# MATLAB® Mathematics

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MATLAB<sup>®</sup> Mathematics

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# **Matrices and Arrays**

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# Matrices and Arrays

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

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"Constructing a Simple Matrix" on page 1-3

"Specialized Matrix Functions" on page 1-4

"Concatenating Matrices" on page 1-6

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"Generating a Numeric Sequence" on page 1-9

#### Overview

. . .

The most basic MATLAB<sup>®</sup> 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
А	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, the string '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:

 $A = [row_1; row_2; \dots; row_n]$ 

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:

A = [12 62 93 -8 22; 16 2 87 43 91; -4 17 -72 95 6] A = 12 62 93 - 8 22 16 2 87 43 91 -4 17 -72 95 6

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 1-52.

For instructions on how to read or overwrite any matrix element, see "Matrix Indexing" on page 1-12.

#### **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,

7 -2 +5	7 - 2 + 5
ans =	ans =
10	10

the next two are *not*:

[7 -2 +5	5]		[7 - 2 + 5]
ans =			ans =
7	-2	5	10

#### **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.
еуе	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.

Function	Description
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 =
        0
                  0
                            0
                                      0
                                                0
                                                          0
        0
                  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 = 

10	12	19	21	3
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];
```

В	=	dia	g(A, -1)				
В	=						
		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:

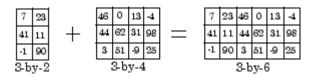
```
A = ones(2, 5) * 6;
                            % 2-by-5 matrix of 6's
                            % 3-by-5 matrix of random values
B = rand(3, 5);
C = [A; B]
                            % Vertically concatenate A and B
C =
    6.0000
              6.0000
                         6.0000
                                    6.0000
                                              6.0000
    6.0000
              6.0000
                         6.0000
                                    6.0000
                                              6.0000
    0.9501
              0.4860
                         0.4565
                                    0.4447
                                              0.9218
```

0.2311	0.8913	0.0185	0.6154	0.7382
0.6068	0.7621	0.8214	0.7919	0.1763

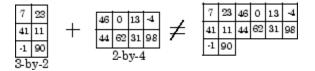
#### **Keeping Matrices Rectangular**

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

T

Function	Description
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 = cat(1, A, B);	% Concatenate along the first dimension
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
             6
        1
        5
   3
             7
   4
        9
              2
B = repmat(A, 2, 4)
B =
   8
        1
             6
                   8
                        1
                             6
                                  8
                                       1
                                            6
                                                 8
                                                      1
                                                           6
   3
        5
             7
                  3
                        5
                             7
                                  3
                                       5
                                            7
                                                 3
                                                      5
                                                           7
             2
                        9
                             2
                                  4
                                       9
                                            2
   4
        9
                   4
                                                 4
                                                      9
                                                           2
   8
        1
              6
                   8
                        1
                             6
                                  8
                                       1
                                            6
                                                 8
                                                      1
                                                           6
```

3	5	7	3	5	7	3	5	7	3	5	7
4	9	2	4	9	2	4	9	2	4	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 = 9 2 0 0 0 0 -5 -6 -9 0 0 -4 -4 -2 

#### **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 increments rather than decrementing. 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

A = 10:5:50 A = 10 15 20 25 30 35 40 45 50

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

A = 3:0.2:3.8 A = 3.0000 3.2000 3.4000 3.6000 3.8000

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

A = 9:-1:1 A = 9 8 7 6 5 4 3 2 1

### **Matrix Indexing**

#### In this section...

"Accessing Single Elements" on page 1-12
"Linear Indexing" on page 1-13
"Functions That Control Indexing Style" on page 1-13
"Accessing Multiple Elements" on page 1-14
"Using Logicals in Array Indexing" on page 1-17
"Single-Colon Indexing with Different Array Types" on page 1-20
"Indexing on Assignment" on page 1-21

#### **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,

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

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

A(4, 2) ans = 14

For arrays with more than two dimensions, specify additional indices following the row and column indices. See the section on "Multidimensional Arrays" on page 1-50.

#### **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

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

is actually stored in memory as the sequence

2, 4, 3, 6, 2, 5, 9, 8, 1

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  $(2-1) \times 3 + 3$ , 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:

#### **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:

B = A;B(1:3:16) = -10B = -10 2 3 -10 5 11 -10 8 9 -10 6 12 - 10 14 15 -10

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

A(:)

ans = . . 

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

1

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
          0
               0.2785
                                0
                                     0.4218
                                                0.0357
    0.1270
                     0
                                0
                                           0
                                                      0
                    0
          0
                          0.4854
                                           0
                                                      0
          0
                     0
                                0
                                           0
                                                      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:

8

1

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

B = isprime(A)B = % Logical indexing A(~B) = 0;A A = find(B) ans = 

#### 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:

 $A = \begin{bmatrix} 1 & 2 & 3; 4 & 5 & 6; 7 & 8 & 9 \end{bmatrix}$   $A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$ 

 $B = logical([0 \ 1 \ 0; \ 1 \ 0 \ 1])$ 

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

#### **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:

n(:)	c{:}	s(:).a
ans =	ans =	ans =
1	1	1
4	ans =	ans =
2	3	2
5	ans =	ans =
3	2	1
6	ans =	ans =
	4	2

# **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.

# **Getting Information About a Matrix**

In this section
"Dimensions of the Matrix" on page 1-22
"Classes Used in the Matrix" on page 1-23
"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:

```
if ndims(A) ~= 2
    return
end
[rows cols] = size(A);
for m = 1:rows
    for n = 1:cols
        x = A(m, n);
        if x >= 5 && x <= 7
            disp(sprintf('A(%d, %d) = %5.2f', m, n, A(m,n)))
        end
    end
end</pre>
```

The code returns the following:

A(1, 3) = 6.15A(3, 1) = 6.07

### **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.

Function	Description
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

"Diminishing the Size of a Matrix" 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 1-7). 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. T

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:
x
y
z
```

#### 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:

A(4,1) A =	= 160			
10	20	30	40	50
60	70	80	90	100
110	120	130	140	150
160	0	0	0	0

**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:

A(4:6,1:3) = magic(3)+100 A =

10	20	30	40	50
60	70	80	90	100
110	120	130	140	150
108	101	106	0	0
103	105	107	0	0
104	109	102	0	0

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:

A(4,8)	= 300						
A =							
10	20	30	40	50	0	0	0
60	70	80	90	100	0	0	0
110	120	130	140	150	0	0	0
0	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}
```

Add a cell to C{3,1} and MATLAB appends an entire row:

$C{3, 1} = \dots$		
<pre>struct('Fund_A',</pre>	.45, 'Fund_E', .35,	'Fund_G', 20);
C =		
'Madison'	' G '	[1x3 double]
[ 46]	'325 Maple Dr'	[3.0153e+003]
[1x1 struct]	[]	[]

**Expanding a Character Array.** 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 a string terminator, you may find that some functions treat the expanded string as if it were less than its full length.

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

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

Closer inspection however reveals string terminators at the point of expansion:

```
uint8(greeting)
ans =
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 =
0
```

### Diminishing the Size of a Matrix

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
                           13
                     З
      5
            11
                   10
                            8
      9
             7
                           12
                     6
      4
            14
                   15
                            1
```

Then, delete the second column of A using

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

This changes matrix A to

A =		
16	3	13
5	10	8
9	6	12
4	15	1

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:

A(2:2:10) = []

results in

A = 16 9 3 6 13 12 1

### **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.

Function	Description
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:

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

**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:

В	=	Α.'		
В	=			
		1	2	3
		4	5	6
		7	8	9
		10	11	12

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 =  $10 \quad 11 \quad 12$   $7 \quad 8 \quad 9$   $4 \quad 5 \quad 6$   $1 \quad 2 \quad 3$ 

Flipping a Matrix. Flip A in a left-to-right direction:

1

2

3

 $B = fliplr(A) \\ B = \\ 10 \quad 7 \quad 4 \\ 11 \quad 8 \quad 5 \\ 12 \quad 9 \quad 6 \\ \end{bmatrix}$ 

### **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,
                                   end;
   % 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.
   evaluate stats(A);
                                    % User-defined function
   % 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 1-35 "Shifting the Location of Matrix Elements" on page 1-35 "Sorting the Data in Each Column" on page 1-37 "Sorting the Data in Each Row" on page 1-37 "Sorting Row Vectors" on page 1-38

## **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 strings 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; 1 <sup>-</sup>	1:18; 2	1:28;	31:38;	41:48]		
A =							
	1 2	2 3	4	5	6	7	8
1	1 12	2 13	14	15	16	17	18
2	1 22	2 23	24	25	26	27	28
3	1 32	2 33	34	35	36	37	38
4	1 42	2 43	44	45	46	47	48
B = c B =	ircshi1	ft(A, [	0, 3])				
	6 7	7 8	1	2	3	4	5
1	6 17	7 18	11	12	13	14	15
2	6 27	7 28	21	22	23	24	25
3	6 37	7 38	31	32	33	34	35
4	6 47	7 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 = 

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	1	73	89	20	74	52
60	82	17	5	19	44	20
48	44	40	35	60	93	67
89	61	93	81	27	46	83
76	79	91	0	19	41	1

Sort each column of A in ascending order:

c = sort(A, 1)с = issorted(c(:, 1)) ans = 

### 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
           74
                  73
                         52
                                23
                                       20
                                               1
    82
           60
                  44
                         20
                                19
                                       17
                                               5
    93
           67
                         48
                                44
                                       40
                                              35
                  60
    93
           89
                  83
                         81
                                61
                                       46
                                              27
    91
           79
                  76
                         41
                                19
                                        1
                                               0
issorted(fliplr(r(1, :)))
ans =
     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
             З
                    7
                            2
                                   4
                                          5
      4
             6
                    3
                            7
                                           5
                                   1
      2
                    6
                            7
                                          3
             1
                                   5
                                   2
     6
             7
                    5
                            1
                                          3
                                   2
      3
             1
                    7
                            4
                                          6
      3
             2
                    1
                            6
                                   5
                                          7
```

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 keeps the elements of each row in its original order, but sorts the entire row of vectors according to the order of the elements in the specified column.

The next example creates a random matrix A:

A=floo A =	r(gall	ery('ur	niformo	lata',∣	[6 7],0	0)*100);
95	45	92	41	13	1	84
23	1	73	89	20	74	52
60	82	17	5	19	44	20
48	44	40	35	60	93	67
89	61	93	81	27	46	83
76	79	91	0	19	41	1

To sort in ascending order based on the values in column 1, you can call sortrows with just the one input argument:

#### sortrows(A)

r =

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

To base the sort on a column other than the first, call sortrows with a second input argument that indicates the column number, column 4 in this case:

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

# **Operating on Diagonal Matrices**

#### In this section ...

"Diagonal Matrix Functions" on page 1-40

"Constructing a Matrix from a Diagonal Vector" on page 1-40

"Returning a Triangular Portion of a Matrix" on page 1-41

"Concatenating Matrices Diagonally" on page 1-41

# **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.
diag	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:

A = diag([12:4:32])

А	-
А	

12	0	0	0	0	0
0	16	0	0	0	0
0	0	20	0	0	0
0	0	0	24	0	0
0	0	0	0	28	0
0	0	0	0	0	32

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
                   1
                          8
           24
                                15
    23
            5
                   7
                         14
                                16
     4
            6
                  13
                         20
                                22
    10
           12
                  19
                         21
                                 3
                          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:

B = tril(A, -1)B = 

A = magic(6);

# **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 1-9 for more information on how this works.

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

#### In this section ...

"Overview" on page 1-42

"The Empty Matrix" on page 1-43

"Scalars" on page 1-45

"Vectors" on page 1-46

### **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 1-43

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 1-45

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 1-46

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
A	0x0	0	double array

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)

#### **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 or 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), ...
all(A), prod(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 =
Empty matrix: 0-by-3
```

#### **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 =
1
false && []
ans =
0
```

**Elementwise Operations.** Unlike the short-circuit operators, all elementwise 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 =
[]
```

**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

ans = 2 size(A) % Check value of row and column dimensions ans = 1 1

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

```
isscalar(A)
ans =
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:

```
A = [5.73 2-4i 9/7 25e3 .046 sqrt(32) 8j];
size(A) % Check value of row and column dimensions
ans =
1 7
```

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
                                                       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 =
 1

# **Full and Sparse Matrices**

#### In this section...

"Overview" on page 1-48

"Sparse Matrix Functions" on page 1-48

### Overview

It is not uncommon to have matrices with a large number of zero-valued elements and, because the MATLAB software stores zeros in the same way it stores any other numeric value, these elements can use memory space unnecessarily and can sometimes require extra computing time.

Sparse matrices provide a way to store data that has a large percentage of zero elements more efficiently. While *full matrices* internally store every element in memory regardless of value, *sparse matrices* store only the nonzero elements and their row indices. Using sparse matrices can significantly reduce the amount of memory required for data storage.

You can create sparse matrices for the double and logical classes. All MATLAB built-in arithmetic, logical, and indexing operations can be applied to sparse matrices, or to mixtures of sparse and full matrices. Operations on sparse matrices return sparse matrices and operations on full matrices return full matrices.

For more information about the computational advantages and construction of sparse matrices, see "Memory Management" on page 4-11 and "Creating Sparse Matrices" on page 4-13.

# **Sparse Matrix Functions**

This table shows some of the functions most commonly used when working with sparse matrices.

Function	Description
full	Convert a sparse matrix to a full matrix.
issparse	Determine if a matrix is sparse.

Function	Description
nnz	Return the number of nonzero matrix elements.
nonzeros	Return the nonzero elements of a matrix.
nzmax	Return the amount of storage allocated for nonzero elements.
spalloc	Allocate space for a sparse matrix.
sparse	Create a sparse matrix or convert full to sparse.
speye	Create a sparse identity matrix.
sprand	Create a sparse uniformly distributed random matrix.

# **Multidimensional Arrays**

#### In this section...

"Overview" on page 1-50 "Creating Multidimensional Arrays" on page 1-52 "Accessing Multidimensional Array Properties" on page 1-56 "Indexing Multidimensional Arrays" on page 1-56 "Reshaping Multidimensional Arrays" on page 1-60 "Permuting Array Dimensions" on page 1-62 "Computing with Multidimensional Arrays" on page 1-64 "Organizing Data in Multidimensional Arrays" on page 1-65 "Multidimensional Cell Arrays" on page 1-67 "Multidimensional Structure Arrays" on page 1-68

# Overview

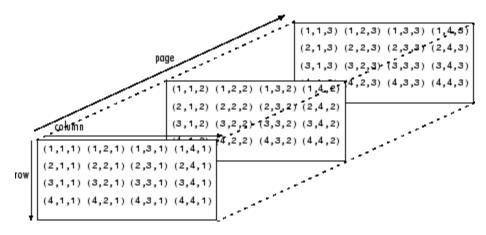
An array having more than two dimensions is called a multidimensional array in the MATLAB application. Multidimensional arrays in MATLAB are an extension of the normal two-dimensional matrix. Matrices have two dimensions: the row dimension and the column dimension.

	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)

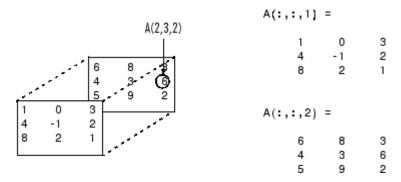
You can access a two-dimensional matrix element with two subscripts: the first representing the row index, and the second representing the column index.

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

T

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 two-dimensional matrices. In addition, MATLAB provides a special concatenation function that is useful for building multidimensional arrays.

This section discusses

- "Generating Arrays Using Indexing" on page 1-52
- "Extending Multidimensional Arrays" on page 1-53
- "Generating Arrays Using MATLAB Functions" on page 1-54
- "Building Multidimensional Arrays with the cat Function" on page 1-54

#### **Generating Arrays Using Indexing**

One way to create a multidimensional array is to create a two-dimensional array and extend it. For example, begin with a simple two-dimensional array A.

A = [5 7 8; 0 1 9; 4 3 6];

A is a 3-by-3 array, that is, its row dimension is 3 and its column dimension is 3. To add a third dimension to A,

 $A(:,:,2) = [1 \ 0 \ 4; \ 3 \ 5 \ 6; \ 9 \ 8 \ 7]$ 

MATLAB responds with

A(:,:,1) =

5	7	8
0	1	9
4	3	6
A(:,:,2)	=	
1	0	4
3	5	6
9	8	7

You can continue to add rows, columns, or pages to the array using similar assignment statements.

#### **Extending Multidimensional Arrays**

To extend A in any dimension:

- Increment or add the appropriate subscript and assign the desired values.
- Assign the same number of elements to corresponding array dimensions. For numeric arrays, all rows must have the same number of elements, all pages must have the same number of rows and columns, and so on.

You can take advantage of the MATLAB scalar expansion capabilities, together with the colon operator, to fill an entire dimension with a single value:

A(:,:,3) = 5; A(:,:,3) ans = 5 5 5 5 5 5 5 5 5 5 5 5

To turn A into a 3-by-3-by-3-by-2, four-dimensional array, enter

 Note that after the first two assignments MATLAB pads A with zeros, as needed, to maintain the corresponding sizes of dimensions.

#### **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) =B(:,:,2) = 

**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:

```
B = cat(3, [2 8; 0 5], [1 3; 7 9])
B(:,:,1) = 2 8 0 5
B(:,:,2) = 1 3 7 9
```

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-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

### **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.

size(C)
ans =
 2 2 1 2
rows columns dim3 dim4

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

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

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

whos Name	Size	Bytes	Class
A B C	2x2x2 2x2x2 4-D	64 64 64	double array double array double array
D	4 - D	192	double array

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)

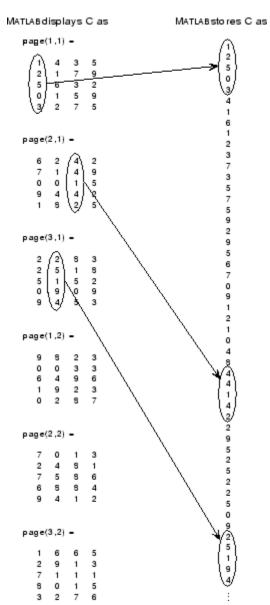
Now assign a 2-by-2 subset of array nddata to the four elements in the center of C.

```
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 1-13 for an introduction to this topic.

1



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

ans = 0

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,

C(3,2,1,1,1,1,1,1,1)

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 respecifying 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 ...])

s1, s2, 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).

м								r	es	hap	e(M,	, [6 ]	5])
			9 3 6	7 5 9	8 8 4	5 5 3	2 1 3		1 9 8 2	3 6 5 4	5 7 2 9	7 5 9 8	5 5 3 2
1 2 9 0 8 1	3 6 5	4 3 0	5 7 2		• • · •				0	3 0	3 6	8 4	1 3

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.

c	reshape(C, [6 2])
9 10	1 6
11 12	3 8
5 0	2 9
7 8	4 11
1 2	5 10
3 4	7 12

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 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:

```
C = squeeze(B);
size(C)
ans =
2 3 4
```

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

# **Permuting Array Dimensions**

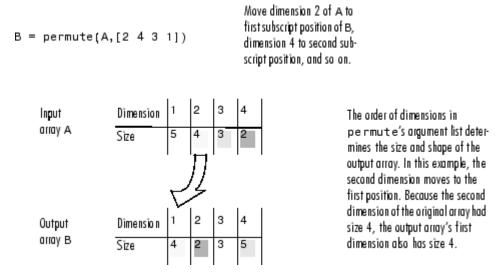
The permute function reorders the dimensions of an array:

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.

Α			B = perm	3])	C = permute(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)	=		lefelbed.
A(:,:,2)	=		B(:,:,2)	=		transposition).				
						nunsposinon).	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.



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 \*,  $\uparrow$ ,  $\backslash$ , 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:

 $A = cat(3, [1 2 3; 9 8 7; 4 6 5], [0 3 2; 8 8 4; 5 3 5], \dots \\ [6 4 7; 6 8 5; 5 4 3]);$ 

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.

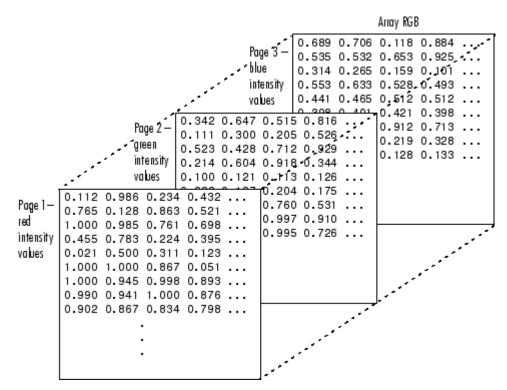
# **Organizing Data in Multidimensional Arrays**

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 four-dimensional 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.



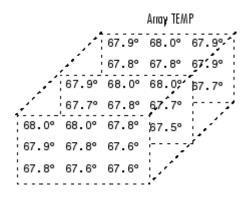
To access an entire plane of the image, use

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,:);

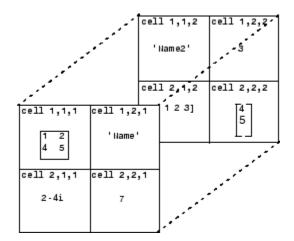
# **Multidimensional Cell Arrays**

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);

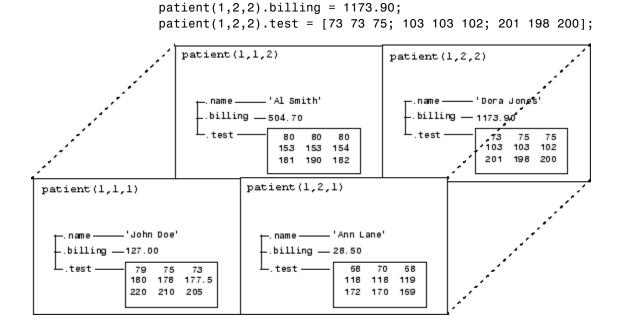
The subscripts for the cells of  ${\tt C}$  look like



# **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';
```



### **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]);
```

1

# **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.

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 Create a Matrix** 

### 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.

### Functions to Modify the Shape of a Matrix (Continued)

Function	Description
flipud	Flip a matrix about a horizontal axis.
reshape	Change the dimensions of a matrix.
rot90	Rotate a matrix by 90 degrees.
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 characters or strings.
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.

### **Functions to Determine Class (Continued)**

Function	Description
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.
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.

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

## Functions for Working with Multidimensional Arrays

# 2

# Linear Algebra

- "Matrices in the MATLAB Environment" on page 2-2
- "Systems of Linear Equations" on page 2-12
- "Inverses and Determinants" on page 2-25
- "Factorizations" on page 2-30
- "Powers and Exponentials" on page 2-39
- "Eigenvalues" on page 2-43
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# **Matrices in the MATLAB Environment**

### In this section...

"Creating Matrices" on page 2-2
"Adding and Subtracting Matrices" on page 2-4
"Vector Products and Transpose" on page 2-4
"Multiplying Matrices" on page 2-6
"Identity Matrix" on page 2-8
"Kronecker Tensor Product" on page 2-9
"Vector and Matrix Norms" on page 2-10
"Using Multithreaded Computation with Linear Algebra Functions" on page 2-11

# **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<sup>TM</sup> 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:

A = pascal(3)

A =

1	1	1
1	2	3
1	3	6

The second example is not symmetric:

В	=	magic(3)			
в	=				
		8	1		6
		3	5		7
		4	9		2

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

```
C = fix(10*rand(3,2))
C =
9 4
2 8
6 7
```

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:

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

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 =
        9
               2
                     7
        4
              7
                     10
        5
              12
                     8
Y = X - A
Y =
        8
               1
                     6
        3
               5
                      7
        4
               9
                      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 plus
Matrix dimensions must agree.
w = v + s
w = 9 7 6
```

# **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
```

 $\begin{array}{c} x = \\ 2 \\ X = u^* v \\ X = \\ 6 & 0 & -3 \\ 2 & 0 & -1 \\ 8 & 0 & -4 \end{array}$ 

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 1 5 6 7

Transposition turns a row vector into a column vector:

4

9

2

If x and y are both real column vectors, the product  $x^{\star}y$  is not defined, but the two products

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 + 2.0000i7.0000 - 3.0000i 3.0000 + 4.0000i 6.0000 - 2.0000i 0 + 9.0000i 4.0000 + 7.0000i then 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

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

2-6

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
       26
                     26
              38
       41
              70
                     39
Y = B*A
Y =
       15
              28
                     47
       15
              34
                     60
       15
              28
                     43
```

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

```
u = [3; 1; 4];
x = A*u
x =
8
```

 $17 \\
 30 \\
 v = [2 \ 0 \ -1]; \\
 y = v*B \\
 y = \\
 12 \ -7 \ 10$ 

Rectangular matrix multiplications must satisfy the dimension compatibility conditions:

C = fix(10\*rand(3,2)); X = A\*C X = 17 19 31 41 51 70 Y = C\*A Error using mtimes

Inner matrix dimensions must agree.

