## **More About**

- "Triangulation Representations" on page 7-3
- "Delaunay Triangulation" on page 7-17
- "Spatial Searching" on page 7-50

# **Delaunay Triangulation**

#### In this section...

"Definition of Delaunay Triangulation" on page 7-17

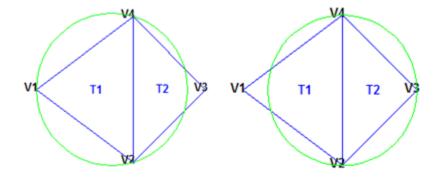
"Creating Delaunay Triangulations" on page 7-19

"Triangulation of Point Sets Containing Duplicate Locations" on page 7-47

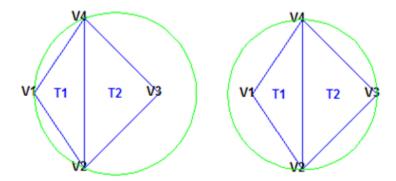
# **Definition of Delaunay Triangulation**

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.

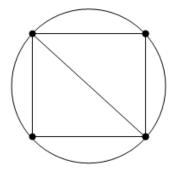


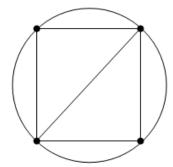
The triangles below are different. The circumcircle associated with T1 is not empty. It contains V3 in its interior. The circumcircle associated with T2 is not empty. It contains V1 in its interior. This triangulation is *not* a Delaunay triangulation.



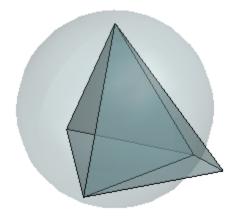
Delaunay triangles are said to be "well shaped" because in fulfilling the empty circumcircle property, triangles with large internal angles are selected over ones with small internal angles. The triangles in the non-Delaunay triangulation have sharp angles at vertices V2 and V4. If the edge {V2, V4} 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

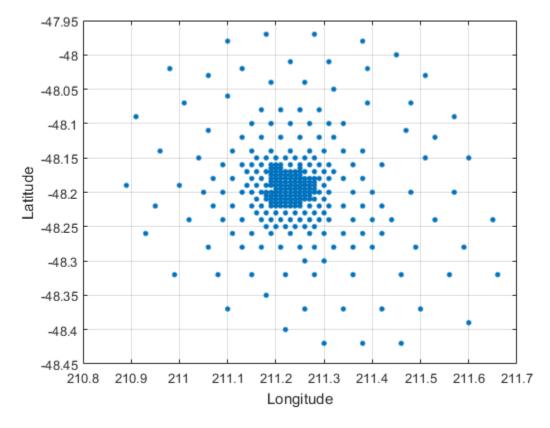
The delaunay and delaunayn functions take a set of points and produce a triangulation in matrix format. Refer to "Triangulation Matrix Format" on page 7-4 for more information on this data structure. In 2-D, the delaunay function is often used to produce a triangulation that can be used to plot a surface 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.

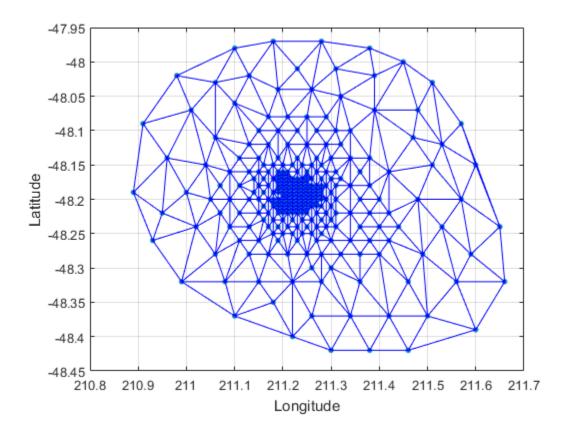
```
load seamount
plot(x,y,'.','markersize',12)
xlabel('Longitude'), ylabel('Latitude')
grid on
```



Construct a Delaunay triangulation from this point set and use triplot to plot the triangulation in the existing figure.

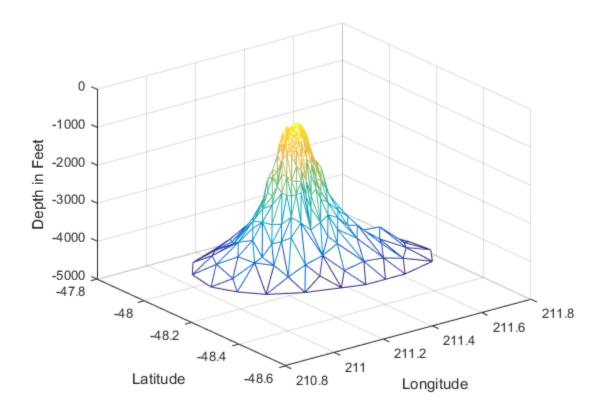
```
tri = delaunay(x,y);
```

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');
```

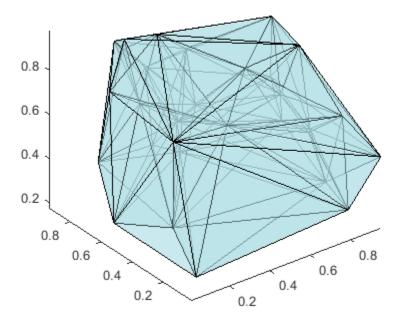


If you want to plot the surface in shaded mode, use trisurf instead of trimesh.

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.

```
X = gallery('uniformdata',[30 3],0);
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 7-50 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 7-3 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 = 205 230 262
```

delaunayTriangulation provides an easy way to index into the ConnectivityList property matrix.

Access the first triangle.

```
DT(1,:)

ans =

205 230 262
```

Examine the first vertex of the first triangle.

```
DT(1,1)
ans =
```

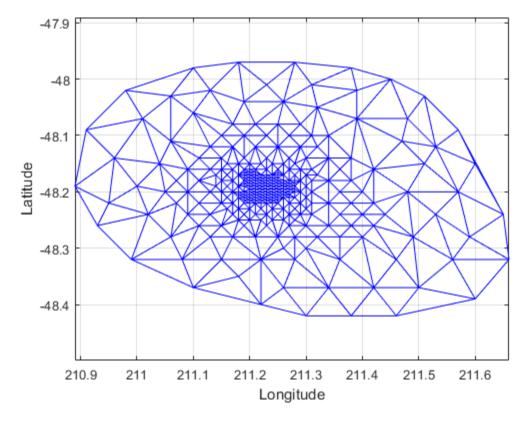
Examine all the triangles in the triangulation.

```
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
```

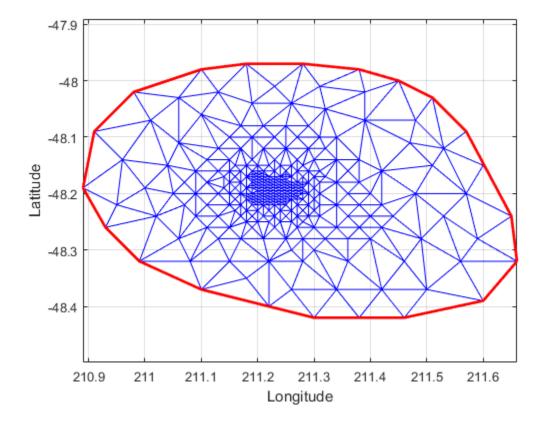


Alternatively, you could use triplot(DT(:,:), DT.Points(:,1), DT.Points(:,2)); to get the same plot.

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
```

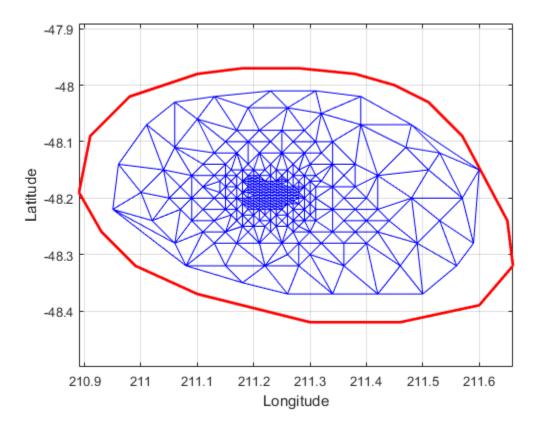


You can incrementally edit the delaunayTriangulation to add or remove points. If you need to add points to an existing triangulation, then an incremental addition is faster than a complete retriangulation of the augmented point set. Incremental removal

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.

```
figure
plot(xHull, yHull, 'r', 'LineWidth', 2);
axis equal
xlabel('Longitude'),ylabel('Latitude')
grid on
% The convex hull topology duplicates the start and end vertex.
% Remove the duplicate entry.
k(end) = [];
% Now remove the points on the convex hull.
DT.Points(k,:) = []
% Plot the new triangulation
hold on
triplot(DT);
hold off
DT =
  delaunayTriangulation with properties:
              Points: [274×2 double]
    ConnectivityList: [528×3 double]
         Constraints: []
```



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 nearest Neighbor method to find the nearest vertex.

```
vertexId = nearestNeighbor(DT, 211.6, -48.15)
```

vertexId =

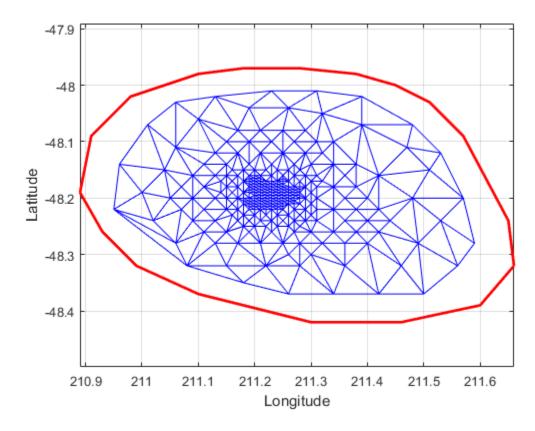
50

axis equal

grid on
hold on
triplot(DT);
hold off

Now remove that vertex from the triangulation.

xlabel('Longitude'),ylabel('Latitude')



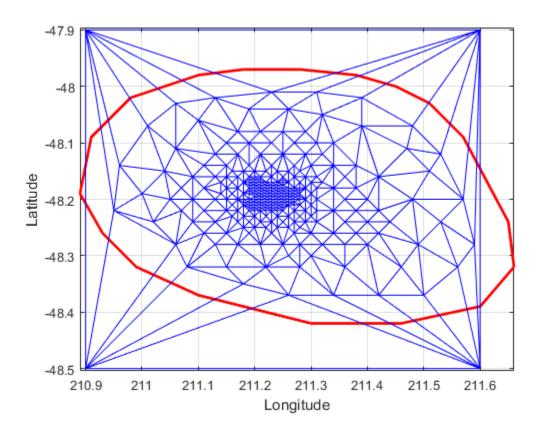
Add points to the existing triangulation. Add 4 points to form a rectangle around the triangulation.

```
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];
```

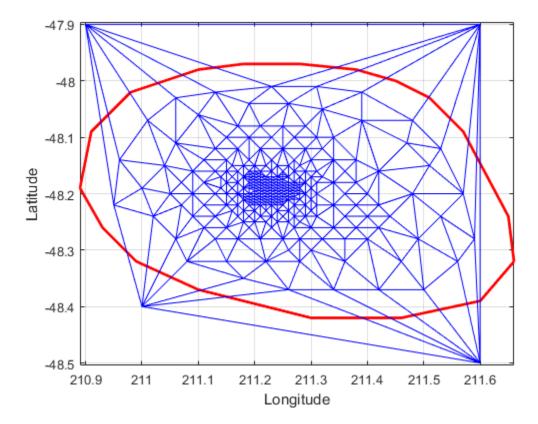
Close all existing figures.

close all

Plot the new triangulation

```
figure
plot(xHull,yHull,'r','LineWidth',2);
axis equal
```

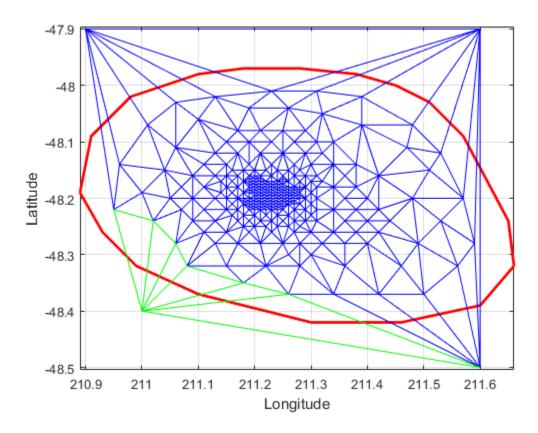
```
xlabel('Longitude'),ylabel('Latitude')
grid on
hold on
triplot(DT);
hold off
```



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.

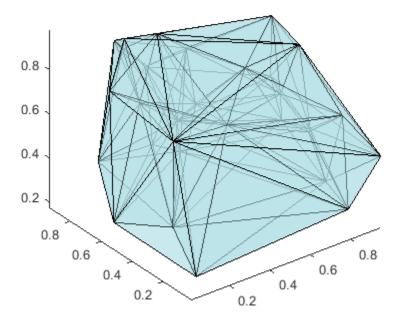
This example shows how to use a delaunayTriangulation to create and plot the triangulation of 3-D points.

```
P = gallery('uniformdata',30,3,0);
DT = delaunayTriangulation(P)
faceColor = [0.6875 0.8750 0.8984];
tetramesh(DT,'FaceColor', faceColor,'FaceAlpha',0.3);
```

DT =

delaunayTriangulation with properties:

Points: [30×3 double]
ConnectivityList: [117×4 double]
Constraints: []

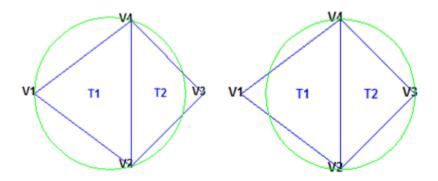


The tetramesh function plots both the internal and external faces of the triangulation. For large 3-D triangulations, plotting the internal faces might be an unnecessary use of resources. A plot of the boundary might be more appropriate. You can use the freeBoundary method to get the boundary triangulation 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.

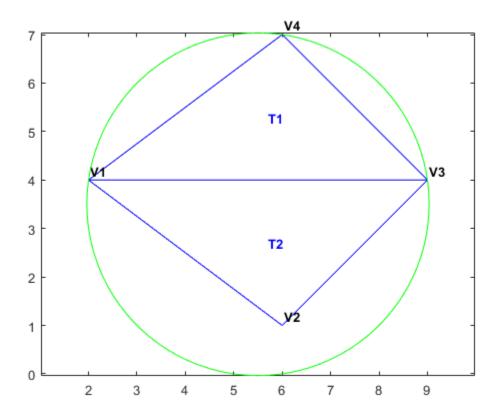
```
C = [1 3];
DT = delaunayTriangulation(P,C);
```

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
```

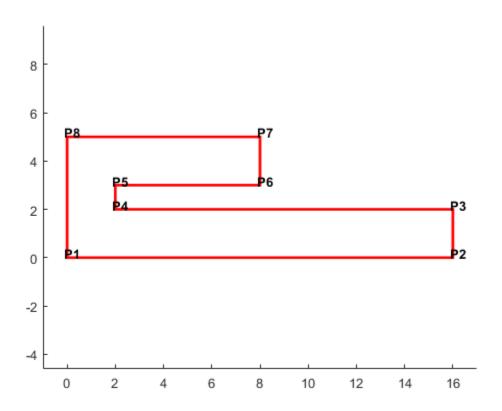


The constraint between vertices (V1, V3) was honored, however, the Delaunay criterion was invalidated. This also invalidates the nearest-neighbor relation that is inherent in a Delaunay triangulation. This means the nearestNeighbor search method provided by delaunayTriangulation cannot be supported if 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.

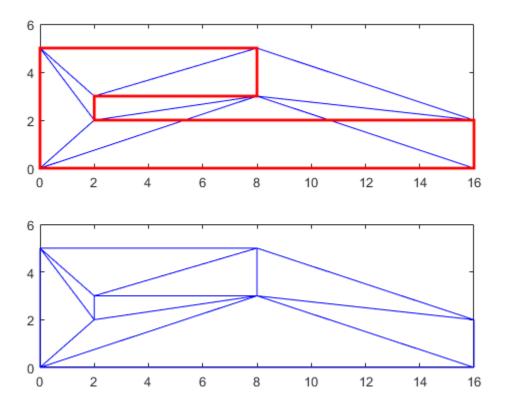
Constrained triangulations are generally used to triangulate a nonconvex polygon. The constraints give us a correspondence between the polygon edges and the triangulation edges. This relationship enables you to extract a triangulation that represents the region. The following example shows how to use a constrained delaunayTriangulation to triangulate a nonconvex polygon.

Define and plot a polygon.



Create and plot the triangulation together with the polygon boundary.

```
% Plot the standalone triangulation in a subplot.
subplot(2,1,2);
axis([-1 17 -1 6]);
axis equal
triplot(DT)
```



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];
```

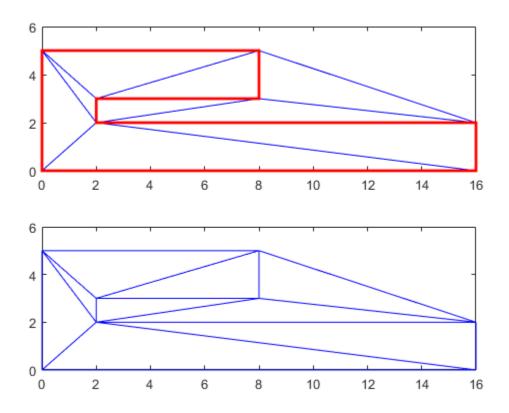
In general, if you have N points in a sequence that define a polygonal boundary, the constraints can be expressed as C = [(1:(N-1))' (2:N)'; N 1];

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.

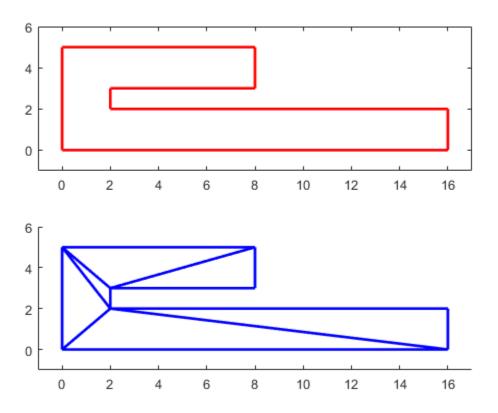


The plot shows that the edges of the triangulation respect the boundary of the polygon. However, the triangulation fills the concavities. What is needed is a triangulation that represents the polygonal domain. You can extract the triangles within the polygon using the delaunayTriangulation method, isInterior. 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(I0, :),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:

```
P = gallery('uniformdata',[25 2],0);
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.

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:

```
P = gallery('uniformdata',[25 2],0);
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
```

## **More About**

• "Spatial Searching" on page 7-50

# **Spatial Searching**

#### In this section...

"Introduction" on page 7-50

"Nearest-Neighbor Search" on page 7-50

"Point-Location Search" on page 7-54

### 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.

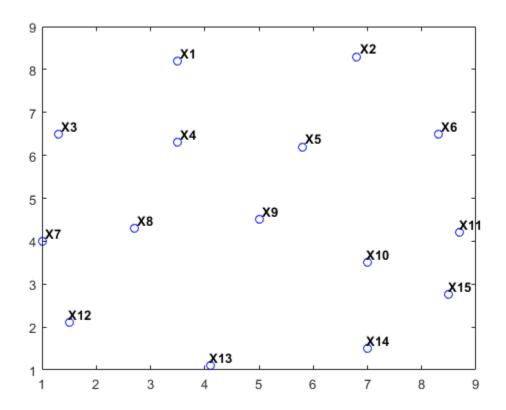
This example shows how to perform a nearest-neighbor search in 2-D with delaunayTriangulation.

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;...
1 4; 2.7 4.3; 5 4.5; 7 3.5; 8.7 4.2; 1.5 2.1; 4.1 1.1; ...
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
```



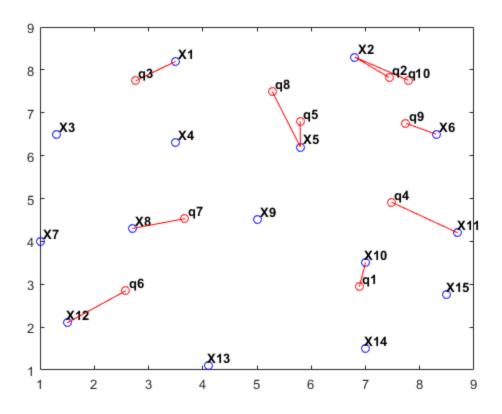
Create a Delaunay triangulation from the points.

```
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.



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:

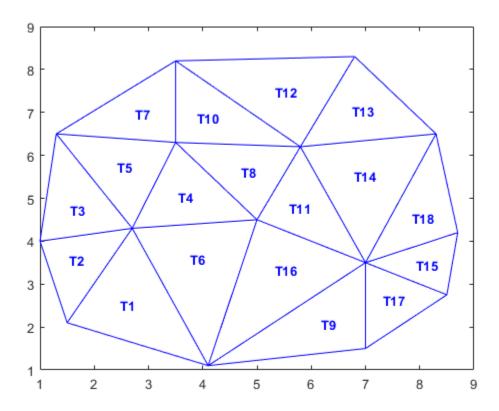
- For 2-D and 3-D, use the class-based approach with the pointLocation method provided by the triangulation class and inherited by the delaunayTriangulation class.
- For 4-D and higher, use the delaunayn function to construct the triangulation and the complementary tsearchn function to perform the point-location 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.

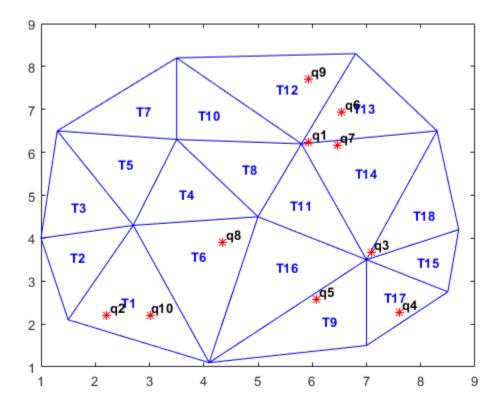
```
X = [3.5 8.2; 6.8 8.3; 1.3 6.5; 3.5 6.3; 5.8 6.2; ...
8.3 6.5; 1 4; 2.7 4.3; 5 4.5; 7 3.5; 8.7 4.2; ...
1.5 2.1; 4.1 1.1; 7 1.5; 8.5 2.75];
```

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 8-54 for further details.

## **Voronoi Diagrams**

```
In this section...

"Plot 2-D Voronoi Diagram and Delaunay Triangulation" on page 7-59

"Computing the Voronoi Diagram" on page 7-63
```

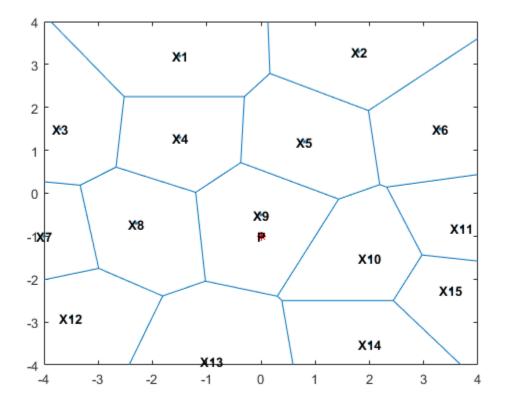
The Voronoi diagram of a discrete set of points X decomposes the space around each point X(i) into a region of influence  $R\{i\}$ . This decomposition has the property that an arbitrary point P within the region  $R\{i\}$  is closer to point i than any other point. The region of influence is called 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.

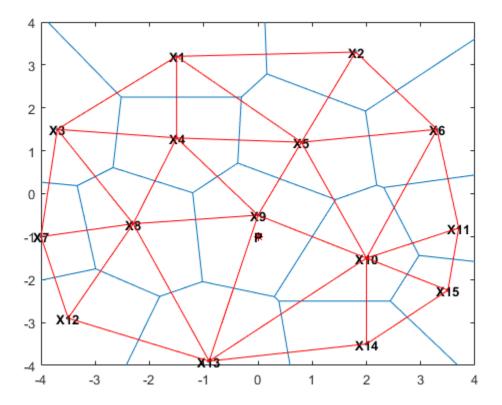


Observe that P is closer to X9 than to any other point in X, which is true for any point P within the region that bounds X9.

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
```



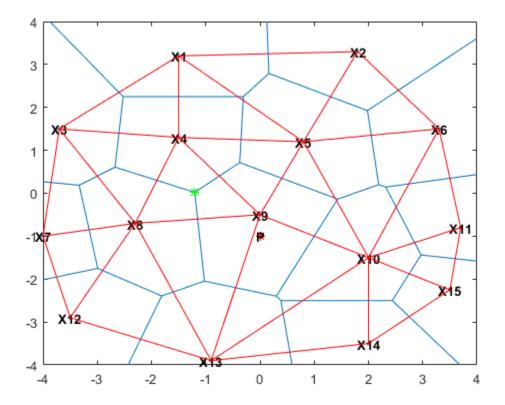
From the plot you can see that the Voronoi region associated with the point X9 is defined by the perpendicular bisectors of the Delaunay edges attached to X9. Also, the vertices of the Voronoi edges are located at the circumcenters of the Delaunay triangles. You can illustrate these associations by plotting 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 MATLAB 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 7-4 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)
```

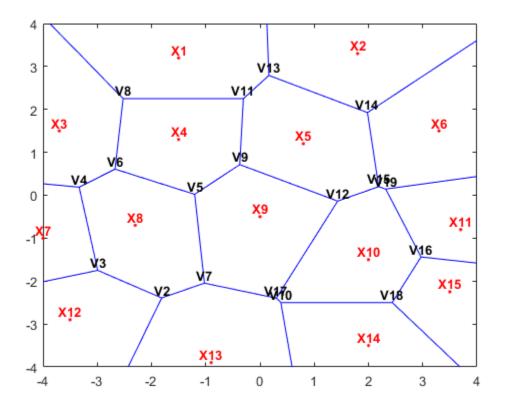
Using the voronoiDiagram method

```
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)');
hold on
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
Hpl = text(V(2:end,1), V(2:end,2)+.2, vlabels, ...
      'FontWeight', 'bold', 'HorizontalAlignment',...
      'center', 'BackgroundColor', 'none');
hold off
```



 $R\{9\}$  gives the indices of the Voronoi vertices associated with the point site X9.  $R\{9\}$ 

The indices of the Voronoi vertices are the indices with respect to the  $\boldsymbol{V}$  array.

Similarly,  $R\{4\}$  gives the indices of the Voronoi vertices associated with the point site X4.  $R\{4\}$ 

```
ans = 5 9 11 8 6
```

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.

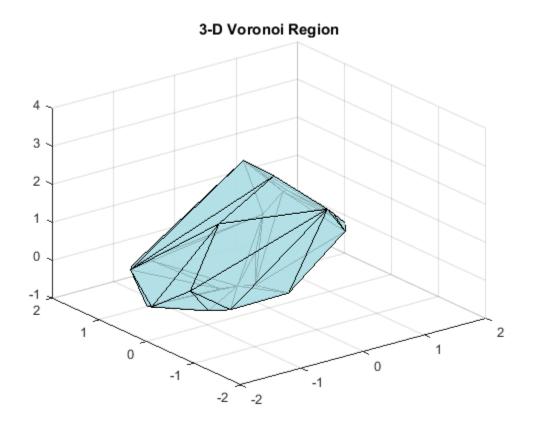
Create a sample of 25 points in 3-D space and compute the topology of the Voronoi diagram for this point set.

```
X = -3 + 6.*gallery('uniformdata',[25 3],0);
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.