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

2-8

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:

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

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

Х =

1 2 3 4

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

kron(X,I)

and

kron(I,X)

are

1	0	2	0
0	1	0	2
3	0	4	0
0	3	0	4

and

Linear Algebra

1	2	0	0
3	4	0	0
0	0	1	2
0	0	3	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.

# **Systems of Linear Equations**

### In this section ...

"Computational Considerations" on page 2-12

"General Solution" on page 2-14

"Square Systems" on page 2-14

"Overdetermined Systems" on page 2-17

"Underdetermined Systems" on page 2-21

"Using Multithreaded Computation with Systems of Linear Equations" on page 2-23

"Iterative Methods for Solving Systems of Linear Equations" on page 2-23

# **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*,  $\setminus$ , 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  $x = A \setminus b$  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 > n	Overdetermined system. Find a least-squares solution.
m < n	Under determined system. Find a basic solution with at most $\boldsymbol{m}$ 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:

- 1 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  ${\sf A}$  and a single right side column vector  ${\sf b}.$ 

### **Nonsingular Coefficient Matrix**

If the matrix A is nonsingular, the solution, x = A 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\b
X =
19 -3 -1
-17 4 13
6 0 -6
```

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\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:

А	=	[1	3	7
		- 1	4	4
		1	10	18 ]

is singular, as you can verify by typing

rank(A)

ans =

2

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

**Note** For information about using pinv to solve systems with rectangular coefficient matrices, see "Pseudoinverses" on page 2-26.

**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

rref([A b]) ans = 1.0000 0 2.2857 0 0 1.0000 1.5714 0 0 0 0 1.0000

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  $\exp(-t)$ . The unknown coefficients,  $c_1$  and  $c_2$ , can be computed by doing a least-squares fit, which minimizes the sum of the squares of the deviations of the data from the model. There are six equations in two unknowns, represented by a 6-by-2 matrix.

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

E =

1.0000	1.0000
1.0000	0.7408
1.0000	0.4493
1.0000	0.3329
1.0000	0.2019
1.0000	0.1003

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

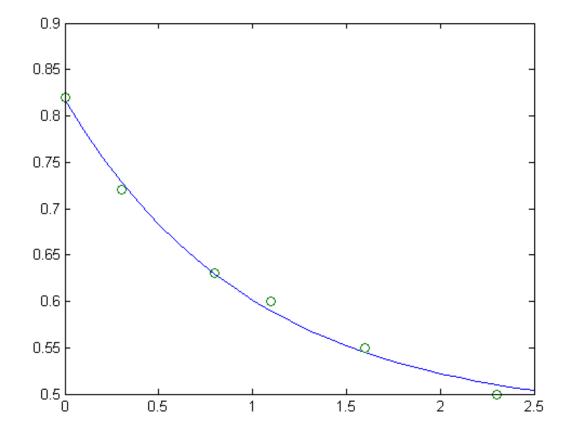
c = E\y c = 0.4760 0.3413

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.

2-20

## **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:

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

rng(0);

b = randi(8,2,1)

<math display="block">R = \frac{6 \ 8 \ 7 \ 3}{3 \ 5 \ 4 \ 1}

b = \frac{7}{8}
```

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

```
format rat
p = R\b
p =
0
17/7
0
-29/7
```

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

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

Z = null(R, 'r') Z = -1/2 -7/6 -1/2 1/2

1

0

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:

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

To illustrate, choose an arbitrary q and construct x.

0

1

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

#### lsqr

LSQR Method

#### minres

Minimum Residual Method. This method is appropriate for Hermitian coefficient matrix A.

#### qmr

Quasi-Minimal Residual Method

#### symmlq

Symmetric LQ Method

#### tfqmr

Transpose-Free QMR Method

# **Inverses and Determinants**

#### In this section...

"Introduction" on page 2-25

"Pseudoinverses" 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:

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

```
A =
        1
                1
                       1
        1
                2
                       3
        1
                3
                       6
d = det(A)
X = inv(A)
d =
        1
X =
        3
               -3
                       1
       - 3
                5
                      -2
        1
               -2
                       1
```

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

B = magic(3)

В =				
	8	1	6	
	3	5	7	
	4	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:

The matrix

Q = X\*C Q = 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:

 $A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \\ 10 & 11 & 12 \end{bmatrix};$ 

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. x = 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. z = -0.8594 1.3438 -0.6875

# **Factorizations**

#### In this section...

"Introduction" on page 2-30

"Cholesky Factorization" on page 2-30

"LU Factorization" on page 2-32

"QR Factorization" on page 2-33

"Using Multithreaded Computation for Factorization" on page 2-37

## 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 offdiagonal 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	1	1	1
1	2	3	4	5	6

1	3	6	10	15	21
1	4	10	20	35	56
1	5	15	35	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

R = chol(A)

<b>D</b>	_
к	=

1	1	1	1	1	1
0	1	2	3	4	5
0	0	1	3	6	10
0	0	0	1	4	10
0	0	0	0	1	5
0	0	0	0	0	1

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:

2-32

	1.0000	0	0
	0.3750	0.5441	1.0000
	0.5000	1.0000	0
U =			
	8.0000	1.0000	6.0000
	0	8.5000	-1.0000
	0	0	5.2941

The LU factorization of A allows the linear system

A\*x = b

to be solved quickly with

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

Determinants and inverses are computed from the LU factorization using

det(A) = det(L)\*det(U)

and

inv(A) = inv(U) \* inv(L)

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

## **QR** Factorization

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

Q'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	-0.5564	0.6869	-0.1478	-0.2008
0.3167	0.6676	0.1351	-0.1729	-0.6370
0.5808	-0.2410	-0.4695	0.5792	-0.2207

1.5346 1.0663 1.	2010 1.403	6
------------------	------------	---

0	0.7245	0.3474	-0.0126
0	0	0.9320	0.6596
0	0	0	0.6648
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:

0.6191	0.1406	-0.1899	-0.5058
0.1506	0.4084	0.5034	0.5974
0.3954	-0.5564	0.6869	-0.1478
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 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 -0.7044 -0.5285 -0.4739 -0.6163 0.1241 0.7777 R = -8.2762 -11.3578 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:

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

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

```
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.

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

# **Powers and Exponentials**

#### In this section...

"Positive Integer Powers" on page 2-39

"Inverse and Fractional Powers" on page 2-39

"Element-by-Element Powers" on page 2-40

"Exponentials" on page 2-40

## **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 1 2 3 1 3 6  $X = A^2$ X = 3 10 6 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:

 $X = A.^{2}$ 

A =			
	1	1	1
	1	4	9
	1	9	36

## **Exponentials**

The function

sqrtm(A)

computes  $A^{(1/2)}$  by a more accurate algorithm. The m in sqrtm distinguishes this function from sqrt(A), which, like A.<sup>(1/2)</sup>, 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

expm(A)

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).

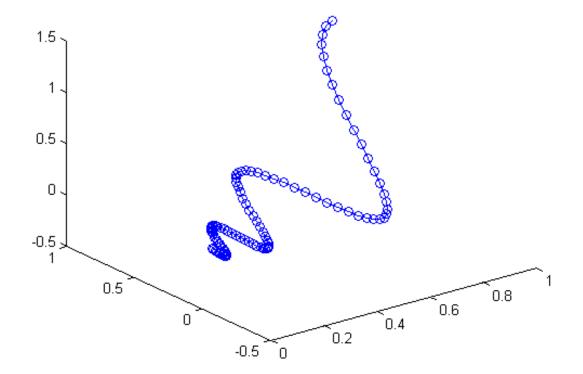
```
x0 = [1 1 1]'
x0 =
1
1
1
```

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,:),'-o')
```



# **Eigenvalues**

#### In this section...

"Eigenvalue Decomposition" on page 2-43

"Multiple Eigenvalues" on page 2-44

"Schur Decomposition" on page 2-45

## **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:

A =		
0	- 6	- 1
6	2	-16
- 5	20	- 10

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 -0.2110 - 0.6447i -0.3553 -0.2110 + 0.6447i -0.4248 -0.6930 -0.6930 D = -3.0710 0 0 0 -2.4645+17.6008i 0 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  $V^D^i V$ , which can be written more succinctly as  $V^D/V$ , is within round-off error of A. And,  $inv(V)^A*V$ , or  $V\setminus A*V$ , is within round-off error of D.

## **Multiple Eigenvalues**

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

A	=	[6	12	19	
		- 9	- 20	-33	
		4	9	15	]

For this matrix

[V,D] = eig(A)produces V = -0.4741-0.4082-0.40820.8127 0.8165 0.8165 -0.3386 -0.4082-0.4082 D = -1.0000 0 0 0 1.0000 0 0 0 1.0000

There is a double eigenvalue at  $\lambda = 1$ . The second and third 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.

## **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

 $Av = \sigma u$  $A'u = \sigma v.$ 

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 have

$$AV = U\Sigma$$
$$A'U = V\Sigma$$

Since U and V are orthogonal, this becomes the singular value decomposition

$$A = U\Sigma V'.$$

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

4 8 7

А	=		
		9	
		6	
		2	

the full singular value decomposition is

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

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

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

U =

0.6105	-0.7174
0.6646	0.2336
0.4308	0.6563

S = 14.9359 0 0 5.1883

V =

0.6925	-0.7214
0.7214	0.6925

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

# 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 3-15
- "Managing the Global Stream" on page 3-17
- "Creating and Controlling a Random Number Stream" on page 3-24
- "Multiple streams" on page 3-32
- "Replace Discouraged Syntaxes of rand and randn" on page 3-35

# **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 can be useful in testing or diagnostic situations.

Although repeatability can be useful, it is possible to accidentally repeat your results 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, randn, randi, or randperm to ensure that you do not repeat a result from a previous MATLAB session.

There also can be situations in which you want to repeat a result that you got at the start of a MATLAB session, but you do not want to restart to do it. You can reset the generator to the startup state at any time in a MATLAB session:

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

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

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

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

See Also

rng

# **Create Arrays of Random Numbers**

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	<ul> <li>"Random Numbers within a Specific Range" on page 3-6</li> <li>"Random Integers" on page 3-7</li> <li>"Random Numbers from Normal Distribution with Specific Mean and Variance" on page 3-8</li> </ul>
Concepts	• "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.

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

```
r_range =
-10 10
```

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

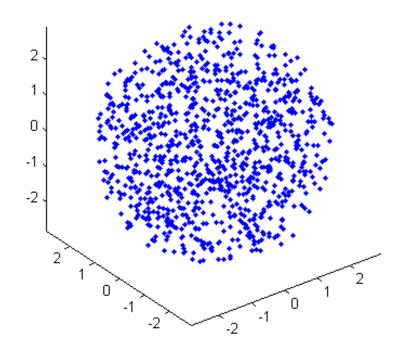
azimuth = 2\*pi\*rand(1000,1);

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.

A = rand(3,3)

A =

0.5388	0.2045	0.6705
0.4192	0.8781	0.4173
0.6852	0.0274	0.5587

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

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

rng(1); A = rand(3,3) A = 0.4170 0.3023 0.1863 0.7203 0.1468 0.3456 0.0001 0.0923 0.3968

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

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

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

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

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

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

### Save and Restore the Generator Settings

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

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, A, of random integer values between 1 and 10.

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

A =

5	4	2
8	2	4
1	1	4

Repeat the same command.

A = randi(10,3,3)

A =

6	3	7
5	9	5
7	1	6

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  $\boldsymbol{s},$  and reproduce the first array,  $\boldsymbol{A}.$ 

rng(s); A = randi(10,3,3) A = 5 4 2 8 2 4 1 1 4

	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
Concepts	• "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
Concepts	<ul> <li>"Random Numbers in MATLAB" on page 3-2</li> <li>"Specifying Startup Options in MATLAB Startup File"</li> </ul>

### **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:

```
get(globalStream)

Type: 'mt19937ar'

NumStreams: 1

StreamIndex: 1

Substream: 1

Seed: 0

State: [625x1 uint32]

NormalTransform: 'Ziggurat'

Antithetic: 0

FullPrecision: 1
```

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 <code>RandStream</code> class. Static methods are indicated with the <code>syntax</code> <code>RandStream.methodName</code>.

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	

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.
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'.

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

Property	Description
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 =
1
```

### **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**

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.

```
RandStream.setGlobalStream(myStream)
RandStream.getGlobalStream
```

ans =

mlfg6331\_64 random stream (current global stream) Seed: O NormalTransform: Ziggurat

RandStream.getGlobalStream==myStream

```
ans =
1
```

### **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 3-26 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.

Keyword	Generator	Multiple Stream and Substream Support	Approximate Period In Full Precision
mt19937ar	Mersenne twister (default)	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	$2^{127}$
shr3cong	Shift-register generator summed with linear congruential generator	No	2 <sup>64</sup>
swb2712	Modified subtract with borrow generator	No	2 <sup>1492</sup>

### **Generator algorithms**

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 generator (mt19937ar) is 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 [10] for an example).

### **Generator Algorithms**

#### mcg16807

A 32-bit multiplicative congruential generator, as described in [11], 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 [8], 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 [5], but with the mlfg6331\_64 generator underneath.

#### mrg32k3a

A 32-bit combined multiple recursive generator, as described in [3]. This generator is similar to the CMRG implemented in the RngStreams package. It has a period of  $2^{127}$ , and supports up to  $2^{63}$  parallel streams, via sequence splitting, and  $2^{51}$  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 [5], but with the mrg32k3a generator underneath.

#### mt19937ar

The Mersenne Twister, as described in [9], with Mersenne prime  $2^{19937} - 1$ . This is the generator documented at http://www.math.sci.hiroshima-u.ac.jp/~m-mat/MT/emt.html. It has a period of  $2^{19937} - 1$ . Each U(0,1) value is created using two 32-bit integers from the generator; the possible values are all multiples of  $2^{-53}$  strictly within 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 [5], 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 using rand('twister',s).

#### 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 [5]) 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 [7], 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 [4] (1999) differs from the one used in [5] (2000). MATLAB uses the most recent version of the generator, presented in [5].

swb2712

A modified Subtract-with-Borrow generator, as described in [6]. 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 [5], 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 [5]. Approximately 2.02 uniform values are consumed per normal value, on average.

### References

[1] Devroye, L. Non-Uniform Random Variate Generation, Springer-Verlag, 1986.

[2] L'Ecuyer, P. and R. Simard. "TestU01: A C Library for Empirical Testing of Random Number Generators," *ACM Transactions on Mathematical Software*, 33(4): Article 22. 2007.

[3] L'Ecuyer, P., R. Simard, E. J. Chen, and W. D. Kelton. "An Objected-Oriented Random-Number Package with Many Long Streams and Substreams." *Operations Research*, 50(6):1073–1075. 2002.

[4] Marsaglia, G. "Random numbers for C: The END?" Usenet posting to sci.stat.math. 1999. Available online at http://groups.google.com/group/sci.crypt/browse\_thread/ thread/ca8682a4658a124d/.

[5] Marsaglia G., and W. W. Tsang. "The ziggurat method for generating random variables." *Journal of Statistical Software*, 5:1–7. 2000. Available online at http://www.jstatsoft.org/v05/i08.

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[7] Marsaglia, G., and W. W. Tsang. "A fast, easily implemented method for sampling from decreasing or symmetric unimodal density functions." *SIAM J.Sci.Stat.Comput.* 5(2):349–359. 1984.

[8] Mascagni, M., and A. Srinivasan. "Parameterizing Parallel Multiplicative Lagged-Fibonacci Generators." *Parallel Computing*, 30: 899–916. 2004.

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[10] Moler, C.B. *Numerical Computing with MATLAB*. SIAM, 2004. Available online at http://www.mathworks.com/moler

[11] 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.

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.

```
r1=rand(s1,10000,1);
r2=rand(s2,100000,1);
r3=rand(s3,100000,1);
corrcoef([r1,r2,r3])
```

ans =

1.0000	0.0030	0.0045
0.0030	1.0000	-0.0015
0.0045	-0.0015	1.0000

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 3-26 for a summary of generator properties.

# **Replace Discouraged Syntaxes of rand and randn**

### In this section...

"Description of the Former Syntaxes" on page 3-35

"Description of Replacement Syntaxes" on page 3-36

"Replacement Syntaxes for Initializing the Generator with an Integer Seed" on page 3-36

"Replacement Syntaxes for Initializing the Generator with a State Vector" on page 3-37

"If You Are Unable to Upgrade from Former Syntax" on page 3-38

### **Description of the Former 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 will be removed in a future release for the following reasons:

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

To assess the impact this change will have on 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 to replace the former syntaxes, take a few moments to understand what the former syntaxes did. This should help you to see which new rng syntax best suits your needs.

The first input to the former syntaxes of 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 former 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 former syntax with rand and randn.
- The second column shows how to exactly reproduce the former 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.

Former rand/randn Syntax	Not Recommended: Reproduce Former Behavior Exactly By Specifying Generator Type	Recommended Alternative: Does Not Override Generator Type
rand('twister',5489)	<pre>rng(5489,'twister')</pre>	<pre>rng('default')</pre>
rand('seed',sd)	ppg(cd_lv4l)	and (cd)
randn('seed',sd)	rng(sd,'v4')	
rand('state',sd)	<pre>rng(sd,'v5uniform') rng(sd,'v5normal')</pre>	
randn('state',sd)		
<pre>rand('seed',sum(100*clock))</pre>	<pre>rng(sum(100*clock),'v4')</pre>	<pre>rng('shuffle')</pre>

# Replacement Syntaxes for Initializing the Generator with a State Vector

The most common use of the state vector (shown here as st) in the previous 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 former 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.

Former Syntax Using rand/randn	New Syntax Using rng
% Save v5 generator state. st = rand('state');	% Get generator settings. s = rng;
% Call rand. x = rand;	% Call rand. x = rand;
% Restore v5 generator state. rand('state',st);	<pre>% Restore previous generator % settings. rng(s);</pre>
% 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 Former Syntax

If there is code that you are not able or not permitted to modify and you know that it uses the former 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**

- "Function Summary" on page 4-2
- "Computational Advantages" on page 4-11
- "Constructing Sparse Matrices" on page 4-13
- "Accessing Sparse Matrices" on page 4-19
- "Sparse Matrix Operations" on page 4-26
- "Selected Bibliography" on page 4-50

# **Function Summary**

#### In this section ...

"Functions That Support Sparse Matrices" on page 4-2

"Functions That Do Not Support Sparse Matrices" on page 4-5

"Functions with Sparse Alternatives" on page 4-10

### **Functions That Support Sparse Matrices**

Sparse matrix functions are located in the MATLAB sparfun directory. For a complete list, brief descriptions, and links to reference pages, type:

help sparfun

Sparse matrix functions fall into the following categories:

- "Elementary Sparse Matrices" on page 4-2
- "Full to Sparse Conversion" on page 4-3
- "Working with Sparse Matrices" on page 4-3
- "Graph Theory" on page 4-4
- "Reordering Algorithms" on page 4-4
- "Linear Algebra" on page 4-4
- "Linear Equations (Iterative Methods)" on page 4-5
- "Other Miscellaneous Functions" on page 4-5

#### **Elementary Sparse Matrices**

Function	Description
speye	Sparse identity matrix
sprand	Sparse uniformly distributed random matrix
sprandn	Sparse normally distributed random matrix

Function	Description
sprandsym	Sparse random symmetric matrix
spdiags	Sparse matrix formed from diagonals

### Full to Sparse Conversion

Function	Description
sparse	Create sparse matrix
full	Convert sparse matrix to full matrix
find	Find indices of nonzero elements
spconvert	Import from sparse matrix external format

### Working with Sparse Matrices

Function	Description
nnz	Number of nonzero matrix elements
nonzeros	Nonzero matrix elements
nzmax	Amount of storage allocated for nonzero matrix elements
spones	Replace nonzero sparse matrix elements with ones
spalloc	Allocate space for sparse matrix
issparse	True for sparse matrix
spfun	Apply function to nonzero matrix elements
spy	Visualize sparsity pattern

### **Graph Theory**

Function	Description
gplot	Plot graph, as in "graph theory"
etree	Elimination tree
etreeplot	Plot elimination tree
treelayout	Lay out tree or forest
treeplot	Plot picture of tree

### **Reordering Algorithms**

Function	Description
colamd	Column approximate minimum degree permutation
symamd	Symmetric approximate minimum degree permutation
symrcm	Symmetric reverse Cuthill-McKee permutation
colperm	Column permutation
randperm	Random permutation
dmperm	Dulmage-Mendelsohn permutation

### Linear Algebra

Function	Description
eigs	A few eigenvalues
svds	A few singular values
ilu	Incomplete LU factorization
ichol	Incomplete Cholesky factorization
normest	Estimate the matrix 2-norm
condest	1-norm condition number estimate
sprank	Structural rank

Function	Description
bicg	Biconjugate gradients method
bicgstab	Biconjugate gradients stabilized method
bicgstabl	Biconjugate gradients stabilized(l) method
cgs	Conjugate gradients squared method
gmres	Generalized minimum residual method
lsqnonneg	Solve nonnegative least-squares constraints problem
lsqr	LSQR method
minres	Minimum residual method
pcg	Preconditioned conjugate gradients method
qmr	Quasi-minimal residual method
tfqmr	Transpose-free quasi-minimal residual method
symmlq	Symmetric LQ method

#### **Linear Equations (Iterative Methods)**

#### **Other Miscellaneous Functions**

Function	Description
spaugment	Form least squares augmented system
spparms	Set parameters for sparse matrix routines
symbfact	Symbolic factorization analysis

### **Functions That Do Not Support Sparse Matrices**

- "Elementary Matrices and Arrays" on page 4-6
- "Elementary Math Functions" on page 4-6
- "Bit-Wise Functions" on page 4-7

- "Eigenvalue and Singular Value Functions" on page 4-7
- "Matrix Analysis Functions" on page 4-8
- "Factorization Functions" on page 4-8
- "Linear Equation Functions" on page 4-8
- "Special Functions" on page 4-8
- "Filtering and Convolution Functions" on page 4-9
- "Fourier Transform Functions" on page 4-9
- "Histogram Plotting Functions" on page 4-9

These built-in functions do not accept sparse matrices as input.

#### **Elementary Matrices and Arrays**

Function	Description
rand	Uniformly distributed pseudorandom numbers

#### **Elementary Math Functions**

#### **Complex Functions.**

Function	Description
complex	Construct complex data from real and imaginary components

#### **Real Array Exponential Functions.**

Function	Description
reallog	Natural logarithm for nonnegative real arrays
realpow	Array power for real-only output
realsqrt	Square root for nonnegative real arrays

### **Bit-Wise Functions**

Function	Description			
bitand	Bitwise AND			
bitcmp	Bitwise complement			
bitget	Bit at specified position			
bitmax	Maximum double-precision floating-point integer			
bitor	Bitwise OR			
bitset	Set bit at specified position			
bitshift	Shift bits specified number of places			
bitxor	Bitwise XOR			

# **Eigenvalue and Singular Value Functions**

Function	Description		
hess	Hessenberg form of matrix		
ordeig	Eigenvalues of quasitriangular matrices		
ordqz	Reorder eigenvalues in QZ factorization		
ordschur	Reorder eigenvalues in Schur factorization		
schur	Schur decomposition		
svd	Singular value decomposition		

### **Matrix Analysis Functions**

Function	Description		
cond	Condition number with respect to inversion		
null	Null space		
orth	Range space of matrix		
rcond	Matrix reciprocal condition number estimate		

### **Factorization Functions**

Function	Description		
cholupdate	Rank 1 update to Cholesky factorization		
gsvd	Generalized singular value decomposition		
qz	QZ factorization for generalized eigenvalues		

#### **Linear Equation Functions**

Function	Description		
linsolve	Solve linear system of equations		
pinv	Moore-Penrose pseudoinverse of matrix		

#### **Special Functions**

Function	Description		
airy	Airy functions		
besselh	Bessel function of third kind (Hankel function)		
besseli	Modified Bessel function of first kind		
besselj	Bessel function of first kind		
besselk	Modified Bessel function of second kind		

Function	Description		
bessely	Bessel function of second kind		
erfc	Error function		
erf	Error function		
erfcx	Error function		
gamma	Gamma function		
gammaln	Gamma function		
psi	Psi (polygamma) function		

### **Filtering and Convolution Functions**

Function	Description	
conv2	2-D convolution	
convn	N-D convolution	
filter	1-D digital filter	
filter2	2-D digital filter	

### **Fourier Transform Functions**

Function	Description		
fft	Discrete Fourier transform		
fftn	N-D discrete Fourier transform		
ifft	Inverse discrete Fourier transform		
ifftn	N-D inverse discrete Fourier transform		

#### **Histogram Plotting Functions**

Function	Description
histc	Histogram count

# **Functions with Sparse Alternatives**

These functions do not accept sparse inputs, but you can use other functions in their place.

Function	Replacement Function Supporting Sparse Inputs		
cond	Use condest instead.		
eig	Syntax d = eig(S) accepts a sparse symmetric matrix S. Otherwise, use eigs in place of eig.		
norm(S,2)	Use normest for the 2-norm of a sparse matrix S.		
svd	Use svds instead.		

# **Computational Advantages**

#### In this section...

"Memory Management" on page 4-11

"Computational Efficiency" on page 4-12

### **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.

<pre>M_full = magic(1100); M_full(M_full &gt; 50) = 0; M_sparse = sparse(M_full);</pre>		% Create 1100-by-1100 matrix. % Set elements >50 to zero. % Create sparse matrix of same.		
whos Name	Size	Bytes	Class	Attributes
M_full	1100x1100	9680000	double	

M_sparse	1100x1100	5004	double	sparse
----------	-----------	------	--------	--------

Notice that the number of bytes used is fewer in the sparse case, because zero-valued elements are not stored.

### **Computational Efficiency**

Sparse matrices also have significant advantages in terms of computational efficiency. Unlike operations with full matrices, operations with sparse matrices do not perform unnecessary low-level arithmetic, such as zero-adds (x+0 is always x). 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 4-26.

# **Constructing Sparse Matrices**

#### In this section ...

"Creating Sparse Matrices" on page  $4\mathchar`-13$ 

"Importing Sparse Matrices" on page 4-18

### **Creating Sparse Matrices**

- "Converting Full to Sparse" on page 4-13
- "Creating Sparse Matrices Directly" on page 4-14
- "Creating Sparse Matrices from Their Diagonal Elements" on page 4-16

MATLAB software 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.

S = sparse(A)

For example:

A = [ 0 0 0 5

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

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 =

(1,1)	-2
(2,1)	1
(1,2)	1
(2,2)	-2
(3,2)	1
(2,3)	1
(3,3)	-2
(4,3)	1
(3,4)	1
(4,4)	-2

(5,4)	1
(4,5)	1
(5,5)	- 2

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

=	full	(S)			
=					
	-2	1	0	0	0
	1	-2	1	0	0
	0	1	-2	1	0
	0	0	1	-2	1
	0	0	0	1	-2
		= -2 1 0 0	-2 1 1 -2 0 1 0 0	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$

#### **Creating Sparse Matrices from Their Diagonal Elements**

Creating sparse matrices based on their diagonal elements is a common operation, so the function spdiags handles this task. Its syntax is

S = spdiags(B,d,m,n)

To create an output matrix **S** of size *m*-by-*n* with elements on **p** diagonals:

- B is a matrix of size  $\min(m,n)$ -by-p. The columns of B are the values to populate the diagonals of S.
- d is a vector of length p whose integer elements specify which diagonals of S to populate.

That is, the elements in column j of B fill the diagonal specified by element j of d.

**Note** If a column of B is longer than the diagonal it's replacing, super-diagonals are taken from the lower part of the column of B, and sub-diagonals are taken from the upper part of the column of B.

As an example, consider the matrix  $\boldsymbol{B}$  and the vector  $\boldsymbol{d}.$ 

 $B = \begin{bmatrix} 41 & 11 & 0 \\ 52 & 22 & 0 \\ 63 & 33 & 13 \\ 74 & 44 & 24 \end{bmatrix};$  $d = \begin{bmatrix} -3 \\ 0 \\ 2 \end{bmatrix};$ 

Use these matrices to create a 7-by-4 sparse matrix A:

A = spdiags(B,d,7,4)

```
A =
```

(1,1)	11
(4,1)	41
(2,2)	22
(5,2)	52
(1,3)	13
(3,3)	33
(6,3)	63
(2,4)	24
(4,4)	44
(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 4-19

"Indices and Values" on page 4-21

"Indexing in Sparse Matrix Operations" on page 4-21

"Visualizing Sparse Matrices" on page 4-24

### **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	1100x1100	9680000	double	
M_sparse	1100x1100	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 (31, 1)-3.7648e-02 (87,1) -3.4424e-01 (26, 2)1.0000e+00 (31,2) -2.4523e-02 (88, 2)-3.7371e-01 (27,3) 1.0000e+00 (31, 3)-3.6613e-02 (89,3) -8.3694e-01 (28, 4)1.3000e+02 • nonzeros(west0479); ans = 1.0000e+00 -3.7648e-02 -3.4424e-01 1.0000e+00 -2.4523e-02 -3.7371e-01 1.0000e+00 -3.6613e-02 -8.3694e-01 1.3000e+02 . . .

Note Use Ctrl+C to stop the nonzeros listing at any time.

Note that initially nnz has the same value as nzmax by default. That is, the number of nonzero elements is equivalent to the number of storage locations allocated for nonzeros. However, MATLAB software 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 indexing into a full matrix. For example, consider the 4-by-4 identity matrix:

A=eye(4);

To replace the 2,1 entry with the number 3, you would do this:

A(2,1)=3 A =

1	0	0	0
3	1	0	0
0	0	1	0
0	0	0	1

Now suppose you were working on a sparse matrix:

B=speye(4);

The find command returns the indices and values of the nonzero components of a matrix:

If you wanted to change a value in this matrix, you might be tempted to use the same indexing:

B(3,1) = 42;

This code does work, however, it is slow. Since MATLAB stores sparse matrices in compressed sparse column format, it needs to overwrite multiple entries in B.

```
[i,j,s]=find(B);
[i,j,s]
ans =
1 1 1 1
```

3	1	42
2	2	1
3	3	1
4	4	1

In order to store the new matrix with '42' at (3,1), MATLAB overwrites all matrix values after 3,1 and adds an additional row to the nonzero values vector and the row indices vectors.

Instead of using subscripted assignment, try using the sparse command to construct the matrix from the triplets. For example, suppose you wanted the sparse form of the coordinate matrix C:

 $C = \begin{array}{ccccc} 4 & 0 & 0 & -1 \\ 0 & 4 & 0 & -1 \\ 0 & 0 & 4 & -1 \\ -1 & -1 & -1 & 4 \end{array}$ 

You can use indexing:

C=4\*speye(4); C(1:3,4)=-1; C(4,1:3)=-1;

but this has the same issue that many of the entries in C need to be overwritten. If you use a loop, you exacerbate the inefficiency:

```
C=4*speye(4);
for k=1:3
C(k,4)=-1;
C(4,k)=-1;
end
```

Instead of rewriting every matrix entry when you want to rewrite one, construct the three-column matrix directly with the sparse function:

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

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.

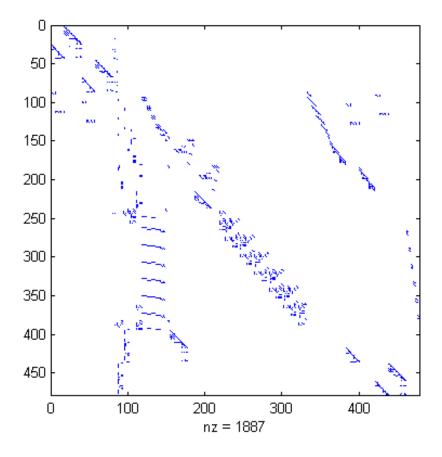
For example:

Load the supplied sparse matrix  ${\tt west0479},$  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 4-26

"Permutations and Reordering" on page 4-27

"Factoring Sparse Matrices" on page 4-31

"Systems of Linear Equations" on page 4-41

"Eigenvalues and Singular Values" on page 4-44

"Performance Limitations" on page 4-47

# **Efficiency of Operations**

- "Computational Complexity" on page 4-26
- "Algorithmic Details" on page 4-26

### **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.
- Submatrix indexing on the right side of an assignment preserves the storage format of the operand unless the result is a scalar. T = S(i,j) produces a sparse result if S is sparse and either i or j is a vector. It produces a full scalar if both i and j are scalars. Submatrix indexing on the left, as in T(i,j) = S, does not change the storage format of the matrix on the left.

### **Permutations and Reordering**

- "Reordering for Sparsity" on page 4-30
- "Reordering to Reduce Bandwidth" on page 4-30
- "Approximate Minimum Degree Ordering" on page 4-30

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
Ρ	=					
		1 0 0 0	0 0 1 0	0 1 0 0	0 0 1 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 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 =

11	1	0	0	0
0	1	33	1	0
0	0	1	44	1

1	22	1	0	0
0	0	0	1	55

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

ans =

11	0	0	1	0
1	1	0	22	0
0	33	1	1	0
0	1	44	0	1
0	0	1	0	55

If P is a sparse matrix, then both representations use storage proportional to n and you can apply either to S in time proportional to nnz(S). The vector representation is slightly more compact and efficient, so the various sparse matrix permutation routines all return full row vectors with the exception of the pivoting permutation in LU (triangular) factorization, which returns a matrix compatible with the full LU factorization.

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

P = I(p,:) P' = I(:,p) p = (1:n)\*P' p = (P\*(1:n)')'

The inverse of P is simply R = P'. You can compute the inverse of p with r(p) = 1:n.

r(p) = 1:5r =1 4 2 3 5

#### **Reordering for Sparsity**

Reordering the columns of a matrix can often make its LU or QR factors sparser. Reordering the rows and columns can often make its Cholesky factors sparser. The simplest such reordering is to sort the columns by nonzero count. This is sometimes a good reordering for matrices with very irregular structures, especially if there is great variation in the nonzero counts of rows or columns.

The function p = colperm(S) computes this column-count permutation. The colperm code has only a single line.

[ignore,p] = sort(sum(spones(S)));

This line performs these steps:

- 1 The inner call to spones creates a sparse matrix with ones at the location of every nonzero element in S.
- **2** The sum function sums down the columns of the matrix, producing a vector that contains the count of nonzeros in each column.
- **3** full converts this vector to full storage format.
- **4** sort sorts the values in ascending order. The second output argument from sort is the permutation that sorts this vector.

#### **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 4-32 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 4-31
- "Cholesky Factorization" on page 4-36
- "QR Factorization" on page 4-37
- "Incomplete Factorizations" on page 4-38

#### LU Factorization

If S is a sparse matrix, the following command returns three sparse matrices L, U, and P such that P\*S = L\*U.

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

Lu obtains the factors by Gaussian elimination with partial pivoting. The permutation matrix P has only n nonzero elements. As with dense matrices, the statement [L,U] = lu(S) returns a permuted unit lower triangular matrix and an upper triangular matrix whose product is S. By itself, lu(S) returns L and U in a single matrix without the pivot information.

The three-output syntax

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

selects P via numerical partial pivoting, but does not pivot to improve sparsity in the LU factors. On the other hand, the four-output syntax

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

selects P via threshold partial pivoting, and selects P and Q to improve sparsity in the LU factors.

You can control pivoting in sparse matrices using

lu(S,thresh)

where thresh is a pivot threshold in [0,1]. Pivoting occurs when the diagonal entry in a column has magnitude less than thresh times the magnitude of any sub-diagonal entry in that column. thresh = 0 forces diagonal pivoting. thresh = 1 is the default. (The default for thresh is 0.1 for the four-output syntax).

When you call 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.

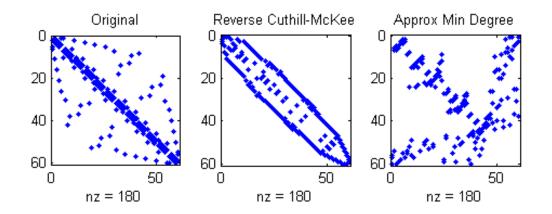
Create two permutations, r and m using symrcm and symamd respectively.

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.

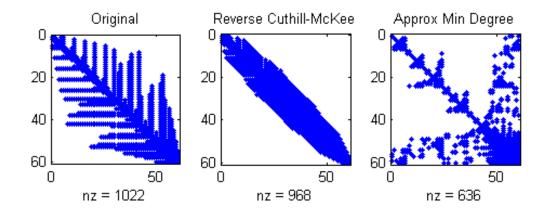
- lu(B) (Original): 1022
- lu(B(r,r)) (Reverse Cuthill-McKee): 968
- lu(B(m,m)) (Approximate minimum degree): 636

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)).

4-36

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

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';
```

These calculations show that the zero-fill factors have 7840 nonzeros, the ILUTP(1e-4) factors have 31147 nonzeros, and the ILUC(1e-4) factors have 31083 nonzeros. Also, the relative error of the product of the zero-fill factors is essentially zero on the pattern of A. Finally, the relative error in the factorizations produced with threshold dropping is on the same order of the drop tolerance, although this is not guaranteed to occur. See the ilu reference page for more options and details.

The ichol function provides *zero-fill incomplete Cholesky factorizations* (IC(0)) as well as threshold-based dropping incomplete Cholesky factorizations (ICT(tau)) of symmetric, positive definite sparse matrices. These factorizations are the analogs of the incomplete LU factorizations above and have many of the same characteristics. For example:

shows that A has 195228 nonzeros, and its complete Cholesky factorization without reordering has 7762589 nonzeros. By contrast:

```
L = ichol(A);
nnz(L)
ans =
117216
norm(A-(L*L').*spones(A),'fro')./norm(A,'fro')
ans =
3.5805e-017
```

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:

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

Now, assuming you have created a permutation vector 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 p.

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

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.

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		

Functions for Iterative Methods for Sparse	Systems
--	---------

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. If sigma is omitted, the eigenvalues largest in magnitude are found. If sigma is zero, the eigenvalues smallest in magnitude are found. A second matrix, B, can be included for the generalized eigenvalue problem:  $Au = \lambda Bu$ .

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 oder and number of nonzero elements.

size(A) nnz(A)

ans =

```
2945 2945
ans =
14473
```

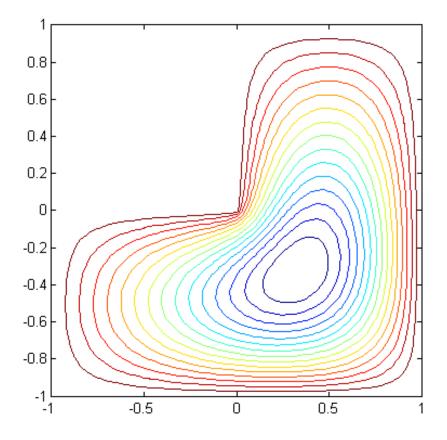
A is a matrix of order 2945 with 14,473 nonzero elements.

Compute the smallest eigenvalue and eigenvector.

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

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].

#### **Performance Limitations**

- "Creating Sparse Matrices" on page 4-48
- "Manipulating Sparse Matrices" on page 4-49

This section describes some limitations of the sparse matrix storage format and their impact on matrix creation, manipulation, and operations.

#### **Creating Sparse Matrices**

The best way to create a sparse matrix is to use the **sparse** function. If you do not have prior knowledge of the nonzero indices or their values, it is much more efficient to create the vectors containing these values, and then create the sparse matrix.

Preallocating the memory for a sparse matrix and filling it in an elementwise manner causes a significant amount of overhead in indexing into the sparse array:

Elapsed time is 26.281000 seconds.

Whereas 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.
```

#### **Manipulating Sparse Matrices**

Sparse matrices are stored in a column-major format. In some cases, accessing the matrix by columns may be more efficient than accessing by rows. To do this, you can transpose the matrix, perform operations on the columns, and then retranspose the result:

```
S = sparse(10000,10000,1);
for n = 1:1000
        A = S(100,:)' + S(200,:)';
        A = A';
end;
```

The time required to transpose the matrix is negligible. Note that the sparse matrix memory requirements could prevent you from transposing a sparse matrix having a large number of rows. This might occur even when the number of nonzero values is small.

Using linear indexing to access or assign an element in a large sparse matrix will fail if the linear index exceeds intmax. To access an element whose linear index is greater than intmax, use array indexing:

```
S = spalloc(216<sup>2</sup>, 216<sup>2</sup>, 2)
S(1) = 1
S(end) = 1
S(216<sup>2</sup>,216<sup>2</sup>) = 1
```

# Selected Bibliography

[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, available at http://www.cise.ufl.edu/submit/files/file\_281.ps.

[6] Saad, Yousef, *Iterative Methods for Sparse Linear Equations*. PWS Publishing Company, 1996.

# 5

# Functions of One Variable

- "Function Summary" on page 5-2
- "Representing Polynomials" on page 5-3
- "Evaluating Polynomials" on page 5-4
- "Roots of Polynomials" on page 5-5
- "Roots of Scalar Functions" on page 5-6
- "Derivatives" on page 5-12
- "Convolution" on page 5-13
- "Partial Fraction Expansions" on page 5-14
- "Polynomial Curve Fitting" on page 5-15
- "Characteristic Polynomials" on page 5-17

# **Function Summary**

The following table lists the MATLAB polynomial functions.

Function	Description
conv	Multiply polynomials
deconv	Divide polynomials
fzero	Find root of continuous function of one variable
poly	Polynomial with specified roots
polyder	Polynomial derivative
polyfit	Polynomial curve fitting
polyval	Polynomial evaluation
polyvalm	Matrix polynomial evaluation
residue	Partial-fraction expansion (residues)
roots	Find polynomial roots

Symbolic Math Toolbox software contains additional specialized support for polynomial operations.

# **Representing Polynomials**

MATLAB software represents polynomials as row vectors containing coefficients ordered by descending powers. For example, consider the equation

$$p(x) = x^3 - 2x - 5$$

This is the celebrated example Wallis used when he first represented Newton's method to the French Academy. To enter this polynomial into MATLAB, use

$$p = [1 \ 0 \ -2 \ -5];$$

# **Evaluating Polynomials**

The polyval function evaluates a polynomial at a specified value. To evaluate p at s = 5, use

polyval(p,5)
ans =
 110

It is also possible to evaluate a polynomial in a matrix sense. In this case  $p(x) = x^3 - 2x - 5$  becomes  $p(X) = X^3 - 2X - 5I$ , where X is a square matrix and I is the identity matrix. For example, create a square matrix X and evaluate the polynomial p at X:

X = [2 4 5; -1 0 3; 7 1 5]; Y = polyvalm(p,X) Y = 377 179 439 111 81 136 490 253 639

# **Roots of Polynomials**

The roots function calculates the roots of a polynomial:

```
r = roots(p)
r =
    2.0946
    -1.0473 + 1.1359i
    -1.0473 - 1.1359i
```

By convention, the MATLAB software stores roots in column vectors. The function poly returns to the polynomial coefficients:

```
p2 = poly(r)
p2 =
1 8.8818e-16 -2 -5
```

 $\operatorname{\texttt{poly}}$  and  $\operatorname{\texttt{roots}}$  are inverse functions, up to ordering, scaling, and roundoff error.

## **Roots of Scalar Functions**

#### In this section ...

"Solving a Nonlinear Equation in One Variable" on page 5-6

"Using a Starting Interval" on page 5-8

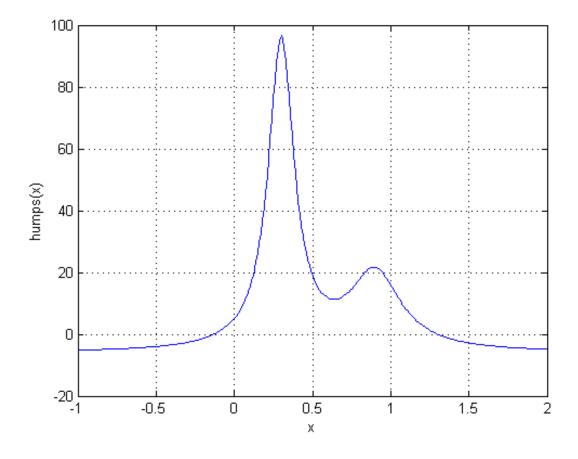
"Using a Starting Point" on page 5-10

#### 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)')
set(gca,'YGrid','on','XGrid','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 8-13, "Using a Starting Interval" on page 5-8, and "Using a Starting Point" on page 5-10.
- Choosing various tolerances that control how fzero determines it is at a root see "Set Options" on page 8-13.

- Choosing a plot function for observing the progress of fzero towards a root
   — see "Plot Functions" on page 8-27.
- Using a custom-programmed output function for observing the progress of fzero towards a root see "Output Functions" on page 8-19.

#### **Using a Starting Interval**

The graph of humps indicates that the function is negative at x = -1 and positive at x = 1. You can confirm this by calculating humps at these two points.

humps(1)

```
ans =
16
humps(-1)
ans =
-5.1378
```

Consequently, you can use  $[-1 \ 1]$  as a starting interval for fzero.

The iterative algorithm for fzero finds smaller and smaller subintervals of [-1 1]. For each subinterval, the sign of humps differs at the two endpoints. As the endpoints of the subintervals get closer and closer, they converge to zero for humps.

To show the progress of fzero at each iteration, set the Display option to iter using the optimset function.