### **More About**

• "Spatial Searching" on page 7-50

## Types of Region Boundaries

```
In this section...

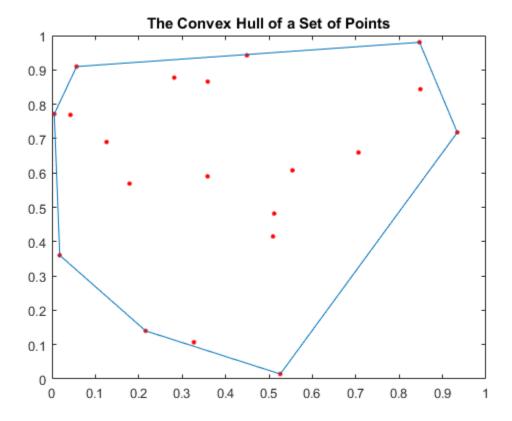
"Convex Hulls vs. Nonconvex Polygons" on page 7-68

"Alpha Shapes" on page 7-72
```

#### Convex Hulls vs. Nonconvex Polygons

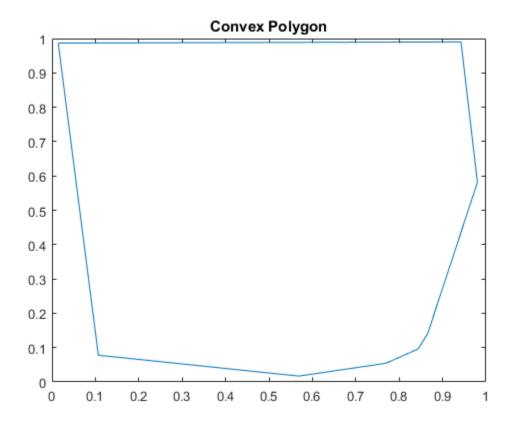
The convex hull of a set of points in N-D space is the smallest convex region enclosing all points in the set. If you think of a 2-D set of points as pegs in a peg board, the convex hull of that set would be formed by taking an elastic band and using it to enclose all the pegs.

```
x = gallery('uniformdata',20,1,20);
y = gallery('uniformdata',20,1,30);
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
```



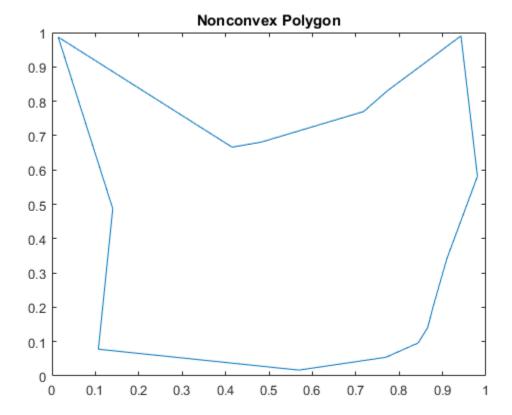
A convex polygon is a polygon that does not have concave vertices, for example:

```
x = gallery('uniformdata',20,1,30);
y = gallery('uniformdata',20,1,40);
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 "vacuum pack" 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.

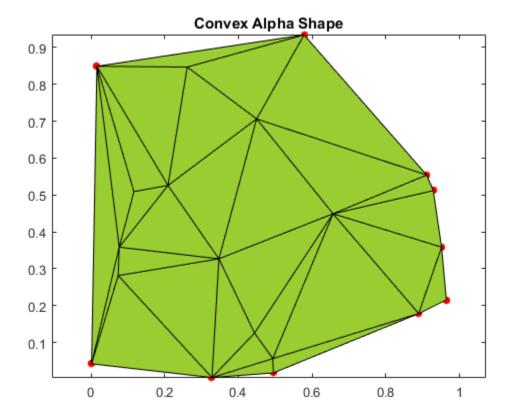
If the convex hulls did not intersect, this would avoid the expense of a more comprehensive intersection test.

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

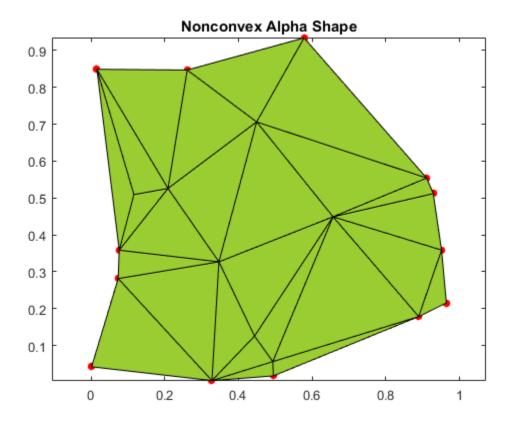
The alpha shape of a set of points is a *generalization* of the convex hull and a subgraph of the Delaunay triangulation. That is, the convex hull is just one type of alpha shape, and the full family of alpha shapes can be derived from the Delaunay triangulation of a given point set.

```
x = gallery('uniformdata',20,1,10);
y = gallery('uniformdata',20,1,20);
plot(x,y,'r.','MarkerSize',20)
hold on
shp = alphaShape(x,y,100);
plot(shp)
title('Convex Alpha Shape')
hold off
```



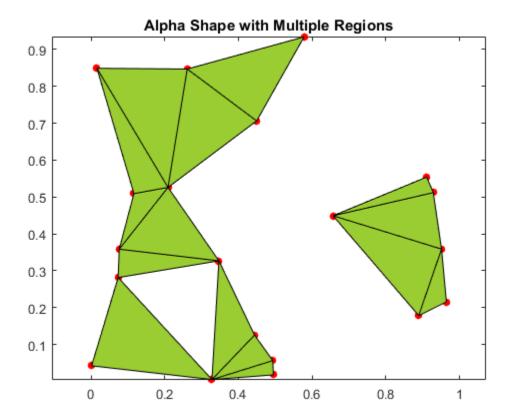
Unlike the convex hull, alpha shapes have a parameter that controls the level of detail, or how tightly the boundary fits around the point set. The parameter is called *alpha* or the *alpha radius*. Varying the alpha radius from 0 to Inf produces a set of different alpha shapes unique for that point 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 alphaShape | convhull

### **More About**

- "Using the delaunayTriangulation Class" on page 7-24
- "Triangulation Matrix Format" on page 7-4
- alphaShape

## **Computing the Convex Hull**

#### In this section...

"Computing the Convex Hull Using convhull and convhulln" on page 7-76

"Convex Hull Computation Using the delaunayTriangulation Class" on page 7-81

"Convex Hull Computation Using alphaShape" on page 7-84

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 convhulln 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
```

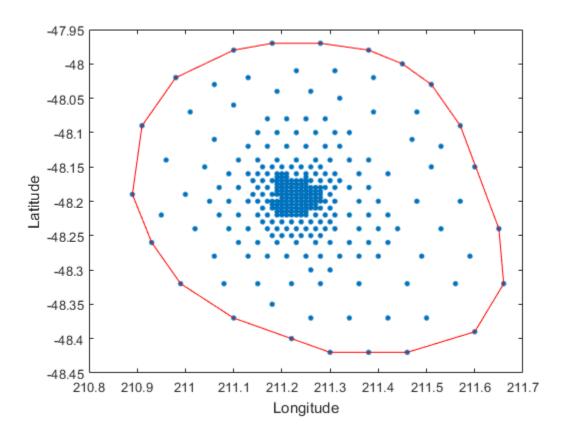
Compute the convex hull of the point set.

```
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.

$$[K,A] = convhull(x,y);$$

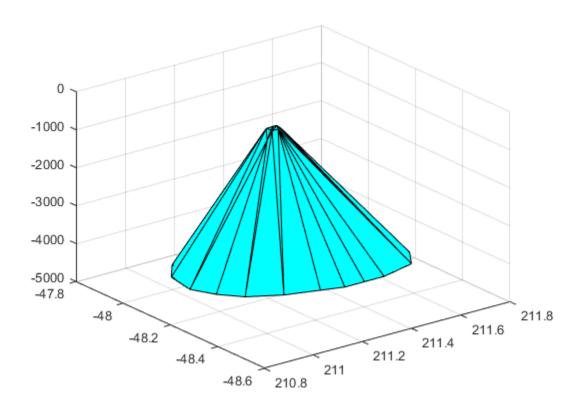
convhull can compute the convex hull of both 2-D and 3-D point sets. You can reuse the seamount dataset to illustrate the computation of the 3-D convex hull.

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.



The volume bounded by the 3-D convex hull can optionally be returned by convhull, the syntax is as follows.

$$[K,V] = convhull(x,y,z);$$

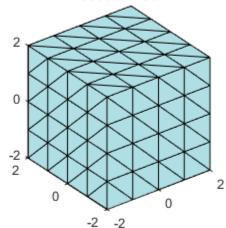
The convhull function also provides the option of simplifying the representation of the convex hull by removing vertices that do not contribute to the area or volume. For example, if boundary facets of the convex hull are collinear or coplanar, you can merge them to give a more concise representation. 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(:);

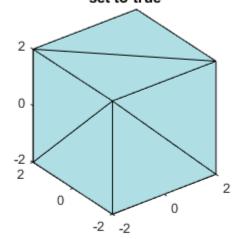
K1 = convhull(x,y,z);
subplot(1,2,1)
defaultFaceColor = [0.6875 0.8750 0.8984];
trisurf(K1,x,y,z,'Facecolor',defaultFaceColor)
axis equal
title(sprintf('Convex hull with simplify\nset to false'))

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'))
```

# Convex hull with simplify set to false



# Convex hull with simplify set 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 delaunayTriangulation Class

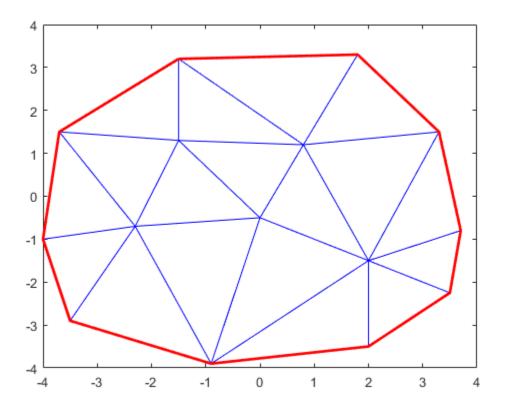
This example shows the relationship between a Delaunay triangulation of a set of points in 2-D and the convex hull of that set of points.

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 <code>convhull</code> function is generally more efficient than a computation based on the <code>convexHull</code> 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.

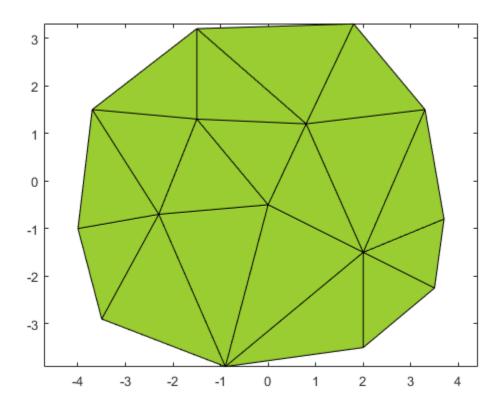
alphaShape computes a regularized alpha shape from a set of 2-D or 3-D points. You can specify the alpha radius, which determines how tightly or loosely the alpha shape envelops the point set. When the alpha radius is set to Inf, the resulting alpha shape is the convux hull of the point set.

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)
```



# Interpolation

- "Gridded and Scattered Sample Data" on page 8-2
- "Interpolating Gridded Data" on page 8-4
- "Interpolation of Multiple 1-D Value Sets" on page 8-50
- "Interpolation of 2-D Selections in 3-D Grids" on page 8-52
- "Interpolating Scattered Data" on page 8-54
- "Interpolation Using a Specific Delaunay Triangulation" on page 8-83
- "Extrapolating Scattered Data" on page 8-86

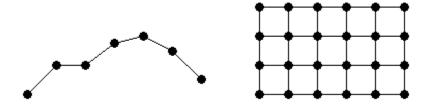
## **Gridded and Scattered Sample Data**

Interpolation is a method for estimating the value at a query location that lies within the domain of a set of sample data points. A sample data set defined by locations X and corresponding values V can be interpolated to produce a function of the form V = F(X). This function can then be used to evaluate a query point Xq, to give Vq = F(Xq). This is a single-valued function; for any query Xq within the domain 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. One other interesting characteristic is that the interpolating function passes through the data points. This is an important distinction between interpolation and curve/surface fitting. In fitting, the function does not necessarily pass through the sample data points.

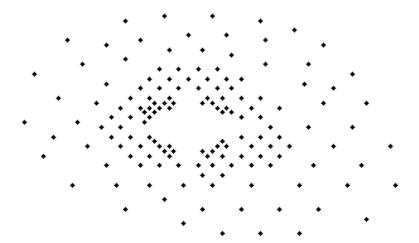
The computation of the value Vq is generally based on the data points in the neighborhood of the query point Xq. There are numerous approaches to performing interpolation. In MATLAB interpolation is classified into two categories depending on the structure of the sample data. The sample data may be ordered in a axis-aligned grid or they may be scattered. In the case of a gridded distribution of sample points, you can leverage the organized structure of the data to efficiently find the sample points in the neighborhood of the query. Interpolation of scattered data on the other hand requires a triangulation of the data points, and this introduces an additional level of computation.

The two approaches to interpolation are covered in the following sections:

• The "Interpolating Gridded Data" on page 8-4 section covers 1-D interpolation, and the N-D ( $N \ge 2$ ) interpolation of sample data in axis-aligned grid format:



The "Interpolating Scattered Data" on page 8-54 section covers the N-D ( $N \ge 2$ ) interpolation of scattered data:



## **Interpolating Gridded Data**

#### In this section...

"Gridded Data Representation" on page 8-4

"Grid-Based Interpolation" on page 8-18

"Interpolation with the interp Family of Functions" on page 8-25

"Interpolation with the griddedInterpolant Class" on page 8-37

#### **Gridded Data Representation**

- "Grid Representation" on page 8-4
- "Types of Grid Representations" on page 8-13
- · "Grid Approximation Techniques" on page 8-15

#### **Grid Representation**

This example shows how to create a 2-D grid using meshgrid and ndgrid.

In MATLAB®, *gridded data* means data *ordered* in a grid. You can understand ordered data by thinking about how MATLAB stores data in matrices.

Define some data.

```
A = gallery('uniformdata',[3 5],0)
A =
                                              0.9218
    0.9501
              0.4860
                         0.4565
                                    0.4447
    0.2311
              0.8913
                         0.0185
                                    0.6154
                                              0.7382
    0.6068
              0.7621
                         0.8214
                                    0.7919
                                              0.1763
```

MATLAB stores the data in a matrix. You can think of A as a set of places for the elements that are ordered by the indices of the matrix. The linear indices of A are:

```
\left[\begin{array}{cccccc} 1 & 4 & 7 & 10 & 13 \\ 2 & 5 & 8 & 11 & 14 \\ 3 & 6 & 9 & 12 & 15 \end{array}\right]
```

Any element in the matrix can be retrieved by indexing, that is, by asking for the element at that place in the matrix. The ith element in A is retrieved by A(i).

Retrieve the 7th element in A.

```
A(7)
ans =
0.4565
```

For an m-by-n matrix, you can find the column elements adjacent to the ith element by offsetting i by 1. To find the row elements adjacent to the ith element, offset i by m.

$$i-1$$
 $i-m$ 
 $i$ 
 $i+m$ 

Retrieve the column elements adjacent to A(7).

```
ans = 0.7621
ans = 0.0185
```

A(6), A(8)

MATLAB uses a similar idea for creating data grids. A grid is not just a set of points that meet certain geometric properties. Rather, a *gridded data set* relies on an ordered relationship among the points in the grid. The adjacency information readily available in the grid structure is very useful for many applications and particularly grid-based interpolation.

MATLAB provides two functions for creating grids:

- meshgrid creates 2-D and 3-D grids that are Cartesian axis aligned. To create a 2-D grid, the syntax is [X,Y] = meshgrid(xgv, ygv) where xgv is a vector of length, and ygv is a vector of length n. meshgrid replicates xgv to form the n-by-|m| matrix X, and it replicates ygv to form another n-by-|m| matrix Y. X and Y represent the coordinates of the grid points. The rows of X are aligned with the horizontal X-axis, and the columns of Y are aligned with the negative Y-axis.
- ndgrid creates N-D grids that are array space aligned. In array space the axes are row, column, page, etc. The calling syntax is [X1, X2, X3,...,Xn] = ndgrid(x1gv, x2gv, x3gv,...,xngv) where x1gv,x2gv,x3gv,...,xngv are vectors that span the grid in each dimension. X1,X2,X3,...,Xn are output arrays that can be used for evaluating functions of multiple variables and for multidimensional interpolation.

Use meshgrid to create a 2-D axis aligned grid from two vectors, xgv and ygv.

```
xav = [1 \ 2 \ 3]:
ygv = [1 2 3 4 5];
[X,Y] = meshgrid(xgv, ygv)
X =
             2
      1
                    3
             2
                    3
      1
             2
                    3
      1
             2
                    3
             2
                    3
Y =
      1
             1
                    1
      2
             2
                    2
      3
             3
                    3
      4
             4
                    4
      5
             5
                    5
```

Now use ndgrid to create a 2-D space aligned grid from the same two vectors, xgv and ygv.

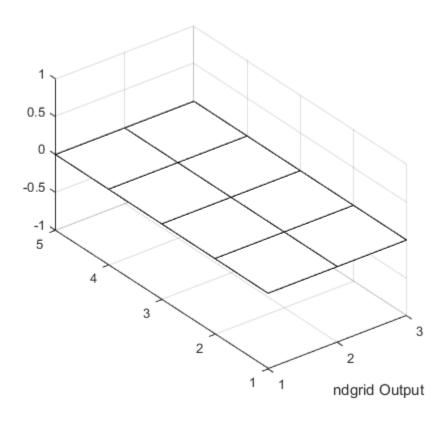
```
[X1,X2] = ndgrid(xgv,ygv)
```

```
X1 =
     1
                  1
                                1
     2
            2
                  2
                         2
                                2
     3
            3
                  3
                         3
                                3
X2 =
     1
            2
                   3
                                5
     1
            2
                   3
                         4
                                5
                   3
                                5
```

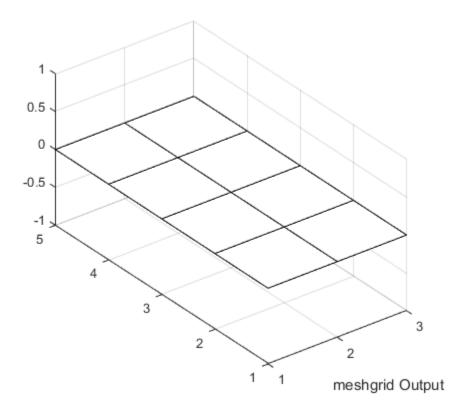
Notice that ndgrid's X1 is the transpose of meshgrid's X. The same is true for X2 and Y.

For a given set of inputs, the meshgrid and ndgrid functions will produce grids with exactly the same coordinates. The only difference between their outputs is the format of the coordinate arrays. Plot both outputs and see that they are the same.

```
figure()
[X1_ndgrid,X2_ndgrid] = ndgrid(1:3,1:5);
Z = zeros(3,5);
mesh(X1_ndgrid,X2_ndgrid,Z,'EdgeColor','black')
axis equal;
% Set the axis labeling and title
h1 = gca;
h1.XTick = [1 2 3];
h1.YTick = [1 2 3 4 5];
xlabel('ndgrid Output')
```



```
figure()
[X_meshgrid,Y_meshgrid] = meshgrid(1:3, 1:5);
mesh(X_meshgrid,Y_meshgrid,Z','EdgeColor','black')
axis equal;
% Set the axis labeling and title
h2 = gca;
h2.XTick = [1 2 3];
h2.YTick = [1 2 3 4 5];
xlabel('meshgrid Output')
```



Depending on how you intend to use your grid, you may prefer one format or the other. Some functions in MATLAB might require your data to have a meshgrid format while others might require an ndgrid format.

### **Converting Between Grid Formats**

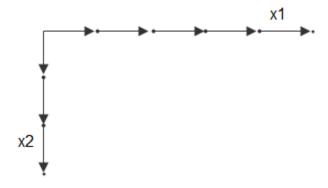
To convert a 2-D grid output from meshgrid to the ndgrid format, transpose the coordinate matrices:

```
[X_meshgrid,Y_meshgrid] = meshgrid(1:3, 1:5);
[X1_ndgrid,X2_ndgrid] = ndgrid(1:3,1:5);
isequal(X_meshgrid',X1_ndgrid)
ans =
```

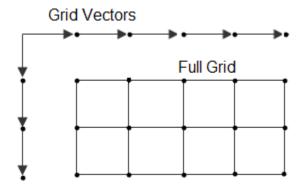
```
isequal(Y meshgrid',X2 ndgrid)
ans =
You can also use the permute function.
isequal(permute(X_meshgrid,[2 1]),X1_ndgrid)
ans =
To convert a 3-D meshgrid to ndgrid, transpose each page of the coordinate array. For
a given array my array, permute(my array, [2 1 3]) interchanges the rows and
columns, and the net effect is the transposition of every page:
[X meshgrid,Y meshgrid,Z meshgrid] = meshgrid(1:3, 1:5, [1 2]);
[X1_ndgrid, X2_ndgrid, X3_ndgrid] = ndgrid(1:3,1:5, [1 2]);
isequal(permute(X_meshgrid,[2 1 3]),X1_ndgrid)
ans =
     1
isequal(permute(Y_meshgrid,[2 1 3]),X2_ndgrid)
ans =
isequal(permute(Z_meshgrid,[2 1 3]),X3_ndgrid)
ans =
     1
```

#### **Grid Vectors**

The inputs that you pass to the grid functions are called grid vectors. The grid vectors implicitly define the grid. Consider two vectors, x1gv = (1:3) and x2gv = (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 x1gv and the other set of coordinates is given by x2gv. When the grid vectors are replicated they form two coordinate arrays that make up the *full grid*:



### Monotonic and Nonmonotonic Grids

Your input grid vectors may 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 8 3 1], ndgrid outputs the following:

[X1,X2]	= ndgri	.d([2	4 6 3	1])
X1 =				
2	2	2	2	2
4	4	4	4	4
6	6	6	6	6
3	3	3	3	3
1	1	1	1	1
X2 =				
2	4	6	3	1
2	4	6	3	1
2	4	6	3	1
2	4	6	3	1
2	4	6	3	1

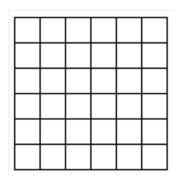
Your grid vectors should be monotonic if you intend to pass the grid to other MATLAB functions.

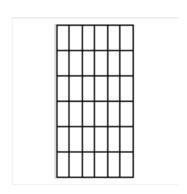
#### **Uniform and Nonuniform Grids**

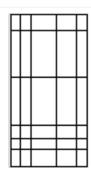
A *uniform* grid is one in which all neighboring points in a given dimension have equal spacing. For example, [X1, X2] = ndgrid([1 3 5 9],[11 13 15]) is a uniform with a spacing of 2 units in each dimension.

It is not necessary for the spacing in a uniform grid to be equal in all dimensions. For example, [X1, X2] = ndgrid([1 2 3 4],[11 13 15]) is considered uniform even though the spacing in X1 and X2 are different.

A grid whose spacing varies within any dimension is a *nonuniform* grid. For example, [X1, X2] = ndgrid([1 5 6 9],[11 13 15]) creates a nonuniform grid because the spacing varies along the first dimension.







Uniform Uniform Nonuniform

### **Types of Grid Representations**

MATLAB allows you to represent a grid in one of three representations: full grid, compact grid, or default grid. The compact grid and default grid are used primarily for convenience and improved efficiency.

#### **Full Grid**

A *full grid* is one in which the points are explicitly defined. The outputs of **ndgrid** and **meshgrid** define a full grid.

### **Compact Grid**

The explicit definition of every point in a grid is expensive in terms of memory. The *compact grid* representation is a way to dispense with the memory overhead of a full grid. The compact grid representation stores just the grid vectors instead of the full grid. (For information on how the griddedInterpolant class uses the compact grid representation, see "Interpolation with the griddedInterpolant Class" on page 8-37.)

#### **Default Grid**

For many cases, when you are analyzing data, you care about both the distances between points in the grid and their value. For example, a data set might represent rainfall at specific points in a geographic area. In this case, you would care about the value at each grid point and the distance between a point and its neighbor. In other cases, you might care only about the value for a given point and not about the relative distances. For example, you could be working with input data from an MRI scan where the distance between the points is completely uniform. In this case, you would care about the values of the points, but you can be certain of a completely uniform grid. In this case, the *default grid* representation is useful. The *default grid representation* stores the value at a grid point explicitly and creates grid point coordinates implicitly.

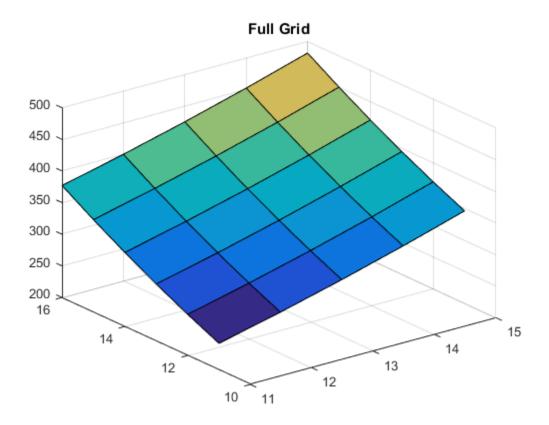
This example shows how you can use the default grid instead of the full grid to produce a plot.

Create a grid and a function that you want to plot.

```
[X,Y] = meshgrid(11:15,11:16);
Z = X.^2 + Y.^2;
```

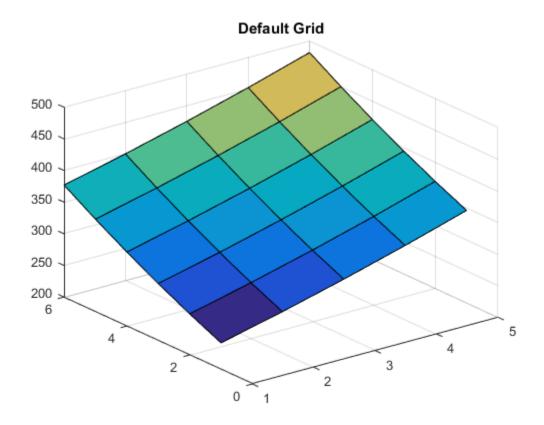
Use the full grid that you created with meshgrid by using X and Y.

```
figure
surf(X,Y,Z)
title('Full Grid')
```



In contrast, have MATLAB create a default grid instead of using the full grid.

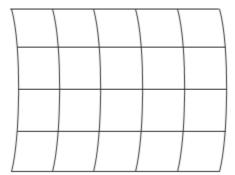
```
figure
surf(Z)
title('Default Grid')
```



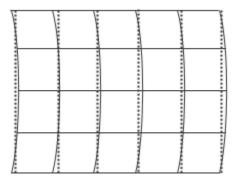
Notice the difference in the scaling of the axes. When you plot the full grid the X- and Y-axis have ranges of 11 to 15 and 10 to 16 respectively. When you plot the default grid the X- and Y-axis have ranges of 1 to m and 1 to n, where Z is m-by-n.

# **Grid Approximation Techniques**

In some cases, you may need to approximate a grid for your data. An approximate grid can be idealized by a standard MATLAB grid by choosing an appropriate set of grid vectors. 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:



In this case, although the input data cannot be gridded directly, you can approximate straight grid lines at appropriate intervals:



You can also use the default grid.

### Degenerate Grid

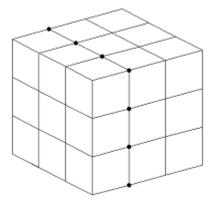
A *degenerate grid* is a special case of grid where one or more dimensions of the grid are singletons. A singleton dimension can be internal, as in 7:7 in this example:

```
[X1,X2,X3] = ndgrid(1:2:10,7:7,1:3:15); or a singleton dimension can be trailing:
```

```
[X1,X2,X3] = ndgrid(1:2:10,1:3:15,7:7);
```

You can create a degenerate grid if you are trying to take a slice of a larger data set. For example, you may want to analyze just a slice of a 3-D MRI scan. In this case, you will

need a slice of data from a multidimensional grid, such as the dotted slice in the following figure:



If you use indexing to extract the desired data, the resultant grid is degenerate in the X3 dimension:

The concept of data gridding is very important for understanding the ways in which MATLAB does grid-based interpolation.

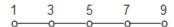
# **Grid-Based Interpolation**

- · "Benefits of Using Grid-Based Interpolation" on page 8-18
- "Interpolation versus Fit" on page 8-21
- "Interpolation Methods" on page 8-21

In grid-based interpolation, the data to be interpolated is represented by an ordered grid. For example, an arrangement of temperature measurements over a rectangular flat surface at 1-cm intervals from top-to-bottom vertically and left-to-right horizontally is considered 2-D gridded data. Grid-based interpolation provides an efficient way to approximate the temperature at any location between the grid points.

### Benefits of Using Grid-Based Interpolation

Grid-based interpolation provides significant savings in computational overhead because the gridded structure allows MATLAB to locate a query point and its adjacent neighbors very quickly. To understand how this works, consider the following points on a 1-D grid:

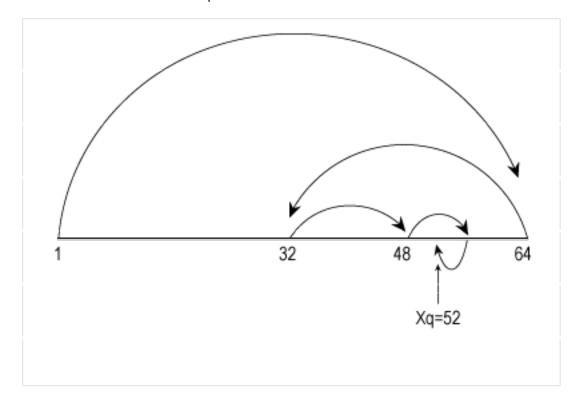


The lines connecting adjacent points represent the *cells* of the grid. The first cell occurs between x=1 and x=3, the second occurs between x=3 and x=5, and so on. Each number represents a coordinate in the grid. If you want to query the grid at x=6, you would have to use interpolation because 6 is not explicitly defined in the grid. Since this grid has a uniform spacing of 2, you can narrow down the location of the query point with a single integer division (6/2=3). This tells you that the point is in the 3rd cell of the grid. Locating a cell in a 2-D grid involves performing this operation once in each dimension. This operation is called a *fast lookup*, and MATLAB uses this technique only when the data is arranged in a uniform grid.

This fast lookup efficiently locates the cell containing a query point Xq. A binary search proceeds as follows:

- 1 Locate the center grid point.
- 2 Compare Xq to the point at the center of the grid.

- **3** If Xq is less than the point found at the center, eliminate all of the grid points greater than central point from the search. Similarly, if Xq is greater than the one found at the center, we eliminate all of the grid points that are less than the central point. Note that by doing this, we have reduced the number of points we must search by half.
- Find the center of the remaining grid points and repeat from Step 2 until you are left with one grid point on either side of your query. These two points mark the boundary of the cell that contains Xq.

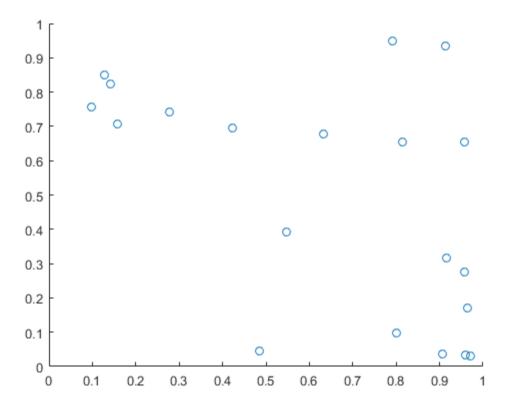


To illustrate the power of binary searches, consider the following example. Before the advent of electronic credit card authorizations, the only protection merchants had against fraudulent credit card purchases was to compare the account number on each customer's credit card against a list of "bad" account numbers. These lists were bound booklets with tens of thousands of card numbers arranged in ascending order. How many comparisons would be required to search through a list of 10,000 account numbers for one sale? It turns out that for any list of n ordered items, the maximum number of

comparisons will be no more than the number of times you can divide the list in half, or log2(n). Therefore, the credit card search will take no more than log2(10e3) or about 13 comparisons. That's a pretty impressive if you consider how many comparisons it would take to perform a sequential search.

By contrast, consider a problem with a scattered data set.