```
options = optimset('Display','iter');
```

Then call fzero as follows:

Func-count	Х	f(x)	Procedure
2	- 1	-5.13779	initial
3	-0.513876	-4.02235	interpolation
4	-0.513876	-4.02235	bisection
5	-0.473635	-3.83767	interpolation
6	-0.115287	0.414441	bisection
7	-0.115287	0.414441	interpolation
8	-0.132562	-0.0226907	interpolation
9	-0.131666	-0.0011492	interpolation
10	-0.131618	1.88371e-07	interpolation
11	-0.131618	-2.7935e-11	interpolation
12	-0.131618	8.88178e-16	interpolation
13	-0.131618	8.88178e-16	interpolation
Zero found i	in the inter	val [-1, 1]	
a =			
-0.1316			

#### a = fzero(@humps,[-1 1],options)

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	а	f(a)	b	f(b)	Procedure
1	-0.2	-1.35385	-0.2	-1.35385	initial i
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
13	-0.168	-0.786636	-0.232	-1.83055	search
15	-0.154745	-0.51962	-0.245255	-2.00602	search
17	-0.136	-0.104165	-0.264	-2.23521	search
18	-0.10949	0.572246	-0.264	-2.23521	search

Search for a zero in the interval [-0.10949, -0.264]: Func-count Х f(x) Procedure 18 -0.109490.572246 initial 19 -0.140984-0.219277interpolation 20 -0.132259 -0.0154224 interpolation 21 -0.131617 3.40729e-05 interpolation 22 -0.131618 -6.79505e-08 interpolation 23 -2.98428e-13 interpolation -0.131618 24 -0.131618 8.88178e-16 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.

### **Derivatives**

The polyder function computes the derivative of any polynomial. To obtain the derivative of the polynomial  $p = [1 \ 0 \ -2 \ -5]$ ,

q = polyder(p) q = 3 0 -2

**polyder** also computes the derivative of the product or quotient of two polynomials. For example, create two polynomials **a** and **b**:

```
a = [1 3 5];
b = [2 4 6];
```

Calculate the derivative of the product **a\*b** by calling **polyder** with a single output argument:

```
c = polyder(a,b)
c =
8 30 56 38
```

Calculate the derivative of the quotient a/b by calling polyder with two output arguments:

[q,d] = polyder(a,b)
q =
 -2 -8 -2
d =
 4 16 40 48 36

q/d is the result of the operation.

### Convolution

Polynomial multiplication and division correspond to the operations convolution and deconvolution. The functions conv and deconv implement these operations.

Consider the polynomials  $a(s) = s^2 + 2s + 3$  and  $b(s) = 4s^2 + 5s + 6$ . To compute their product,

```
a = [1 2 3]; b = [4 5 6];
c = conv(a,b)
c =
4 13 28 27 18
```

Use deconvolution to divide a(s) back out of the product:

[q,r] = deconv(c,a) q = 4 5 6 r = 0 0 0 0 0

# **Partial Fraction Expansions**

residue finds the partial fraction expansion of the ratio of two polynomials. This is particularly useful for applications that represent systems in transfer function form. For polynomials b and a, if there are no multiple roots,

$$\frac{b(s)}{a(s)} = \frac{r_1}{s - p_1} + \frac{r_2}{s - p_2} + \dots + \frac{r_n}{s - p_n} + k_s$$

where r is a column vector of residues, p is a column vector of pole locations, and k is a row vector of direct terms. Consider the transfer function

```
\frac{-4s+8}{s^2+6s+8}
b = [-4 8];
a = [1 6 8];
[r,p,k] = residue(b,a)
r =
-12
8
p =
-4
-2
k =
[]
```

Given three input arguments (r, p, and k), residue converts back to polynomial form:

# **Polynomial Curve Fitting**

polyfit finds the coefficients of a polynomial that fits a set of data in a least-squares sense:

p = polyfit(x,y,n)

x and y are vectors containing the x and y data to be fitted, and n is the degree of the polynomial to return. For example, consider the *x*-*y* test data

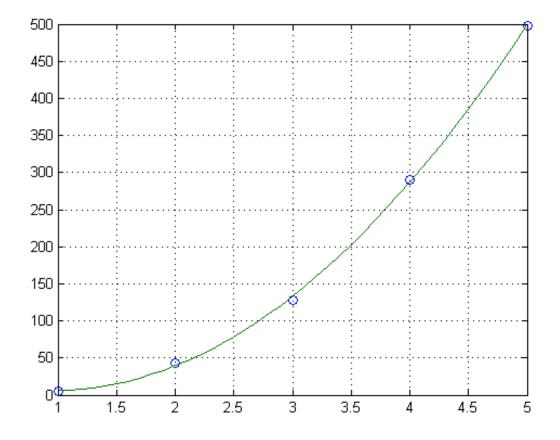
x = [1 2 3 4 5]; y = [5.5 43.1 128 290.7 498.4];

A third degree polynomial that approximately fits the data is

p = polyfit(x,y,3)
p =
 -0.1917 31.5821 -60.3262 35.3400

Compute the values of the polyfit estimate over a finer range, 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 "Programmatic Fitting" | polyfit | polyval

# **Characteristic Polynomials**

The poly function also computes the coefficients of the characteristic polynomial of a matrix:

```
A = [1.2 3 -0.9; 5 1.75 6; 9 0 1];
poly(A)
ans =
1.0000 -3.9500 -1.8500 -163.2750
```

The roots of this polynomial, computed with roots, are the *characteristic roots*, or eigenvalues, of the matrix A. (Use eig to compute the eigenvalues of a matrix directly.)

# 6

# **Computational Geometry**

- "Overview" on page 6-2
- "Triangulation Representations" on page 6-3
- "Delaunay Triangulation" on page 6-20
- "Spatial Searching" on page 6-56
- "Voronoi Diagrams" on page 6-70
- "Convex Hulls" on page 6-80

#### **Overview**

MATLAB software 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.

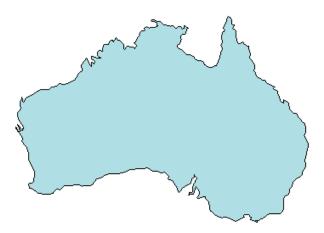
MATLAB provides both function-based and class-based tools for computational geometry. The function-based tools are convenient when the output from the function is sufficiently complete to get you to the solution. The class-based tools are more versatile because they provide complementary methods that 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 delaunayTriangulation 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.

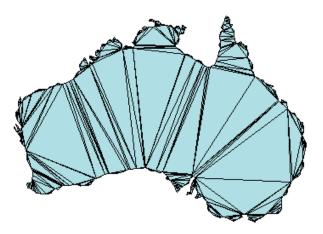
# **Triangulation Representations**

#### 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

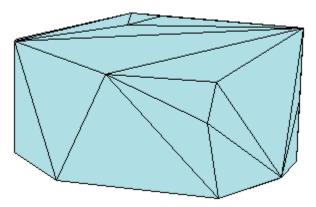


can be represented by the triangulation on the map shown below.



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.



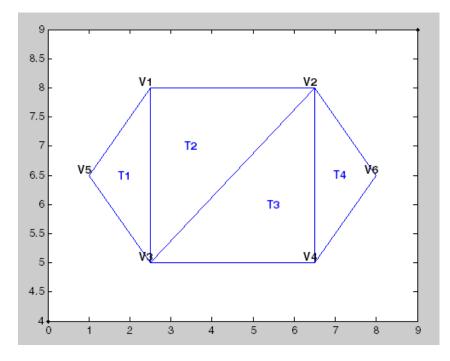
6-4

## **Triangulation Matrix Format**

MATLAB software 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

Vertices		
V2	6.5	8.0
V3	2.5	5.0
V4	6.5	5.0
V5	1.0	6.5
V6	8.0	6.5

The data in the previous table is stored as a matrix in the MATLAB environment. The vertex IDs are labels used for identifying specific vertices. They are shown to illustrate the concept of a vertex ID, but they are not stored explicitly. Instead, the row numbers of the matrix serve as the vertex IDs.

The triangulation connectivity data is shown in this table.

Connectivity			
Triangle ID	IDs of Bounding	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).

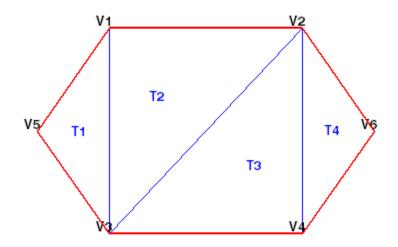
You can represent and query the following types of triangulations using MATLAB software:

- 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.

;

Ρ	=	[	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.

3 2 1; 3 4 2; 4 6 2];

Create a triangulation from this data.

```
TR = triangulation(T,P)
```

TR =

triangulation with properties:

Points: [6x2 double] ConnectivityList: [4x3 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 = 3

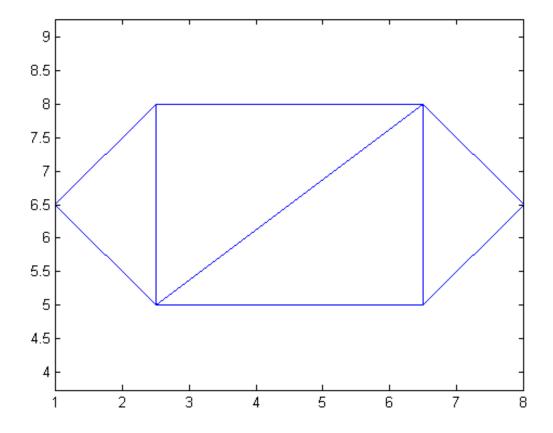
Now, examine all the triangles in the triangulation.

TR(:,:)

ans	=		
	5	3	1
	3	2	1
	3	4	2
	4	6	2

Use triplot to plot the triangulation. The triplot function is not a triangulation method, but it accepts and can plot a triangulation.

triplot(TR);
axis equal



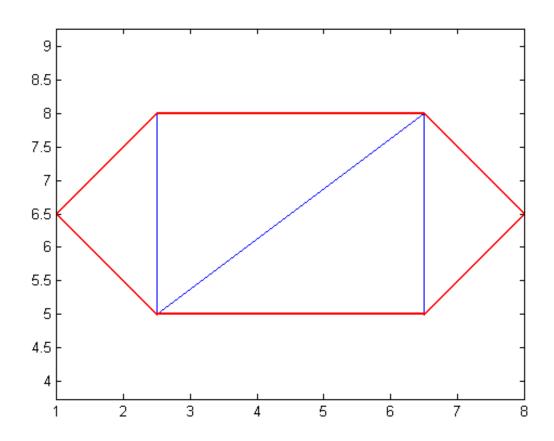
Use the triangulation method, freeBoundary, to query the free boundary and highlight it in a plot. This method returns the edges of the triangulation that are shared by only one triangle. The returned edges are expressed in terms of the vertex IDs.

```
boundaryedges = freeBoundary(TR)';
```

Now plot the boundary edges as a red line.

```
hold on;
plot(P(boundaryedges,1),P(boundaryedges,2),'-r','LineWidth',2);
```

6-12



hold off;

You can use the freeBoundary method to validate a triangulation. For example, if you observed red edges in the interior of the triangulation, then it would indicate a problem in how the triangles are connected.

#### Creating a triangulation Using delaunayTriangulation.

This example shows how to create a Delaunay triangulation using delaunayTriangulation.

When you create a Delaunay triangulation using the delaunayTriangulation class, you automatically get access to the triangulation methods because delaunayTriangulation is a subclass of triangulation.

Create a delaunayTriangulation from a set of points.

Ρ	=	[	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: [6x2 double]
ConnectivityList: [4x3 double]
Constraints: []
```

The resulting delaunayTriangulation object has the properties, Points and ConnectivityList, just like a triangulation object.

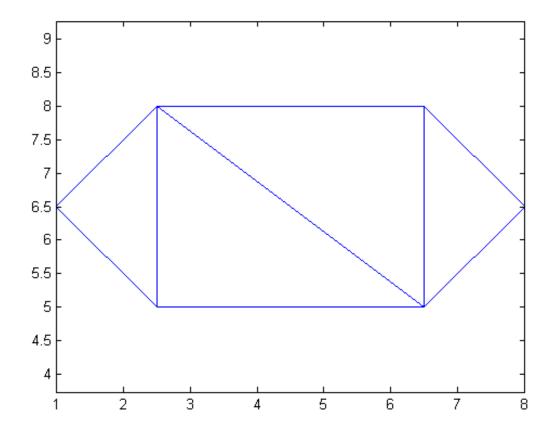
You can access the triangulation using direct indexing, just like triangulation. For example, examine the connectivity of the first triangle.

```
DT(1,:)
ans =
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 =

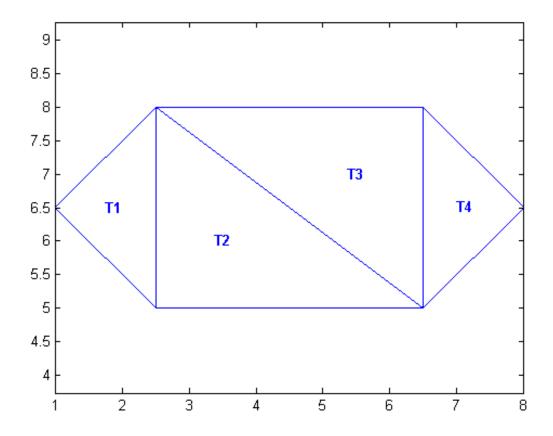
1.8787	6.5000
3.5000	6.0000

5.50007.00007.12136.5000

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,

Ρ	=	[	2.5	8.0
			6.5	8.0
			2.5	5.0
			6.5	5.0
			1.0	6.5
			8.0	6.5];

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	T = delaunay(P); TR = triangulation(T,P); IC = incenter(TR);
	Both approaches are valid in this example, but if you want to create a Delaunay triangulation and perform queries on it, then you should use delaunayTriangulation for these reasons:
	• The delaunayTriangulation class provides additional methods that are useful for working with triangulations. For example, you can to perform nearest-neighbor and point-in-triangle searches.
	• It allows you to edit the triangulation to add, move, or remove points.
	• It allows you to create constrained Delaunay triangulations. This allows you to create a triangulation for a 2-D domain.
See Also	delaunay   delaunayTriangulation   freeBoundary   triangulation   triplot
Concepts	<ul> <li>"Triangulation Representations" on page 6-3</li> <li>"Delaunay Triangulation" on page 6-20</li> <li>"Spatial Segrething" on page 6-56</li> </ul>

• "Spatial Searching" on page 6-56

# **Delaunay Triangulation**

#### In this section...

"Definition of Delaunay Triangulation" on page 6-20

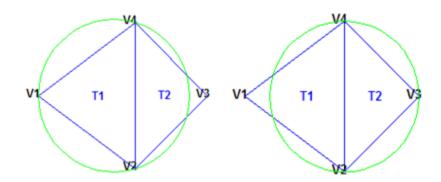
"Creating Delaunay Triangulations" on page 6-22

"Triangulation of Point Sets Containing Duplicate Locations" on page 6-53

## **Definition of Delaunay Triangulation**

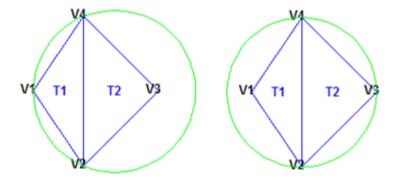
Delaunay triangulations are widely used in scientific computing in many diverse applications. While there are numerous algorithms for computing triangulations, it is the favorable geometric properties of the Delaunay triangulation that make it so useful.

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. This triangulation is a Delaunay triangulation.



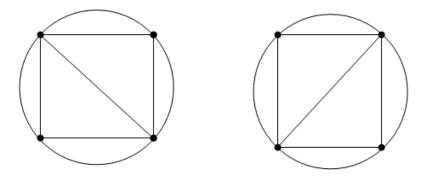
The triangles below are different. The circumcircle associated with T1 is not empty. It contains V3 in its interior. The circumcircle associated with T2 is

not empty. It contains V1 in its interior. This triangulation is not a Delaunay triangulation.

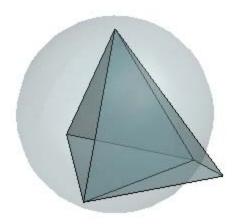


Delaunay triangles are said to be "well shaped" because in fulfilling the empty circumcircle property, triangles with large internal angles are selected over ones with small internal angles. The triangles in the non-Delaunay triangulation have sharp angles at vertices V2 and V4. If the edge {V2, V4} 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.

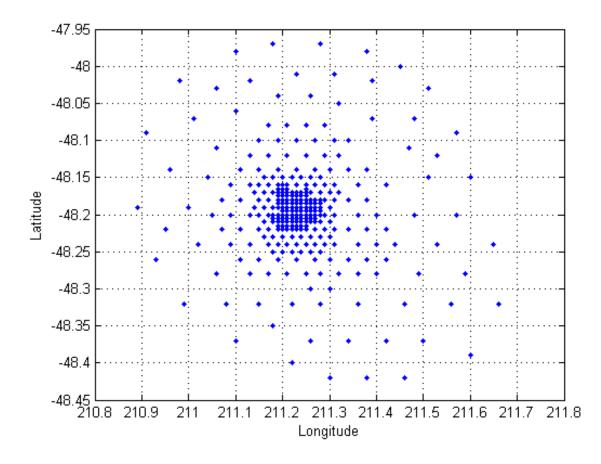
## Using the delaunay and delaunayn functions

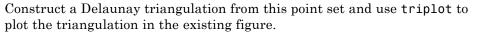
The delaunay and delaunayn functions take a set of points and produce a triangulation in matrix format. Refer to "Triangulation Matrix Format" on page 6-5 for more information on this data structure. In 2-D, the delaunay function is often used to produce a triangulation that can be used to plot a surface 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.

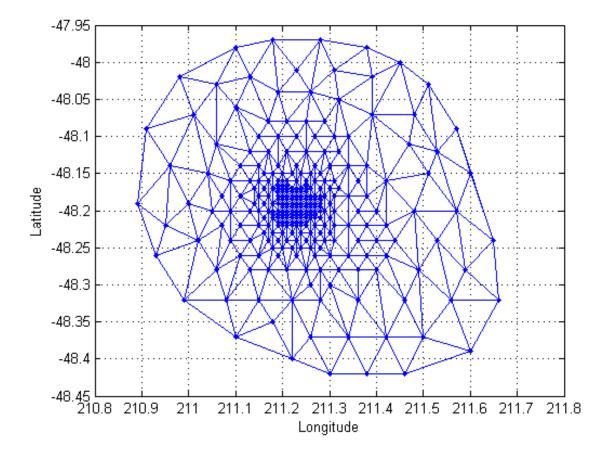
Load the seamount data set and view the (x, y) data as a scatter plot.

```
load seamount
plot(x,y,'.','markersize',12)
xlabel('Longitude'), ylabel('Latitude')
grid on
```



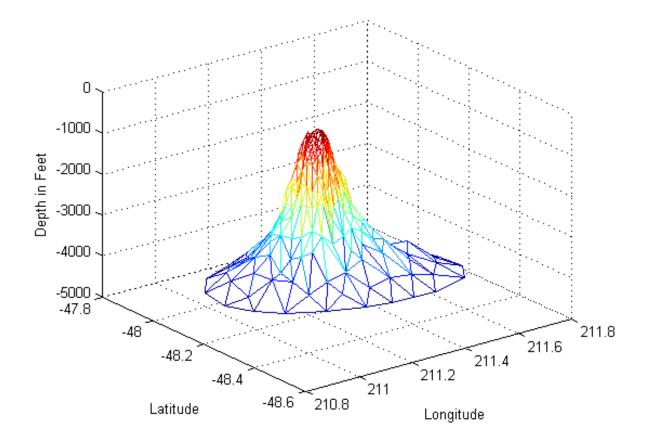


tri = delaunay(x,y); hold on, triplot(tri,x,y), hold off



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');
```

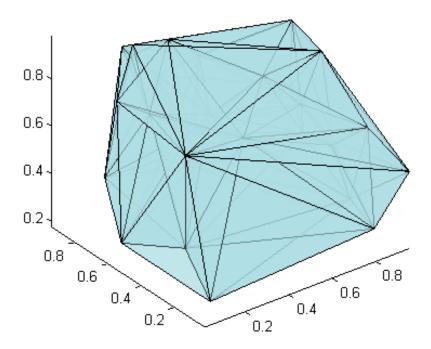


If you want to plot the surface in shaded mode, use  $\verb"trisurf"$  instead of trimesh.

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 6-56 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 6-3 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.

```
load seamount
DT = delaunayTriangulation(x,y)
```

DT =

delaunayTriangulation with properties:

```
Points: [294x2 double]
ConnectivityList: [566x3 double]
Constraints: []
```

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 =
205
```

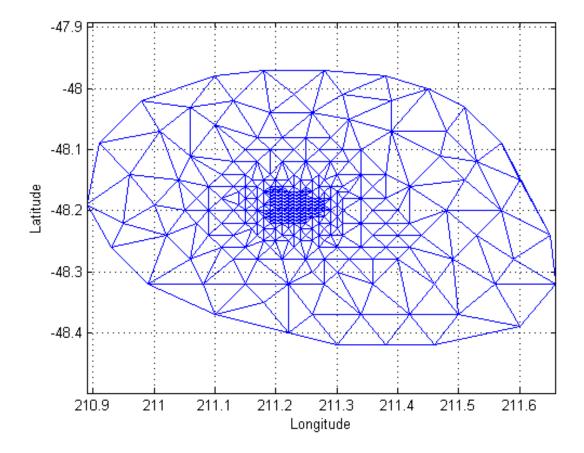
Examine all the triangles in the triangulation.

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.

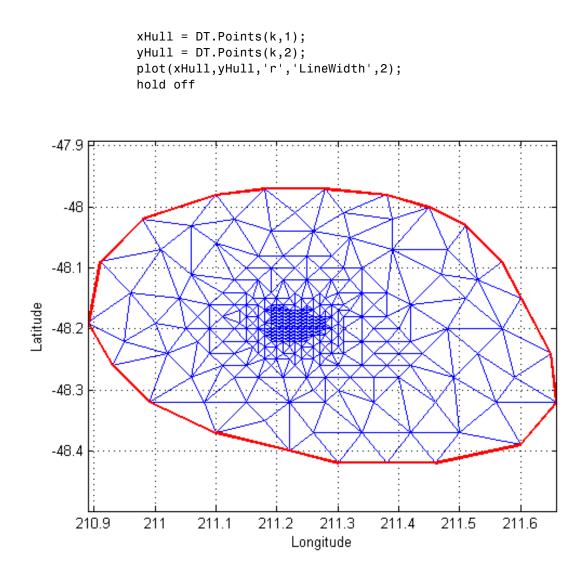
```
triplot(DT);
axis equal
xlabel('Longitude'), ylabel('Latitude')
grid on
```



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);

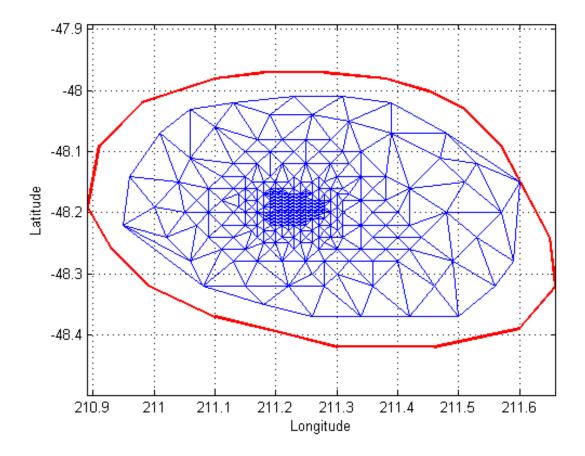


You can incrementally edit the delaunayTriangulation to add or remove points. If you need to add points to an existing triangulation, then an incremental addition is faster than a complete retriangulation of the augmented point set. Incremental removal of points is more efficient when

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: [274x2 double]
    ConnectivityList: [528x3 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 nearestNeighbor method to find the nearest vertex.

```
vertexId = nearestNeighbor(DT, 211.6, -48.15)
```

```
vertexId = 50
```

Now remove that vertex from the triangulation.

```
DT.Points(vertexId,:) = []
```

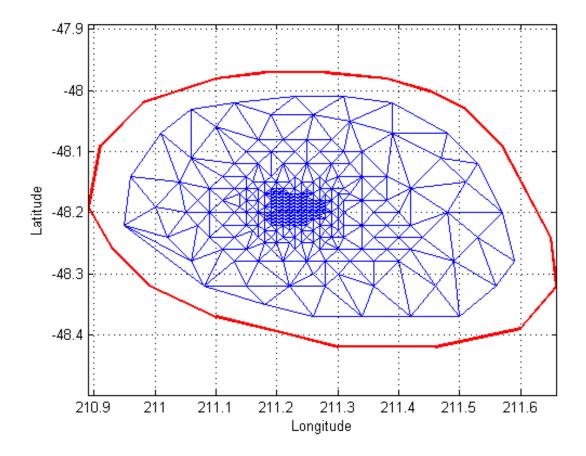
DT =

delaunayTriangulation with properties:

```
Points: [273x2 double]
ConnectivityList: [525x3 double]
Constraints: []
```

Plot the new triangulation.

```
figure
plot(xHull,yHull,'r','LineWidth',2);
axis equal
xlabel('Longitude'),ylabel('Latitude')
grid on
hold on
triplot(DT);
hold off
```



Add points to the existing triangulation. Add 4 points to form a rectangle around the triangulation.