```
x = rand(20,1);
y = rand(20,1);
scatter(x,y)
```



To find the points in close proximity to a query point would require many more operations. If your data can be approximated as a grid, grid-based interpolation will provide substantial savings in computation and memory usage.

If your data is scattered, you can use the tools detailed in "Interpolating Scattered Data" on page 8-54.

### Interpolation versus Fit

The interpolation methods available in MATLAB create interpolating functions that pass though the sample data points. If you were to query the interpolation function at a sample location, you would get back the value at that sample data point. By contrast, curve and surface fitting algorithms do not necessarily pass through the sample data points.

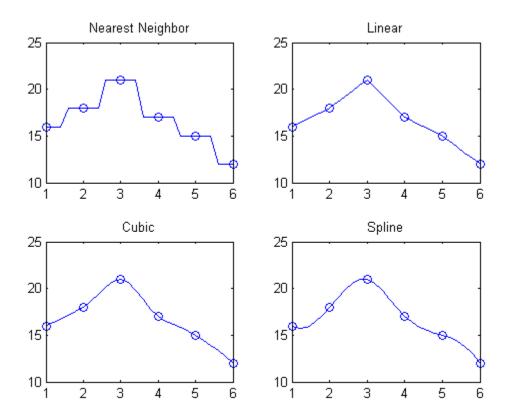
### Interpolation Methods

Grid-based interpolation offers several different methods for interpolation. When choosing an interpolation method, keep in mind that some require more memory or longer computation time than others. However, you may need to trade off these resources to achieve the desired smoothness in the result. The following table provides an overview of the benefits, trade-offs, and requirements for each method.

Method	Description	Continuity	Memory Usage and Performance	Requirements
Nearest Neighbor	The interpolated value at a query point is the value at the nearest sample grid point.	Discontinuous	<ul> <li>Modest memory requirements</li> <li>Fastest computation time</li> </ul>	• Requires 2 grid points in each dimension.
Next Neighbor	The interpolated value at a query point is the value at the next sample grid point.	Discontinuous	Same memory requirements and computation time as nearest neighbor.	<ul> <li>Available for 1D interpolation only.</li> <li>Requires at least 2 grid points.</li> </ul>
Previous Neighbor	The interpolated value at a query point is the value at the previous sample grid point.	Discontinuous	Same memory requirements and computation time as nearest neighbor.	• Available for 1D interpolation only.

Method	Description	Continuity	Memory Usage and Performance	Requirements
				• 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.	Co	<ul> <li>Requires more memory than nearest neighbor.</li> <li>Requires more computation time than nearest neighbor.</li> </ul>	• 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.	C1	<ul> <li>Requires more memory than linear.</li> <li>Requires more computation time than linear.</li> </ul>	<ul> <li>Available for 1D interpolation only.</li> <li>Requires at least 4 grid points.</li> </ul>
Cubic	The interpolated value at a query point is based on cubic interpolation of the values at neighboring grid points in each respective dimension.	C1	<ul> <li>Requires more memory than linear.</li> <li>Requires more computation time than linear.</li> </ul>	<ul> <li>Grid must have uniform spacing, though the spacing in each dimension does not have to be the same.</li> <li>Requires at least 4 points in each dimension.</li> </ul>

Method	Description	Continuity	Memory Usage and Performance	Requirements
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	<ul> <li>Requires more memory than cubic.</li> <li>Requires more computation time than cubic.</li> </ul>	• Requires 4 points in each dimension.



# **Comparison of Four Interpolation Methods**

MATLAB provides support for grid-based interpolation in several ways:

- The interp family of functions: interp1, interp2, interp3, and interpn.
- The  $griddedInterpolant\ class.$

Both the interp family of functions and griddedInterpolant support N-D grid-based interpolation. However, there are memory and performance benefits to using the griddedInterpolant class over the interp functions. Moreover, the griddedInterpolant class provides a single consistent interface for working with gridded data in any number of dimensions.

# Interpolation with the interp Family of Functions

- "The interp1 Function" on page 8-25
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### The interp 1 Function

This example shows how the interp1 function can be used to interpolate a set of sample values using the 'pchip' method.

The function interp1 performs one-dimensional interpolation. Its most general form is:

```
Vq = interp1(X,V,Xq,method)
```

where X is a vector of coordinates and V is a vector containing the values at those coordinates. Xq is a vector containing the query points at which to interpolate, and method optionally specifies any of four interpolation methods: 'nearest', 'linear', 'pchip', or 'spline'.

Create a set of 1-D grid points X and corresponding sample values V.

```
X = [1 \ 2 \ 3 \ 4 \ 5];

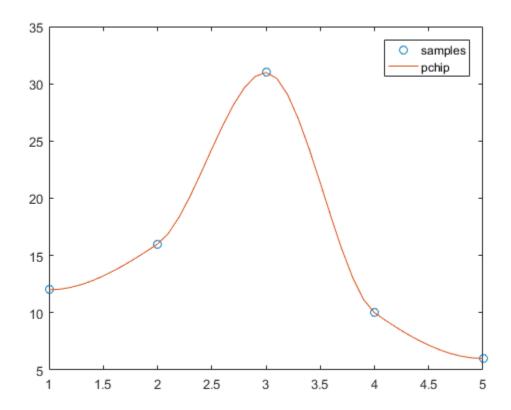
V = [12 \ 16 \ 31 \ 10 \ 6];
```

Interpolate over finer intervals with 0.1 spacing.

```
Xq = (1:0.1:5);
Vq = interp1(X,V,Xq,'pchip');
```

Plot the samples and interpolated values.

```
plot(X,V,'o');
hold on
plot(Xq,Vq,'-');
legend('samples','pchip');
hold off
```



## 1-D Extrapolation With interp1

This example shows how to use the 'extrap' option to interpolate beyond the domain of your sample points.

Define the sample points and values.

```
X = [1 \ 2 \ 3 \ 4 \ 5];

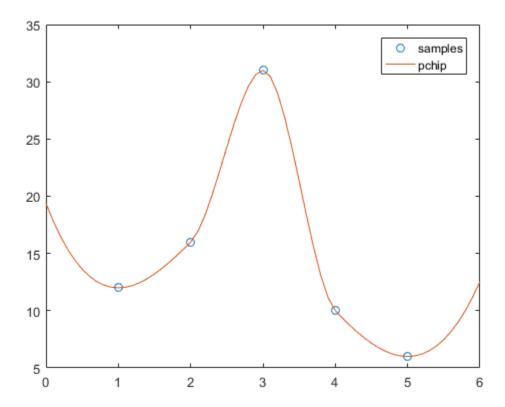
V = [12 \ 16 \ 31 \ 10 \ 6];
```

Specify the query points, Xq, that extend beyond the domain of X.

```
Xq = (0:0.1:6);
Vq = interp1(X,V,Xq,'pchip','extrap');
```

Plot the results.

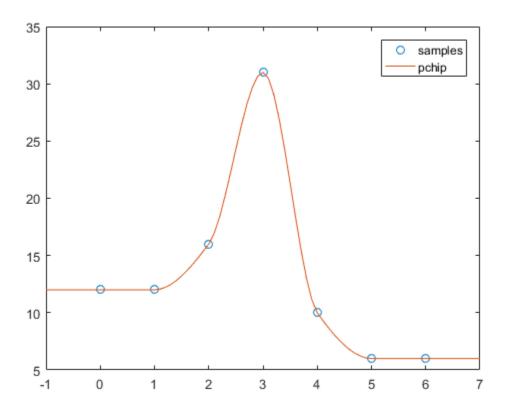
```
figure
plot(X,V,'o');
hold on
plot(Xq,Vq,'-');
legend('samples','pchip');
hold off
```



In an alternative approach, you can introduce additional points to gain more control over the behavior in the extrapolated regions. For example, you can constrain the curve to remain flat in the extrapolated region by extending the domain with repeated values.

```
X = [0 \ 1 \ 2 \ 3 \ 4 \ 5 \ 6];
```

```
V = [12 12 16 31 10 6 6];
Specify the query points, Xq, that extend further beyond the domain of X.
Xq = (-1:0.1:7);
Interpolate using 'pchip'. You can omit the 'extrap' option because it is the default with the 'pchip' and 'spline' methods.
Vq = interp1(X,V,Xq,'pchip');
Plot the results.
figure
plot(X,V,'o');
hold on
plot(Xq,Vq,'-');
legend('samples','pchip');
hold off
```



### The interp2 Function

This example shows how the interp2 function can be used to interpolate the coarsely sampled peaks function over a finer grid.

The interp2 and interp3 functions perform two and three-dimensional interpolation respectively, and they interpolate grids in the meshgrid format. The calling syntax for interp2 has the general form:

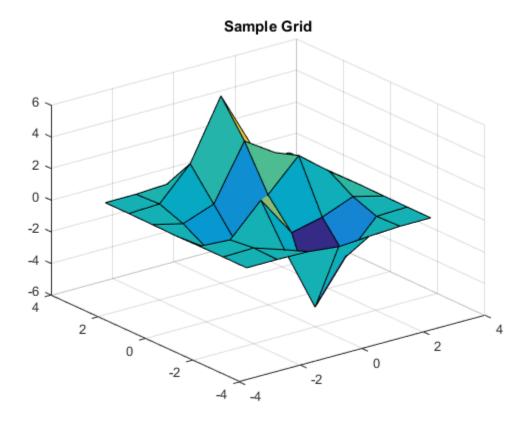
where X and Y are arrays of coordinates that define a grid in meshgrid format, and V is an array containing the values at the grid points. Xq and Yq are arrays containing the

coordinates of the query points at which to interpolate. method optionally specifies any of four interpolation methods: 'nearest', 'linear', 'cubic', or 'spline'.

The grid points that comprise X and Y must be monotonically increasing and should conform to the meshgrid format.

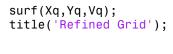
Create a coarse grid and corresponding sample values.

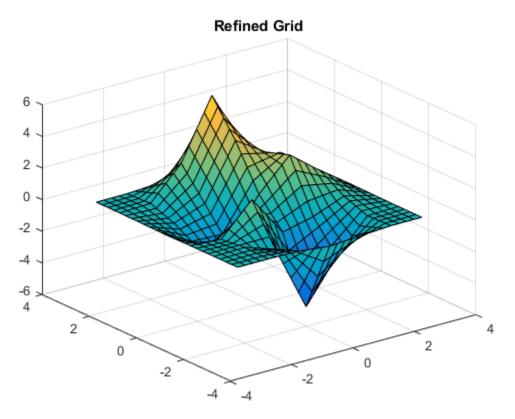
```
[X,Y] = meshgrid(-3:1:3);
V = peaks(X,Y);
Plot the sample values.
surf(X,Y,V)
title('Sample Grid');
```



Generate a finer grid for interpolation.

```
[Xq,Yq] = meshgrid(-3:0.25:3);
Use interp2 to interpolate at the query points.
Vq = interp2(X,Y,V,Xq,Yq,'linear');
Plot the results.
```





### The interp3 Function

This example shows how to use interp3 to interpolate a 3-D function at a single query point and compare it to the value generated by an analytic expression.

interp3 works in the same way as interp2 except that it takes two additional arguments: one for the third dimension in the sample grid and the other for the third dimension in the query points,

```
Vq = interp3(X,Y,Z,V,Xq,Yq,Zq,method).
```

As is the case with interp2, the grid points you supply to interp3 must be monotonically increasing and should conform to the meshgrid format.

Define a function that generates values for X, Y, and Z input.

```
generatedvalues = @(X,Y,Z)(X.^2 + Y.^3 + Z.^4);
Create the sample data.
[X,Y,Z] = meshgrid((-5:.25:5));
V = generatedvalues(X,Y,Z);
Interpolate at a specific query point.
Vq = interp3(X,Y,Z,V,2.35,1.76,0.23,'cubic')
```

```
Vq = 10.9765
```

Compare Vq to the value generated by the analytic expression.

# The interpn Function

This example shows how the interpn function can be used to interpolate a coarsely sampled function over a finer grid using the 'cubic' method.

The function interpn performs n-dimensional interpolation on grids that are in the ndgrid format. Its most general form is:

```
Vq = interpn(X1, X2, X3, ... Xn, V, Y1, Y2, Y3, ..., Yn, method)
```

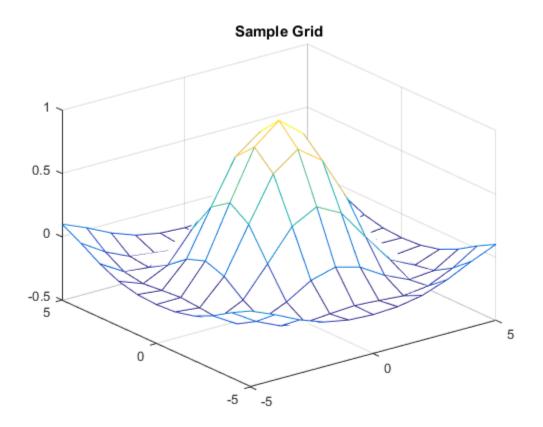
where X1,X2,X3,...,Xn are arrays of coordinates that define a grid in ndgrid format, and V is an array containing the values at the grid points. Y1,Y2,Y3,...,Yn are arrays containing the coordinates of the query points at which to interpolate. method optionally specifies any of four interpolation methods: 'nearest', 'linear', 'cubic', or 'spline'.

The grid points that comprise  $X1, X2, X3, \ldots Xn$  must be monotonically increasing and should conform to the ndgrid format.

Create a set of grid points and corresponding sample values.

```
[X1,X2] = ndgrid((-5:1:5));
R = sqrt(X1.^2 + X2.^2)+ eps;
V = sin(R)./(R);
Plot the sample values.
mesh(X1,X2,V)
```

title('Sample Grid');

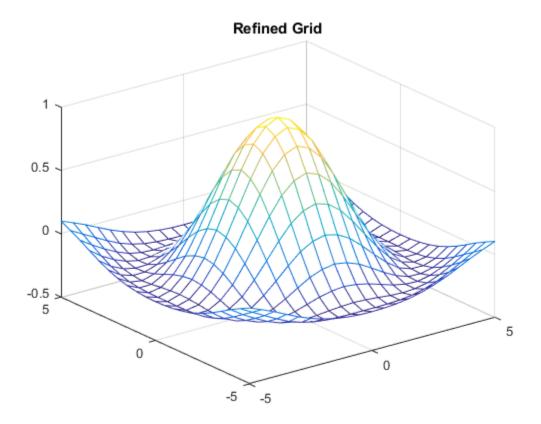


Create a finer grid for interpolation.

```
[Y1,Y2] = ndgrid((-5:.5:5));
```

Interpolate over the finer grid and plot the results.

```
Vq = interpn(X1,X2,V,Y1,Y2,'cubic');
mesh(Y1,Y2,Vq)
title('Refined Grid');
```



interpn has an alternate syntax: Vq = interpn(V,ntimes,method) that allows you to interpolate over a grid that is an integer number of times finer than the sample grid. In the previous code, Y1 and Y2 queried the interpolant over a grid that contained one extra point between each of the samples. The following code demonstrates how you can achieve the same result with ntimes=1.

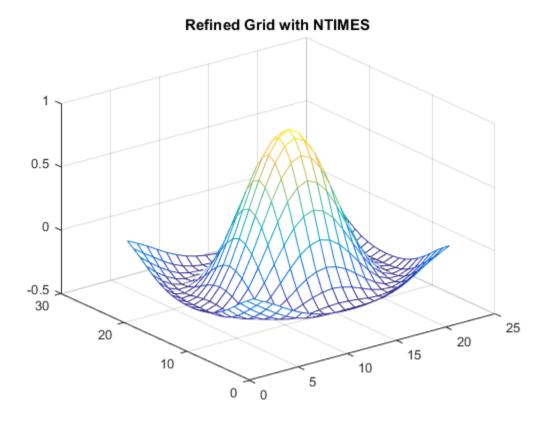
Interpolate over a finer grid using ntimes=1.

Vq = interpn(V,1,'cubic');

Plot the result.

mesh(Vq)

### title('Refined Grid with NTIMES');

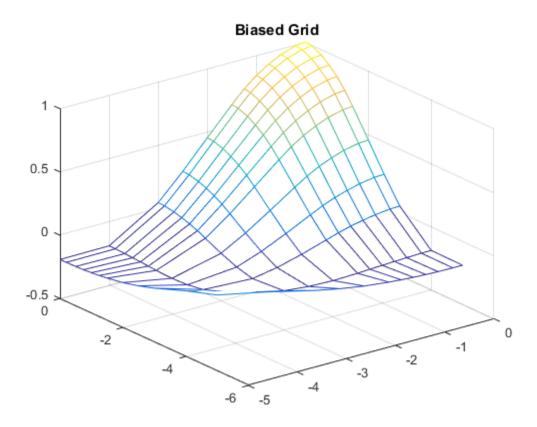


Notice that the plot is scaled differently than in the previous example. This is because we called mesh and passed the values only. The mesh function used a default grid based on the dimensions of Vq. The output values are the same in both cases.

You can also supply a nonuniform grid of query points. This can be useful if you are interested in querying the interpolant at a higher resolution in one region of the grid. The following code shows how this can be done.

Interpolate over a biased grid.

```
Vq = interpn(X1,X2,V,Y1,Y2,'cubic');
Plot the result.
mesh(Y1,Y2,Vq);
title('Biased Grid');
```



# Interpolation with the griddedInterpolant Class

Like the interpn function, the griddedInterpolant class provides a single interface for grid-based interpolation in n dimensions. However griddedInterpolant offers the following additional benefits:

- It offers substantial performance improvements for repeated queries to the interpolant.
- It offers additional performance improvements and savings in memory consumption because it stores the sample points as a compact grid.

griddedInterpolant accepts sample data that conforms to the ndgrid format. If you wish to create a griddedInterpolant with meshgrid data, you will need to convert the data to the ndgrid format. See "Converting meshgrid Data to the ndgrid Format" on page 8-39 for a demonstration of how to convert 2-D and 3-D meshgrids.

The griddedInterpolant class supports the five interpolation methods that are also supported by interpn: nearest, linear, pchip, cubic, and spline. However griddedInterpolant offers greater performance with less overhead.

### Constructing the Interpolant

An *interpolant* is a function that performs interpolation. You create the interpolant by calling the <code>griddedInterpolant</code> constructor and passing the sample data: the grid and corresponding sample values. You can also specify the interpolation method if you wish to override the default "linear" method. The calling syntax has the following forms:

• For 1-D interpolation, you can pass X, a set of points, and V, a vector of the same length containing the corresponding values.

```
F = griddedInterpolant(x,v)
```

For higher dimensions, you can supply a full grid. X1, X2,..., Xn specify the grid as
a set of n n-D arrays. These arrays conform to the ndgrid format and are the same
size as the sample array V.

```
F = griddedInterpolant(X1, X2, ..., Xn, V)
```

• If you know that the distances between adjacent sample points are uniform, you can let griddedInterpolant create a default grid by passing only the sample points V.

```
F = griddedInterpolant(V)
```

You can also specify the coordinates of your sample data as a compact grid. The
compact grid is represented by a set of vectors. These vectors are then packaged into a
cell array by enclosing them in curly braces; for example, {x1g,x2g,...,xng} where
vectors x1g,x2g,...,xng define the grid coordinates in each dimension.

```
F = griddedInterpolant({x1g,x2g,...,xng},V)
```

• You can also specify the interpolation method as a final input argument with any of the calling syntaxes. This example specifies nearest neighbor interpolation.

```
F = griddedInterpolant({x1g,x2g,x3g},V,'nearest')
```

### Querying the Interpolant

The griddedInterpolant, F, is evaluated in the same way as you would call a function. Your query points may be scattered or gridded, and you can pass them to F in any of the following ways:

• You can specify an m-by-n matrix Xq, which contains m scattered points in n dimensions. The interpolated values Vq are returned as an m-by-1 vector.

```
Vq = F(Xq)
```

 You can also specify the query points as a series of n column vectors x1q,x2q,...,xnq of length m. These vectors represent m points in n dimensions. The interpolated values Vq are returned as an m-by-1 vector.

```
Vq = F(x1q, x2q, ..., xnq)
```

 You can specify the query points as a series of n n-dimensional arrays representing a full grid. The arrays X1q, X2q,..., Xnq are all the same size and conform to the ndgrid format. The interpolated values Vq will also be the same size.

```
Vq = F(X1q, X2q, ..., Xnq)
```

You can also specify the query points as a compact grid. x1gq, x2gq,...,xngq are vectors that define the grid points in each dimension.

```
Vq = F(\{x1gq, x2gq, ..., xngq\})
For example, in 2-D:
Vq = F(\{(0:0.2:10), (-5:0.5:5)\});
```

# Converting meshgrid Data to the ndgrid Format

The griddedInterpolant class accepts ndgrid formatted sample data. If you want to create a griddedInterpolant with meshgrid data, you should convert it to the ndgrid format first.

The following example outlines the steps for converting 2-D meshgrid data to the ndgrid format. We begin by creating the meshgrid and corresponding sample values:

```
[X,Y] = meshgrid(-2:.1:2,-1:.1:1);
V=0.75*Y.^3-3*Y-2*X.^2;
```

To convert X, Y, and V to ndgrid format, follow these steps:

1 Transpose each array in the grid as well as the sample data.

```
X=X';
Y=Y';
V=V';
```

**2** Now create the interpolant.

```
F = griddedInterpolant(X,Y,V);
```

To convert a 3-D meshgrid, we use the permute function. Again, we'll start by creating the meshgrid and corresponding sample values:

```
[X,Y,Z] = meshgrid(-5:5,-3:3,-10:10);
V = X.^3 + Y.^2 + Z;
```

To convert X, Y, Z, and V to ndgrid format, follow these steps:

1 Use the permute function to interchange the rows and columns of each array. The net effect will be the transpose of every page.

```
P = [2 1 3];
X = permute(X,P);
Y = permute(Y,P);
Z = permute(Z,P);
V = permute(V,P);
```

2 Now create the interpolant.

```
F = griddedInterpolant(X,Y,Z,V);
```

### griddedInterpolant in One Dimension

This example shows how to create and plot a 1-D interpolant using griddedInterpolant with a cubic interpolation method.

Create a coarse grid and sample values.

```
X = [1 \ 2 \ 3 \ 4 \ 5];

V = [12 \ 6 \ 15 \ 9 \ 6];
```

Construct the griddedInterpolant using a cubic interpolation method.

```
F = griddedInterpolant(X,V,'cubic')

F =
    griddedInterpolant with properties:
        GridVectors: {[1 2 3 4 5]}
        Values: [12 6 15 9 6]
        Method: 'cubic'
    ExtrapolationMethod: 'cubic'
```

The GridVectors property contains the compact grid specifying the coordinates of the sample values V. The Method property specifies the interpolation method. Notice that we specified 'cubic' when we created F. If you omit the Method argument, the default interpolation method, linear, will be assigned to F.

You can access any of the properties of F in the same way you would access the fields in a struct.

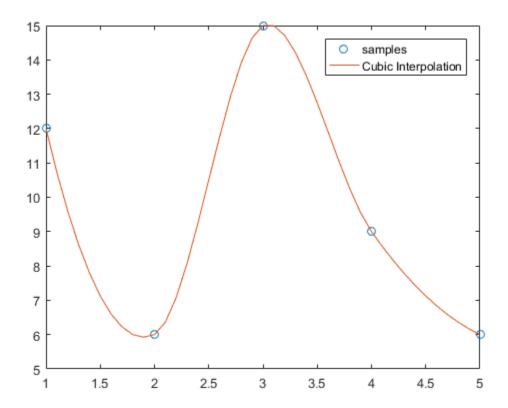
```
F.GridVectors; % Displays the grid vectors as a cell array
F.Values; % Displays the sample values
F.Method; % Displays the interpolation method
```

Interpolate over finer intervals with 0.1 spacing.

```
Xq = (1:0.1:5);
Vq = F(Xq);

Plot the result.

plot(X,V,'o');
hold on
plot(Xq,Vq,'-');
legend('samples','Cubic Interpolation');
```



### griddedInterpolant in Two Dimensions

This example shows how to create and plot a 2-D interpolant using griddedInterpolant.

In two dimensions and higher, you can specify the sample coordinates as an ndgrid, a compact grid, or a default grid. In this example, we'll supply an ndgrid.

Create a coarse grid and sample values.

$$[X,Y] = ndgrid(-1:.3:1,-2:.3:2);$$
  
V = 0.75\*Y.^3 - 3\*Y - 2\*X.^2;

 $Construct\ the\ {\tt griddedInterpolant}.$ 

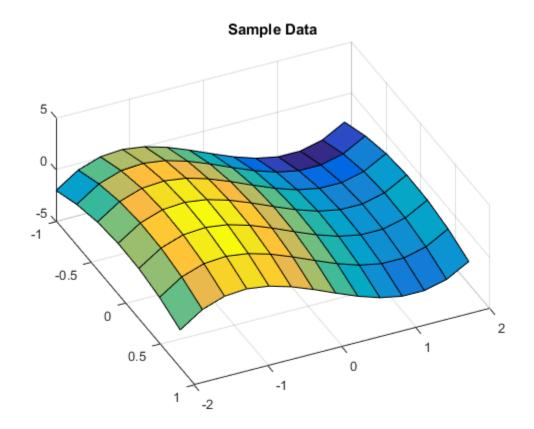
```
F = griddedInterpolant(X,Y,V,'spline');
Interpolate over finer intervals with 0.1 spacing.

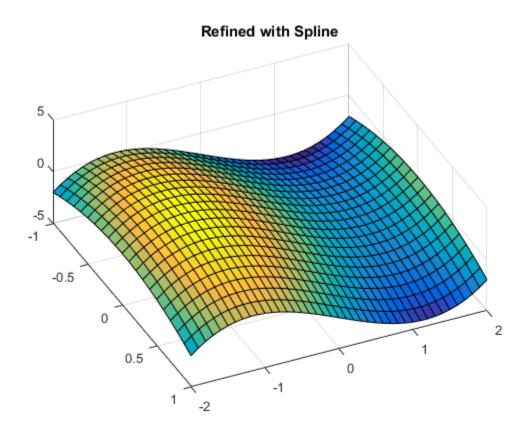
[Xq,Yq] = ndgrid(-1:.1:1,-2:.1:2);
Vq = F(Xq,Yq);

Plot the result.

figure()
surf(X,Y,V);
view(65,60)
title('Sample Data');

figure()
surf(Xq,Yq,Vq);
view(65,60)
title('Refined with Spline');
```





### griddedInterpolant in Three Dimensions

This example shows how to create a 3-D interpolant and evaluate over a slice plane so you can plot the values on that plane.

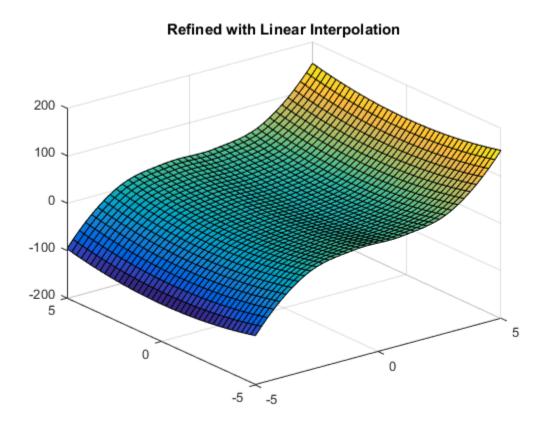
Create a full grid and sample values.

Construct the griddedInterpolant.

```
F = griddedInterpolant(X,Y,Z,V,'cubic');
```

Since we already created the full grid to generate our sample values, we had nothing to lose in passing it to <code>griddedInterpolant</code>. In practice however, it's common to load the sample data into MATLAB from disk. The compact grid can very beneficial in such cases because it allows you to specify the entire grid in a form that is much more economical in terms of memory. If we had loaded V into MATLAB instead of calculating it from a full grid, we could have created a compact grid to conserve memory in our workspace. For example,

```
gv = {(-5:2:5),(-5:2:5),(-5:2:5)};
F = griddedInterpolant(gv,V,'cubic');
Now interpolate over a plane at Z = 2 with 0.25 spacing.
[Xq,Yq,Zq] = ndgrid((-5:.25:5),(-5:.25:5),2:2);
Vq = F(Xq,Yq,Zq);
Plot the result.
surf(Xq,Yq,Vq);
title('Refined with Linear Interpolation');
```



### griddedInterpolant in Four Dimensions

In this example, we'll create a 4-D interpolant and evaluate it at a single point

1 Create a coarse grid and sample values.

2 Construct the griddedInterpolant.

F = griddedInterpolant(X1,X2,X3,X4,V,'linear');

3 Query the griddedInterpolant at a single point.

$$Vq = F([-3.2 \ 2.1 \ 4.7 \ -1.3])$$

MATLAB outputs the following:

```
ans = -10.1000
```

.

#### Other Ways of Working with griddedInterpolant

Depending on the arrangement of your query points, you may prefer one evaluation syntax over the others. For example, if we create the following interpolant:

```
[X,Y]=ndgrid(-1:.25:1,-2:.25:2);
V=0.75*Y.^3-3*Y-2*X.^2;
F = griddedInterpolant(X,Y,V);
We can query F using a full grid to give the values at the grid points:
[Xq, Yq] = ndgrid(-1:.1:0, -2:.1:0);
Vq = F(Xq, Yq);
We can also interpolate over the same grid using the compact grid format:
gvq = \{-1:.1:0, -2:.1:0\};
Vq = F(gvq);
We can also query a single point:
Vq = F(.315,.738)
which returns:
Vq =
   -2.1308
or a random set of scattered points:
rng('default')
Vq = F(rand(3,2))
which returns:
```

Vq =

```
-3.4919
   -3.3557
   -0.3515
We can also examine the Values in F:
 F.Values(1,3)
which returns:
 ans =
   -0.0313
Now we'll replace the Values array:
F.Values = 2*V;
You can edit the properties in F on-the-fly. For example, you can replace the interpolation
method as follows:
 F.Method = 'cubic';
You can also replace the GridVectors in F. First, we'll examine GridVectors:
gv = F.GridVectors;
gv{1}
gv is a cell array, and gv\{1\} displays the first grid vector:
ans =
  -1.0000
          -0.7500
                  -0.5000
                          -0.2500
                                        0.2500
                                                0.5000
                                                        0.7500
                                                                 1.0000
Now we'll replace the GridVectors in F by creating a new cell array new_gv:
new_gv = \{(0:0.3:1), (0:0.3:1)\};
F.GridVectors = new_gv;
```

# Interpolation of Multiple 1-D Value Sets

This example shows how to interpolate three 1-D data sets in a single pass using griddedInterpolant. 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 a 2-D grid of sample points.

```
samplePoints = \{x, 1: size(V,2)\};
```

This compact notation specifies a full 2-D grid. The first element, samplePoints{1}, contains the *x*-coordinates for V, and samplePoints{2} contains the *y*-coordinates. The orientation of each coordinate vector does not matter.

Create the interpolant, F, by passing the sample points and sample values to griddedInterpolant.

```
F = griddedInterpolant(samplePoints,V);
Create a 2-D query grid with 0.5 spacing along X over all columns of V.
queryPoints = {(1:0.5:5),1:size(V,2)};
Evaluate the interpolant at the x-coordinates for each value set.
Vq = F(queryPoints)
```

```
Vq =
    1.0000
               2.0000
                         3.0000
    1.5000
               3.0000
                         4.5000
    2.0000
               4.0000
                         6.0000
    2.5000
               5.0000
                         7.5000
    3.0000
               6.0000
                         9.0000
    3.5000
               7.0000
                        10.5000
    4.0000
               8.0000
                        12.0000
    4.5000
               9.0000
                        13.5000
    5.0000
              10.0000
                        15.0000
```

## See Also

griddedInterpolant

# **Related Examples**

• "Interpolation with the griddedInterpolant Class" on page 8-37

# 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,:);
```

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.

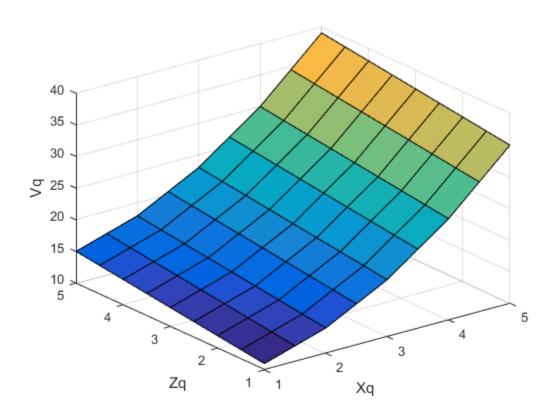
```
x = squeeze(x);
z = squeeze(z);
v = squeeze(v);
```

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');
zlabel('Vq');
```



## **See Also**

interpn | squeeze

## **More About**

• "Gridded Data Representation" on page 8-4

# **Interpolating Scattered Data**

```
In this section...

"Scattered Data" on page 8-54

"Interpolating Scattered Data Using griddata and griddatan" on page 8-57

"scatteredInterpolant Class" on page 8-61

"Interpolating Scattered Data Using the scatteredInterpolant Class" on page 8-61

"Interpolation of Complex Scattered Data" on page 8-71

"Addressing Problems in Scattered Data Interpolation" on page 8-73
```

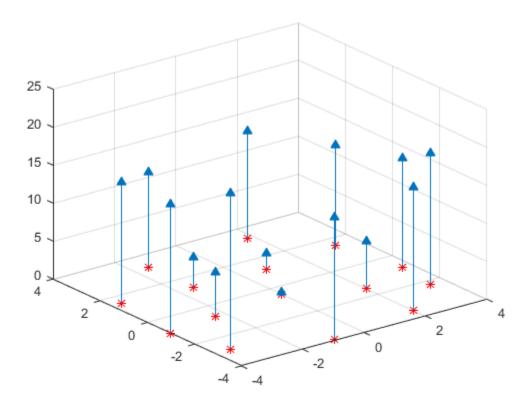
### Scattered Data

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.

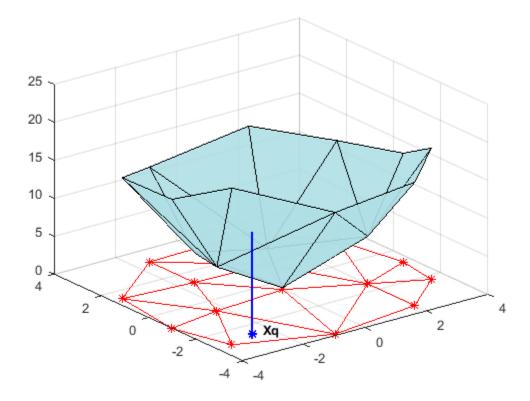


Create a Delaunay triangulation, lift the vertices, and evaluate the interpolant at the query point Xq.

```
axis([-4, 4, -4, 4, 0, 25]);
grid
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.

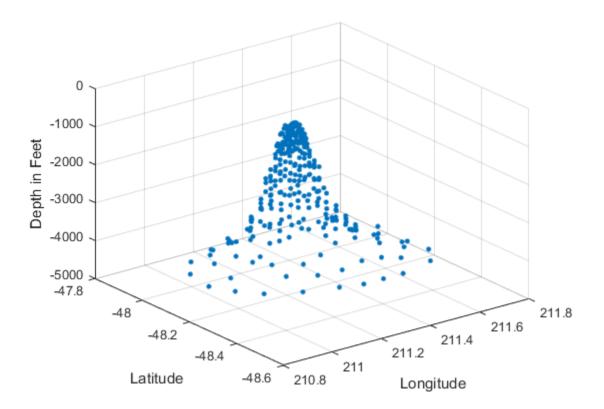
## Interpolating Scattered Data Using griddata and griddatan

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 grid-point 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.

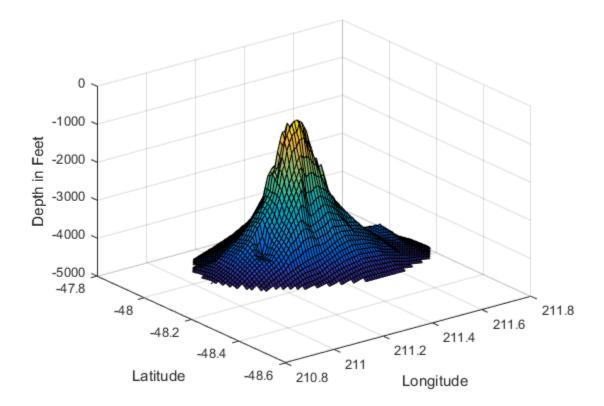
Plot the seamount data set (a *seamount* is an underwater mountain). The data set consists of a set of longitude (x) and latitude (y) locations, and corresponding seamount elevations (z) measured at those coordinates.

```
load seamount
plot3(x,y,z,'.','markersize',12)
xlabel('Longitude')
ylabel('Latitude')
zlabel('Depth in Feet')
grid on
```



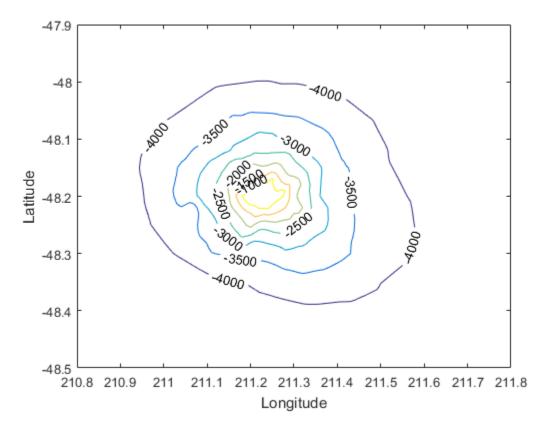
Use meshgrid to create a set of 2-D grid points in the longitude-latitude plane and then use griddata to interpolate the corresponding depth at those points.

```
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 scatteredInterpolant class described in "Interpolating Scattered Data Using the scatteredInterpolant Class" on page 8-61 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 8-86 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.

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 query 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 =
1.3966
```

You can also pass individual coordinates:

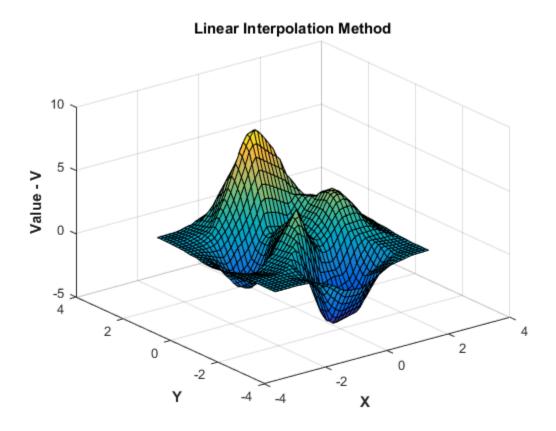
```
Vq = F(1.5, 1.25)
Vq =
1.3966
```

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 =
1.0880
1.8127
2.3472
```

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');
```



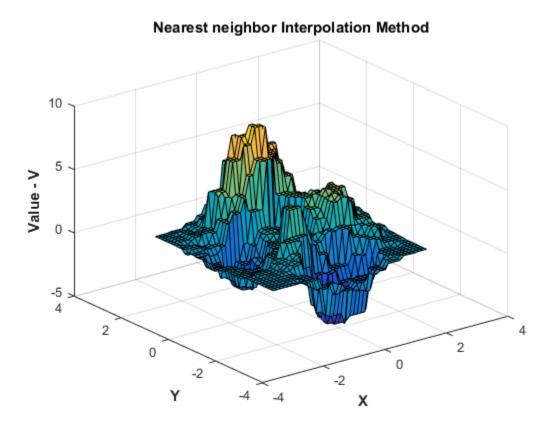
### Change the interpolation method.

You can change the interpolation method on the fly. Set the method to 'nearest'.

```
F.Method = 'nearest';
```

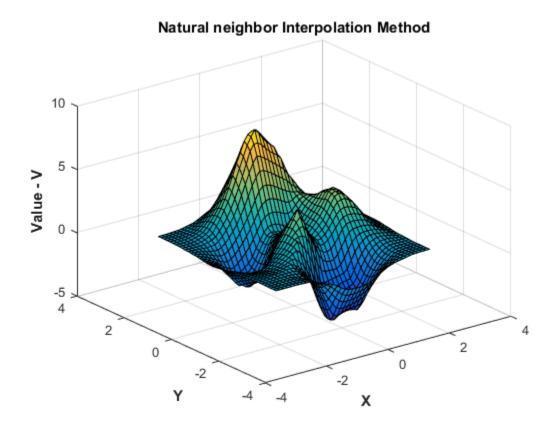
Reevaluate and plot the interpolant as before.

```
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.

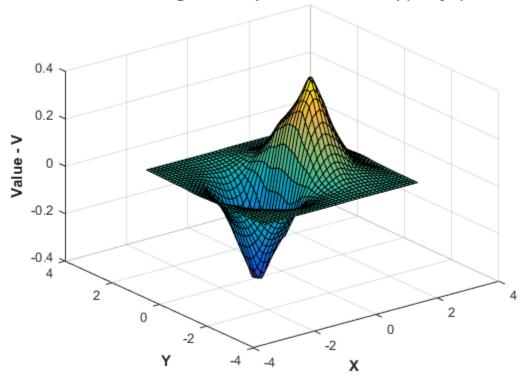
The following steps show how to change the values in our example. You will compute the values using the expression,  $v = xe^{-x^2-y^2}$ .

```
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)')
```

## 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);

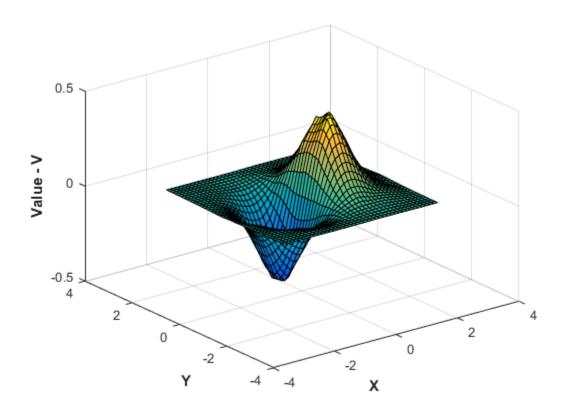
V = X(:,1).*exp(-X(:,1).^2-X(:,2).^2);
```

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.

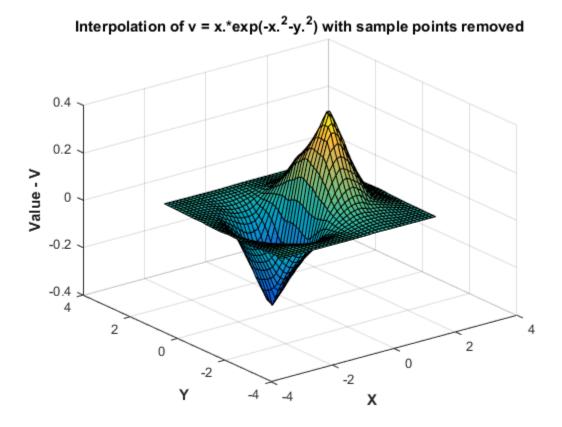
F.Points(5:15,:) = [];
F.Values(5:15) = [];

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 Complex Scattered Data

This example shows how to interpolate scattered data when the value at each sample location is complex.

Create the sample data.

```
X = -3 + 6 .* gallery('uniformdata',[250 2],0);

V = complex(X(:,1).*X(:,2), X(:,1).^2 + X(:,2).^2);
```

Create the interpolant.

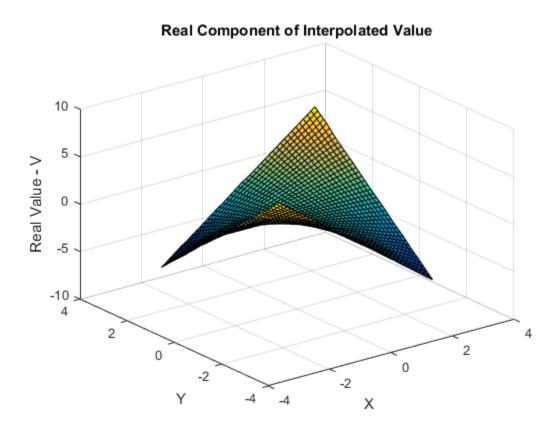
F = scatteredInterpolant(X,V);

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.

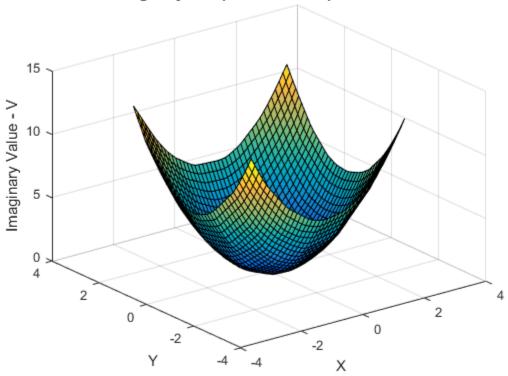
VqReal = real(Vq);
figure
surf(Xq,Yq,VqReal);
xlabel('X');
ylabel('Y');
zlabel('Real Value - V');
title('Real Component of Interpolated Value');
```



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');
```

## **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;
V = x.^2 + y.^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)) | isnan(X(:,2)) | isnan(V);
X(nan_flags,:) = [];
V(nan_flags) = [];
F = scatteredInterpolant(X,V);
```

#### Interpolant Outputs NaN Values

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 8-86 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.

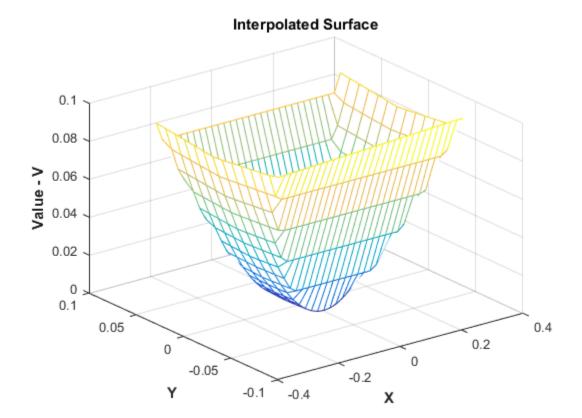
```
t = 0.4*pi:0.02:0.6*pi;
x1 = cos(t)';
y1 = sin(t)'-1.02;
x2 = x1;
y2 = y1*(-1);
x3 = linspace(-0.3,0.3,16)';
y3 = zeros(16,1);
```

```
x = [x1;x2;x3];

y = [y1;y2;y3];
```

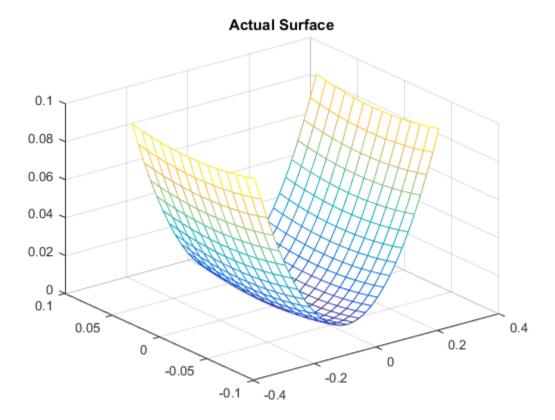
Now lift these sample points onto the surface  $z = x^2 + y^2$  and interpolate the surface.

```
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:

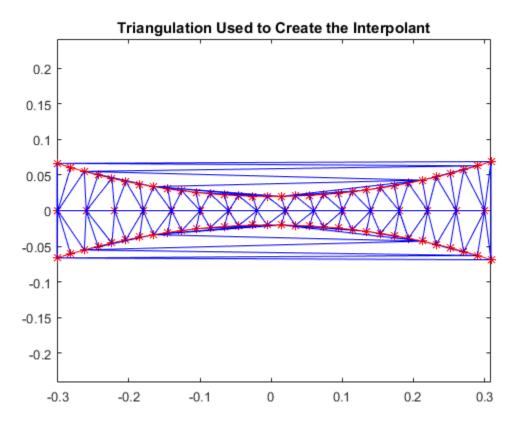
```
zi = xi.^2 + yi.^2;
figure
mesh(xi,yi,zi)
title('Actual Surface')
```



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
```

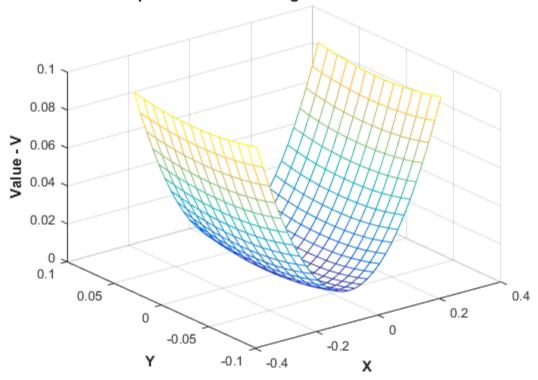


The triangles within the red boundaries are relatively well shaped; they are constructed from points that are in close proximity and the interpolation works well in this region. Outside the red boundary, the triangles are sliver-like and connect points that are remote from each other. There is not sufficient 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');
```

#### Interpolated surface from griddata with v4 method



The interpolated surface from 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 8-83

"Linear Interpolation Using a delaunay Triangulation Query" on page 8-84

#### 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*gallery('uniformdata',[10 2],1);
```

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 =

5.3163
0.3453
4.3026
1.2579
1.9435
5.9194
3.9030
0.4172
11.7282
0.8641
```

## 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 V3, V3, then the interpolated value is V3, V4, V4, V5, V5

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*gallery('uniformdata',[10 2],1);
```

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 =
```

5.9456

1.1222

4.7963

0.9373

2.3533

3.4219

2.3104

0.7728

8.0479

1.0886

#### **See Also**

delaunayTriangulation | nearestNeighbor | pointLocation

#### **More About**

"Interpolating Scattered Data" on page 8-54

# **Extrapolating Scattered Data**

#### In this section...

"Factors That Affect the Accuracy of Extrapolation" on page 8-86

"Compare Extrapolation of Coarsely and Finely Sampled Scattered Data" on page 8-86

"Extrapolation of 3-D Data" on page 8-90

#### 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 8-78 for more information.

You should inspect your extrapolation results visually using your knowledge of the behavior outside the domain.

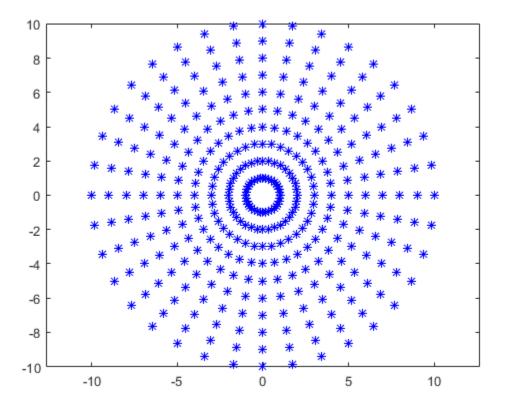
#### Compare Extrapolation of Coarsely and Finely Sampled Scattered Data

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);
```

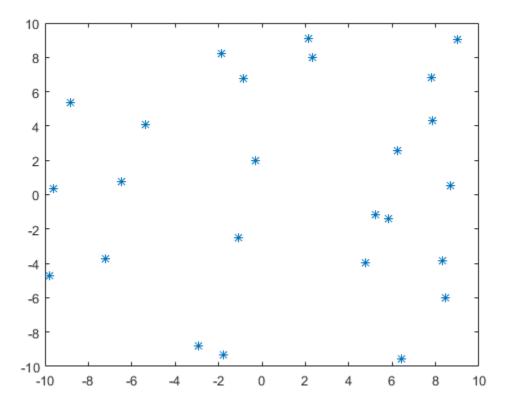
```
r = 1:10;
x1 = bsxfun(@times,r.',c);
y1 = bsxfun(@times,r.',s);
figure
plot(x1,y1,'*b')
axis equal
```



Create a second, more coarsely distributed set of points. Use the gallery function to create random samplings in the range, [-10, 10].

```
x2 = -10 + 20*gallery('uniformdata',[25 1],0);
y2 = -10 + 20*gallery('uniformdata',[25 1],1);
```

```
figure
plot(x2,y2,'*')
```



Sample a parabolic function,  $V\left( x,y\right) ,$  at both sets of points.

Create a scatteredInterpolant for each sampling of v(x,y).

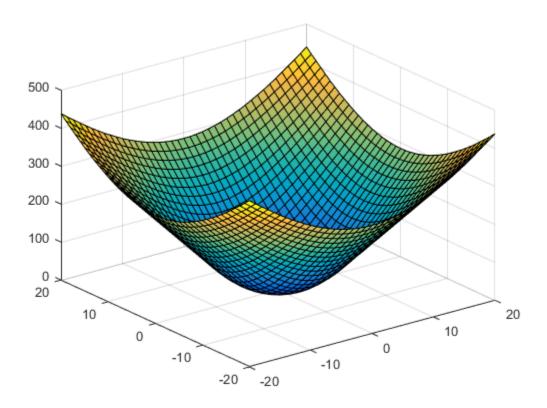
```
F1 = scatteredInterpolant(x1(:),y1(:),v1(:));
F2 = scatteredInterpolant(x2(:),y2(:),v2(:));
```

Create a grid of query points that extend beyond each domain.

```
[xq,yq] = ndgrid(-20:20);
```

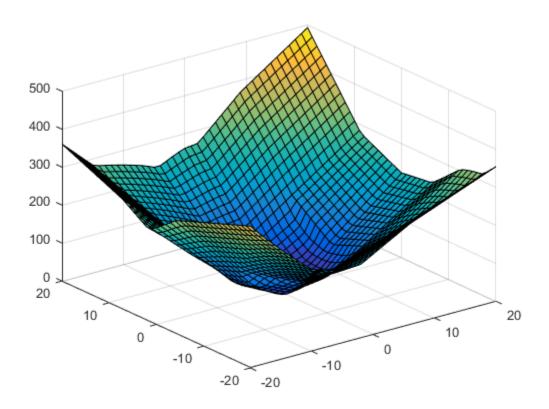
Evaluate F1 and plot the results.

```
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.

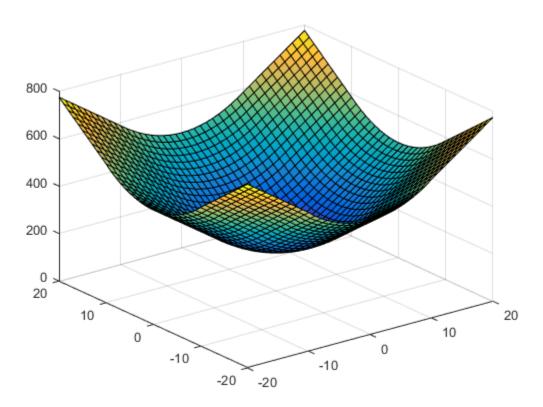
```
v = x.^2 + y.^2 + z.^2;
```

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.

# **Optimization**

- "Optimizing Nonlinear Functions" on page 9-2
- "Curve Fitting via Optimization" on page 9-8
- "Set Options" on page 9-11
- "Iterative Display" on page 9-15
- "Output Functions" on page 9-17
- "Plot Functions" on page 9-25
- "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 9-4

"Maximizing Functions" on page 9-5

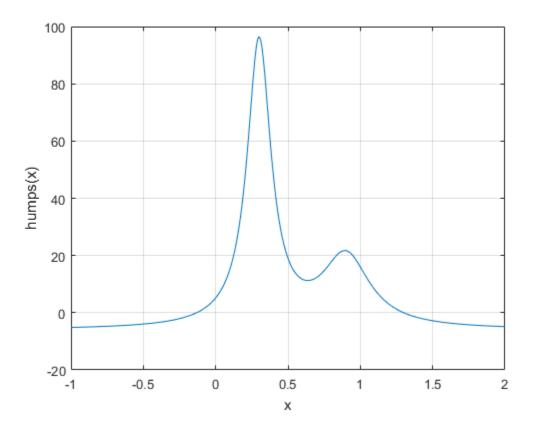
"fminsearch Algorithm" on page 9-5

"Reference" on page 9-7
```

### 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 ask for a tabular display of output by passing a fourth argument created by the optimset command to fminbnd:

```
opts = optimset('Display','iter');
```

#### x = fminbnd(@humps, 0.3, 1, opts)

```
Func-count
                            f(x)
                                           Procedure
                Χ
   1
            0.567376
                           12.9098
                                            initial
   2
                           13.7746
            0.732624
                                            aolden
   3
            0.465248
                           25.1714
                                            golden
   4
                           11.2693
            0.644416
                                            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
```

This 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 what procedure is being used at each iteration, either a golden section search or a parabolic interpolation. For more information, see "Iterative Display" on page 9-15.

#### **Minimizing Functions of Several Variables**

The fminsearch function is similar to fminbnd except that it handles functions of many variables, and you 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.

```
v = [-0.6,-1.2,0.135];
a = fminsearch(@three_var,v)
a =
     0.0000   -1.5708     0.1803
```

#### **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  $x_0$ , and using these n vectors as elements of the simplex in addition to  $x_0$ . (It 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).

```
where m = \sum x(i)/n, i = 1...n,
```

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 ss = m + 2(m - x(n+1)),

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**
- **6** If  $f(r) \ge f(x(n))$ , perform a *contraction* between m and the better of x(n+1) and r:
  - **a** If f(r) < f(x(n+1)) (i.e., r is better than x(n+1)), calculate c = m + (r m)/2

and calculate f(c). If f(c) < f(r), accept c and terminate the iteration. **Contract outside** Otherwise, continue with Step 7 (Shrink).

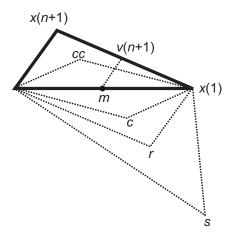
**b** If 
$$f(r) \ge f(x(n+1))$$
, calculate  $cc = m + (x(n+1) - m)/2$ 

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

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 might 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.

# **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  $\lambda$  are the parameters to fit. Fitting the curve means finding parameters A and  $\lambda$  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".

```
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".