```
Padditional = [210.9 -48.5; 211.6 -48.5; ...
211.6 -47.9; 210.9 -47.9];
DT.Points(end+(1:4),:) = Padditional
```

DT =

```
delaunayTriangulation with properties:
```

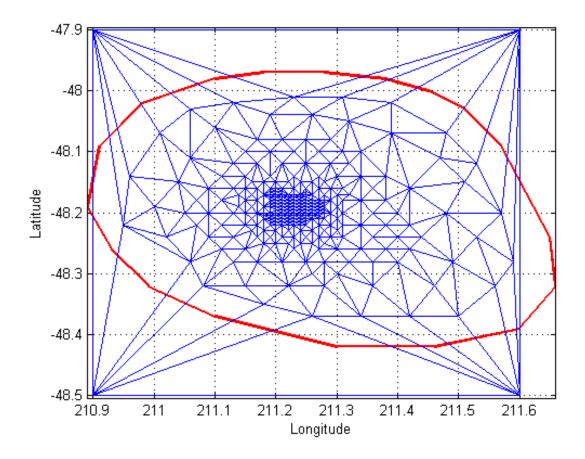
```
Points: [277x2 double]
ConnectivityList: [548x3 double]
Constraints: []
```

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).

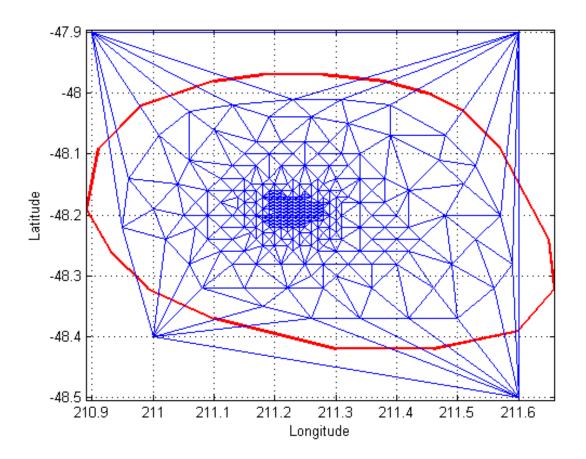
DT.Points(274,:) = [211 -48.4];

Close all existing figures.

close all

Plot the new triangulation

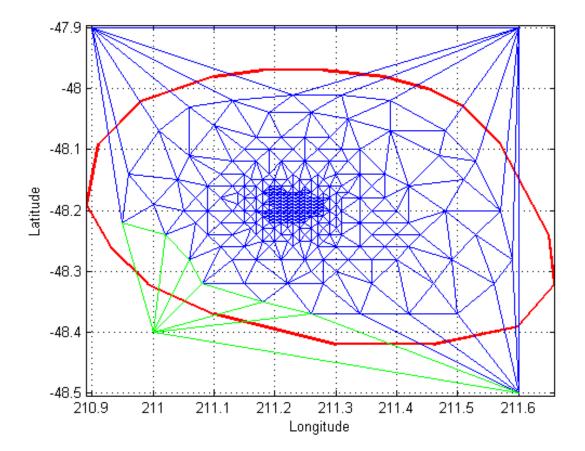
```
figure
plot(xHull,yHull,'r','LineWidth',2);
axis equal
xlabel('Longitude'),ylabel('Latitude')
grid on
hold on
triplot(DT);
hold off
```



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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.

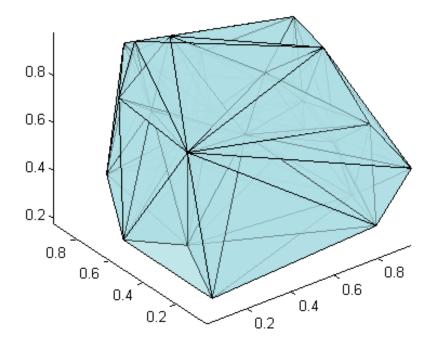
This example shows how to use a delaunayTriangulation to create and plot the triangulation of 3-D points.

```
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: [30x3 double]
ConnectivityList: [117x4 double]
Constraints: []
```



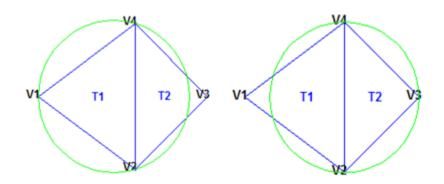
The tetramesh function plots both the internal and external faces of the triangulation. For large 3-D triangulations, plotting the internal faces might be an unnecessary use of resources. A plot of the boundary might be more appropriate. You can use the freeBoundary method to get the boundary triangulation 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 chose 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];

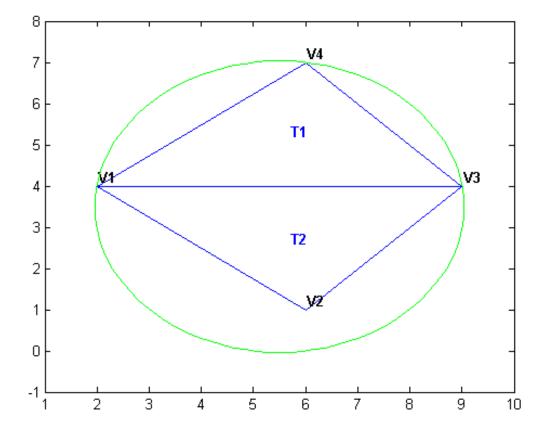
Define a constraint, C, between V1 and V3.

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 th
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');
hold off
```

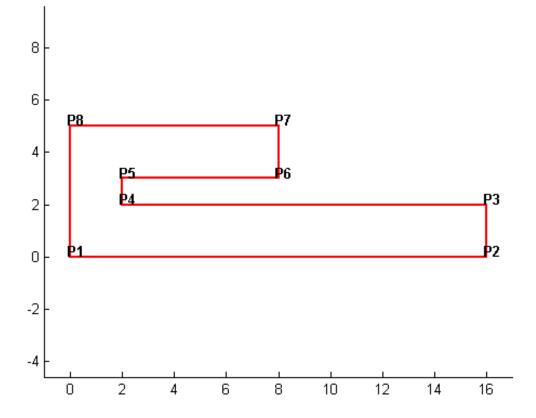


The constraint between vertices (V1, V3) was honored, however, the Delaunay criterion was invalidated. This also invalidates the nearest-neighbor relation that is inherent in a Delaunay triangulation. This means the nearestNeighbor search method provided by delaunayTriangulation cannot be supported if 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.

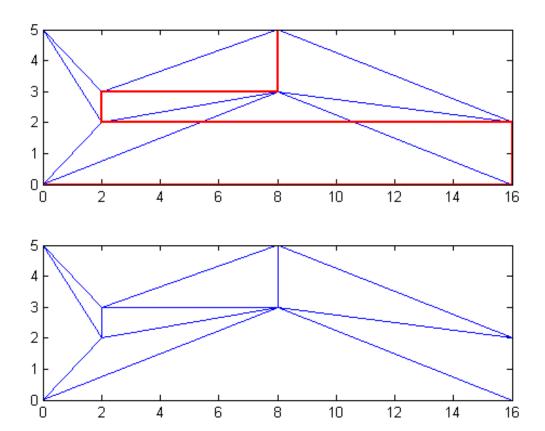
Define and plot a polygon.



Create and plot the triangulation together with the polygon boundary.

```
figure()
subplot(2,1,1);
axis([-1 17 -1 6]);
axis equal
P = [0 0; 16 0; 16 2; 2 2; 2 3; 8 3; 8 5; 0 5];
DT = delaunayTriangulation(P);
triplot(DT)
```

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This triangulation cannot be used to represent the domain of the polygon because some triangles cut across the boundary. You need to impose a constraint on the edges that are cut by triangulation edges. Since all edges have to be respected, you need to constrain all edges. The steps below show how to constrain all the edges.

Enter the constrained edge definition. Observe from the annotated figure where you need constraints (between (V1, V2), (V2, V3), and so on).

C = [1 2; 2 3; 3 4; 4 5; 5 6; 6 7; 7 8; 8 1];

In general, if you have N points in a sequence that define a polygonal boundary, the constraints can be expressed as C = [(1:(N-1))' (2:N)'; N 1];

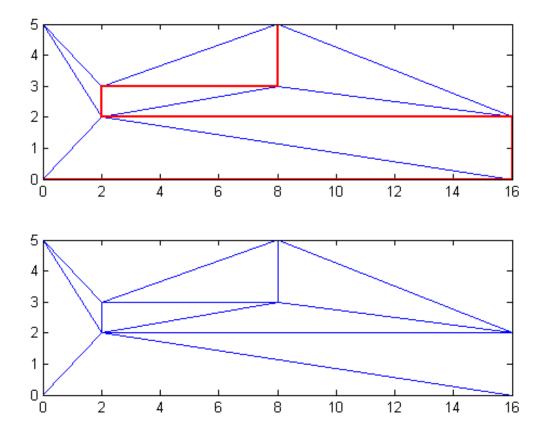
Specify the constraints when you create the delaunayTriangulation.

DT = delaunayTriangulation(P,C);

Alternatively, you can impose constraints on an existing triangulation by setting the Constraints property: DT.Constraints = C;.

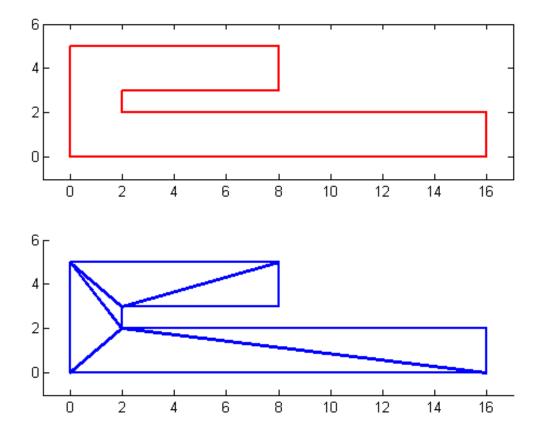
Plot the triangulation and polygon.

```
figure('Color','white')
subplot(2,1,1);
axis([-1 17 -1 6]);
axis equal
triplot(DT)
hold on;
patch(P(:,1),P(:,2),'-r','LineWidth',2, ...
            'FaceColor','none','EdgeColor','r');
hold off
% Plot the standalone triangulation in a subplot.
subplot(2,1,2);
axis([-1 17 -1 6]);
axis equal
triplot(DT)
```



The plot shows that the edges of the triangulation respect the boundary of the polygon. However, the triangulation fills the concavities. What is needed is a triangulation that represents the polygonal domain. You can extract the triangles within the polygon using the delaunayTriangulation method, isInterior. This method returns a logical array whose true and false values that indicate whether the triangles are inside a bounded geometric domain. The analysis is based on the Jordan Curve theorem, and the boundaries are defined by the edge constraints. The ith triangle in the triangulation is considered to be inside the domain if the ith logical flag is true, otherwise it is outside. Now use the isInterior method to compute and plot the set of domain triangles.

```
% Plot the constrained edges in red
figure('Color','white')
subplot(2,1,1);
plot(P(C'),P(C'+size(P,1)),'-r','LineWidth', 2);
axis([-1 17 -1 6]);
% Compute the in/out status
I0 = isInterior(DT);
subplot(2,1,2);
hold on;
axis([-1 17 -1 6]);
% Use triplot to plot the triangles that are inside.
% Uses logical indexing and dt(i,j) shorthand
% format to access the triangulation.
triplot(DT(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.

DT =

delaunayTriangulation with properties:

```
Points: [22x2 double]
ConnectivityList: [31x3 double]
Constraints: []
```

If for example, the Delaunay triangulation is used to compute the convex hull, the indices of the points on the hull are indices with respect to the unique point set, DT.Points. Therefore, use the following code to compute and plot the convex hull:

```
K = DT.convexHull();
plot(DT.Points(:,1),DT.Points(:,2),'.');
hold on
plot(DT.Points(K,1),DT.Points(K,2),'-r');
```

If the original data set containing the duplicates were used in conjunction with the indices provided by delaunayTriangulation, then the result would be incorrect. The delaunayTriangulation works with indices that are based on the unique data set DT.Points. For example, the following would produce an incorrect plot, because K is indexed with respect to DT.Points and not P:

K = DT.convexHull();
plot(P(:,1),P(:,2),'.');
hold on
plot(P(K,1),P(K,2),'-r');

It's often more convenient to create a unique data set by removing duplicates prior to creating the delaunayTriangulation. Doing this eliminates the potential for confusion. This can be accomplished using the unique function as follows:

```
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
```

Concepts

• "Spatial Searching" on page 6-56

# **Spatial Searching**

#### In this section...

"Introduction" on page 6-56

"Nearest-Neighbor Search" on page 6-56

"Point Location" on page 6-61

"Searching Non-Delaunay Triangulations" on page 6-66

## Introduction

MATLAB provides you with the necessary functions to perform a spatial search using a Delaunay triangulation. The Delaunay-based 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 Xand a query point qin 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 Delaunay triangulation of X, the point location search locates the triangle or tetrahedron that contains the query point q.

While MATLAB supports these search schemes in N dimensions, exact spatial searches usually become prohibitive in 6 dimensions. You should consider approximate alternatives for large problems in up to 10 dimensions.

### **Nearest-Neighbor Search**

There are two Delaunay-based approaches to computing nearest neighbors in MATLAB, depending on the dimensionality of the problem:

• For 2-D and 3-D search, use the nearestNeighbor method provided 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 efficient as the search methods provided by delaunayTriangulation.

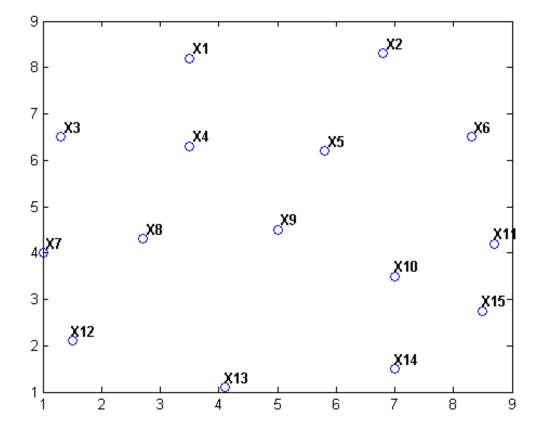
This example shows how to perform a nearest-neighbor search in 2-D with delaunayTriangulation.

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);

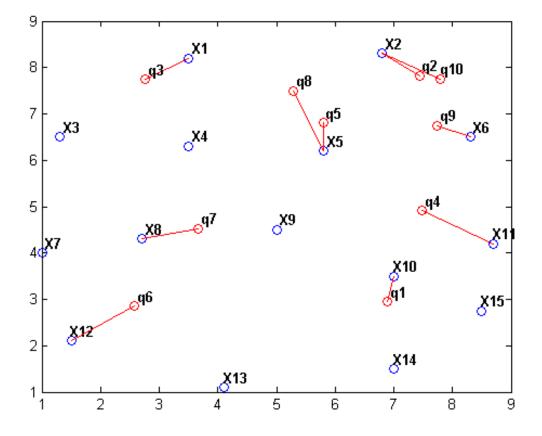
Create some query points and for each query point find the index of its corresponding nearest neighbor in X using the nearestNeighbor method.

```
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.

```
xnn = X(xi,:);
hold on
plot(q(:,1),q(:,2),'or');
plot([xnn(:,1) q(:,1)]',[xnn(:,2) q(:,2)]','-r');
vxlabels = arrayfun(@(n) {sprintf('q%d', n)}, (1:numq)');
Hpl = text(q(:,1)+0.2, q(:,2)+0.2, vxlabels, 'FontWeight', ...
        'bold', 'HorizontalAlignment','center', ...
        'BackgroundColor','none');
```

```
hold off
```



Performing a nearest-neighbor search in 3-D is a direct extension of the 2-D example based on delaunayTriangulation.

For 4-D and higher, use the delaunayn and dsearchn functions as illustrated in the following example:

Create a random sample of points in 4-D and triangulate the points using delaunayn:

X = 20\*rand(50,4) - 10;

```
tri = delaunayn(X);
```

Create some query points and for each query point find the index of its corresponding nearest neighbor in X using the dsearchn function:

q = rand(5,4); xi = dsearchn(X,tri, q)

The nearestNeighbor method and the dsearchn function allow the Euclidean distance between the query point and its nearest neighbor to be returned as an optional argument. In the 4-D example, you can compute the distances (dnn) as follows:

[xi dnn] = dsearchn(X,tri, q)

## **Point Location**

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 two approaches to performing a point-location search in MATLAB, depending on the dimensionality of the problem:

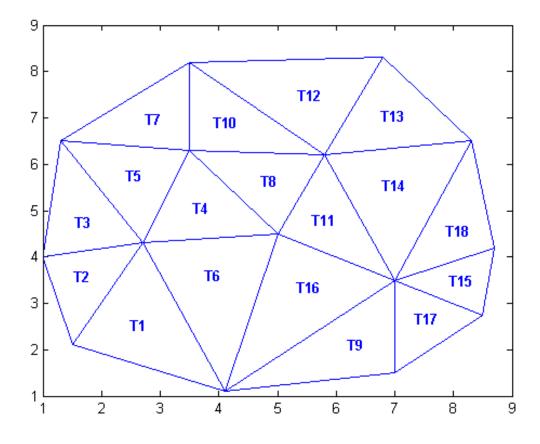
- For 2-D and 3-D, use the class-based approach with the pointLocation method provided by the delaunayTriangulation class.
- For 4-D and higher, use the delaunayn function to construct the triangulation and the complementary tsearchn function performs the point location search. Although supporting 2-D and 3-D, these N-D functions are not as efficient as the search methods provided by delaunayTriangulation.

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];

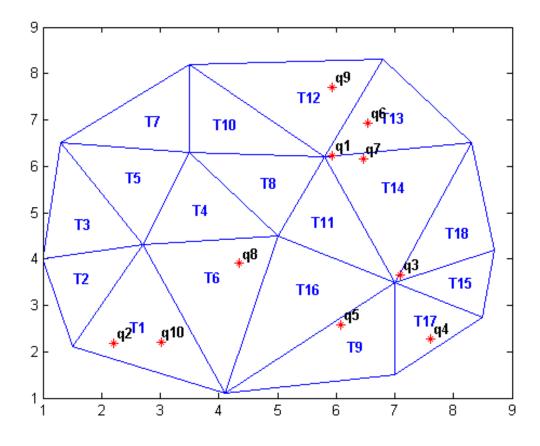
Create the triangulation and plot it showing the triangle ID labels at the incenters of the triangles.



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;

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 7-59 for further details.

#### **Searching Non-Delaunay Triangulations**

You only can use the search functions tsearchn and dsearchn to search convex, fully connected Delaunay triangulations that were created in MATLAB. If you create a Delaunay triangulation using delaunayn and subsequently modify the location of the coordinates, then the Delaunay criterion could be invalid. Therefore, you should not use the search functions as they may not converge. The search functions do not check the validity of the Delaunay triangulation as this would introduce a significant performance penalty. Imported triangulations, such as triangulations used for finite element analysis, tend to be nonconvex. They could have holes, or they might not respect the Delaunay criterion. Hence, you cannot reliably use the search functions tsearchn and dsearchn on triangulations like these.

The class delaunayTriangulation is more secure in this respect because you only can use the search methods to search a delaunayTriangulation. However, you cannot perform a nearestNeighbor search on a delaunayTriangulation that has constrained edges as it is locally non-Delaunay. To perform a nearest-neighbor search on a constrained delaunayTriangulation, do one of the following:

- Delete the constraints
- Create a new unconstrained delaunayTriangulation using the same point set, and use the unconstrained triangulation to perform the search.

Similarly, to perform a nearest-neighbor search on a triangulation that is represented in matrix format, create a delaunayTriangulation from the vertex coordinates and use it to perform the search.

MATLAB does not provide dedicated functions for performing a point location search on a 2-D (triangle) or 3-D (tetrahedral) triangulations that are in matrix format and do not meet the search function requirements. However, for relatively small triangulations, a brute-force search might be viable. For a 2-D triangulation, you might recreate the triangulation topology using a constrained delaunayTriangulation.

You can perform the brute-force search by checking the query point against every triangle (or tetrahedron) and selecting the one that contains the point. For example, suppose you have the following triangulation in matrix format and you want to perform a brute-force point location search that finds a triangle enclosing a point.

```
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];
```

```
tri = delaunay(X);
% Remove first triangle to make the triangulation nonconvex
tri(1,:) = [];
```

The first thing you can do is create a triangulation to represent this triangulation:

tr = triangulation(tri,X);

The triangulation class has many useful query methods, but it does not have a pointLocation or a nearestNeighbor method. A triangulation

can represent a nonconvex triangulation with holes and non-Delaunay triangulations, but the search algorithms preclude these.

The triangulation class provides a useful method that you can use to check if a query point lies within a specified triangle (or tetrahedron). The method is cartesianToBarycentric. Given a point expressed in Cartesian coordinates and a specified triangle in the triangulation, this method returns the barycentric coordinates of the point with respect to the triangle. If all three barycentric coordinates are positive, the point is within the triangle . Otherwise, the point is outside the triangle. Plot the triangulation to explore this method:

Search for the triangle enclosing (6,3):

```
numtri = size(tr,1);
B = cartesianToBarycentric(tr, (1:numtri)', repmat([6 3], numtri,1));
posB = (B >= 0);
enclosingTri = find(posB(:,1) & posB(:,2) & posB(:,3))
```

You can now use a constrained delaunayTriangulation to perform the search. You should start with the triangulation you created in the brute-force search and use it to find all edges in the triangulation so you can constrain them.

```
Cedges = edges(tr);
```

Now create the constrained delaunayTriangulation and plot it in a separate figure so you can compare both triangulations.:

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```
dt = delaunayTriangulation(X, Cedges)
figure
triplot(dt)
axis equal
hold on
ic = incenter(dt);
numtri = size(dt,1);
trilabels = arrayfun(@(x) {sprintf('T%d', x)}, (1:numtri)');
Htl = text(ic(:,1), ic(:,2), trilabels, 'FontWeight', ...
                     'bold', 'HorizontalAlignment', 'center', 'Color', ...
                    'blue');
hold off
```

Since the triangle numbering is different in each triangle, you need to build an array of indices to map triangle IDs from the delaunayTriangulation to the triangulation. To do this mapping, you will compute the incenters of the triangulation and find the corresponding enclosing triangles in the delaunayTriangulation:

```
dtTotrIndex = nan(size(dt,1),1);
ic = incenter(tr);
dtid = pointLocation(dt,ic);
```

dtTotrIndex(dtid) = 1:size(tr,1);

Now you use the delaunayTriangulation to perform the point location search. Next, use the map to find the corresponding triangle in the triangulation:

```
trid = pointLocation(dt, 6,3);
if isfinite(trid)
    trid = dtTotrIndex(trid);
end
trid
```

## Voronoi Diagrams

#### In this section...

"Plot 2-D Voronoi Diagram and Delaunay Triangulation" on page 6-70

"Computing the Voronoi Diagram" on page 6-75

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.

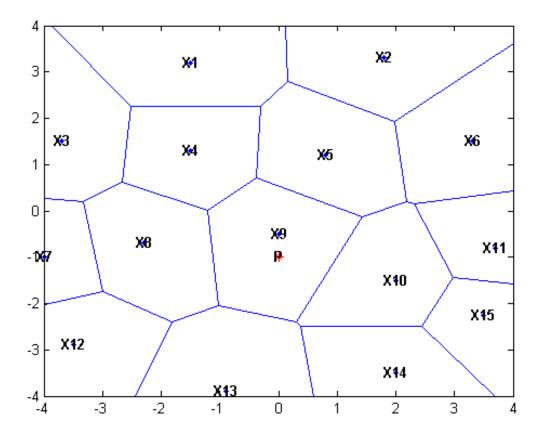
The Voronoi diagram is an N-D geometric construct, but most practical applications are in 2-D and 3-D space. The properties of the Voronoi diagram are best understood using an example.

#### 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.

```
'BackgroundColor', 'none');
% Add a query point, P, at (0, -1.5).
P = [0 -1];
plot(P(1),P(2), '*r');
text(P(1), P(2), 'P', 'FontWeight', 'bold', ...
'HorizontalAlignment','center', ...
'BackgroundColor', 'none');
hold off
```

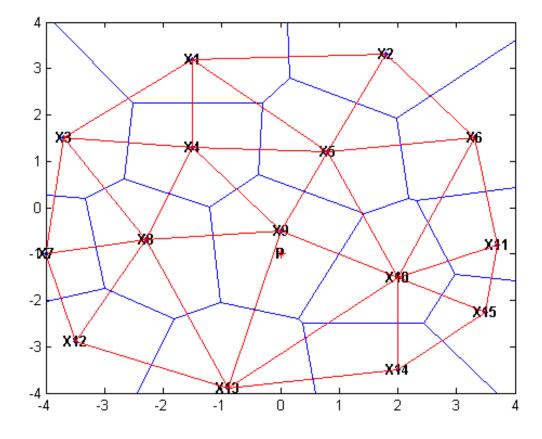


Observe that P is closer to X9 than to any other point in X, which is true for any point P within the region that bounds X9.

The Voronoi diagram of a set of points X is closely related to the Delaunay triangulation of X. To see this relationship, construct a Delaunay triangulation of the point set X and superimpose the triangulation plot on the Voronoi diagram.