#### 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.

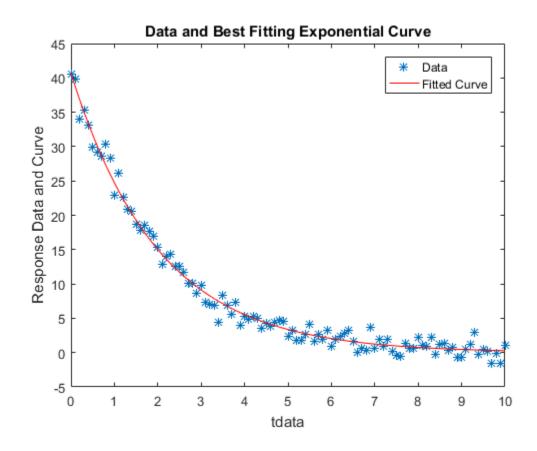
```
x0 = rand(2,1);
bestx = fminsearch(fun,x0)
bestx =
    40.6877
    0.4984
```

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
```



# **Set Options**

# In this section... "How to Set Options" on page 9-11 "Options Table" on page 9-11 "Tolerances and Stopping Criteria" on page 9-12 "Output Structure" on page 9-13

#### **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 1sqnonneg). See "Iterative Display" on page 9-15.	
	· 'off' displays no intermediate steps.	
	• 'final' displays just the final output.	

Option	Description	Solvers
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.  • 'off' (default) displays no error.	fminbnd, fminsearch, fzero
MaxFunEvals	The maximum number of function evaluations allowed. The default value is 500 for fminbnd and 200*length(x0) for fminsearch.	fminbnd, fminsearch
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 "Output Functions" on page 9-17.	fminbnd, fminsearch, fzero
PlotFcns	Plot information on the iterations of the solver. The default is [ ] (none). For available predefined functions, see "Plot Functions" on page 9-25.	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 9-12.	fminsearch
TolX	The termination tolerance for <i>x</i> . The default value is 1.e-4. See "Tolerances and Stopping Criteria" on page 9-12.	fminbnd, fminsearch, fzero, lsqnonneg

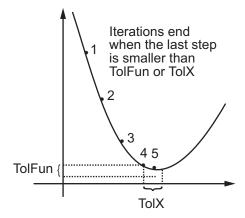
# **Tolerances and Stopping Criteria**

The number of iterations in an optimization depends on a solver's *stopping criteria*. 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 doesn't 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.

• 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 sometimes 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 sometimes 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 each solver's output structure 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.

# **Iterative Display**

You obtain details of the steps solvers take by setting the <code>Display</code> option to 'iter' with <code>optimset</code>. 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 9-5.	
	initial (initial point)	fzero
	• search (search for an interval containing a zero)	
	• bisection	

Heading	Information Displayed	Solvers
	• 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

# **Output Functions**

```
In this section...

"What Is an Output Function?" on page 9-17

"Creating and Using an Output Function" on page 9-17

"Structure of the Output Function" on page 9-19

"Example of a Nested Output Function" on page 9-19

"Fields in optimValues" on page 9-22

"States of the Algorithm" on page 9-22

"Stop Flag" on page 9-23
```

#### What Is an Output Function?

An *output function* is a function that an optimization function calls at each iteration of its algorithm. Typically, you might 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

$$\min_{x} f(x) = \min_{x} e^{x_1} \left( 4x_1^2 + 2x_2^2 + x_1 x_2 + 2x_2 \right).$$

To do so,

- 1 Create a file containing the preceding code and save it as outfun.m in a directory on the MATLAB path.
- 2 Enter the command

```
options = optimset('OutputFcn', @outfun);
```

to set the value of the Outputfon field of the options structure to a function handle to outfun.

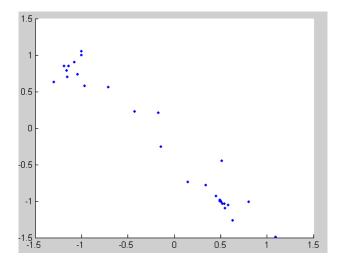
**3** Enter the following commands:

```
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
```

This returns the solution

```
x =
     0.1290 -0.5323
fval =
     -0.5689
```

and displays 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 should quit or continue. See "Stop Flag" on page 9-23.
- 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 9-22 describes the structure in detail.
- state is the current state of the algorithm. "States of the Algorithm" on page 9-22 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 9-17 does not require the output function to preserve data from one iteration to the next. When this

is the case, you can write the output function as a function file and call the optimization function directly from the command line. However, if you want your output function to record data from one iteration to the next, you should 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, although you could also write the objective function as a separate file or as an anonymous function.

Since the nested function has access to variables in the file that contains it, 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 points generated by fminsearch in solving the optimization problem

$$\min_{x} f(x) = \min_{x} e^{x_1} \left( 4x_1^2 + 2x_2^2 + x_1x_2 + 2x_2 \right).$$

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)
```

```
\label{eq:z} \begin{array}{ll} z &=& \exp(x(1))^*(4^*x(1)^2 + 2^*x(2)^2 + x(1)^*x(2) + 2^*x(2));\\ \text{end} \\ \end{array} end
```

- **3** Save the file as myproblem.m in a directory 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 all three optimization functions, fminbnd, fminsearch, and fzero.

The "Command-Line Display Headings" column of the table lists the headings, corresponding to the optimValues fields that are displayed at the command line 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 interrupt the current iteration of the optimization. You might want the output function to do this to improve the efficiency of the computations. When state is set to 'interrupt', the values of x and <code>OptimValues</code> are the same as at the last call to the output function, in which <code>state</code> 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 might use 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 should quit or continue. 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 make the output function stop an optimization when a user clicks a **Stop** button. The following code shows how to do this, assuming 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');
```

# **Plot Functions**

#### In this section...

"What Is A Plot Function?" on page 9-25

"Example: Plot Function" on page 9-25

#### 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 while the algorithm executes. 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 "Output Functions" on page 9-17.

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

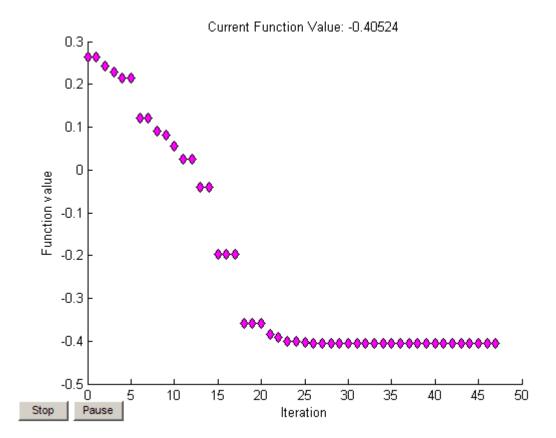
# **Example: Plot Function**

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 = 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
    ffinal =
       -0.4052
```



# **Troubleshooting and Tips**

Here is a list of typical problems and recommendations for dealing with them.

Problem	Recommendation
The solution found by fminbnd or fminsearch does not appear to be a global minimum.	There is no guarantee that you have a global minimum unless your problem is continuous and has only one minimum. Starting the optimization from a number of different starting points (or intervals in the case of fminbnd) may help to locate the global minimum or verify that there is only one minimum. Use different methods, where possible, to verify results.
Sometimes an optimization problem has values of X for which it is impossible to evaluate f.	Modify your function to include a penalty function to give a large positive value to f when infeasibility is encountered.
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).	Your objective function (fun) may be returning NaN or complex values. The optimization routines expect only real numbers to be returned. Any other values may cause unexpected results. To determine whether this is the case, set  options = optimset('FunValCheck', 'on')  and call the optimization function with options as an input argument. This displays an error when the objective function returns NaN or complex values.

Optimization problems may take many iterations to converge. Most optimization problems benefit from good starting guesses. Providing good starting guesses improves the execution efficiency and may help locate the global minimum instead of a local minimum.

Sophisticated problems are best solved by an evolutionary approach, whereby a problem with a smaller number of independent variables is solved first. Solutions from lower order problems can generally be used as starting points for higher order problems by using an appropriate mapping.

The use of simpler cost functions and less stringent termination criteria in the early stages of an optimization problem can also reduce computation time. Such an approach often produces superior results by avoiding local minima.

# **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 cubicpoly.m 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);
```

#### More About

- "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 11-13
- "ODE Event Location" on page 11-15
- "Solve Nonstiff ODEs" on page 11-22
- "Solve Stiff ODEs" on page 11-28
- "Solve Differential Algebraic Equations (DAEs)" on page 11-36
- "Nonnegative ODE Solution" on page 11-43
- "Troubleshoot Common ODE Problems" on page 11-47

# **Choose an ODE Solver**

#### In this section...

"Ordinary Differential Equations" on page 11-2

"Types of ODEs" on page 11-3

"Systems of ODEs" on page 11-3

"Higher-Order ODEs" on page 11-4

"Complex ODEs" on page 11-5

"Basic Solver Selection" on page 11-6

"Summary of ODE Examples and Files" on page 11-9

# **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;
```

# **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

$$y_1 = y$$

$$y_2 = y'$$

$$y_3 = y''$$

$$\vdots$$

$$y_n = y^{(n-1)}$$

The result of these substitutions is a system of *n* first-order equations

$$\begin{cases} y'_1 = y_2 \\ y'_2 = y_3 \\ \vdots \\ y'_n = f(t, y_1, y_2, ..., y_n). \end{cases}$$

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

$$\begin{cases} y'_1 = y_2 \\ y'_2 = y_3 \\ y'_3 = y_1 y_3 - 1. \end{cases}$$

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

$$yv = [\text{Real}(y) \text{ Imag}(y)]$$
$$fv = [\text{Real}(f(t, y)) \text{ Imag}(f(t, y))].$$

For example, if the ODE is y' = yt + 2i, then you can represent the equation using a function file.

```
function f = complexf(t,y)
% Define function that takes and returns complex values
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)];
```

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.

```
y0 = 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 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		Medium	Most of the time. ode45 should be the first solver you try.
ode23	Nonstiff	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.
ode15s	Stiff	Low to Medium	Try ode15s when ode45 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.

Solver	Problem Type	Accuracy	When to Use
			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.

Solver	Problem Type	Accuracy	When to Use
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.

Example File	Solver Used	Options Specified	Description	Documentation Link
amp1da	ode23t	• 'Mass'	Stiff DAE — electrical circuit with constant, singular mass matrix	"Solve Stiff Differential Algebraic Equation"
ballod	ode23	<ul><li>'Events'</li><li>'OutputFcn'</li><li>'OutputSel'</li><li>'Refine'</li></ul>	Simple event location — bouncing ball	"ODE Event Location" on page 11-15

Example File	Solver Used	Options Specified	Description	Documentation Link
		• 'InitialStep'		
		<ul><li>'MaxStep'</li></ul>		
batono	ode45	· 'Mass'	ODE with time- and state-dependent mass matrix — motion of a baton	
brusso	ode15s	<ul><li>'JPattern'</li><li>'Vectorized'</li></ul>	Stiff large problem — diffusion in a chemical reaction (the Brusselator)	"Solve Stiff ODEs" on page 11-28
burger	ode15s	<ul><li>'Mass'</li><li>'MStateDependence</li><li>'JPattern'</li><li>'MvPattern'</li><li>'RelTol'</li><li>'AbsTol'</li></ul>	ODE with strongly state-dependent mass matrix — Burgers' equation solved using a moving mesh technique	
fem1od	ode15s	<ul><li>'Mass'</li><li>'MStateDependenc</li><li>'Jacobian'</li></ul>	Stiff problem with a time-dependent mass matrix — finite element method	_
fem2od	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	<ul><li>'Mass'</li><li>'RelTol'</li><li>'AbsTol'</li><li>'Vectorized'</li></ul>	Stiff, linearly implicit DAE from a conservation law — Robertson chemical reaction	"Solve Robertson Problem as Semi-Explicit Differential Algebraic Equations (DAEs)"

Example File	Solver Used	Options Specified	Description	Documentation Link
ihb1da	ode15i	<ul><li>'RelTol'</li><li>'AbsTol'</li><li>'Jacobian'</li></ul>	Stiff, fully implicit DAE  — Robertson chemical reaction	"Solve Robertson Problem as Implicit Differential Algebraic Equations (DAEs)"
iburge	ode15i	<ul><li>'RelTol'</li><li>'AbsTol'</li><li>'Jacobian'</li><li>'JPattern'</li></ul>	Implicit ODE system — Burgers' equation	
kneeod	ode15s	• 'NonNegative'	The "knee problem" with nonnegativity constraints	"Nonnegative ODE Solution" on page 11-43
orbito	ode45	<ul><li>'RelTol'</li><li>'AbsTol'</li><li>'Events'</li><li>'OutputFcn'</li></ul>	Advanced event location — restricted three body problem	"ODE Event Location" on page 11-15
rigido	ode45	_	Nonstiff problem — Euler equations of a rigid body without external forces	"Solve Nonstiff ODEs" on page 11-22
vdpode	ode15s	• 'Jacobian'	Parameterizable van der Pol equation (stiff for large $\mu$ )	"Solve Stiff ODEs" on page 11-28

# **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 11-22
- "Solve Stiff ODEs" on page 11-28
- "Solve Differential Algebraic Equations (DAEs)" on page 11-36

#### **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. Use the odeset function to create an options structure that you then pass to the solver. The odeget function queries the value of an option in an existing structure, which can be used to dynamically change option values based on conditions.

This table summarizes the compatibility of each option with the different solvers.

Option	ode45	ode23	ode113	ode15s	ode23s	ode23t	ode23tb	ode15i
RelTol AbsTol NormCon	√	V	√	√	√	V	V	V
OutputF OutputS Refine Stats		V	V	V	V	V	V	V
NonNega	√	√	√	√ *	_	√ *	√*	_
Events	√	√	√	√	√	√	√	√**
MaxStep Initial		√	√	√	√	√	√	<b>V</b>
Jacobia JPatter Vectori	_	_	_	√	√	<b>V</b>	V	√
Mass MStateD MvPatte MassSin		\frac{\frac{1}{\sqrt{1}}}{}	\ \ -	\ \ \ \	<del>-</del>	\ \ \ \	\ \ \ \ -	_ _ _ _
Initial	_	_	_	√	_	√	_	_
MaxOrde BDF	_	_	_	√	_	_	_	<del>\</del>

**Note:** \* — You can 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.

# **See Also**

odeget | odeset

#### **More About**

- "Choose an ODE Solver" on page 11-2
- "ODE Event Location" on page 11-15
- "Nonnegative ODE Solution" on page 11-43

## **ODE Event Location**

#### In this section...

"What is Event Location?" on page 11-15

"Writing an Event Function" on page 11-15

"Event Information" on page 11-16

"Limitations" on page 11-17

"Simple Event Location: A Bouncing Ball" on page 11-17

"Advanced Event Location: Restricted Three Body Problem" on page 11-18

#### 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
```

# **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.
- · ye 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

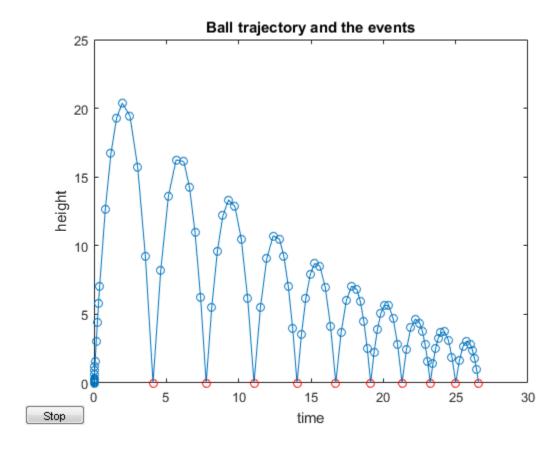
```
y'_1 = y_2

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

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 <code>orbitode</code> 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

$$\begin{array}{ll} y_1' &= y_3 \\ y_2' &= y_4 \\ y_3' &= 2y_4 + y_1 - \frac{\mu^*(y_1 + \mu)}{r_1^3} - \frac{\mu(y_1 - \mu^*)}{r_2^3} \\ y_4' &= -2y_3 + y_2 - \frac{\mu^* y_2}{r_2^3} - \frac{\mu y_2}{r_2^3}, \end{array}$$

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 <code>orbitode.m</code> 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)
% 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
```

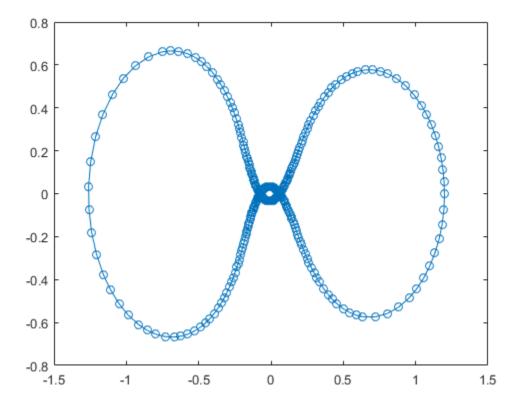
Type orbitode to run the example.

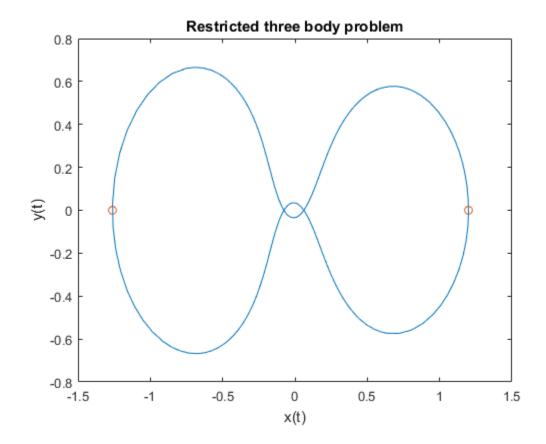
orbitode

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 odeget | odeset

# **More About**

- "Choose an ODE Solver" on page 11-2
- "Summary of ODE Options" on page 11-13
- "Parameterizing Functions" on page 10-2

# **Solve Nonstiff ODEs**

This page contains two examples of solving nonstiff ordinary differential equations using ode45. MATLAB® has three solvers for nonstiff ODEs.

- ode45
- ode23
- 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 stringent error tolerances.

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" for more information.

#### **Example: Nonstiff van der Pol Equation**

The van der Pol equation is a second order ODE

$$y_1'' - \mu (1 - y_1^2) y_1' + y_1 = 0,$$

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.

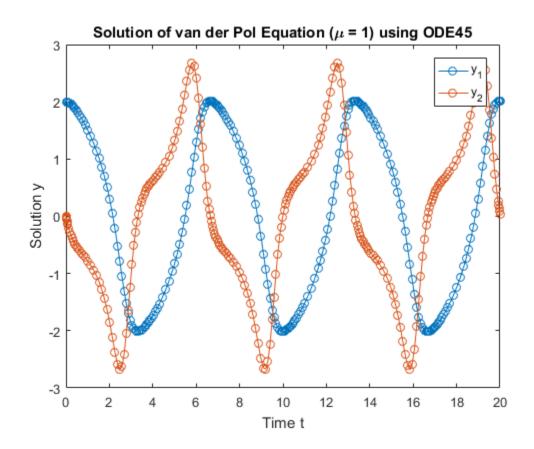
The function file vdp1.m codes the van der Pol equation using  $\mu = 1$ . The variables  $y_1$  and  $y_2$  are represented by y(1) and y(2), and the two-element column vector dydt contains the expressions for  $y_1$  and  $y_2$ .

```
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  $y_1$ , and the second column to  $y_2$ .

```
[t,y] = ode45(@vdp1,[0 20],[2; 0]);
Plot the solutions for $\mathcal{Y}$1 and $\mathcal{Y}$2 against t.

plot(t,y(:,1),'-o',t,y(:,2),'-o')
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  $\mu$ . The van der Pol equations become stiff as  $\mu$  increases. For example, with the value  $\mu=1000$  you 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.
```

function rigidode

function dydt = f(t,y)

-0.51\*y(1)\*y(2) ];

-y(1)\*y(3)

y(2)\*y(3)

dydt = [

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.

%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.

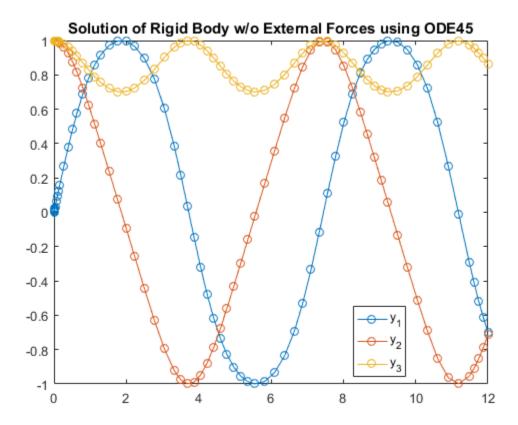
Mark W. Reichelt and Lawrence F. Shampine, 3-23-94, 4-19-94 Copyright 1984-2014 The MathWorks, Inc.

tspan = [0 12];
y0 = [0; 1; 1];

solve the problem using ODE45 figure; ode45(@f,tspan,y0);
```

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 ode113 | ode23 | ode45

# **More About**

• "Choose an ODE Solver" on page 11-2

• "Parameterizing Functions" on page 10-2

# **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 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  $\partial f_i/\partial y_j$  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

$$y_1'' - \mu (1 - y_1^2) y_1' + y_1 = 0,$$

where  $\mu \geq 0$  is a scalar parameter. When  $\mu = 1$ , the resulting system of ODEs is nonstiff and easily solved using ode45. However, if you increase  $\mu$  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

$$\begin{array}{ll} y_1' &= y_2 \\ y_2' &= \mu (1 - y_1^2) y_2 - y_1. \end{array}$$

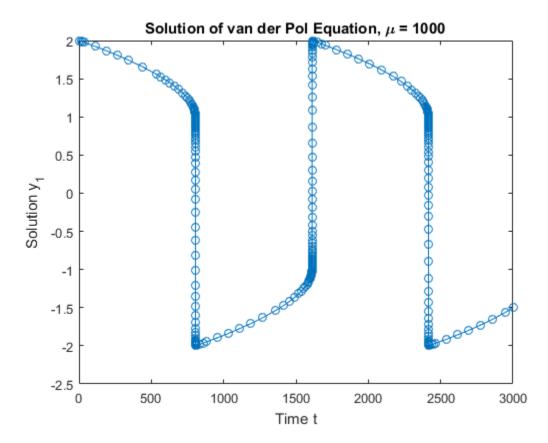
The vdp1000 function evaluates the van der Pol equation using  $\mu = 1000$ .

```
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  $\mu$ . The equations become increasingly stiff as  $\mu$  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  $N \ge 2$ , 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 >= 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

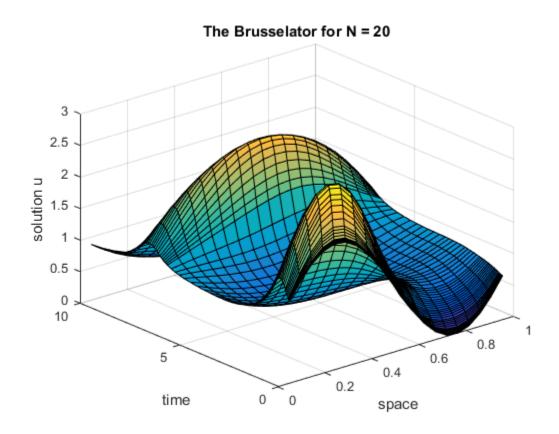
sparse matrix. Providing a sparsity pattern can significantly reduce the

```
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
  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
```

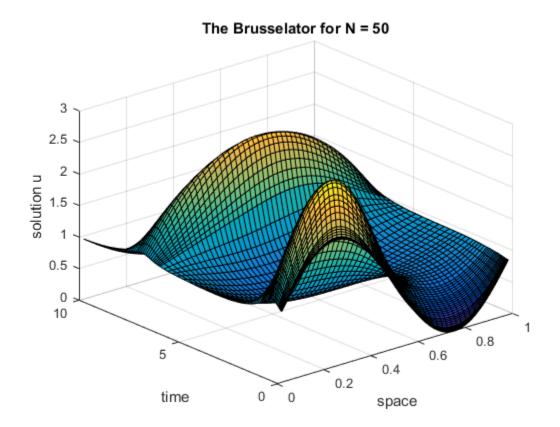
```
c = 0.02 * (N+1)^2;
      dydt = zeros(2*N,size(y,2)); % preallocate dy/dt
      % Evaluate the 2 components of the function at one edge of the grid
      % (with edge conditions).
      i = 1;
      dydt(i,:) = 1 + y(i+1,:).*y(i,:).^2 - 4*y(i,:) + c*(1-2*y(i,:)+y(i+2,:));
      dydt(i+1,:) = 3*y(i,:) - 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;
      dydt(i,:) = 1 + y(i+1,:).*y(i,:).^2 - 4*y(i,:) + c*(y(i-2,:)-2*y(i,:)+1);
      dydt(i+1,:) = 3*v(i,:) - v(i+1,:).*v(i,:).^2 + c*(v(i-1,:)-2*v(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);
end
```

Solve the Brusselator system for N=20 by running the function brussode.

brussode



Solve the system for  $N=50\,\mathrm{by}$  specifying an input to brussode.  $\mathrm{brussode}(50)$ 



# **See Also**

ode15s | ode23s | ode23t | ode23tb

# **More About**

- "Choose an ODE Solver" on page 11-2
- "Summary of ODE Options" on page 11-13
- "Parameterizing Functions" on page 10-2

# Solve Differential Algebraic Equations (DAEs)

#### In this section...

"What is a Differential Algebraic Equation?" on page 11-36

"Consistent Initial Conditions" on page 11-37

"Differential Index" on page 11-38

"Solve Robertson Problem as Semi-Explicit Differential Algebraic Equations (DAEs)" on page 11-39

# 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 forms:

• 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 guess 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

$$y(t) = k(t)$$
.

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 "Check and Reduce Differential Index" for more information.

# 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

$$\begin{array}{ll} y_1' &= -0.04y_1 + 10^4 y_2 y_3 \\ y_2' &= 0.04y_1 - 10^4 y_2 y_3 - (3 \times 10^7) y_2^2 \\ y_3' &= (3 \times 10^7) y_2^2. \end{array}$$

hb1ode 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  $y_3$ . 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 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 hbldae.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.

$$\left(\begin{array}{c} y_1' \\ y_2' \\ 0 \end{array}\right) = My' \to M = \left(\begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{array}\right)$$

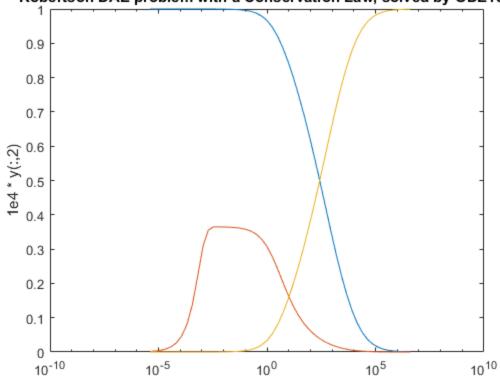
- Set the relative error tolerance to 1e-4.
- Use an absolute tolerance of 1e-10 for the second solution component, since the scale varies dramatically from the other components.
- Leave the 'MassSingular' option at its default value 'maybe' to test the automatic detection of a DAE.

```
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');
```





# **See Also**

ode15i | ode15s | ode23t | odeset

### **More About**

- "Choose an ODE Solver" on page 11-2
- "Summary of ODE Options" on page 11-13
- "Equation Solving"

# **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.

### **Example: Absolute Value Function**

Consider the initial value problem

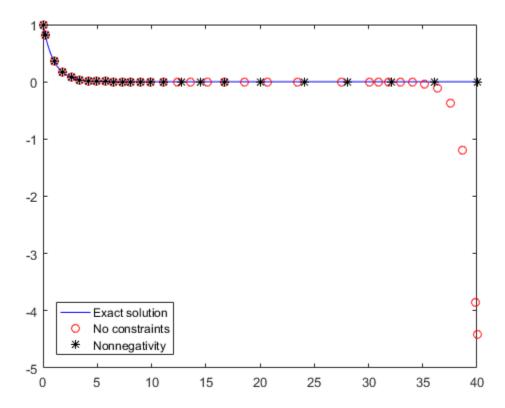
$$y' = -|y|,$$

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**

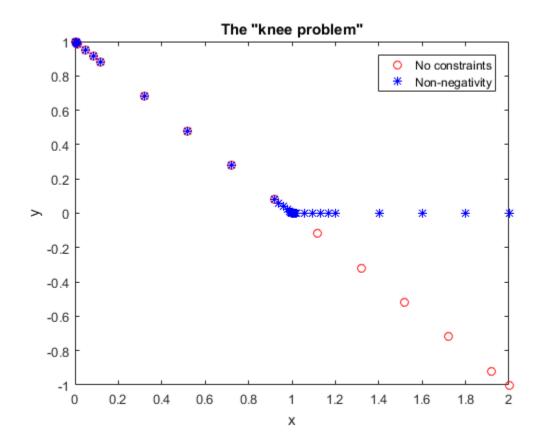
Another example of a problem that requires a nonnegative solution is the *knee problem* coded in the example file kneeode. The equation is

$$\epsilon y' = (1 - x)y - y^2,$$

solved on the interval [0,2] with the initial condition y(0)=1. The parameter  $\epsilon$  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-x for 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('v')
```



### 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 11-13

# **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
	e(i)  ≤ max(RelTol*abs(y(i)),AbsTol(i))
	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

Question or Problem	Answer
	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

Question or Problem	Answer
	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.

Question or Problem	Answer
My plots are not smooth enough.	Increase the value of Refine from its default of 4 in ode45 or 1 in the other solvers. The bigger the value of Refine, the more output points the solver generates. Execution speed is not affected much by the value of Refine.
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 globals, or calculate them once and pass them to nested functions.
I know that the solution undergoes a radical change at time t, where to <= 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**

deval | odeget | odeset | odextend

# More About

- "Choose an ODE Solver" on page 11-2
- "Summary of ODE Options" on page 11-13
- "ODE Event Location" on page 11-15
- "Nonnegative ODE Solution" on page 11-43

# **Boundary Value Problems (BVPs)**

# **Boundary-Value Problems**

### In this section...

"Function Summary" on page 12-2

"Boundary Value Problems" on page 12-3

"BVP Solver" on page 12-3

"Integrator Options" on page 12-6

"Examples" on page 12-7

# **Function Summary**

- "BVP Solver" on page 12-2
- "BVP Helper Functions" on page 12-2
- "BVP Solver Options" on page 12-2

#### **BVP Solver**

Solver	Description
bvp4c	Solve boundary value problems for ordinary differential equations.
bvp5c	Solve boundary value problems for ordinary differential equations.

### **BVP Helper Functions**

Function	Description
bvpinit	Form the initial guess for bvp4c.
deval	Evaluate the numerical solution using the output of bvp4c.

### **BVP Solver Options**

An options structure contains named properties whose values are passed to bvp4c, and which affect problem solution. Use these functions to create, alter, or access an options structure.

Function	Description
bvpset	Create/alter the BVP options structure.

Function	Description
bvpget	Extract properties from options structure created with bvpset.