```
dt = delaunayTriangulation(X);
hold on
triplot(dt,'-r');
hold off
```

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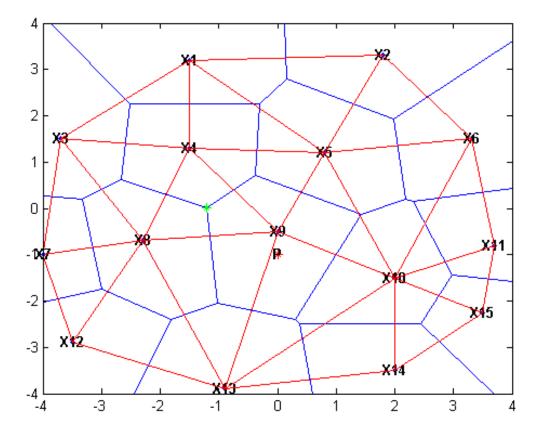
From the plot you can see that the Voronoi region associated with the point X9 is defined by the perpendicular bisectors of the Delaunay edges attached to X9. Also, the vertices of the Voronoi edges are located at the circumcenters of the Delaunay triangles. You can illustrate these associations by plotting 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 = dt.pointLocation(-1, 0);

Now, find the circumcenter of this triangle and plot it in green.

cc = dt.circumcenter(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.

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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 software 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 the delaunayTriangulation method, voronoiDiagram.

The voronoin function supports the computation of the Voronoi topology for discrete points in N-D (N  $\geq$  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 6-5 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

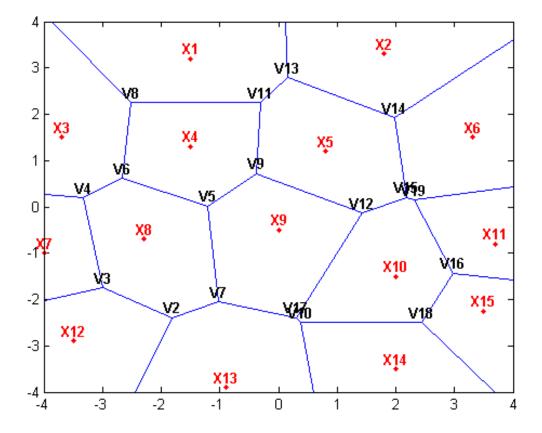
```
dt = delaunayTriangulation(X);
```

[V, R] = dt.voronoiDiagram(X)

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');
set(h(1:end-1),'xliminclude','off','yliminclude','off')
% 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] = dt.voronoiDiagram();
% Assign labels to the Voronoi vertices V.
% By convention the first vertex is at infinity.
numv = size(V,1);
```



 $R\{9\}$  gives the indices of the Voronoi vertices associated with the point site X9.  $R\{9\}$ 

ans = 5 7 17 12 9

The indices of the Voronoi vertices are the indices with respect to the V array.

Similarly,  $R{4}$  gives the indices of the Voronoi vertices associated with the point site X4.

R{4} ans = 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.

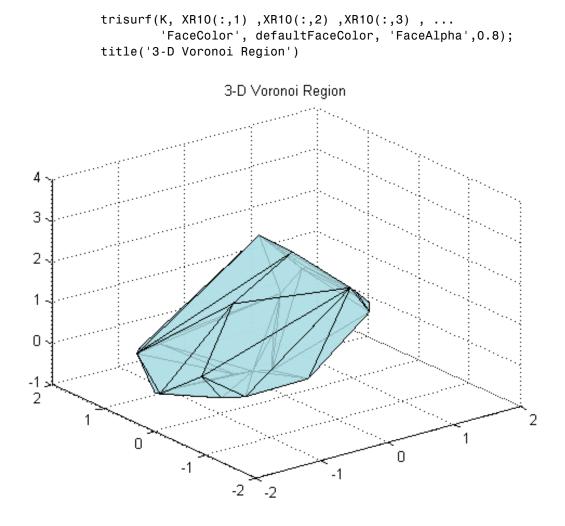
```
X = -3 + 6.*gallery('uniformdata',[25 3],0);
dt = delaunayTriangulation(X);
```

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.

```
tid = nearestNeighbor(dt,0,0,0);
XR10 = V(R{tid},:);
K = convhull(XR10);
defaultFaceColor = [0.6875 0.8750 0.8984];
```

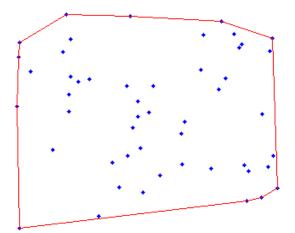


## Concepts

• "Spatial Searching" on page 6-56

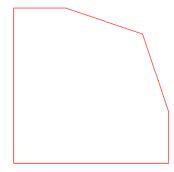
## **Convex Hulls**

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.



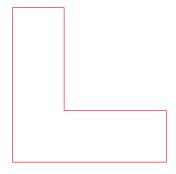
#### The Convex Hull of a Set of Points

A convex polygon is a polygon that does not have concave vertices, for example:



**Convex Polygon** 

A nonconvex polygon has concave vertices:



#### **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.

## **Computing the Convex Hull**

MATLAB provides two ways to compute the convex hull:

- Using the MATLAB functions convhull and convhulln
- Using the  ${\tt convexHull}$  method provided by the  ${\tt delaunayTriangulation}$  class

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  $\geq$  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.

## Computing the Convex Hull Using convhull and convhulln

The convhull and convhulln functions take a set of points and output the indices of the points that lie on the boundary of the convex hull. The point index-based representation of the convex hull supports plotting and convenient data access. The following examples illustrate the computation and representation of the convex hull.

The first example uses a 2-D point set from the seamount dataset as input to the convhull function.

Load the data.

load seamount

Compute the convex hull of the point set.

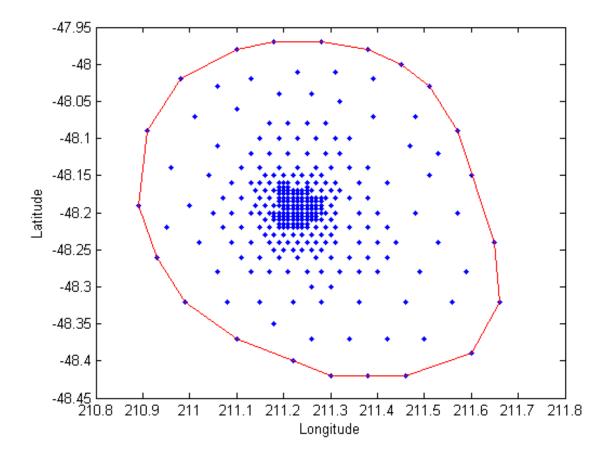
K = convhull(x, y);

K represents the indices of the points arranged in a counter-clockwise cycle around the convex hull.

Plot the data and its convex hull.

```
plot(x,y,'.','markersize',12)
xlabel('Longitude'), ylabel('Latitude')
hold on
```

plot(x(K),y(K),'r')



Add point labels to the points on the convex hull to observe the structure of K.

[K A] = convhull(x, y);

convhull can compute the convex hull of both 2-D and 3-D point sets. You can reuse the seamount dataset to illustrate the computation of the 3-D convex hull.

Include the seamount z-coordinate data elevations.

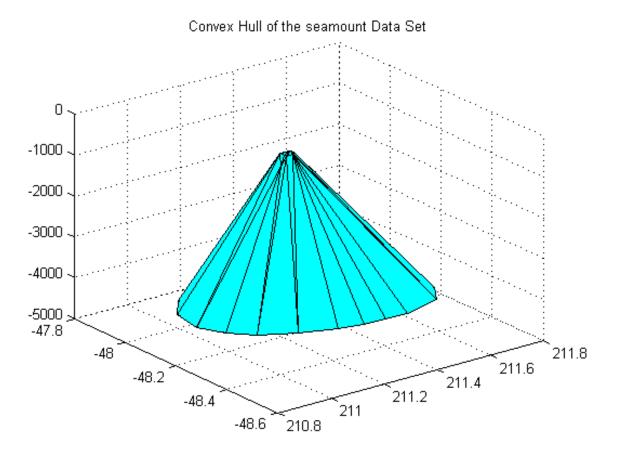
close(gcf)

K = convhull(x,y,z);

In 3-D the boundary of the convex hull, K, is represented by a triangulation. This is a set of triangular facets in matrix format that is indexed with respect to the point array. Each row of the matrix K represents a triangle.

Since the boundary of the convex hull is represented as a triangulation, you can use the triangulation plotting function trisurf.

trisurf(K,x,y,z, 'Facecolor','cyan'); title('Convex Hull of the seamount Data Set')

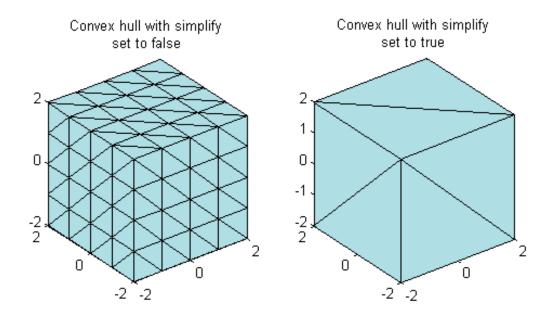


The volume bounded by the 3-D convex hull can optionally be returned by convhull, the syntax is as follows.

[K V] = convhull(x,y,z);

The convhull function also provides the option of simplifying the representation of the convex hull by removing vertices that do not contribute to the area or volume. For example, if boundary facets of the convex hull are collinear or coplanar, you can merge them to give a more concise representation. The following example illustrates use of this option.

```
[x,y,z] = meshgrid(-2:1:2, -2:1:2, -2:1:2);
x = x(:); y = y(:); z = z(:);
K1 = convhull(x,y,z);
subplot(1,2,1);
defaultFaceColor = [0.6875 0.8750 0.8984];
trisurf(K1,x,y,z, 'Facecolor', defaultFaceColor); axis equal;
title(sprintf('Convex hull with simplify\nset to false'));
K2 = convhull(x,y,z, 'simplify',true);
subplot(1,2,2);
trisurf(K2,x,y,z, 'Facecolor', defaultFaceColor); axis equal;
title(sprintf('Convex hull with simplify\nset to true'));
```



MATLAB provides the convhulln function to support the computation of convex hulls and hypervolumes in higher dimensions. Though convhulln supports N-D, problems in more than 10 dimensions present challenges due to the rapidly growing memory requirements.

The convhull function is superior to convhulln in 2-D and 3-D as it is more robust and gives better performance.

## Convex Hull Computation Using the 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.

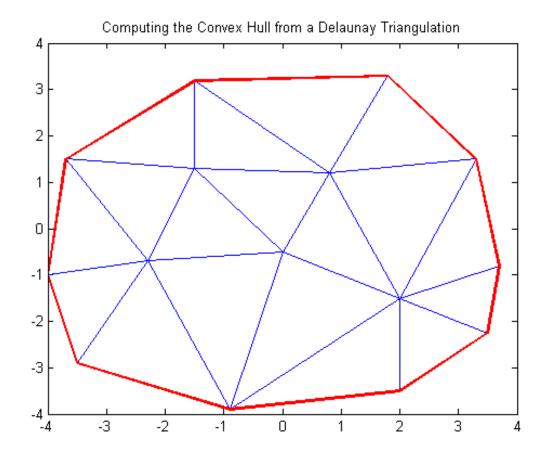
The delaunayTriangulation class supports computation of Delaunay triangulations in 2-D and 3-D space. This class also provides a convexHull method to derive the convex hull from the triangulation.

Create a Delaunay triangulation of a set of points in 2-D.

```
dt = delaunayTriangulation(X);
```

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);
title('Computing the Convex Hull from a Delaunay Triangulation')
hold off;
```



In 3-D, the facets of the triangulation that are shared only by one tetrahedron represent the boundary of the convex hull.

The dedicated convhull function is generally more efficient than a computation based on the convexHull method. However, the triangulation based approach is appropriate if:

• You have a delaunayTriangulation of the point set already and the convex hull is also required.

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• 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.

## Concepts

- "Using the delaunayTriangulation Class" on page 6-29
- "Triangulation Matrix Format" on page 6-5



# Interpolation

- "Gridded and Scattered Sample Data" on page 7-2
- "Interpolating Gridded Data" on page 7-4
- "Interpolation of Multiple 1-D Value Sets" on page 7-55
- "Interpolation of 2-D Selections in 3-D Grids" on page 7-57
- "Interpolating Scattered Data" on page 7-59
- "Interpolation Using a Specific Delaunay Triangulation" on page 7-93
- "Extrapolating Scattered Data" on page 7-96

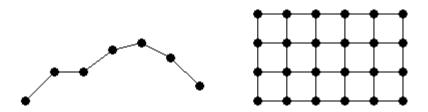
## **Gridded and Scattered Sample Data**

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.

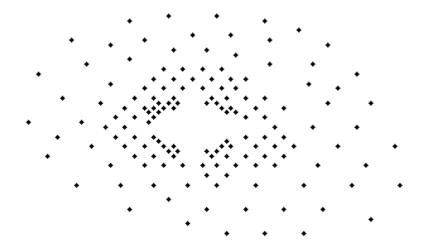
The computation of the value Vq is generally based on the data points in the neighborhood of the query point Xq. There are numerous approaches to performing interpolation. In MATLAB interpolation is classified into two categories depending on the structure of the sample data. The sample data may be ordered 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 7-4 section covers 1-D interpolation, and the N-D (N  $\geq$  2) interpolation of sample data in axis-aligned grid format:



• The "Interpolating Scattered Data" on page 7-59 section covers the N-D (N  $\geq$  2) interpolation of scattered data:



## **Interpolating Gridded Data**

#### In this section ...

"Gridded Data Representation" on page 7-4  $\,$ 

"Grid-Based Interpolation" on page 7-19

"Interpolation with the interp Family of Functions" on page 7-26

"Interpolation with the griddedInterpolant Class" on page 7-41

## **Gridded Data Representation**

- "Grid Representation" on page 7-4
- "Types of Grid Representations" on page 7-13
- "Grid Approximation Techniques" on page 7-16

### **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 =

0.9501	0.4860	0.4565	0.4447	0.9218
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:

Γ	1	4	7	10	13
	2	5	8	11	14
L	3	6	9	12	13 14 15

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-1i-m i i+mi+1

Retrieve the column elements adjacent to A(7).

A(6),A(8)

```
ans =
0.7621
ans =
0.0185
```

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.

```
xgv = [1 2 3];
ygv = [1 2 3 4 5];
[X, Y] = meshgrid(xgv, ygv)
```

```
Х =
```

1	2	3
1	2	3
1	2	3
1	2	3
1	2	3

Y = 1 1 2 2 3 3 4 4 5 5

1

2

3

4

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	1	1
	2	2	2	2	2
	3	3	3	3	3
X2 =					
	1	2	3	4	5
	1	2	3	4	5
	1	2	3	4	5

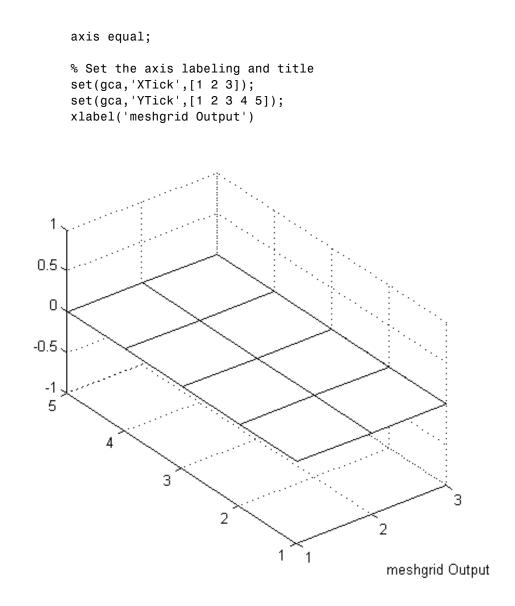
Notice that ndgrid's X1 is the transpose of meshgrid's X. The same is true for X2 and Y.

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
     set(gca, 'XTick', [1 2 3]);
     set(gca, 'YTick', [1 2 3 4 5]);
     xlabel('ndgrid Output')
  1
0.5
  0
-0.5
 -1
  5
          4
                   З
                                                             3
                           2
                                                  2
                                    1
                                       1
                                                   ndgrid Output
```

figure()
[X\_meshgrid,Y\_meshgrid] = meshgrid(1:3, 1:5);
mesh(X\_meshgrid,Y\_meshgrid,Z','EdgeColor','black')



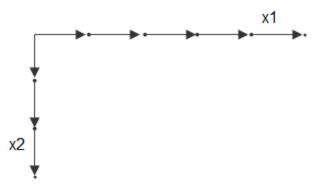
Depending on how you intend to use your grid, you may prefer one format or the other. Some functions in MATLAB might require your data to have a meshgrid format while others might require an ndgrid format. **Converting Between Grid Formats.** To convert a 2-D grid output from meshgrid to the ndgrid format, transpose the coordinate matrices:

You can also use the permute function.

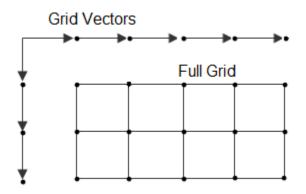
```
isequal(permute(X_meshgrid,[2 1]),X1_ndgrid)
ans =
    1
```

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:

**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:

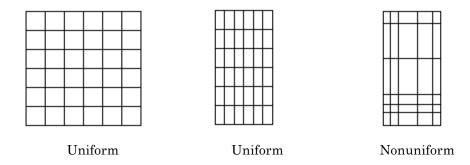
[X1,X2] = ndgrid([2 4 6 3 1])						
X1 =						
2	2	2	2	2		
4	4	4	4	4		
6	6	6	6	6		
3	3	3	3	3		
1	1	1	1	1		
X2 =						
2	4	6	3	1		
2	4	6	3	1		
2	4	6	3	1		
2	4	6	3	1		
2	4	6	3	1		

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.



## **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 7-41.)

**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.

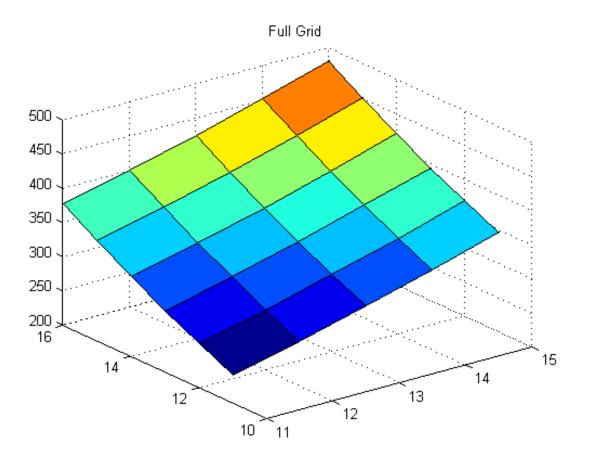
This example shows how you can use the default grid instead of the full grid to produce a plot.

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.

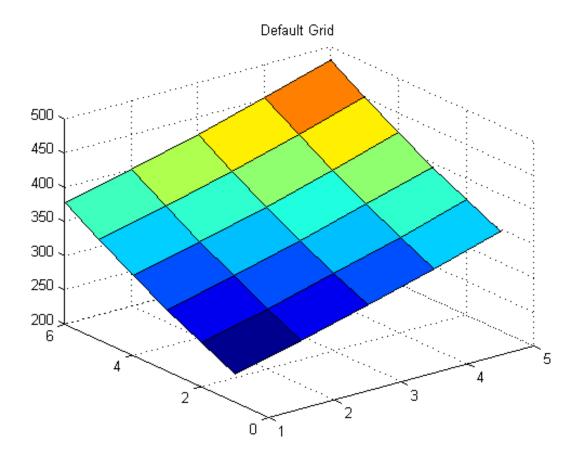
figure()
surf(X,Y,Z)
title('Full Grid')



In contrast, have MATLAB create a default grid instead of using the full grid.

```
figure()
surf(Z)
title('Default Grid')
```

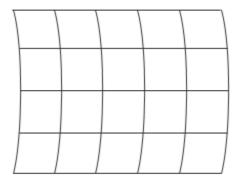
7



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:

	i i i i i i i i i i i i i i i i i i i	 1111111	1000000000

You can also use the default grid.

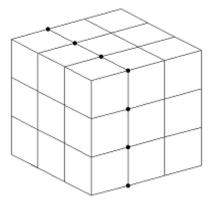
**Degenerate Grid.** A *degenerate grid* is a special case of grid where one or more dimensions of the grid are singletons. A singleton dimension can be internal, as in 7:7 in this example:

[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:

```
[X1, X2, X3] = ndgrid(1:3);
X1_slice = X1(:,:,2)
X1_slice =
     1
                   1
            1
     2
            2
                   2
     3
            3
                   3
X2_slice = X2(:,:,2)
X2 slice =
     1
            2
                   3
            2
     1
                   3
     1
            2
                   3
X3_slice = X3(:,:,2)
X3 slice =
     2
            2
                   2
     2
            2
                   2
```

2 2 2

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 7-19
- "Interpolation versus Fit" on page 7-23
- "Interpolation Methods" on page 7-23

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:

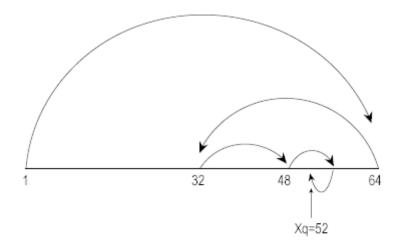
1 3 5 7 9 0 0 0 0 0

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:

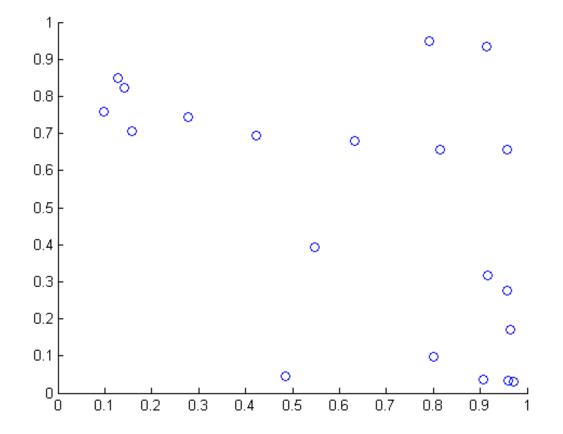
- **1** Locate the center grid point.
- 2 Compare Xq to the point at the center of the grid.
- **3** If Xq is less than the point found at the center, eliminate all of the grid points greater than central point from the search. Similarly, if Xq is greater than the one found at the center, we eliminate 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.
- **4** 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 7-59.

# 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.

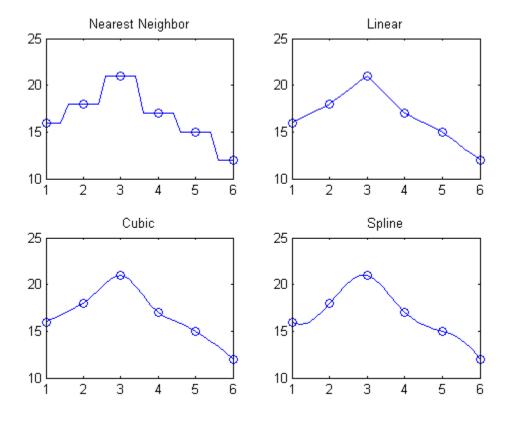
# **Interpolation Methods**

Grid-based interpolation offers five 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.
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.

# (Continued)

Method	Description	Continuity	Memory Usage and Performance	Requirements
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>
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 7-26
- "1-D Extrapolation With interp1" on page 7-27
- "The interp2 Function" on page 7-31
- "The interp3 Function" on page 7-34
- "The interpn Function" on page 7-35

### The interp1 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 is an optional string specifying any of four interpolation methods: 'nearest', 'linear', 'pchip', or 'spline'.

Create a set of 1-D grid points X and corresponding sample values V.

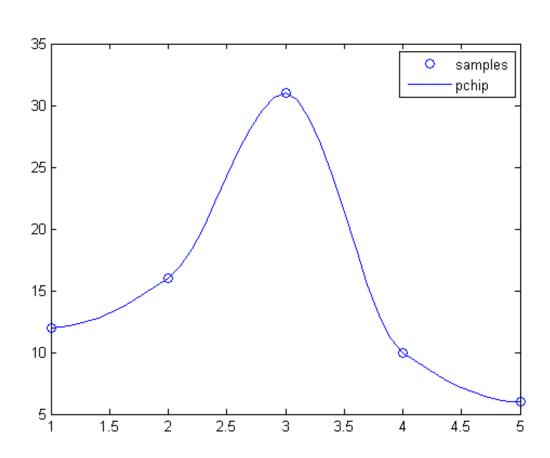
X = [1 2 3 4 5]; V = [12 16 31 10 6];

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.