# **Boundary Value Problems**

The BVP solver is designed to handle systems of ordinary differential equations y' = f(x, y)

where x is the independent variable, y is the dependent variable, and y' represents the derivative of y with respect to  $x \, dy/dx$ .

See "Choose an ODE Solver" on page 11-2 for general information about ODEs.

### **Boundary Conditions**

In a boundary value problem, the solution of interest satisfies certain boundary conditions. These conditions specify a relationship between the values of the solution at more than one x. In its basic syntax, bvp4c is designed to solve two-point BVPs, i.e., problems where the solution sought on an interval [a, b] must satisfy the boundary conditions

$$g(y(a), y(b)) = 0$$

Unlike initial value problems, a boundary value problem may not have a solution, may have a finite number of solutions, or may have infinitely many solutions. As an integral part of the process of solving a BVP, you need to provide a guess for the required solution. The quality of this guess can be critical for the solver performance and even for a successful computation.

There may be other difficulties when solving BVPs, such as problems imposed on infinite intervals or problems that involve singular coefficients. Often BVPs involve unknown parameters p that have to be determined as part of solving the problem

$$y' = f(x, y, p)$$
  
 
$$g(y(a), y(b), p) = 0$$

In this case, the boundary conditions must suffice to determine the value of p.

# **BVP Solver**

- "The BVP Solver" on page 12-4
- "BVP Solver Syntax" on page 12-4

"BVP Solver Options" on page 12-6

#### The BVP Solver

The function bvp4c solves two-point boundary value problems for ordinary differential equations (ODEs). It integrates a system of first-order ordinary differential equations y' = f(x, y)

on the interval [a, b], subject to general two-point boundary conditions bc(y(a), y(b)) = 0

It can also accommodate other types of BVP problems, such as those that have any of the following:

- Unknown parameters
- · Singularities in the solutions
- Multipoint conditions

In this case, the number of boundary conditions must be sufficient to determine the solution and the unknown parameters.

bvp4c produces a solution that is continuous on [a,b] and has a continuous first derivative there. You can use the function deval and the output of bvp4c to evaluate the solution at specific points on the interval of integration.

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, the solver adapts the mesh and repeats the process. The user *must* provide the points of the initial mesh as well as an initial approximation of the solution at the mesh points.

### **BVP Solver Syntax**

The basic syntax of the BVP solver is

sol = bvp4c(odefun,bcfun,solinit)

The input arguments are

odefun

A function handle that evaluates the differential equations. It has the basic form

dydx = odefun(x,y)

where x is a scalar, and dydx and y are column vectors. Odefun can also accept a vector of unknown parameters and a variable number of known parameters, (see "BVP Solver Options" on page 12-6).

bcfun

Handle to a function that evaluates the residual in the boundary conditions. It has the basic form

res = bcfun(ya,yb)

where ya and yb are column vectors representing y(a) and y(b), and res is a column vector of the residual in satisfying the boundary conditions. bcfun can also accept a vector of unknown parameters and a variable number of known parameters, (see "BVP Solver Options" on page 12-6).

solinit

Structure with fields x and y:

Ordered nodes of the initial mesh. Boundary conditions are imposed at a = solinit.x(1) and b = solinit.x(end).

y Initial guess for the solution with solinit.y(:,i) a guess for the solution at the node solinit.x(i).

The structure can have any name, but the fields must be named X and y. It can also contain a vector that provides an initial guess for unknown parameters. You can form solinit with the helper function bypinit. See the bypinit reference page for details.

The output argument sol is a structure created by the solver. In the basic case the structure has fields x, y, yp, and solver.

sol.x	Nodes of the mesh selected by bvp4c
sol.y	Approximation to $y(x)$ at the mesh points of sol.x
sol.yp	Approximation to $y'(x)$ at the mesh points of sol.x

```
sol.solver 'bvp4c'
```

The structure **sol** returned by **bvp4c** contains an additional field if the problem involves unknown parameters:

sol.parameters Value of unknown parameters, if present, found by the solver.

The function deval uses the output structure sol to evaluate the numerical solution at any point from [a,b].

### **BVP Solver Options**

For more advanced applications, you can specify solver options by passing an input argument options.

options	Structure of optional parameters that change the default integration properties. This is the fourth input argument.
	sol = bvp4c(odefun,bcfun,solinit,options)
	You can create the structure options using the function bvpset. The bvpset reference page describes the properties you can specify.

# **Integrator Options**

The default integration properties in the BVP solver bvp4c are selected to handle common problems. In some cases, you can improve solver performance by overriding these defaults. You do this by supplying bvp4c with an options structure that specifies one or more property values.

For example, to change the value of the relative error tolerance of bvp4c from the default value of 1e-3 to 1e-4,

1 Create an options structure using the function bypset by entering

```
options = bvpset('RelTol', 1e-4);
```

2 Pass the options structure to bvp4c as follows:

```
sol = bvp4c(odefun,bcfun,solinit,options)
```

For a complete description of the available options, see the reference page for bvpset.

# **Examples**

- "Mathieu's Equation" on page 12-7
- "Continuation" on page 12-11
- "Singular BVPs" on page 12-19
- "Multipoint BVPs" on page 12-23
- · "Additional Examples" on page 12-27

## Mathieu's Equation

- "Solving the Problem" on page 12-7
- "Finding Unknown Parameters" on page 12-10
- "Evaluating the Solution" on page 12-11

## Solving the Problem

This example determines the fourth eigenvalue of Mathieu's Equation. It illustrates how to write second-order differential equations as a system of two first-order ODEs and how to use bvp4c to determine an unknown parameter  $\lambda$ .

The task is to compute the fourth (q = 5) eigenvalue lambda  $\lambda$  of Mathieu's equation  $y'' + (\lambda - 2 q \cos 2x)y = 0$ 

Because the unknown parameter  $\lambda$  is present, this second-order differential equation is subject to *three* boundary conditions

y(0) = 1

y'(0) = 0

 $y'(\Pi) = 0$ 

**Note:** The file, mat4bvp.m, contains the complete code for this example. All the functions required by bvp4c are coded in this file as nested or local functions. To see the code in an editor, type edit mat4bvp at the command line. To run it, type mat4bvp at the command line.

**Rewrite the problem as a first-order system.** To use bvp4c, you must rewrite the equations as an equivalent system of first-order differential equations. Using a substitution  $y_1 = y$  and  $y_2 = y'$ , the differential equation is written as a system of two first-order equations

$$y_1' = y_2$$

```
y_2' = -(\lambda - 2q \cos 2x)y_1
```

Note that the differential equations depend on the unknown parameter  $\lambda$ . The boundary conditions become

```
y_1(0) - 1 = 0
y_2(0) = 0
y_2(\Pi) = 0
```

2 Code the system of first-order ODEs. Once you represent the equation as a firstorder system, you can code it as a function that bvp4c can use. Because there is an unknown parameter, the function must be of the form

```
dydx = odefun(x,y,parameters)
```

The following code represents the system in the function, mat4ode. Variable q is shared with the outer function:

```
function dydx = mat4ode(x,y,lambda)
dydx = [y(2)
         -(lambda - 2*q*cos(2*x))*y(1)];
      % End nested function mat4ode
```

3 Code the boundary conditions function. You must also code the boundary conditions in a function. Because there is an unknown parameter, the function must be of the form

```
res = bcfun(ya,yb,parameters)
```

The code below represents the boundary conditions in the function, mat4bc.

```
function res = mat4bc(ya,yb,lambda)
res = [ya(2)]
         yb(2)
       ya(1)-1];
```

4 Create an initial guess. To form the guess structure solinit with bypinit, you need to provide initial guesses for both the solution and the unknown parameter.

The function mat4init provides an initial guess for the solution. mat4init uses y  $=\cos 4x$  because this function satisfies the boundary conditions and has the correct qualitative behavior (the correct number of sign changes).

```
function yinit = mat4init(x)
vinit = [cos(4*x)]
          -4*sin(4*x) ];
```

In the call to bvpinit, the third argument, lambda, provides an initial guess for the unknown parameter  $\lambda$ .

```
lambda = 15;
solinit = bvpinit(linspace(0,pi,10),@mat4init,lambda);
```

This example uses the @ symbol to pass mat4init as a function handle to bvpinit.

5 Apply the BVP solver. The mat4bvp example calls bvp4c with the functions mat4ode and mat4bc and the structure solinit created with bvpinit.

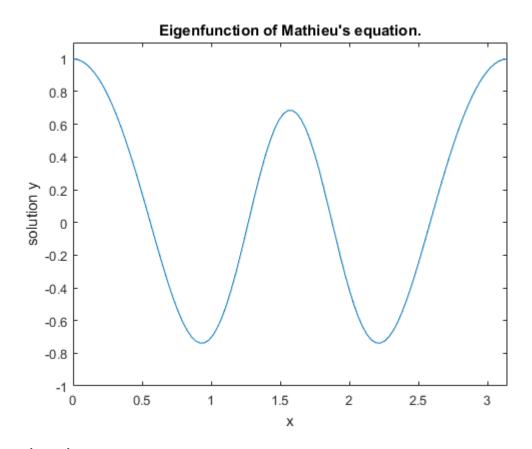
```
sol = bvp4c(@mat4ode,@mat4bc,solinit);
```

- **6** View the results. Complete the example by displaying the results:
  - **a** Print the value of the unknown parameter  $\lambda$  found by bvp4c.

**b** Use deval to evaluate the numerical solution at 100 equally spaced points in the interval  $[0, \pi]$ , and plot its first component. This component approximates y(x).

```
xint = linspace(0,pi);
Sxint = deval(sol,xint);
plot(xint,Sxint(1,:))
axis([0 pi -1 1.1])
title('Eigenfunction of Mathieu''s equation.')
xlabel('x')
ylabel('solution y')
```

The following plot shows the eigenfunction associated with the final eigenvalue  $\lambda = 17.097$ .



## **Finding Unknown Parameters**

The bvp4c solver can find unknown parameters p for problems of the form y' = f(x,y,p) bc(y(a), y(b),p) = 0

You must provide bvp4c an initial guess for any unknown parameters in the vector solinit.parameters. When you call bvpinit to create the structure solinit, specify the initial guess as a vector in the additional argument parameters.

solinit = bvpinit(x,v,parameters)

The bvp4c function arguments odefun and bcfun must each have a third argument.

```
dydx = odefun(x,y,parameters)
res = bcfun(ya,yb,parameters)
```

While solving the differential equations, bvp4c adjusts the value of unknown parameters to satisfy the boundary conditions. The solver returns the final values of these unknown parameters in sol.parameters.

#### **Evaluating the Solution**

The collocation method implemented in bvp4c produces a  $C^1$ -continuous solution over the whole 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 bvp4c.

```
Sxint = deval(sol,xint)
```

The deval function is vectorized. For a vector xint, the ith column of Sxint approximates the solution y(xint(i)).

#### Continuation

- "Introduction" on page 12-11
- "Using Continuation to Solve a BVP" on page 12-11
- "Using Continuation to Verify Consistency" on page 12-14

#### Introduction

To solve a boundary value problem, you need to provide an initial guess for the solution. The quality of your initial guess can be critical to the solver performance, and to being able to solve the problem at all. However, coming up with a sufficiently good guess can be the most challenging part of solving a boundary value problem. Certainly, you should apply the knowledge of the problem's physical origin. Often a problem can be solved as a sequence of relatively simpler problems, i.e., a *continuation*.

This example shows how to use continuation to:

- Solve a difficult BVP
- Verify a solution's consistent behavior

#### Using Continuation to Solve a BVP

This example solves the differential equation  $\varepsilon y'' + xy' = \varepsilon \pi^2 \cos(\pi x) - \pi x \sin(\pi x)$ 

for  $\varepsilon = 10^{-4}$ , on the interval [-1 1], with boundary conditions y(-1) = -2 and y(1) = 0. For  $0 < \varepsilon < 1$ , the solution has a transition layer at x = 0. Because of this rapid change in the solution for small values of  $\varepsilon$ , the problem becomes difficult to solve numerically.

The example solves the problem as a sequence of relatively simpler problems, i.e., a continuation. The solution of one problem is used as the initial guess for solving the next problem.

**Note:** The file, shockbvp.m, contains the complete code for this example. All required functions are coded as nested functions in this file. To see the code in an editor, type edit shockbvp at the command line. To run it, type shockbvp at the command line.

**Note:** This problem appears in [1] to illustrate the mesh selection capability of a well established BVP code COLSYS.

1 Code the ODE and boundary condition functions. Code the differential equation and the boundary conditions as functions that bvp4c can use:

The code below represents the differential equation and the boundary conditions in the functions shockODE and shockBC. Note that shockODE is vectorized to improve solver performance. The additional parameter  $\epsilon$  is represented by e and is shared with the outer function.

**Provide analytical partial derivatives.** For this problem, the solver benefits from using analytical partial derivatives. The code below represents the derivatives in functions shockJac and shockBCJac.

```
function jac = shockJac(x,y)
jac = [ 0     1
```

shockJac shares **e** with the outer function.

Tell bvp4c to use these functions to evaluate the partial derivatives by setting the options FJacobian and BCJacobian. Also set 'Vectorized' to 'on' to indicate that the differential equation function ShockODE is vectorized.

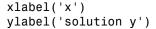
**3 Create an initial guess.** You must provide bvp4c with a guess structure that contains an initial mesh and a guess for values of the solution at the mesh points. A constant guess of  $y(x) \equiv 1$  and  $y'(x) \equiv 0$ , and a mesh of five equally spaced points on  $[-1\ 1]$  suffice to solve the problem for  $\varepsilon = 10^{-2}$ . Use bvpinit to form the guess structure.

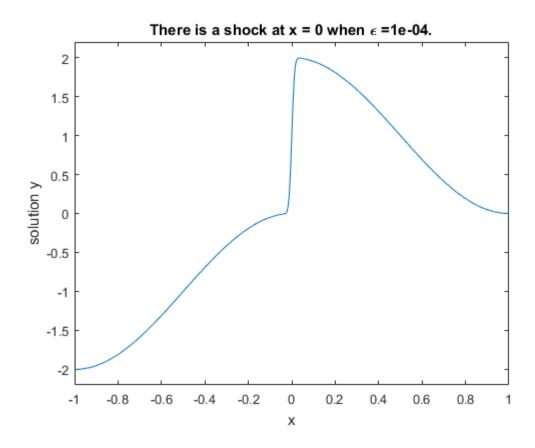
```
sol = bvpinit([-1 -0.5 0 0.5 1],[1 0]);
```

**4 Use continuation to solve the problem.** To obtain the solution for the parameter  $\varepsilon = 10^{-4}$ , the example uses continuation by solving a sequence of problems for  $\varepsilon = 10^{-2}$ ,  $10^{-3}$ ,  $10^{-4}$ . The solver bvp4c does not perform continuation automatically, but the code's user interface has been designed to make continuation easy. The code uses the output sol that bvp4c produces for one value of  $\mathbf{e}$  as the guess in the next iteration.

```
e = 0.1;
for i=2:4
    e = e/10;
    sol = bvp4c(@shockODE,@shockBC,sol,options);
end
```

**5 View the results.** Complete the example by displaying the final solution





## **Using Continuation to Verify Consistency**

Falkner-Skan BVPs arise from similarity solutions of viscous, incompressible, laminar flow over a flat plate. An example is

$$f''' + ff'' + \beta(1 - (f')^2) = 0$$

for  $\beta = 0.5$  on the interval  $[0, \infty]$  with boundary conditions f(0) = 0, f'(0) = 0, and  $f'(\infty) = 1$ .

The BVP cannot be solved on an infinite interval, and it would be impractical to solve it for even a very large finite interval. So, the example tries to solve a sequence of problems

posed on increasingly larger intervals to verify the solution's consistent behavior as the boundary approaches  $\infty$ .

The example imposes the infinite boundary condition at a finite point called infinity. The example then uses continuation in this end point to get convergence for increasingly larger values of infinity. It uses bypinit to extrapolate the solution sol for one value of infinity as an initial guess for the new value of infinity. The plot of each successive solution is superimposed over those of previous solutions so they can easily be compared for consistency.

**Note:** The file, fsbvp.m, contains the complete code for this example. All required functions are coded as nested functions in this file. To see the code in an editor, type edit fsbvp at the command line. To run it, type fsbvp at the command line.

1 Code the ODE and boundary condition functions. Code the differential equation and the boundary conditions as functions that bvp4c can use. The problem parameter beta is shared with the outer function.

**2** Create an initial guess. You must provide bvp4c with a guess structure that contains an initial mesh and a guess for values of the solution at the mesh points. A crude mesh of five points and a constant guess that satisfies the boundary conditions are good enough to get convergence when infinity = 3.

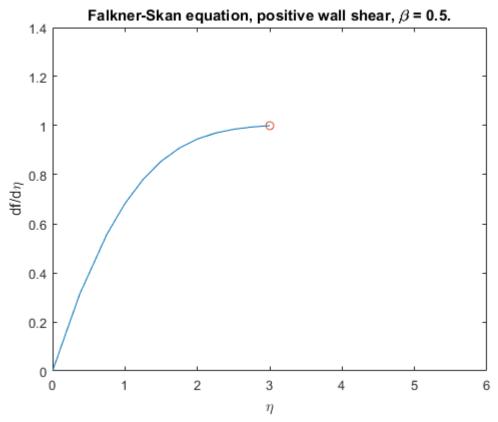
```
infinity = 3;
maxinfinity = 6;
solinit = bvpinit(linspace(0,infinity,5),[0 0 1]);
```

ylabel('df/d\eta')

hold on drawnow shg

**Solve on the initial interval.** The example obtains the solution for infinity = 3. It then prints the computed value of f''(0) for comparison with the value reported by Cebeci and Keller [2]:

```
sol = bvp4c(@fsode,@fsbc,solinit);
eta = sol.x;
f = sol.y;
fprintf('\n');
fprintf('Cebeci & Keller report that f''''(0) = 0.92768.\n')
fprintf('Value computed using infinity = %g is %7.5f.\n', ...
         infinity, f(3,1)
The example prints
Cebeci & Keller report that f''(0) = 0.92768.
Value computed using infinity = 3 is 0.92915.
Setup the figure and plot the initial solution.
figure
plot(eta, f(2,:), eta(end), f(2, end), 'o');
axis([0 maxinfinity 0 1.4]);
title('Falkner-Skan equation, positive wall shear, \beta = 0.5.')
xlabel('\eta')
```

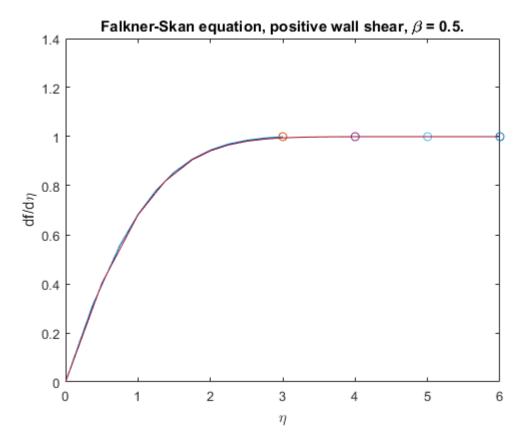


5 Use continuation to solve the problem and plot subsequent solutions. The example then solves the problem for infinity = 4, 5, 6. It uses bypinit to extrapolate the solution sol for one value of infinity as an initial guess for the next value of infinity. For each iteration, the example prints the computed value of f''(0) and superimposes a plot of the solution in the existing figure.

```
for Bnew = infinity+1:maxinfinity

solinit = bvpinit(sol,[0 Bnew]); % Extend solution to Bnew.
sol = bvp4c(@fsode,@fsbc,solinit);
eta = sol.x;
f = sol.y;
```

Note that the values approach 0.92768 as reported by Cebeci and Keller. The superimposed plots confirm the consistency of the solution's behavior.



## Singular BVPs

- "Introduction" on page 12-19
- "Emden's equation" on page 12-20

## Introduction

The function bvp4c solves a class of singular BVPs of the form

$$y' = \frac{1}{x}Sy + f(x, y)$$
$$0 = g(y(0), y(b))$$

It 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 byp4c as the value of the 'SingularTerm' integration property. Boundary conditions at x = 0 must be consistent with the necessary condition for a smooth solution, Sy(0) = 0. An initial guess should also satisfy this necessary condition.

When you solve a singular BVP using

sol = bvp4c(@odefun,@bcfun,solinit,options)

bvp4c requires that your function odefun(x,y) return only the value of the f(x, y) term in Equation 5-2.

#### **Emden's equation**

Emden's equation arises in modeling a spherical body of gas. The PDE of the model is reduced by symmetry to the ODE

$$y'' + \frac{2}{x}y' + y^5 = 0$$

on an interval [0,1]. The coefficient 2/x is singular at x = 0, but symmetry implies the boundary condition y'(0) = 0. With this boundary condition, the term

$$\frac{2}{x}y'(0)$$

is well-defined as x approaches 0. For the boundary condition  $\sqrt{y(1)}=\sqrt{3/\sqrt{2}}$  , this BVP has the analytical solution

$$y(x) = \left(1 + \frac{x^2}{3}\right)^{-1/2}$$

**Note:** The file, emdenbyp.m, contains the complete code for this example. It contains all the required functions coded as local functions. To see the code in an editor, type edit emdenbyp at the command line. To run it, type emdenbyp at the command line.

Rewrite the problem as a first-order system and identify the singular term. Using a substitution  $y_1 = y$  and  $y_2 = y'$ , write the differential equation as a system of two first-order equations

$$y_1' = y_2$$
  
 $y_2' = -\frac{2}{x}y_2 - y_1^5$ 

The boundary conditions become

$$y_2(0) = 0$$
  
 $y_1(1) = \sqrt{3/2}$ 

Writing the ODE system in a vector-matrix form

$$\begin{bmatrix} y_1' \\ y_2' \end{bmatrix} = \frac{1}{x} \begin{bmatrix} 0 & 0 \\ 0 & -2 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} + \begin{bmatrix} y_2 \\ -y_1^5 \end{bmatrix}$$

the terms of Equation 5-2 are identified as

$$S = \begin{bmatrix} 0 & 0 \\ 0 & -2 \end{bmatrix}$$

and

$$f(x,y) = \begin{bmatrix} y_2 \\ -y_1^5 \end{bmatrix}$$

**2 Code the ODE and boundary condition functions.** Code the differential equation and the boundary conditions as functions that bvp4c can use.

```
function dydx = emdenode(x,y)

dydx = [ y(2)

-y(1)^5 ];

function res = emdenbc(ya,yb)

res = [ ya(2)

yb(1) - sqrt(3)/2 ];
```

**3 Setup integration properties.** Use the matrix as the value of the 'SingularTerm' integration property.

```
S = [0,0;0,-2];
options = bvpset('SingularTerm',S);
```

**4 Create an initial guess.** This example starts with a mesh of five points and a constant guess for the solution.

$$y_1(x) \equiv \sqrt{3/2}$$
$$y_2(x) \equiv 0$$

Use bypinit to form the guess structure

```
guess = [sqrt(3)/2;0];
solinit = bvpinit(linspace(0,1,5),guess);
```

**5 Solve the problem.** Use the standard bvp4c syntax to solve the problem.

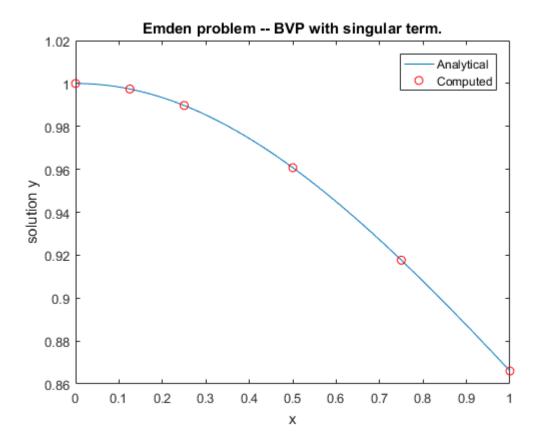
```
sol = bvp4c(@emdenode,@emdenbc,solinit,options);
```

**6** View the results. This problem has an analytical solution

$$y(x) = \left(1 + \frac{x^2}{3}\right)^{-1/2}$$

The example evaluates the analytical solution at 100 equally spaced points and plots it along with the numerical solution computed using bvp4c.

```
x = linspace(0,1);
truy = 1 ./ sqrt(1 + (x.^2)/3);
plot(x,truy,sol.x,sol.y(1,:),'ro');
title('Emden problem -- BVP with singular term.')
legend('Analytical','Computed');
xlabel('x');
ylabel('solution y');
```



## **Multipoint BVPs**

In multipoint boundary value problems, the solution of interest satisfies conditions at points inside the interval of integration. The bvp4c function is useful in solving such problems.

The following example shows how the multipoint capability in bvp4c can improve efficiency when you are solving a nonsmooth problem. The following equations are solved on  $0 \le x \le \lambda$  for constant parameters n,  $\kappa$ ,  $\lambda > 1$ , and  $\eta = \lambda^2/(n \times \kappa^2)$ . These are subject to boundary conditions v(0) = 0 and  $C(\lambda) = 1$ :

$$v' = (C - 1)/n$$

```
C' = (v * C - min(x,1))/\eta
```

The term min(x,1) is not smooth at xc = 1, and this can affect the solver's efficiency. By introducing an interface point at xc = 1, smooth solutions can be obtained on [0,1] and  $[1,\lambda]$ . To get a continuous solution over the entire interval  $[0,\lambda]$ , the example imposes matching conditions at the interface.

**Note:** The file, threebvp.m, contains the complete code for this example, and it solves the problem for  $\lambda = 2$ , n = 0.05, and several values of  $\kappa$ . All required functions are coded as nested functions in threebvp.m. To see the code in an editor, type edit threebvp at the command line. To run it, type threebvp at the command line.

The example takes you through the following steps:

1 Determine the interfaces and divide the interval of integration into regions. Introducing an interface point at xc = 1 divides the problem into two regions in which the solutions remain smooth. The differential equations for the two regions are

```
Region 1: 0 \le x \le 1

v' = (C - 1)/n

C' = (v * C - x)/\eta

Region 2: 1 \le x \le \lambda

v' = (C - 1)/n

C' = (v * C - 1)/\eta
```

Note that the interface xc = 1 is included in both regions. At xc = 1, bvp4c produces a *left* and *right* solution. These solutions are denoted as v(1-), C(1-) and v(1+), C(1+) respectively.

**2 Determine the boundary conditions.** Solving two first-order differential equations in two regions requires imposing four boundary conditions. Two of these conditions come from the original formulation; the others enforce the continuity of the solution across the interface xc = 1:

$$v(0) = 0$$
  
 $C(\lambda) - 1 = 0$   
 $v(1-) - v(1+) = 0$ 

```
C(1-) - C(1+) = 0
```

Here, V(1-), C(1-) and V(1+), C(1+) denote the left and right solution at the interface.

**3** Code the derivative function. In the derivative function, y(1) corresponds to v(x), and y(2) corresponds to C(x). The additional input argument region identifies the region in which the derivative is evaluated. bvp4c enumerates regions from left to right, starting with 1. Note that the problem parameters n and q are shared with the outer function:

```
function dydx = f(x,y,region) 

dydx = zeros(2,1); 

dydx(1) = (y(2) - 1)/n; 

% The definition of C'(x) depends on the region. 

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 % End nested function f
```

4 Code the boundary conditions function. For multipoint BVPs, the arguments of the boundary conditions function, YL and YR, become matrices. In particular, the kth column YL(:,k) represents the solution at the left boundary of the kth region. Similarly, YR(:,k) represents the solution at the right boundary of the kth region.

In the example, y(0) is approximated by YL(:,1), while  $y(\lambda)$  is approximated by YR(:,end). Continuity of the solution at the internal interface requires that YR(:,1) = YL(:,2). Nested function bc computes the residual in the boundary conditions:

5 Create an initial guess. For multipoint BVPs, when creating an initial guess using bypinit, use double entries in xinit for the interface point xc. This example uses a constant guess yinit = [1;1]:

```
xc = 1;
xinit = [0, 0.25, 0.5, 0.75, xc, xc, 1.25, 1.5, 1.75, 2];
solinit = bvpinit(xinit,yinit)
```

For multipoint BVPs, you can use different guesses in different regions. To do that, you specify the initial guess for y as a function using the following syntax:

```
solinit = bvpinit(xinit,@yinitfcn)
```

The initial guess function must have the following general form:

```
function y = yinitfcn(x,region) switch region case 1 % x in [0, 1] y = [1;1]; \qquad \% \text{ initial guess for } y(x) \quad 0 \leq x \leq 1 case 2 % x in [1, \lambda] y = [1;1]; \qquad \% \text{ initial guess for } y(x), \quad 1 \leq x \leq \lambda end
```

**6 Apply the solver.** The bvp4c function uses the same syntax for multipoint BVPs as it does for two-point BVPs:

```
sol = bvp4c(@f,@bc,solinit);
```

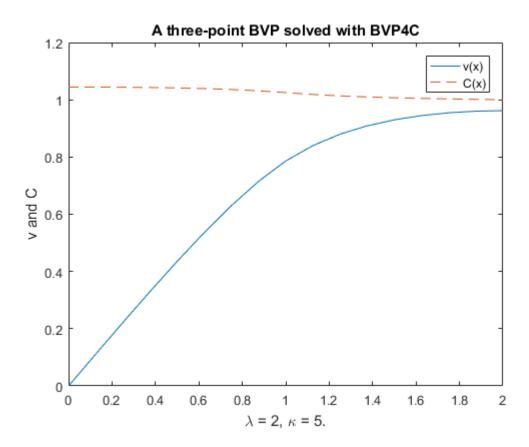
The mesh points returned in Sol.x are adapted to the solution behavior, but the mesh still includes a double entry for the interface point xc = 1. Corresponding columns of Sol.y represent the left and right solution at xc.