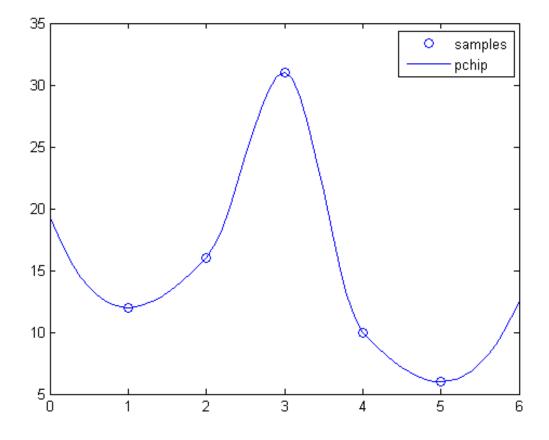
Define the sample points and values.

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.

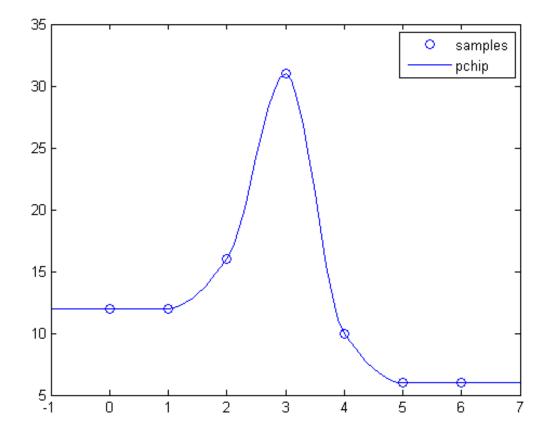
$$Xq = (-1:0.1:7);$$

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:

Vq = interp2(X,Y,V,Xq,Yq,method)

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 is an optional string specifying any of four interpolation methods: 'nearest', 'linear', 'cubic', or 'spline'.

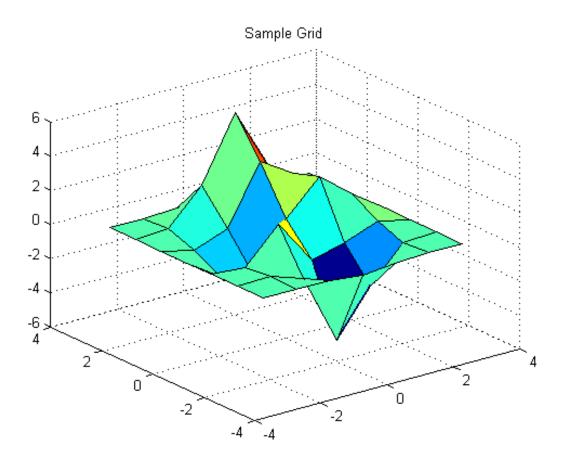
The grid points that comprise X and Y must be monotonically increasing and should conform to the meshgrid format.

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.

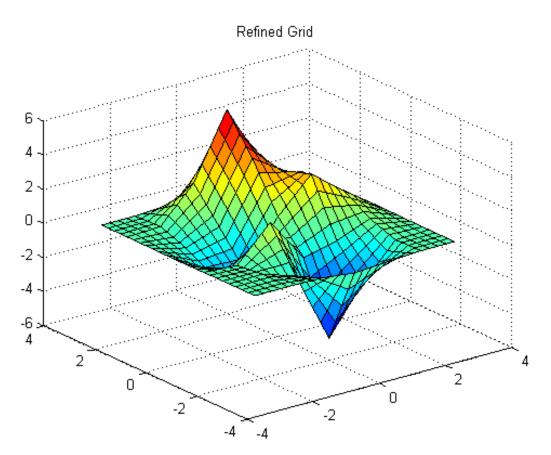
[Xq,Yq] = meshgrid(-3:0.25:3);

Use interp2 to interpolate at the query points.

Vq = interp2(X,Y,V,Xq,Yq,'linear');

Plot the results.

surf(Xq,Yq,Vq);



#### title('Refined Grid');

### 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,

7-34

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.

generated values =  $@(X,Y,Z)(X.^2 + Y.^3 + Z.^4);$ 

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.

```
V_actual = generatedvalues(2.35,1.76,0.23)
```

V\_actual =

10.9771

#### 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 is an optional string specifying any of four interpolation methods: 'nearest', 'linear', 'cubic', or 'spline'.

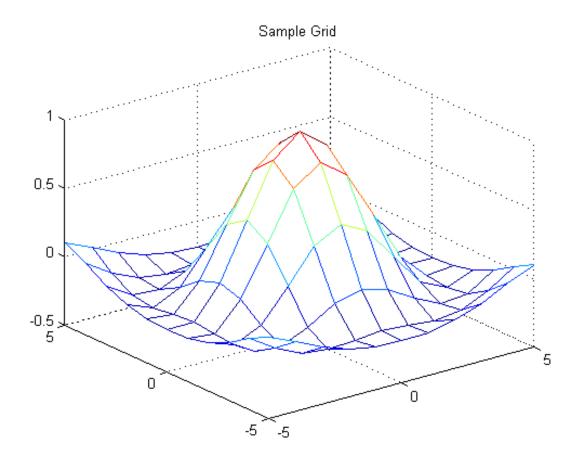
The grid points that comprise X1,X2,X3,...Xn must be monotonically increasing and should conform to the ndgrid format.

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');



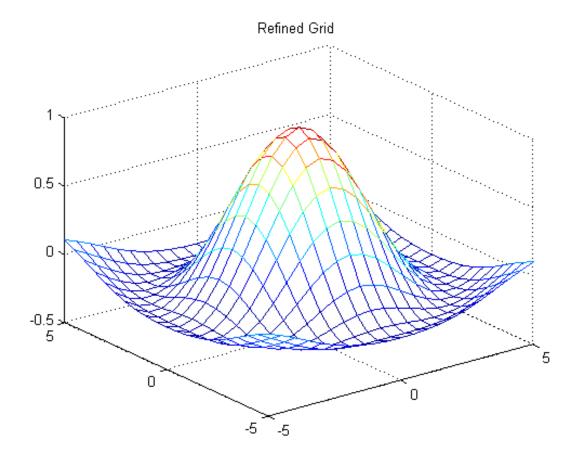
Create a finer grid for interpolation.

[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');
```

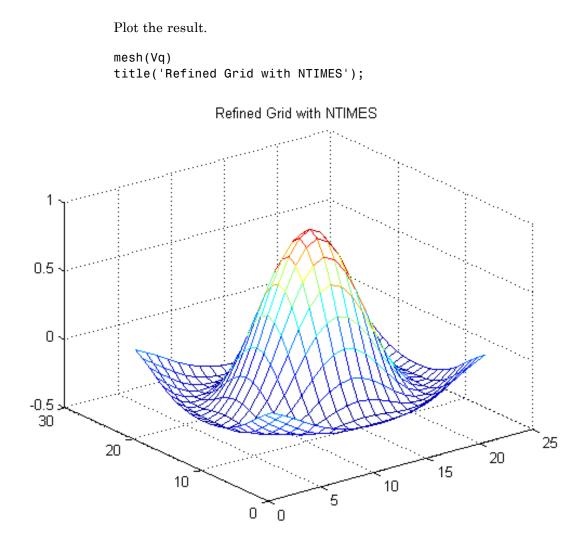
7



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');



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.

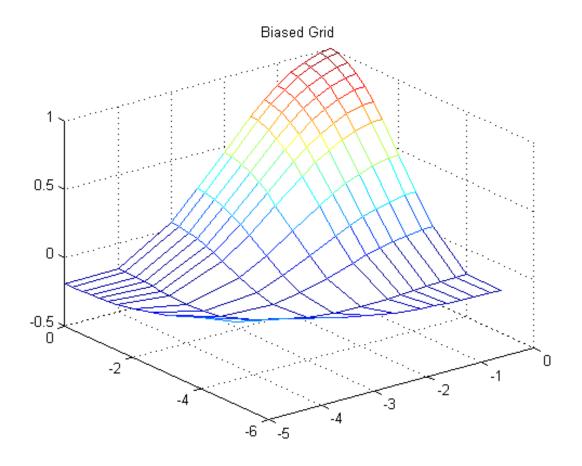
You can also supply nonunifom grid of query points. This can be useful if you are interested in querying the interpolant at a higher resolution in one region of the grid. The following code shows how this can be done.

Interpolate over a biased grid.

```
[Y1, Y2] = ndgrid([-5 -4 -3 -2.5 -2 -1.5 -1.25 -1 -0.75 -0.5 -0.20 0]);
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 7-44 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 preforms interpolation. You create the interpolant by calling the griddedInterpolant constructor and passing the sample data: the grid and corresponding sample values. You can also specify the inerpolation 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.

 $Vq = F(x1q, x2q, \dots, xnq)$ 

• 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.

 $Vq = F(X1q, X2q, \dots, Xnq)$ 

• 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'
```

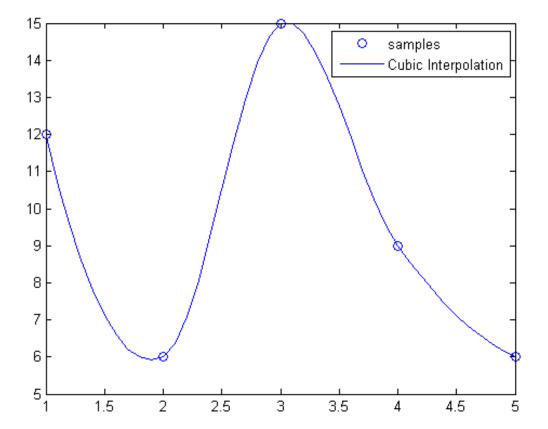
The GridVectors property contains the compact grid specifying the coordinates of the sample values V. The Method property is a string specifying the interpolation method. Notice that we specified 'cubic' when we created F. If you omit the Method argument, the default interpolation method, linear, will be assigned to F.

You can access any of the properties of  ${\sf F}$  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. 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 griddedInterpolant.

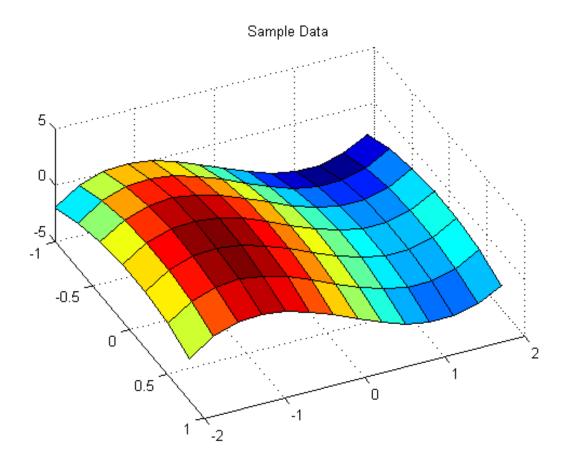
F = griddedInterpolant(X,Y,V,'spline');

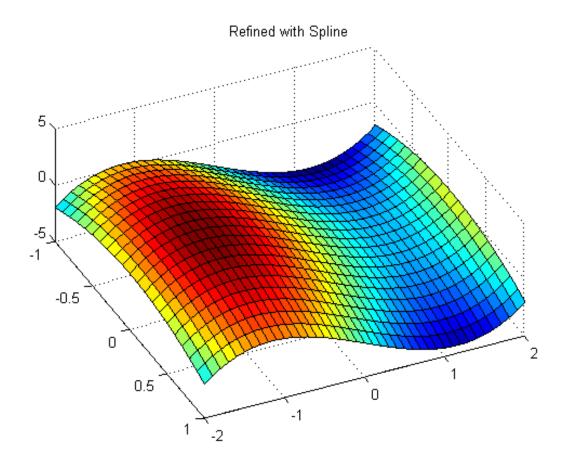
Interpolate over finer intervals with 0.1 spacing.

[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.

[X,Y,Z] = ndgrid((-5:2:5)); V = X.^3 + Y.^2 + Z.^2;

 $Construct \ the \ {\tt griddedInterpolant}.$ 

```
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 griddedInterpolant. 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,

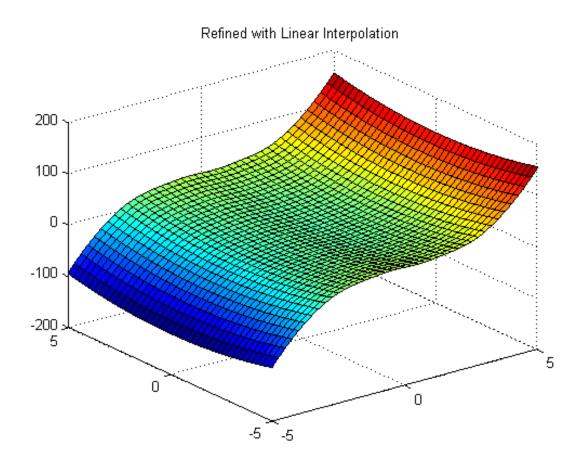
gv = {(-5:2:5),(-5:2:5),(-5:2:5)}; F = griddedInterpolant(gv,V,'cubic');

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.

[X1,X2,X3,X4] = ndgrid((-5:2:5)); V = X1.^3 + X2.^2 + X3.^2 + X4;

**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 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 values sets.

x = (1:5)';

Define the sets of sample points along the columns of matrix V.

V	=	[×,	2*x,	3*x]
V	=			
		1	2	3
		2	4	6
		3	6	9
		4	8	12
		5	10	15

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,  ${\tt F},$  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** • "Interpolation with the griddedInterpolant Class" on page 7-41 **Examples** 

# 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.

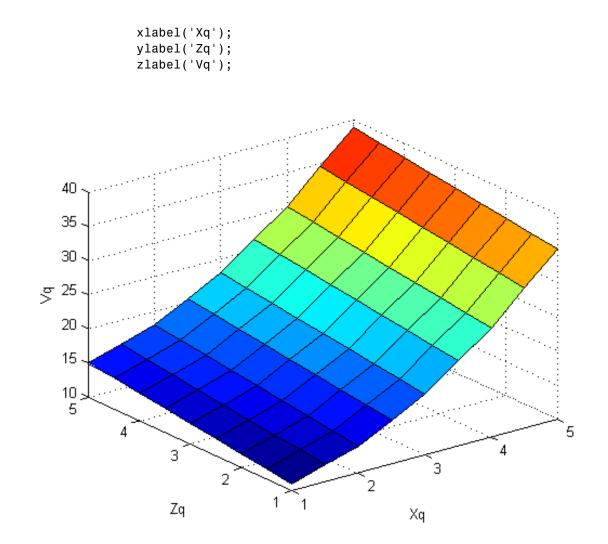
x = squeeze(x); z = squeeze(z); v = squeeze(v);

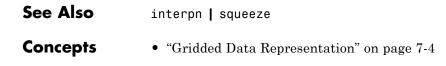
Interpolate the 2-D slice over a finer grid of query points.

[Xq,Zq] = ndgrid(1:0.5:5); Vq = interpn(x,z,v,Xq,Zq);

Plot the results.

figure
surf(Xq,Zq,Vq);





## **Interpolating Scattered Data**

#### In this section ...

"Scattered Data" on page 7-59

"Interpolating Scattered Data Using griddata and griddatan" on page 7-63

"scatteredInterpolant Class" on page 7-67

"Interpolating Scattered Data Using the scatteredInterpolant Class" on page 7-68

"Interpolation of Complex Scattered Data" on page 7-79

"Addressing Problems in Scattered Data Interpolation" on page 7-82

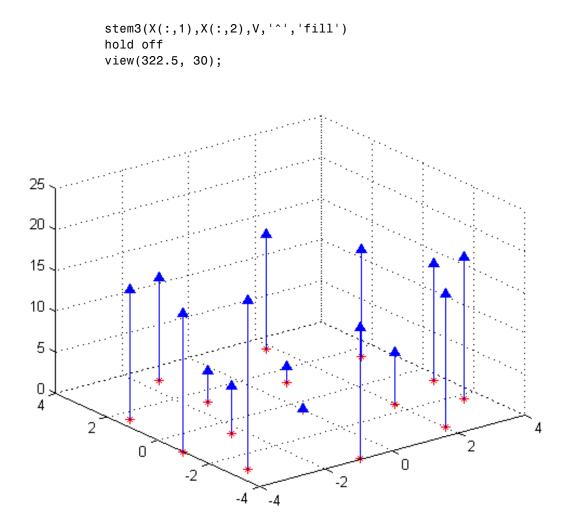
## **Scattered Data**

Scattered data consists of a set of points X and corresponding values V, where the points have no structure or order between their relative locations. There are various approaches to interpolating scattered data. One widely used approach uses a Delaunay triangulation of the points.

This example shows how to construct an interpolating surface by triangulating the points and lifting the vertices by a magnitude V into a dimension orthogonal to X.

There are variations on how you can apply this approach. In this example, the interpolation is broken down into separate steps; typically, the overall interpolation process is accomplished with one function call.

Create a scattered data set on the surface of a paraboloid.



Create a Delaunay triangulation, lift the vertices, and evaluate the interpolant at the query point Xq.

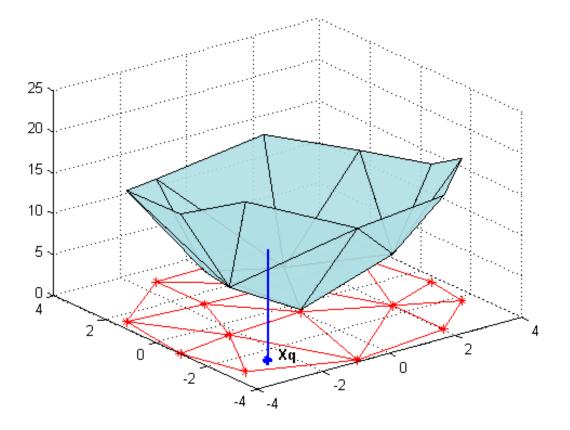
```
figure('Color', 'white')
t = delaunay(X(:,1),X(:,2));
```

hold on

```
trimesh(t,X(:,1),X(:,2), zeros(15,1), ...
        'EdgeColor','r', 'FaceColor','none')
defaultFaceColor = [0.6875 0.8750 0.8984];
trisurf(t,X(:,1),X(:,2), V, 'FaceColor', ...
        defaultFaceColor, 'FaceAlpha',0.9);
plot3(X(:,1),X(:,2),zeros(15,1), '*r')
axis([-4, 4, -4, 4, 0, 25]);
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');

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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

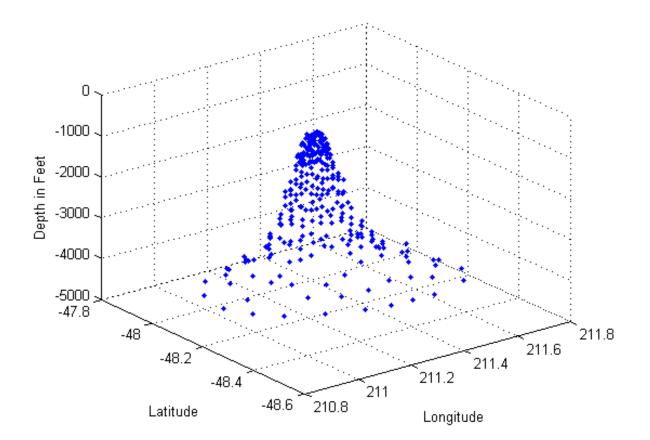
The griddata and griddatan functions take a set of sample points, X, corresponding values, V, and query points, Xq, and return the interpolated values, Vq. The calling syntax is similar for each function; the distinction is the 2-D griddata function lets you define the points in terms of X, Y coordinates. 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.

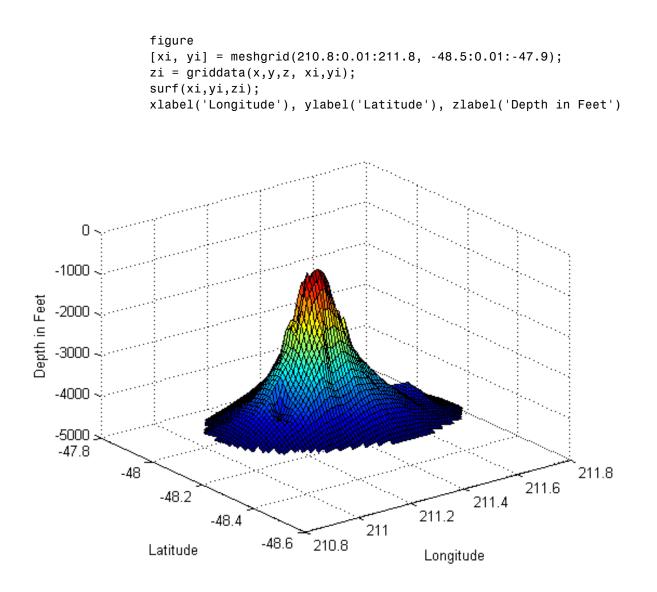
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Plot the seamount data set (a *seamount* is an underwater mountain). The data set consists of a set of longitude (x) and latitude (y) locations, and corresponding seamount elevations (z) measured at those coordinates.

```
load seamount
plot3(x,y,z,'.','markersize',12)
xlabel('Longitude'), ylabel('Latitude'), zlabel('Depth in Feet')
grid on
```

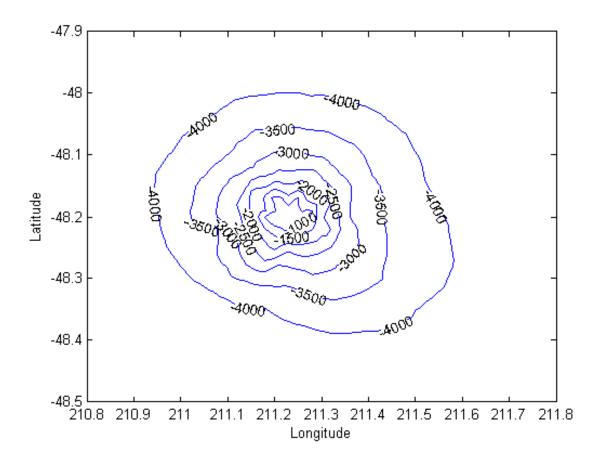


Use meshgrid to create a set of 2-D grid points in the longitude-latitude plane and then use griddata to interpolate the corresponding depth at those points.



Now that the data is in a gridded format, compute and plot the contours.

figure
[c h] = contour(xi,yi,zi, 'b-');
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 griddata 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 7-68 is more efficient in this respect.

MATLAB software also provides griddatan to support interpolation in higher dimensions. The calling syntax is similar to griddata.

The griddata function supports 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.
- 'cubic' Cubic interpolation, where the interpolating surface is C2 continuous.

The griddatan function supports the following interpolation methods:

- 'nearest' Nearest-neighbor interpolation, where the interpolating surface is discontinuous, and
- 'linear' Linear interpolation (default), where the interpolating surface is C0 continuous.

The 'nearest'and 'linear' methods are computationally more efficient than the 'cubic' method. The 'cubic' method is generally used when higher order continuity of the interpolating function is required. However, 'cubic' is not supported by the higher dimensional griddatan function.

## 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 supports natural-neighbor interpolation (which is an improvement over linear interpolation) and works well with larger data sets that have uneven sampling.
- It provides extrapolation functionality for approximating values at points that fall outside the convex hull. See "Extrapolating Scattered Data" on page 7-96 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.

```
X = -3 + 6.*gallery('uniformdata',[250 2],0);
V = peaks(X(:,1),X(:,2));
```

#### Create the interpolant.