**7 View the results.** Using **deval**, the solution can be evaluated at any point in the interval of integration.

Note that, with the left and right values computed at the interface, the solution is not uniquely defined at xc = 1. When evaluating the solution exactly at the interface, deval issues a warning and returns the average of the left and right solution values. Call deval at xc-eps(xc) and xc+eps(xc) to get the limit values at xc.

The example plots the solution approximated at the mesh points selected by the solver:

```
plot(sol.x,sol.y(1,:),sol.x,sol.y(2,:),'--') legend('v(x)','C(x)') title(['A three-point BVP solved with BVP4C'])
```



## **Additional Examples**

The following additional examples are available. Type  $\,$ 

edit examplename

to view the code and

examplename

to run the example.

Example Name	Description
emdenbvp	Emden's equation, a singular BVP
fsbvp	Falkner-Skan BVP on an infinite interval
mat4bvp	Fourth eigenfunction of Mathieu's equation
shockbvp	Solution with a shock layer near x = 0
twobvp	BVP with exactly two solutions
threebvp	Three-point boundary value problem

 $Additional\ examples\ are\ provided\ by\ "Tutorial\ on\ Solving\ BVPs\ with\ BVP4C,"\ available\ at\ http://www.mathworks.com/bvp\_tutorial.$ 

# References

- [1] Ascher, U., R. Mattheij, and R. Russell, "Numerical Solution of Boundary Value Problems for Ordinary Differential Equations," SIAM, Philadelphia, PA, 1995, p. 372.
- [2] 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.

# Partial Differential Equations (PDEs)

# **Partial Differential Equations**

## In this section...

"Function Summary" on page 13-2

"Initial Value Problems" on page 13-2

"PDE Solver" on page 13-3

"Integrator Options" on page 13-6

"Examples" on page 13-7

# **Function Summary**

- "PDE Solver" on page 13-2
- "PDE Helper Function" on page 13-2

#### **PDE Solver**

This is the MATLAB PDE solver.

PDE Initial-Boundary Value Problem Solver	Description
pdepe	Solve initial-boundary value problems for systems of parabolic and elliptic PDEs in one space variable and time.

## **PDE Helper Function**

PDE Helper Function	Description
pdeval	Evaluate the numerical solution of a PDE using the output of pdepe.

# **Initial Value Problems**

pdepe solves systems of parabolic and elliptic PDEs in one spatial variable x and time t, 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 PDEs hold for  $t_0 \le t \le t_f$  and  $a \le x \le b$ . The 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.

In Equation 13-1,  $f(x,t,u,\partial u/\partial x)$  is a flux term and  $s(x,t,u,\partial u/\partial x)$  is a source term. The flux term must depend on  $\partial u/\partial x$ . The coupling of the partial derivatives with respect to time is restricted to multiplication by a diagonal matrix  $c(x,t,u,\partial u/\partial x)$ . The diagonal elements of this matrix are either identically zero or positive. An element that is identically zero corresponds to an elliptic equation and otherwise 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 c if they are mesh points. Discontinuities in c and/or c due to material interfaces are permitted provided that a mesh point is placed at each interface.

At the initial time  $t = t_0$ , for all x the solution components satisfy initial conditions of the form

$$u(x,t_0) = u_0(x).$$

At the boundary x = a or x = b, for all t the solution components satisfy a boundary condition of the form

$$p(x,t,u) + q(x,t)f\left(x,t,u,\frac{\partial u}{\partial x}\right) = 0.$$

q(x,t) is a diagonal matrix with elements that are either identically zero or never zero. Note that the boundary conditions are expressed in terms of the f rather than partial derivative of u with respect to  $x \partial u/\partial x$ . Also, of the two coefficients, only p can depend on u.

## **PDE Solver**

#### The PDE Solver

The MATLAB PDE solver, pdepe, solves initial-boundary value problems for systems of parabolic and elliptic PDEs in the one space variable x and time t. There must be at least one parabolic equation in the system.

The pdepe solver converts the PDEs to ODEs using a second-order accurate spatial discretization based on a fixed set of user-specified nodes. The discretization method is described in [1]. The time integration is done with ode15s. The pdepe solver exploits the

capabilities of ode15s for solving the differential-algebraic equations that arise when Equation 13-1 contains elliptic equations, and for handling Jacobians with a specified sparsity pattern. ode15s changes both the time step and the formula dynamically.

After discretization, elliptic equations give rise to algebraic equations. If the elements of the initial conditions vector that correspond to elliptic equations are not "consistent" with the discretization, pdepe tries to adjust them before beginning the time integration. For this reason, the solution returned for the initial time may have a discretization error comparable to that at any other time. If the mesh is sufficiently fine, pdepe can find consistent initial conditions close to the given ones. If pdepe displays a message that it has difficulty finding consistent initial conditions, try refining the mesh. No adjustment is necessary for elements of the initial conditions vector that correspond to parabolic equations.

## **PDE Solver Syntax**

The basic syntax of the solver is:

```
sol = pdepe(m,pdefun,icfun,bcfun,xmesh,tspan)
```

**Note:** Correspondences given are to terms used in "Initial Value Problems" on page 13-2.

The input arguments are

m Specifies the symmetry of the problem. m can be 0 = slab,

1 =cylindrical, or 2 =spherical. It corresponds to m in

Equation 13-1.

pdefun Function that defines the components of the PDE. It computes

the terms c, f, and s in Equation 13-1, and has the form

[c,f,s] = pdefun(x,t,u,dudx)

where x and t are scalars, and u and dudx are vectors that approximate the solution u and its partial derivative with respect to x. c, f, and s are column vectors. c stores the diagonal

elements of the matrix c.

icfun Function that evaluates the initial conditions. It has the form

u = icfun(x)

When called with an argument x, icfun evaluates and returns the initial values of the solution components at x in the column vector u.

Function that evaluates the terms p and q of the boundary conditions. It has the form

[pl,ql,pr,qr] = bcfun(xl,ul,xr,ur,t)

where ul is the approximate solution at the left boundary x1 = a and ur is the approximate solution at the right boundary xr = b. pl and ql are column vectors corresponding to p and the diagonal of q evaluated at x1. Similarly, pr and qr correspond to xr. When m > 0 and a = 0, boundedness of the solution near x = 0 requires that the f vanish at a = 0. pdepe imposes this boundary condition automatically and it ignores values returned in pl and q1.

Vector [x0, x1, ..., xn] specifying the points at which a numerical solution is requested for every value in tspan. x0 and xn correspond to a and b, respectively.

Second-order approximation to the solution is made on the mesh specified in xmesh. Generally, it is best to use closely spaced mesh points where the solution changes rapidly. Pdepe does *not* select the mesh in x automatically. You must provide an appropriate fixed mesh in xmesh. The cost depends strongly on the length of xmesh. When m > 0, it is not necessary to use a fine mesh near x = 0 to account for the coordinate singularity.

The elements of xmesh must satisfy x0 < x1 < ... < xn. The length of xmesh must be  $\geq 3$ .

bcfun

xmesh

tspan

Vector [t0, t1, ..., tf] specifying the points at which a solution is requested for every value in xmesh. t0 and tf correspond to  $t_0$  and  $t_f$ , respectively.

pdepe performs the time integration with an ODE solver that selects both the time step and formula dynamically. The solutions at the points specified in tspan are obtained using the natural continuous extension of the integration formulas. The elements of tspan merely specify where you want answers and the cost depends weakly on the length of tspan.

The elements of tspan must satisfy t0 < t1 < ... < tf. The length of tspan must be  $\geq 3$ .

The output argument sol is a three-dimensional array, such that

- sol(:,:,k) approximates component k of the solution u.
- sol(i,:,k) approximates component k of the solution at time tspan(i) and mesh points xmesh(:).
- sol(i, j, k) approximates component k of the solution at time tspan(i) and the mesh point xmesh(j).

## **PDE Solver Options**

For more advanced applications, you can also specify as input arguments solver options and additional parameters that are passed to the PDE functions.

options

Structure of optional parameters that change the default integration properties. This is the seventh input argument.

See "Integrator Options" on page 13-6 for more information.

# **Integrator 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 defaults. You do this by supplying pdepe with one or more property values in an options structure.

sol = pdepe(m,pdefun,icfun,bcfun,xmesh,tspan,options)

Use odeset to create the options structure. Only those options of the underlying ODE solver shown in the following table are available for pdepe. The defaults obtained by leaving off the input argument options are generally satisfactory.

## **PDE Properties**

Properties Category	Property Name
Error control	RelTol, AbsTol, NormControl
Step-size	InitialStep, MaxStep

# **Examples**

- "Single PDE" on page 13-7
- "System of PDEs" on page 13-13
- "Additional Examples" on page 13-17

# **Single PDE**

- "Solving the Equation" on page 13-7
- "Evaluating the Solution" on page 13-12

## **Solving the Equation**

This example illustrates the straightforward formulation, solution, and plotting of the solution of a single PDE

$$\pi^2 \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}.$$

This equation holds on an interval  $0 \le x \le 1$  for times  $t \ge 0$ . At t = 0, the solution satisfies the initial condition

$$u(x,0) = \sin \pi x$$
.

At x = 0 and x = 1, the solution satisfies the boundary conditions

$$u(0,t) = 0$$
  
$$\pi e^{-t} + \frac{\partial u}{\partial x}(1,t) = 0.$$

**Note:** The file, pdex1.m, contains the complete code for this example. It contains all the required functions coded as local functions. To see the code in an editor, type edit pdex1 at the command line. To run it, type pdex1 at the command line. See "PDE Solver Syntax" on page 13-4 for more information.

1 Rewrite the PDE. Write the PDE in the form

$$c\left(x,t,u,\frac{\partial u}{\partial x}\right)\frac{\partial u}{\partial t} = x^{-m}\frac{\partial}{\partial x}\left(x^{m}f\left(x,t,u,\frac{\partial u}{\partial x}\right)\right) + s\left(x,t,u,\frac{\partial u}{\partial x}\right).$$

This is the form shown in Equation 13-1 and expected by pdepe. See "Initial Value Problems" on page 13-2 for more information. For this example, the resulting equation is

$$\pi^2 \frac{\partial u}{\partial t} = x^0 \frac{\partial}{\partial x} \left( x^0 \frac{\partial u}{\partial x} \right) + 0$$

with parameter m = 0 and the terms

$$c\left(x,t,u,\frac{\partial u}{\partial x}\right) = \pi^2$$

$$f\left(x,t,u,\frac{\partial u}{\partial x}\right) = \frac{\partial u}{\partial x}$$

$$s\left(x,t,u,\frac{\partial u}{\partial x}\right) = 0.$$

**2** Code the PDE. Once you rewrite the PDE in the form shown above (Equation 13-1) and identify the terms, you can code the PDE in a function that pdepe can use. The function must be of the form

```
[c,f,s] = pdefun(x,t,u,dudx)
```

where c, f, and s correspond to the c, f, and s terms. The code below computes c, f, and s for the example problem.

```
function [c,f,s] = pdex1pde(x,t,u,DuDx)
c = pi^2;
f = DuDx;
s = 0;
```

**3** Code the initial conditions function. You must code the initial conditions in a function of the form

```
u = icfun(x)
```

The code below represents the initial conditions in the function pdex1ic.

```
function u0 = pdex1ic(x)
u0 = sin(pi*x);
```

**4** Code the boundary conditions function. You must also code the boundary conditions in a function of the form

```
[pl,ql,pr,qr] = bcfun(xl,ul,xr,ur,t)
```

The boundary conditions, written in the same form as Equation 13-3, are

$$u(0,t) + 0 \cdot \frac{\partial u}{\partial x}(0,t) = 0$$
 at  $x = 0$ 

and

$$\pi e^{-t} + 1 \cdot \frac{\partial u}{\partial x}(1,t) = 0$$
 at  $x = 1$ .

The code below evaluates the components p(x,t,u) and q(x,t) of the boundary conditions in the function pdex1bc.

```
function [pl,ql,pr,qr] = pdex1bc(xl,ul,xr,ur,t)
pl = ul;
ql = 0;
pr = pi * exp(-t);
ar = 1;
```

In the function pdex1bc, pl and ql correspond to the left boundary conditions (x = 0), and pr and qr correspond to the right boundary condition (x = 1).

**5 Select mesh points for the solution.** Before you use the MATLAB PDE solver, 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 (see "PDE Solver" on page 13-3). In particular, the cost and the 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.

This example requests the solution on the mesh produced by 20 equally spaced points from 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);
```

**6 Apply the PDE solver.** The example calls pdepe with m = 0, the functions pdex1pde, pdex1ic, and pdex1bc, and the mesh defined by x and t at which pdepe is to evaluate the solution. The pdepe function returns the numerical solution in a three-dimensional array sol, where sol(i,j,k) approximates the kth component of the solution,  $u_k$ , evaluated at t(i) and x(j).

```
m = 0;
sol = pdepe(m,@pdex1pde,@pdex1ic,@pdex1bc,x,t);
```

This example uses @ to pass pdex1pde, pdex1ic, and pdex1bc as function handles to pdepe.

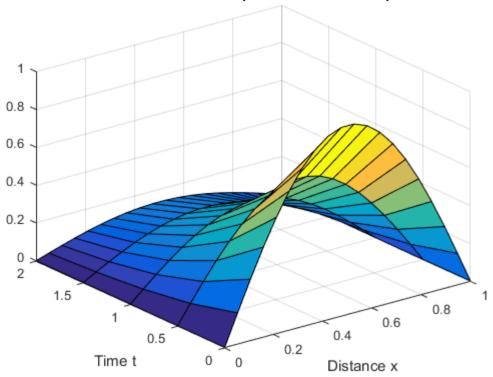
**Note:** See "Function Handles" for more information about function handles.

- **7** View the results. Complete the example by displaying the results:
  - Extract and display the first solution component. In this example, the solution *u* has only one component, but for illustrative purposes, the example "extracts" it from the three-dimensional array. The surface plot shows the behavior of the solution.

```
u = sol(:,:,1);
surf(x,t,u)
title('Numerical solution computed with 20 mesh points')
```

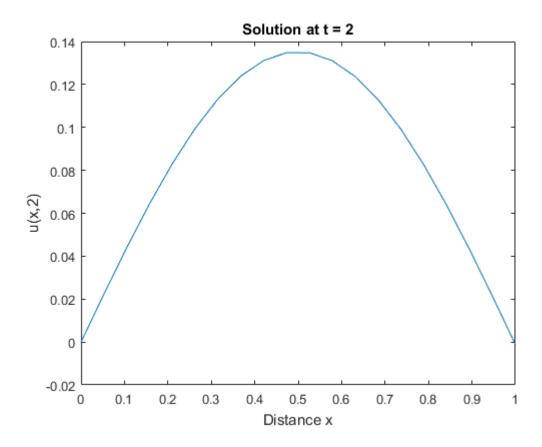
```
xlabel('Distance x')
ylabel('Time t')
```

# Numerical solution computed with 20 mesh points.



**b** Display a solution profile at  $t_f$ , the final value of t. In this example,  $t_f = t = 2$ .

```
figure
plot(x,u(end,:))
title('Solution at t = 2')
xlabel('Distance x')
ylabel('u(x,2)')
```



### **Evaluating the Solution**

After obtaining and plotting the solution above, you might be interested in a solution profile for a particular value of t, or the time changes of the solution at a particular point x. The kth column u(:,k) (of the solution extracted in step 7) contains the time history of the solution at x(k). The jth row u(j,:) contains the solution profile at t(j).

Using the vectors x and u(j,:), and the helper function pdeval, you can evaluate the solution u and its derivative  $\partial u/\partial x$  at any set of points xout

```
[uout,DuoutDx] = pdeval(m,x,u(j,:),xout)
```

The example pdex3 uses pdeval to evaluate the derivative of the solution at xout = 0. See pdeval for details.

## System of PDEs

This example illustrates the solution of a system of partial differential equations. The problem is taken from electrodynamics. It has boundary layers at both ends of the interval, and the solution changes rapidly for small t.

The PDEs are

$$\frac{\partial u_1}{\partial t} = 0.024 \frac{\partial^2 u_1}{\partial x^2} - F(u_1 - u_2)$$
$$\frac{\partial u_2}{\partial t} = 0.170 \frac{\partial^2 u_2}{\partial x^2} + F(u_1 - u_2)$$

where  $F(y) = \exp(5.73y) - \exp(-11.46y)$ . The equations hold on an interval  $0 \le x \le 1$  for times  $t \ge 0$ .

The solution *u* satisfies the initial conditions

$$u_1(x,0) \equiv 1$$
$$u_2(x,0) \equiv 0$$

and boundary conditions

$$\begin{split} &\frac{\partial u_1}{\partial x}(0,t) \equiv 0 \\ &u_2(0,t) \equiv 0 \\ &u_1(1,t) \equiv 1 \\ &\frac{\partial u_2}{\partial x}(1,t) \equiv 0. \end{split}$$

**Note:** The file, pdex4.m, contains the complete code for this example. It contains all the required functions coded as local functions. To see the code in an editor, type edit pdex4 at the command line. To run it, type pdex4 at the command line.

1 Rewrite the PDE. In the form expected by pdepe, the equations are

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix} \cdot * \frac{\partial}{\partial t} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \frac{\partial}{\partial x} \begin{bmatrix} 0.024 \left( \partial u_1 \ / \ \partial x \right) \\ 0.170 \left( \partial u_2 \ / \ \partial x \right) \end{bmatrix} + \begin{bmatrix} -F \left( u_1 - u_2 \right) \\ F \left( u_1 - u_2 \right) \end{bmatrix}.$$

The boundary conditions on the partial derivatives of u have to be written in terms of the flux. In the form expected by pdepe, the left boundary condition is

$$\begin{bmatrix} 0 \\ u_2 \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \end{bmatrix} \cdot * \begin{bmatrix} 0.024 \left( \frac{\partial u_1}{\partial u_2} / \frac{\partial x}{\partial x} \right) \\ 0.170 \left( \frac{\partial u_2}{\partial u_2} / \frac{\partial x}{\partial x} \right) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

and the right boundary condition is

$$\begin{bmatrix} u_1 - 1 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} \cdot * \begin{bmatrix} 0.024(\partial u_1 / \partial x) \\ 0.170(\partial u_2 / \partial x) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

**2 Code the PDE.** After you rewrite the PDE in the form shown above, you can code it as a function that pdepe can use. The function must be of the form

$$[c,f,s] = pdefun(x,t,u,dudx)$$

where c, f, and s correspond to the c, f, and s terms in Equation 13-1.

```
function [c,f,s] = pdex4pde(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];
```

**3** Code the initial conditions function. The initial conditions function must be of the form

```
u = icfun(x)
```

The code below represents the initial conditions in the function pdex4ic.

```
function u0 = pdex4ic(x);
u0 = [1; 0];
```

**4 Code the boundary conditions function.** The boundary conditions functions must be of the form

```
[pl,ql,pr,qr] = bcfun(xl,ul,xr,ur,t)
```

The code below evaluates the components p(x,t,u) and q(x,t) (Equation 13-3) of the boundary conditions in the function pdex4bc.

```
function [pl,ql,pr,qr] = pdex4bc(xl,ul,xr,ur,t)
pl = [0; ul(2)];
ql = [1; 0];
pr = [ur(1)-1; 0];
qr = [0; 1];
```

**Select mesh points for the solution.** The solution changes rapidly for small *t*. The program selects the step size in time to resolve this sharp change, but to see this behavior in the plots, output times must be selected accordingly. There are boundary layers in the solution at both ends of [0,1], so mesh points must be placed there to resolve these sharp changes. Often some experimentation is needed to select the mesh that reveals the behavior of the solution.

```
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];
```

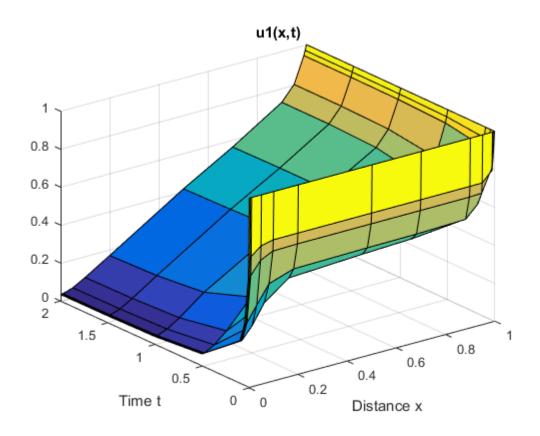
**6 Apply the PDE solver.** The example calls pdepe with m = 0, the functions pdex4pde, pdex4ic, and pdex4bc, and the mesh defined by x and t at which pdepe is to evaluate the solution. The pdepe function returns the numerical solution in a three-dimensional array sol, where sol(i,j,k) approximates the kth component of the solution,  $\mu_k$ , evaluated at t(i) and x(j).

```
m = 0;
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
```

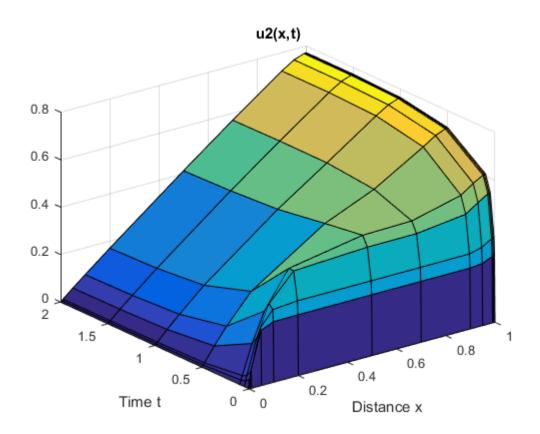
**7 View the results.** The surface plots show the behavior of the solution components.

```
u1 = sol(:,:,1);
u2 = sol(:,:,2);

figure
surf(x,t,u1)
title('u1(x,t)')
xlabel('Distance x')
ylabel('Time t')
```



```
figure
surf(x,t,u2)
title('u2(x,t)')
xlabel('Distance x')
ylabel('Time t')
```



#### **Additional Examples**

The following additional examples are available. Type

edit examplename

to view the code and

examplename

to run the example.

Example Name	Description	
pdex1	Simple PDE that illustrates the straightforward formulation, computation, and plotting of the solution	
pdex2	Problem that involves discontinuities	
pdex3	Problem that requires computing values of the partial derivative	
pdex4	System of two PDEs whose solution has boundary layers at both ends of the interval and changes rapidly for small $t$ .	
pdex5	System of PDEs with step functions as initial conditions	

## **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.

# **Delay Differential Equations (DDEs)**

- "Types of DDEs" on page 14-2
- "Discontinuities in DDEs" on page 14-5
- "DDE with Constant Delays" on page 14-6
- "State-Dependent Delay Problem" on page 14-9
- "Cardiovascular Model with Discontinuities" on page 14-13
- "DDE of Neutral Type" on page 14-17
- "Initial Value DDE of Neutral Type" on page 14-21

# Types of DDEs

#### In this section...

"Constant Delay DDEs" on page 14-2

"Time-Dependent and State-Dependent DDEs" on page 14-2

"DDEs of Neutral Type" on page 14-3

"Evaluating the Solution at Specific Points" on page 14-3

"History and Initial Values" on page 14-3

"Propagation of Discontinuities" on page 14-3

#### **Constant Delay DDEs**

A system of differential equations (DDEs) with constant delays has the following 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 of the form given by Equation 14-1 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**

Equation 14-1 is a special case of

$$y'(t) = f(t, y(t), y(dy_1), ..., y(dy_n))$$

that involves delays,  $dy_1,...,dy_k$ , which 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 DDEs of the form given by Equation 14-2 with history y(t) = S(t) for  $t < t_0$ . The ddesd function integrates with the classic fourstage, 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 by Equation 14-2. 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, Equation 14-1 shows that  $y'(t_0)$  depends on  $y(t_0 - \tau_1),...,y(t_0 - \tau_k)$  for positive constants  $\tau_j$ . 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  $t < t_0$ .

#### **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  $\tau_1, \ldots, \tau_k$  when the delays are constant, as in Equation 14-1. If the delays are not constant, the propagation of discontinuities is more complicated. For neutral DDEs of the form given by Equation 14-1 or Equation 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 by Equation 14-3 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  $[t_0, t_{\rm f}]$ .

#### References

[1] Shampine, L.F. "Dissipative Approximations to Neutral DDEs." *Applied Mathematics & Computation*, Vol. 203, 2008, pp. 641–648.

## **Discontinuities in DDEs**

If your problem has discontinuities, it's 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 <i>t</i> of the discontinuities in a vector as the value of the Jumps property. Applies only to dde23.
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.

# **DDE with Constant Delays**

This example shows how to use dde23 to solve a system of DDEs with constant delays.

Click ddex1.m or type edit ddex1.m in a command window to view the code for this example in an editor.

The differential equations are:

$$\begin{aligned} y_1'(t) &= y_1(t-1) \\ y_2'(t) &= y_1(t-1) + y_2(t-0.2) \\ y_3'(t) &= y_2(t). \end{aligned}$$

The history of this problem is constant:

```
y_1(t) = 1

y_2(t) = 1

y_3(t) = 1
```

for  $t \leq 0$ .

- 1 Create a new program file in the editor. This file will contain a main function and two local functions.
- **2** Define the first-order DDE as a local function.

```
function dydt = ddex1de(t,y,Z)
  ylag1 = Z(:,1);
  ylag2 = Z(:,2);
  dydt = [ylag1(1); ylag1(1)+ylag2(2); y(2)];
end
```

**3** Define the solution history as a local function.

```
function S = ddex1hist(t)
  S = ones(3,1);
end
```

**4** Define the delays,  $\tau_1,...,\tau_k$  in the main function.

```
lags = [1,0.2];
```

5 Solve the DDE by calling dde23 in the main function. Pass the DDE function, the delays, the solution history, and interval of integration, [0,5], as inputs.

```
sol = dde23(@ddex1de,lags,@ddex1hist,[0,5]);
```

The dde23 function produces a continuous solution over the whole interval of integration  $[t_0, t_f]$ .

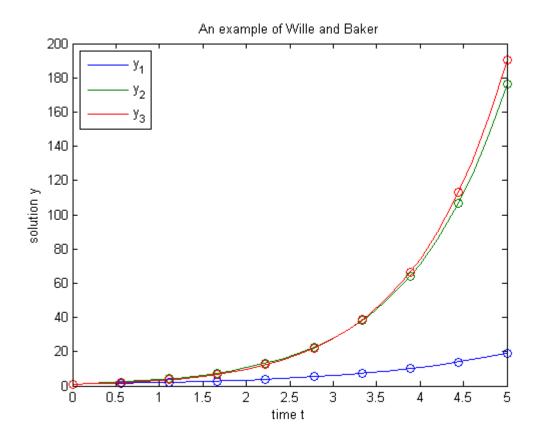
**6** Plot the solution returned by dde23. Add this code to your main function.

```
plot(sol.x,sol.y);
title('An example of Wille and Baker');
xlabel('time t');
ylabel('solution y');
legend('y_1','y_2','y_3','Location','NorthWest');
```

**7** Evaluate the solution at 10 equally spaced points over the interval of integration. Then plot the results on the same axes as sol.y. Add this code to the main function.

```
tint = linspace(0,5,10);
Sint = deval(sol,tint)
hold on
plot(tint,Sint,'o');
```

**8** Run your program to generate and plot the results.



# **Related Examples**

- "Create Functions in Files"
- "Run Functions in the Editor"

## **More About**

• "Create Function Handle"

# State-Dependent Delay Problem

This example shows how to use **ddesd** to solve a system of two DDEs with a state-dependent delay. This system of DDEs was used as a test problem by Enright and Hayashi [1].

Click ddex3.m or type edit ddex3.m in a command window to view the complete code for this example in an editor.

The equations for this system are:

$$\begin{aligned} y_1'(t) &= y_2(t) \\ y_2'(t) &= -y_2(e^{(1-y_2(t))}) \cdot y_2(t)^2 \cdot e^{(1-y_2(t))}. \end{aligned}$$

The analytical solution

$$y_1(t) = \log(t)$$
$$y_2(t) = 1/t$$

is used as the history for  $t \le 0.1$  and the equations are solved on [0.1, 5] with ddesd rather than dde23. The ddesd function is appropriate in this case because the first factor in the second equation has the form  $y_2(d(y))$  with a delay that depends on the second component of the solution.

- 1 Create a new program file in the editor. This file will contain a main function and three local functions.
- **2** Code the system of DDEs as a local function.

```
function dydt = ddex3de(t,y,Z)
  dydt = [y(2); -Z(2)*y(2)^2*exp(1 - y(2))];
end
```

**3** Define the delay as a local function.

```
function d = ddex3delay(t,y)
  d = exp(1 - y(2));
end
```

**4** Define the solution history as a local function.

```
function v = ddex3hist(t)
 v = [log(t); 1./t];
end
```

5 Define the interval of integration and solve the system. Add this code to the main function in your program file.

```
tspan = [0.1 5];
sol = ddesd(@ddex3de,@ddex3delay,@ddex3hist,tspan);
```

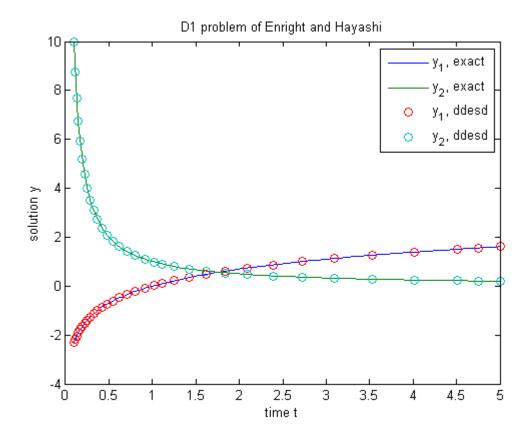
Use the history function to calculate the analytical solution within the integration interval. Add this code to the main function.

```
texact = linspace(0.1,5);
yexact = ddex3hist(texact);
```

7 Plot the numerical solution on the same axes as the analytical solution. Add this code to the main function.

```
figure
plot(texact,yexact,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')
```

8 Run your program to generate and plot the results.



## **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.

## **Related Examples**

- "Create Functions in Files"
- "Run Functions in the Editor"

## **More About**

"Create Function Handle"

## Cardiovascular Model with Discontinuities

This example shows how to use dde23 to solve a cardiovascular model that has a discontinuous derivative as presented by Ottesen [1].

Click ddex2.m or type edit ddex2.m in a command window to view the code for this example in an editor.

This is a problem with 1 delay, constant history, and 3 differential equations with 14 physical parameters. The system is heavily influenced by peripheral pressure, R, which decreases exponentially from 1.05 to 0.84, beginning at t = 600. As a result, the system has a discontinuity in a low-order derivative at t = 600.

- 1 Create a new program file in the editor. This file will contain a main function and a nested function. The main function accepts no inputs and returns no outputs.
- **2** Define the physical parameters. Add this code to the main function.

```
= 1.55;
p.ca
p.cv
         = 519;
         = 1.05;
p.R
         = 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;
```

**3** Define the solution history. Add this code to the main function.

```
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];
```

**4** Define the delay, tau. Add this code to the main function.

```
tau = 4;
```

5 Define the location of discontinuity, which occurs at t = 600. Add this code to the main function.

```
options = ddeset('Jumps',600);
```

When your DDE has discontinuities in low-order derivatives, and you know the locations in advance, it is better to use ddeset with the Jumps property.

6 Solve the DDE over the interval [0, 1000]. Add this code to the main function.

```
sol = dde23(@ddex2de,tau,history,[0,1000],options);
```

The function, @ddex2de, which defines the system of DDEs, is the first input argument. You define this function in 8.

7 Plot the solution. Add this code to the main function.

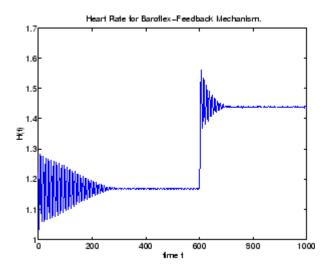
```
figure
plot(sol.x,sol.y(3,:))
title('Heart Rate for Baroflex-Feedback Mechanism.')
xlabel('time t')
vlabel('H(t)')
```

8 Define the system of DDEs as a nested function inside the main function.

```
function dydt = ddex2de(t,y,Z)
    if t <= 600
     p.R = 1.05;
      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);
```

This function is nested so that the main function can access the 14 parameters defined in 2.

**9** Run your program to calculate the solution and display the plot.



#### References

[1] Ottesen, J. T. "Modelling of the Baroflex-Feedback Mechanism with Time-Delay." J.  $Math.\ Biol.\ Vol.\ 36$ , Number 1, 1997, pp. 41–63.

#### **Related Examples**

- "Create Functions in Files"
- "Run Functions in the Editor"

## **More About**

"Create Function Handle"

# **DDE of Neutral Type**

This example shows how to use ddensd to solve the neutral DDE presented by Paul [1] for  $0 \le t \le \pi$ .

Click ddex4.m or type edit ddex4.m in a command window to view the code for this example in an editor.

```
The equation is y'(t) = 1 + y(t) - 2y(t/2)^2 - y'(t - \pi) with history: y(t) = \cos(t) for t \le 0.
```

- 1 Create a new program file in the editor. This file will contain a main function and four local functions.
- **2** Define the first-order DDE as a local function.

```
function yp = ddefun(t,y,ydel,ypdel)
    yp = 1 + y - 2*ydel^2 - ypdel;
end
```

**3** Define the solution delay as a local function.

```
function dy = dely(t,y)
    dy = t/2;
end
```

**4** Define the derivative delay as a local function.

```
function dyp = delyp(t,y)
    dyp = t-pi;
end
```

**5** Define the solution history as a local function.

```
function y = history(t)
    y = cos(t);
end
```

**6** Define the interval of integration and solve the DDE using the ddensd function. Add this code to the main function.

```
tspan = [0 pi];
sol = ddensd(@ddefun,@dely,@delyp,@history,tspan);
```

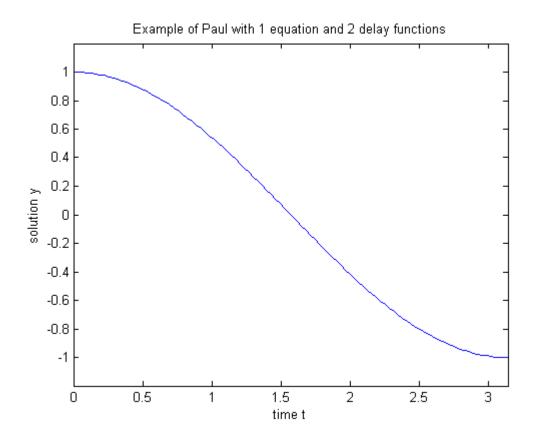
Evaluate the solution at 100 equally spaced points between 0 and  $\pi$ . Add this code to 7 the main function.

```
tn = linspace(0,pi);
yn = deval(sol,tn);
```

8 Plot the results. Add this code to the main function.

```
figure
plot(tn,yn);
xlim([0 pi]);
ylim([-1.2 1.2])
xlabel('time t');
ylabel('solution y');
title('Example of Paul with 1 equation and 2 delay functions')
```

9 Run your program to calculate the solution and display the plot.



#### **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.

## **Related Examples**

- "Create Functions in Files"
- "Run Functions in the Editor"

## **More About**

"Create Function Handle"

# **Initial Value DDE of Neutral Type**

This example shows how to use **ddensd** to solve the initial value DDE presented by Jackiewicz [1] for  $0 \le t \le 0.1$ .

Click ddex5.m or type edit ddex5.m in a command window to view the code for this example in an editor.

```
The equation is y'(t) = 2\cos(2t) y(t/2)^{2\cos(t)} + \log(y'(t/2)) - \log(2\cos(t)) - \sin(t).
```

This is an initial value DDE because the delays are zero at  $t_0$ . The initial conditions are: y(0) = 1 y'(0) = s, where s is the solution of:

 $2 + \log(s) - \log(2) = 0.$ 

This equation is satisfied by  $s_1 = 2$  and  $s_2 = 0.4063757399599599$ .

- 1 Create a new program file in the editor. This file will contain a main function and one local function.
- **2** Define the DDE as a local function.

```
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
```

**3** Define the solution delay and derivative delay. Add this line to the main function.

```
delay = @(t,y) t/2;
```

You can use one anonymous function to handle both delays since they are the same in the equation.

Define the initial conditions, y0 and s1, and the interval of integration, tspan. Add this code to the main function.

```
y0 = 1;
s1 = 2;
tspan = [0 0.1];
```

**5** Solve the DDE for  $0 \le t \le 0.1$ , with initial conditions y(0) = 1, and y'(0) = 2. Add this code to the main function.

```
sol1 = ddensd(@ddefun,delay,delay,{y0,s1},tspan);
```

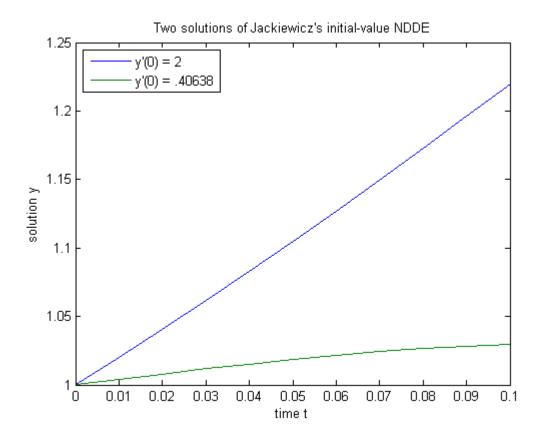
**6** Solve the equation again, this time using y'(0) = 0.4063757399599599. Add this code to the main function.

```
s2 = 0.4063757399599599;
sol2 = ddensd(@ddefun,delay,delay,{y0,s2},tspan);
```

**7** Plot the results. Add this code to the main function.

```
figure
plot(sol1.x,sol1.y,sol2.x,sol2.y);
legend('y''(0) = 2','y''(0) = .40638','Location','NorthWest');
xlabel('time t');
ylabel('solution y');
title('Two solutions of Jackiewicz''s initial-value NDDE');
```

**8** Run your program to calculate and plot the solutions for each value of *s*.



#### **References**

[1] Jackiewicz, Z. "One step Methods of any Order for Neutral Functional Differential Equations." *SIAM J. Numer. Anal.* Vol. 21, Number 3, 1984, pp. 486–511.

## **Related Examples**

- "Create Functions in Files"
- "Run Functions in the Editor"

## **More About**

"Create Function Handle"

# **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 15-6
- "Analytic Solution to Integral of Polynomial" on page 15-8
- "Integration of Numeric Data" on page 15-9
- "Calculate Tangent Plane to Surface" on page 15-13

# 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.

$$\int_{0}^{3\pi} \sqrt{4\cos(2t)^2 + \sin(t)^2 + 1} dt.$$

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.

# **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)

q1 =
    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 =
    3.3307e-16 - 7.7716e-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  ${\tt q1}$  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
```

# 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  $-1 \le y \le 1$ .

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 =
   3.771236166328259 - 3.771236166328255i
```

The integration succeeds when the singular values are on the boundary.

The exact value of this integral is

$$\frac{8\sqrt{2}}{3}\left(1-i\right)$$

8/3\*sqrt(2)\*(1-i)

ans =

3.771236166328253 - 3.771236166328253i

# **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,

$$\int (4x^5 - 2x^3 + x + 4) \ dx$$

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.

# Integration of Numeric Data

This example shows how to integrate a set of discrete velocity data numerically using trapz to approximate the total distance traveled. The integral family only accepts function handles as inputs, so those functions cannot be used with discrete data sets. Use trapz when a functional expression is not available for integration.

#### View the Velocity Data

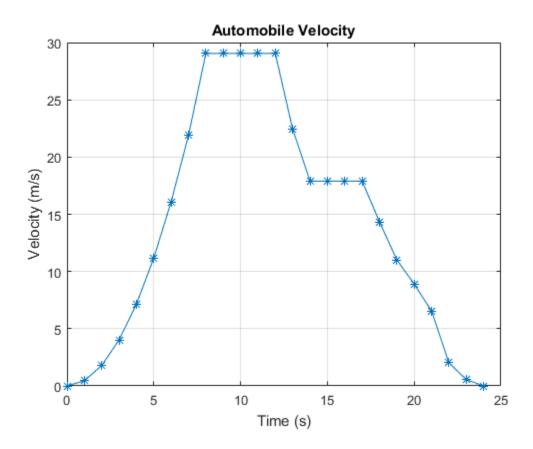
Consider the following velocity data and corresponding time data.

```
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)')
```



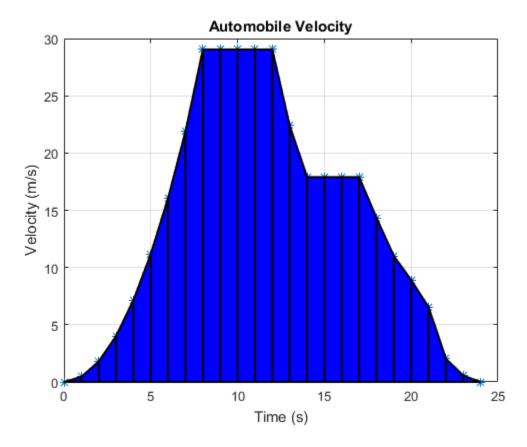
The slope is positive during periods of acceleration, zero during periods of constant velocity, and negative during periods of deceleration. At time t=0, the vehicle is at rest with vel(1)=0 m/s. The vehicle accelerates until reaching a maximum velocity at t=8 s of vel(9)=29.05 m/s and maintains this 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)];
yverts = [zeros(1,24);vel(1:end-1);vel(2:end);zeros(1,24)];
hold on
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.

```
distance = trapz(time,vel)
distance =
  345.2200
```

The distance traveled by the automobile in  $t = 24 \mathrm{\ s}$  is about  $345.22 \mathrm{\ m}$ .

# 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.

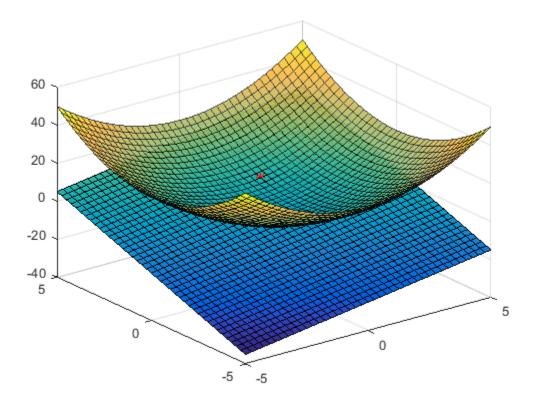
```
x0 = 1;
y0 = 2;
t = (xx == x0) & (yy == y0);
indt = find(t);
fx0 = fx(indt);
fy0 = fy(indt);
```

Create a function handle with the equation of the tangent plane  ${\tt z}$ .

```
z = @(x,y) f(x0,y0) + fx0*(x-x0) + fy0*(y-y0);
```

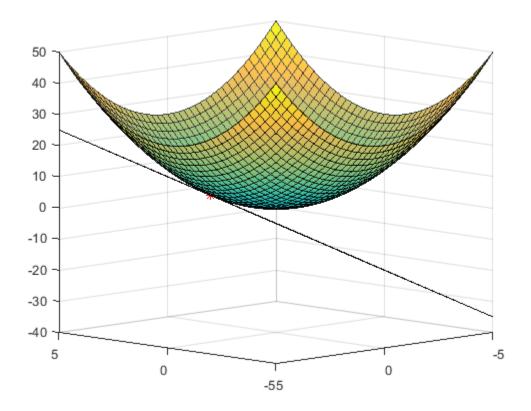
Plot the original function f(x, y), the point P, and a piece of plane z that is tangent to the function at P.

```
\begin{array}{l} 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*') \end{array}
```



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 16-7
- "Polynomial Interpolation Using FFT" on page 16-15
- "Analyze 2-D Optics with the Fourier Transform" on page 16-19

## **Fourier Transforms**

This topic describes the discrete Fourier transform and its implementations, and introduces an example of basic Fourier analysis for signal processing applications.

#### **Discrete Fourier Transform**

The Fourier transform is a mathematical formula that relates a signal sampled in time or space to the same signal sampled in frequency. For a vector x that has n uniformly sampled points, the following formula defines the discrete Fourier transform (DFT) of x:

$$y_{k+1} = \sum_{j=0}^{n-1} \omega^{jk} x_{j+1}$$

i is the imaginary unit,  $\omega = e^{-2\pi i/n}$  is one of n complex roots of unity, and j and k are indices that run from 0 to n-1. The indices for x and y are shifted by 1 in this formula to reflect vector indices in MATLAB®.

The inverse Fourier transform converts a signal sampled in frequency back to a signal sampled in time or space. The inverse Fourier transform of a vector y with n data points is defined as the following:

$$x_{j+1} = \frac{1}{n} \sum_{k=0}^{n-1} \omega^{-jk} y_{k+1}$$

In signal processing, the Fourier transform can reveal important characteristics of a signal, namely, its frequency components. Modern signal and image processing applications often need to handle signals with millions of discrete data points. To compute each element of y, on the order of  $n^2$  floating-point operations are required. This is not computationally optimal, and the DFT is commonly computed with a faster algorithm.

#### **Fast Fourier Transform**

The fast Fourier transform (FFT) is a computationally efficient implementation of the DFT. While a one-dimensional DFT requires on the order of  $n^2$  floating-point operations

for a vector of n data points, the FFT requires on the order of  $n \log n$  operations, a significant reduction in computational complexity. There are many specialized implementations of the FFT algorithm, such as ones that gain efficiency when n is a power of 2.

In MATLAB®, the fft and ifft functions compute the 1-D fast Fourier transform and inverse transform, respectively. For two-dimensional data, you can compute the 2-D transform and inverse transform using fft2 and ifft2. For higher dimensional arrays, use the fftn and ifftn functions. For any of these FFT implementations, you can also use the fftw function, which optimizes speed based on a heuristic tuning algorithm. The fftshift function shifts the output of a Fourier transform so that the zero-frequency component is in the center, and the ifftshift function reverses this shift. Since the zero-frequency component is always the first element of the output, shifting it to the center can be useful for visualizing the spectrum.

#### **Basic Fourier Analysis**

This example uses the Fourier transform to identify component frequencies in a simple signal.

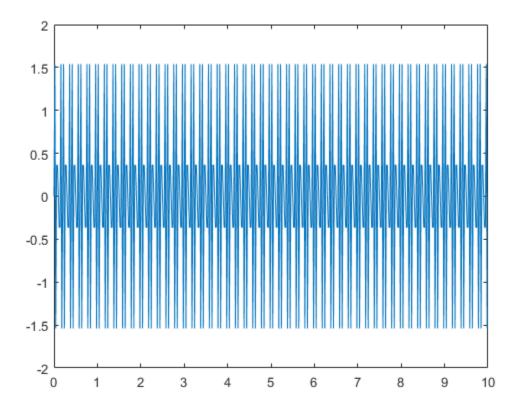
Create a time vector t and a sinusoidal signal x that is a function of t.

```
t = 0:1/50:10-1/50;

x = \sin(2*pi*15*t) + \sin(2*pi*20*t);
```

Plot the signal as a function of time.

```
plot(t,x)
```



Compute the Fourier transform of the signal, and then compute the magnitude  $\boldsymbol{m}$  and phase  $\boldsymbol{p}$  of the signal.

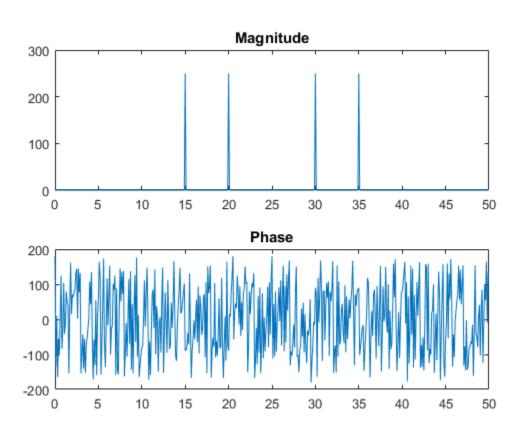
```
y = fft(x);
m = abs(y);
p = angle(y);
```

Compute the frequency vector associated with the signal y, which is sampled in frequency space.

```
f = (0:length(y)-1)*50/length(y);
```

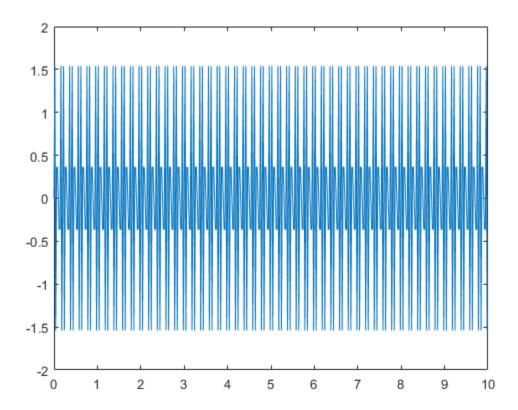
Plot the magnitude and phase of the signal as a function of frequency. The spikes in magnitude correspond to the signal's frequency components.

```
subplot(2,1,1)
plot(f,m)
title('Magnitude')
subplot(2,1,2)
plot(f,rad2deg(p))
title('Phase')
```



Compute and plot the inverse transform of  $\mathcal{Y}$ , which reproduces the original data in x up to round-off error.

```
figure
x2 = ifft(y);
plot(t,x2)
```



# **Basic Spectral Analysis**

This topic introduces frequency and power spectrum analysis of two time-domain signals.

#### In this section...

"Spectral Analysis Quantities" on page 16-7

"Noisy Signal" on page 16-7

"Audio Signal" on page 16-10

### **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	
X	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**

This example computes 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.

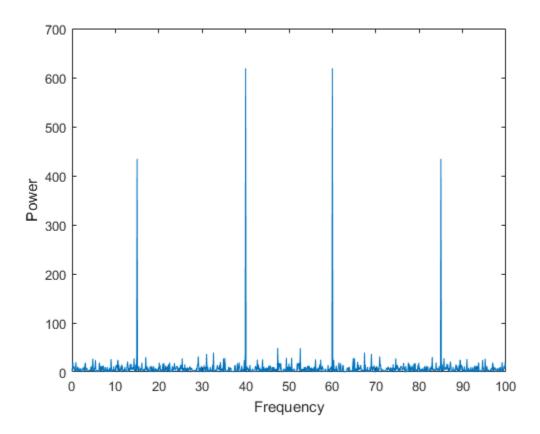
The Fourier transform of the signal identifies its frequency components. In MATLAB®, the fft function computes the Fourier transform using a fast Fourier transform algorithm. Use fft to compute the discrete Fourier transform of the signal.

```
y = fft(x);
```

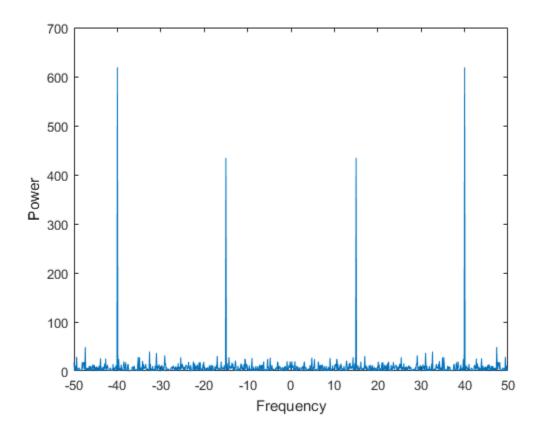
Plot the power spectrum as a function of frequency. While noise disguises a signal's frequency components in time-based space, the Fourier transform reveals them as spikes in power.

```
n = length(x); % number of samples
f = (0:n-1)*(fs/n); % frequency range
power = abs(y).^2/n; % power of the DFT

plot(f,power)
xlabel('Frequency')
ylabel('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.



### **Audio Signal**

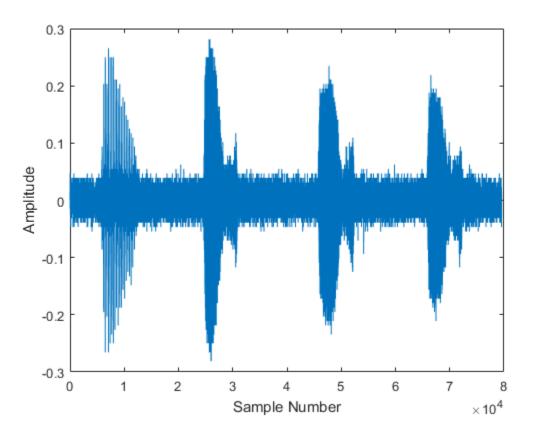
This example analyzes the frequency spectrum of audio data.

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 = fullfile(matlabroot, 'examples', 'matlab', 'bluewhale.au');
[x,fs] = audioread(whaleFile);

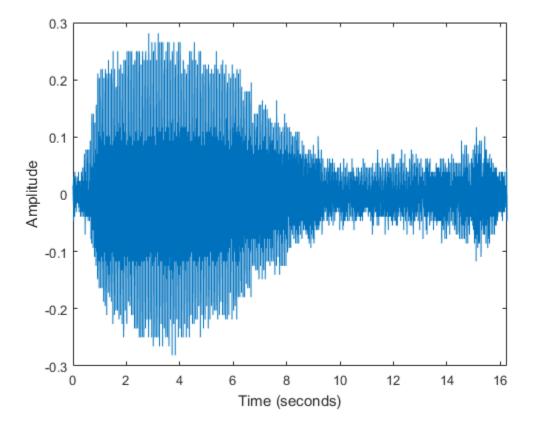
plot(x)
xlabel('Sample Number')
ylabel('Amplitude')
```



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)])
```



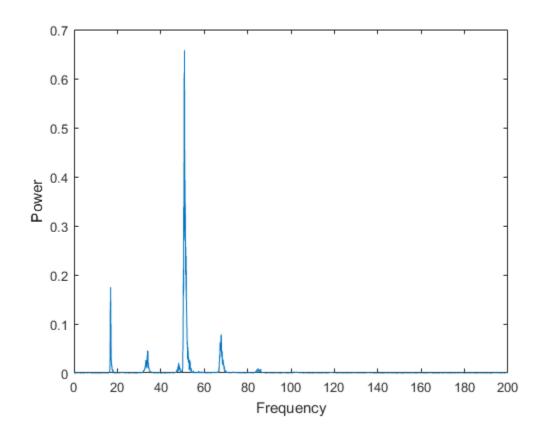
The Fourier transform of the data identifies frequency components of the audio signal. In some applications that process large amounts of data with fft, it is common to resize the input so that the number of samples is a power of 2. This can make the transform computation significantly faster, particularly 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')
```



# Polynomial Interpolation Using FFT

This example shows how to use the fast Fourier transform (FFT) to estimate the coefficients of a trigonometric polynomial that interpolates asteroid orbit data.

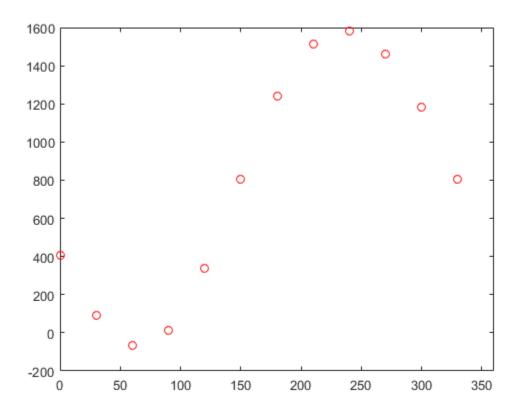
#### **FFT in Mathematics**

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.

$$y = a_0 + a_1 \cos(2\pi(x/360)) + b_1 \sin(2\pi(x/360))$$

$$a_2 \cos(2\pi(2x/360)) + b_2 \sin(2\pi(2x/360))$$

$$\vdots$$

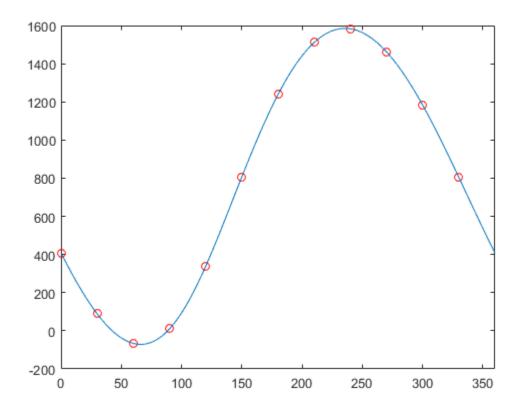
$$a_5 \cos(2\pi(5x/360)) + b_5 \sin(2\pi(5x/360))$$

$$a_6 \cos(2\pi(6x/360))$$

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.

# Analyze 2-D Optics with the Fourier Transform

This topic defines the two-dimensional Fourier transform, and uses the fft2 function to transform a 2-D optical mask into frequency space, revealing its diffraction pattern.

#### **Two-Dimensional Fourier Transform**

The following formula defines the discrete Fourier transform Y of an m-by-n matrix X.

$$Y_{p+1,q+1} = \sum_{j=0}^{m-1} \sum_{k=0}^{n-1} \omega_m^{jp} \omega_n^{kq} X_{j+1,k+1}$$

 $\omega_m$  and  $\omega_n$  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.

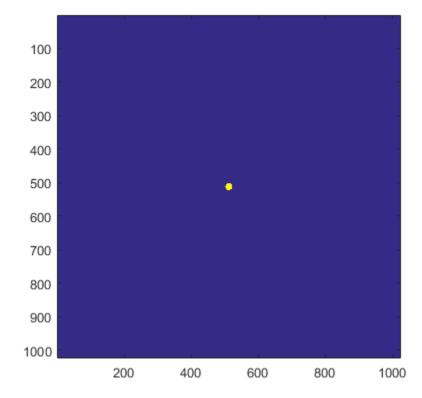
Computing the 2-D Fourier transform of X is equivalent to first computing the 1-D transform of each column of X, and then taking the 1-D transform of each row of the result. In other words, the command fft2(X) is equivalent to Y = fft(fft(X).').'. The ifft2 function computes the 2-D inverse Fourier transform. In general, you can compute the fast Fourier transform of an N-dimensional array with the fftn function and compute the inverse transform with ifftn.

#### 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.

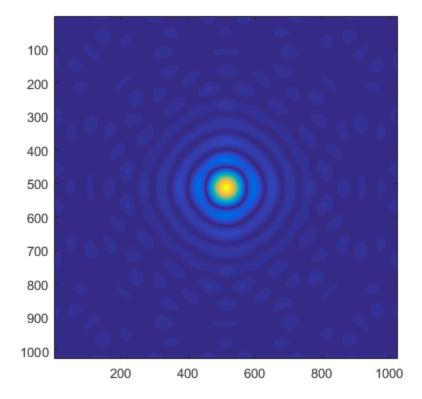
```
n = 2^10;
                           % size of mask
M = zeros(n);
I = 1:n;
x = I - n/2;
                           % mask x-coordinates
y = n/2-I;
                           % mask y-coordinates
[X,Y] = meshgrid(x,y);
                           % create 2-D mask grid
R = 10;
                           % aperture radius
A = (X.^2 + Y.^2 \le R^2); % circular aperture of radius R
M(A) = 1;
                           % set mask elements inside aperture to 1
                           % plot mask
imagesc(M)
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

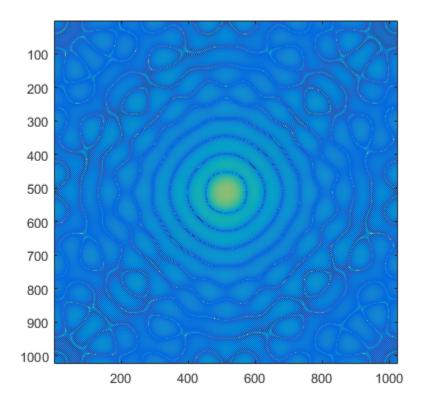
resulting diffraction pattern frequencies. Blue indicates small amplitudes and yellow indicates large amplitudes.

```
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.