```
F = scatteredInterpolant(X,V)
```

F =

scatteredInterpolant with properties:

```
Points: [250x2 double]
Values: [250x1 double]
Method: 'linear'
ExtrapolationMethod: 'linear'
```

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:

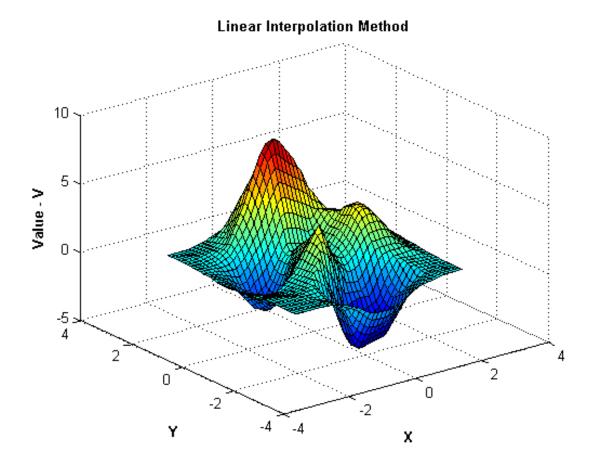
Xq = [0.5 0.25; 0.75 0.35; 1.25 0.85]; Vq = F(Xq)

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 <code>'nearest'</code>.

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');
```

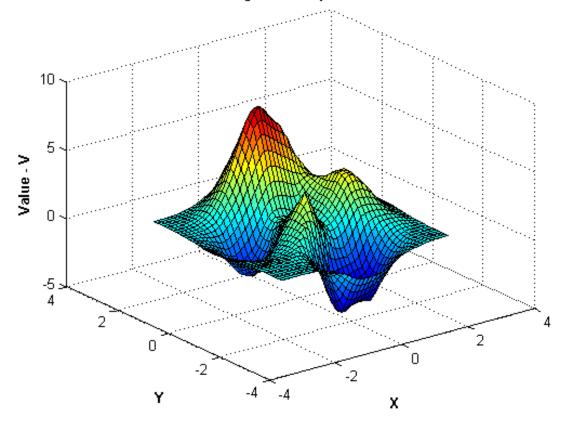
## Nearest neighbor Interpolation Method 10 5 Value - V 0 -5 4 2 Δ 2 0 0 -2 -2 -4 -4 Y х

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');
```

#### Natural neighbor Interpolation Method



#### 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

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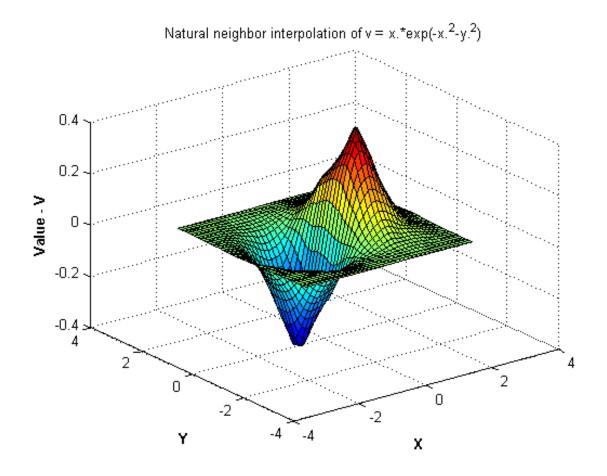
a 3-D velocity field that is defined by locations (x, y, z) and corresponding componentized velocity vectors (Vx, Vy, Vz). You can interpolate each of the velocity components by assigning them to the values property (V) in turn. This has important performance benefits, because it allows you to reuse the same interpolant without incurring the overhead of computing a new one each time.

The following steps show how to change the values in our example. You will compute the values using the expression,  $v = xe^{-x^2-y^2}$ .

V = X(:,1).\*exp(-X(:,1).^2-X(:,2).^2);
F.Values = V;

Evaluate the interpolant and plot the result.

```
Vq = F(Xq,Yq);
figure
surf(Xq,Yq,Vq);
xlabel('X','fontweight','b'), ylabel('Y','fontweight','b')
zlabel('Value - V','fontweight','b')
title('Natural neighbor interpolation of v = x.*exp(-x.^2-y.^2)')
```



#### Add additional point locations and values to the existing interpolant.

This performs an efficient update as opposed to a complete recomputation using the augmented data set.

When adding sample data, it is important to add both the point locations and the corresponding values.

Continuing the example, create new sample points as follows:

X = -1.5 + 3.\*rand(100,2);

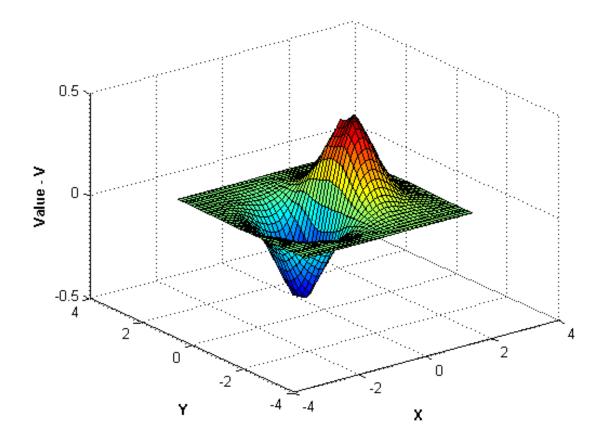
```
V = X(:,1).*exp(-X(:,1).^2-X(:,2).^2);
```

Add the new points and corresponding values to the triangulation.

F.Points(end+(1:100),:) = X; F.Values(end+(1:100)) = V;

Evaluate the refined interpolant and plot the result.

```
Vq = F(Xq,Yq);
figure
surf(Xq,Yq,Vq);
xlabel('X','fontweight','b'), ylabel('Y','fontweight','b');
zlabel('Value - V','fontweight','b');
```



#### Remove data from the interpolant.

You can incrementally remove sample data points from the interpolant. You also can remove data points and corresponding values from the interpolant. This is useful for removing spurious outliers.

When removing sample data, it is important to remove both the point location and the corresponding value.

Remove the 25th point.

F.Points(25,:) = [];
F.Values(25) = [];

Remove points 5 to 15.

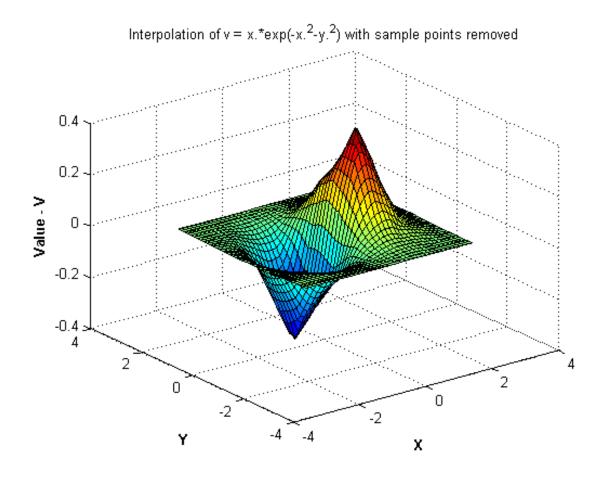
F.Points(5:15,:) = []; F.Values(5:15) = [];

Retain 150 points and remove the rest.

F.Points(150:end,:) = [];
F.Values(150:end) = [];

This creates a coarser surface when you evaluate and plot:

```
Vq = F(Xq,Yq);
figure
surf(Xq,Yq,Vq);
xlabel('X','fontweight','b'), ylabel('Y','fontweight','b');
zlabel('Value - V','fontweight','b');
title('Interpolation of v = x.*exp(-x.^2-y.^2) with sample points removed')
```



## **Interpolation of Complex Scattered Data**

This example shows how to interpolate scattered data when the value at each sample location is complex.

Create the sample data.

Create the interpolant.

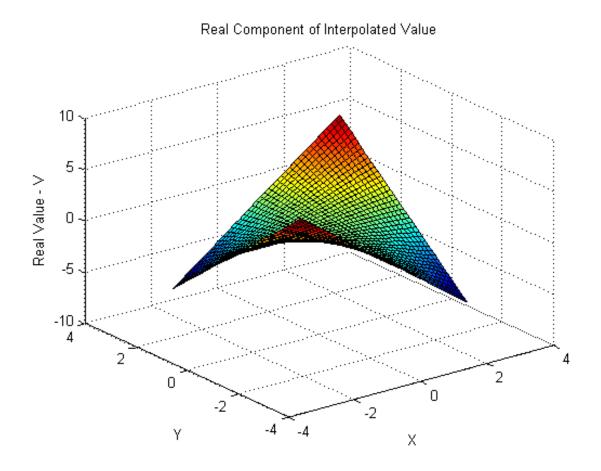
F = scatteredInterpolant(X,V);

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.

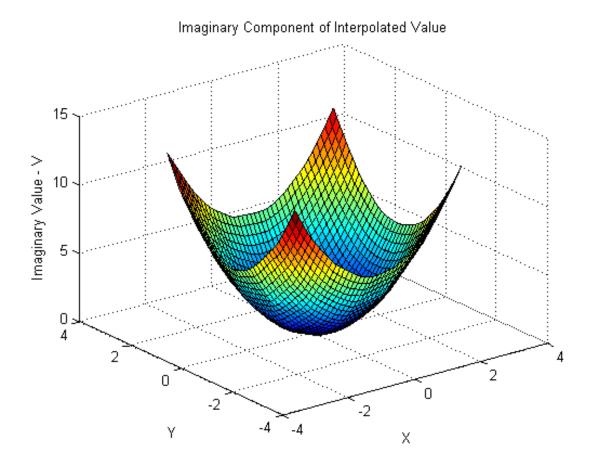
```
VqReal = real(Vq);
figure
surf(Xq,Yq,VqReal);
xlabel('X');
ylabel('Y');
zlabel('Real Value - V');
title('Real Component of Interpolated Value');
```



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');
```

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## **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

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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 7-96 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 = A1A1(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.

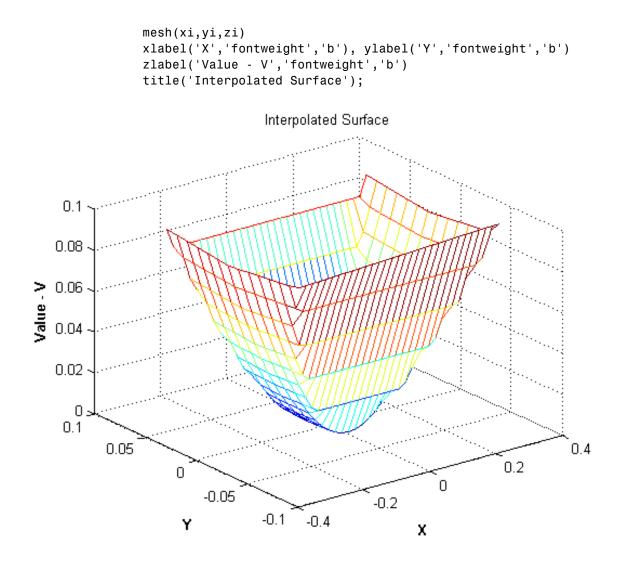
Create a sample data set that will exhibit problems near the boundary.

```
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.

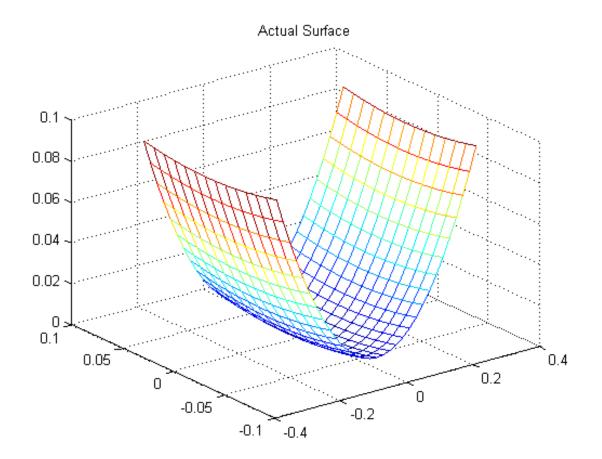
```
z = x.^2 + y.^2;
F = scatteredInterpolant(x,y,z);
[xi,yi] = meshgrid(-0.3:.02:0.3, -0.0688:0.01:0.0688);
zi = F(xi,yi);
```

7-88



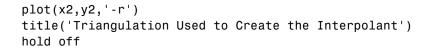
The actual surface is:

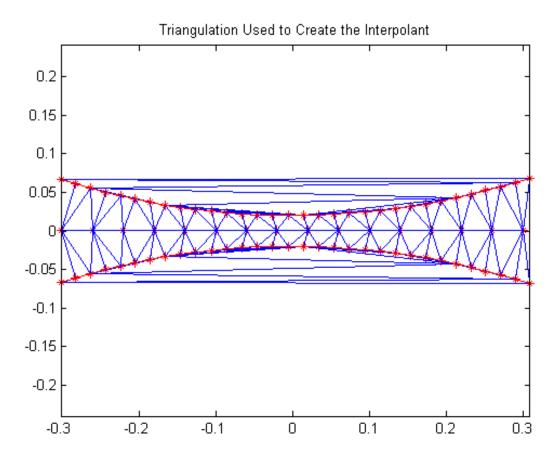
zi = xi.^2 + yi.^2; figure mesh(xi,yi,zi) title('Actual Surface')



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')
```





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.

# Interpolation Using a Specific Delaunay Triangulation

#### In this section ...

"Nearest-Neighbor Interpolation Using a delaunayTriangulation Query" on page 7-93

"Linear Interpolation Using a delaunayTriangulation Query" on page 7-94

# 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.

```
P = -2.5 + 5*gallery('uniformdata',[50 2],0);
DT = delaunayTriangulation(P)
```

DT =

delaunayTriangulation with properties:

```
Points: [50x2 double]
ConnectivityList: [87x3 double]
Constraints: []
```

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 delaunayTriangulation method, pointLocation, to compute the enclosing triangle of a query point and the magnitudes of the vertex weights. The weights are called barycentric coordinates, and they represent a partition of unity. That is, the sum of the three weights equals 1. The interpolated value of a function, V, at a query point is the sum of the weighted values of V at the three vertices. That is, if the function has values, V1, V2, V3 at the three vertices, and the weights are B1, B2, B3, then the interpolated value is (V1)(B1) + (V2)(B2) + (V3)(B3).

Create a delaunayTriangulation of a set of scattered points in 2-D.

```
P = -2.5 + 5*gallery('uniformdata',[50 2],0);
DT = delaunayTriangulation(P)
```

DT =

delaunayTriangulation with properties:

Points: [50x2 double] ConnectivityList: [87x3 double] Constraints: []

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 | pointLocation | nearestNeighbor

**Concepts** • "Interpolating Scattered Data" on page 7-59

# **Extrapolating Scattered Data**

#### In this section ...

"Factors That Affect the Accuracy of Extrapolation" on page 7-96

"Compare Extrapolation of Coarsely and Finely Sampled Scattered Data" on page 7-96

"Extrapolation of 3-D Data" on page 7-102

# 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 7-88 for more information.

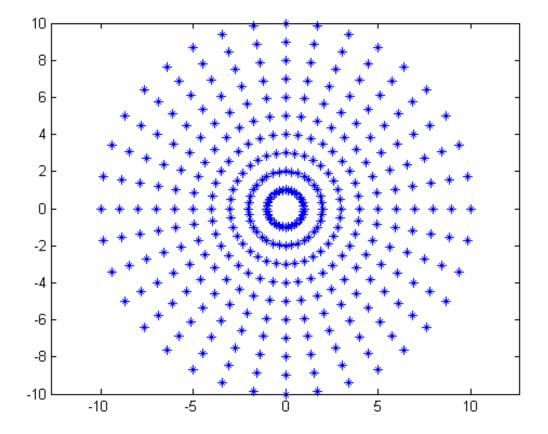
You should inspect your extrapolation results visually using your knowledge of the behavior outside the domain.

#### 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.

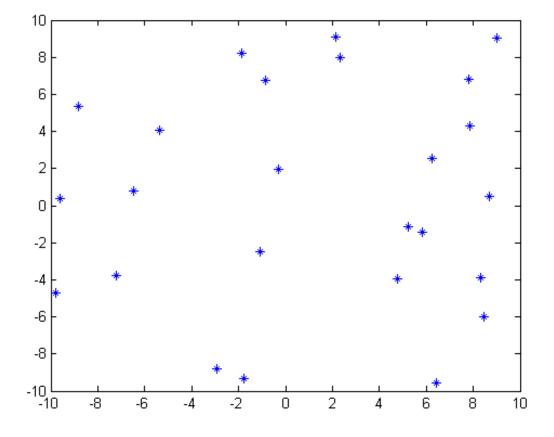
Create a radial distribution of points spaced 10 degrees apart around 10 concentric circles. Use bsxfun to compute the coordinates,  $x = \cos \theta$  and  $y = \sin \theta$ .

```
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(x,y), at both sets of points.

v1 = x1.^2 + y1.^2; v2 = x2.^2 + y2.^2;

Create a scatteredInterpolant for each sampling of v(x,y).

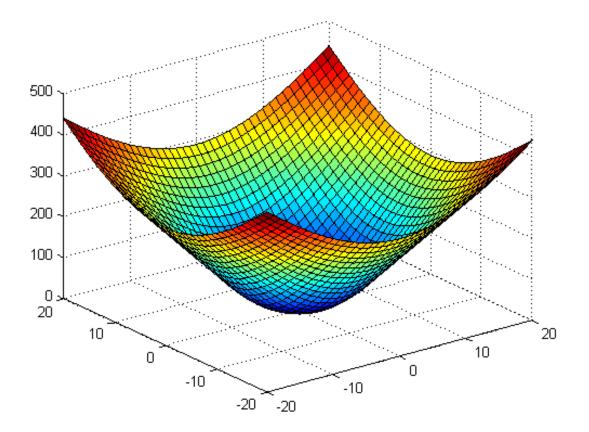
F1 = scatteredInterpolant(x1(:),y1(:),v1(:));
F2 = scatteredInterpolant(x2(:),y2(:),v2(:));

Create a grid of query points that extend beyond each domain.

[xq,yq] = ndgrid(-20:20);

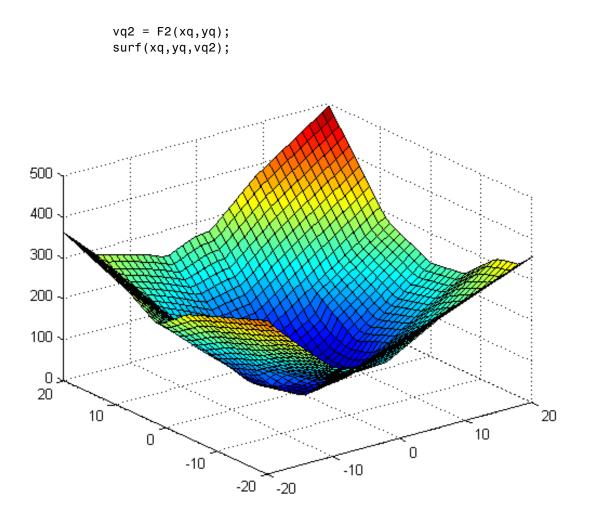
Evaluate F1 and plot the results.

figure
vq1 = F1(xq,yq);
surf(xq,yq,vq1);



Evaluate F2 and plot the results.

figure



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.

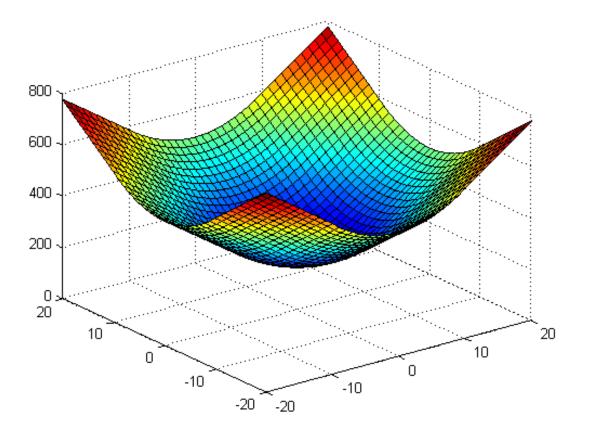
 $v = x.^2 + y.^2 + z.^2;$ 

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); surf(xq,yq,vq);



The extrapolation returned good results because the function is well sampled.

# Optimization

- "Function Summary" on page 8-2
- "Optimizing Nonlinear Functions" on page 8-3
- "Curve Fitting via Optimization" on page 8-10
- "Set Options" on page 8-13
- "Iterative Display" on page 8-17
- "Output Functions" on page 8-19
- "Plot Functions" on page 8-27
- "Troubleshooting and Tips" on page 8-30
- "Reference" on page 8-32

# **Function Summary**

The following table lists the MATLAB optimization functions.

Function	Description
fminbnd	Minimize a function of one variable on a fixed interval
fminsearch	Minimize a function of several variables
fzero	Find zero of a function of one variable
lsqnonneg	Linear least squares with nonnegativity constraints
optimget	Get optimization options structure parameter values
optimset	Create or edit optimization options parameter structure

To maximize a function, see "Maximizing Functions" on page 8-6. For information on solving single-variable nonlinear equations, see "Roots of Scalar Functions" on page 5-6.

# **Optimizing Nonlinear Functions**

#### In this section ...

"Minimizing Functions of One Variable" on page 8-3

"Minimizing Functions of Several Variables" on page 8-5

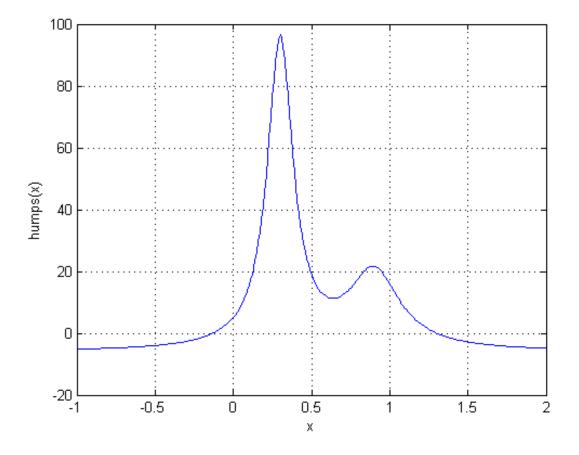
"Maximizing Functions" on page 8-6

"fminsearch Algorithm" on page 8-7

# **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)')
set(gca,'YGrid','on','XGrid','on')
```



To find the minimum of the humps function in the range (0.3,1), use x = fminbnd(@humps,0.3,1)

х =

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	Х	f(x)	Procedure
1	0.567376	12.9098	initial
2	0.732624	13.7746	golden
3	0.465248	25.1714	golden
4	0.644416	11.2693	parabolic
5	0.6413	11.2583	parabolic
6	0.637618	11.2529	parabolic
7	0.636985	11.2528	parabolic
8	0.637019	11.2528	parabolic
9	0.637052	11.2528	parabolic

Optimization terminated:

```
the current x satisfies the termination criteria using OPTIONS.TolX of 1.0
```

х =

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 8-17.

#### **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.

#### **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:

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.
- **2** 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

 $m = \Sigma x(i)/n, i = 1...n,$ 

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 *s*

s = 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

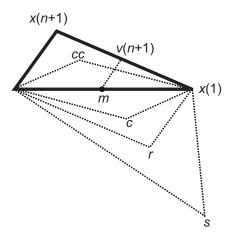
and calculate f(cc). If f(cc) < f(x(n+1)), accept cc and terminate the iteration. **Contract inside** Otherwise, continue with Step 7 (Shrink).

**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.



# **Curve Fitting via Optimization**

#### In this section ...

"Curve Fitting by Optimization" on page 8-10

"Creating an Example File" on page 8-10

"Running the Example" on page 8-11

"Plotting the Results" on page 8-11

# **Curve Fitting by Optimization**

This section gives an example that shows how to fit an exponential function of the form  $Ae^{-\lambda t}$  to some data. The example uses the fminsearch solver to minimize the sum of squares of errors between the data and an exponential function  $Ae^{-\lambda t}$  for varying parameters A and  $\lambda$ .

# **Creating an Example File**

To run the example, first create a file that:

- Accepts vectors corresponding to the *x* and *y*-coordinates of the data
- Returns the parameters of the exponential function that best fits the data

To do so, copy and paste the following code into a file and save it as fitcurvedemo in a directory on the MATLAB path.

```
function [estimates, model] = fitcurvedemo(xdata, ydata)
% Call fminsearch with a random starting point.
start_point = rand(1, 2);
model = @expfun;
estimates = fminsearch(model, start_point);
% expfun accepts curve parameters as inputs, and outputs sse,
% the sum of squares error for A*exp(-lambda*xdata)-ydata,
% and the FittedCurve. FMINSEARCH only needs sse, but we want
% to plot the FittedCurve at the end.
function [sse, FittedCurve] = expfun(params)
A = params(1);
lambda = params(2);
```

```
FittedCurve = A .* exp(-lambda * xdata);
ErrorVector = FittedCurve - ydata;
sse = sum(ErrorVector .^ 2);
end
end
```

The file calls the function fminsearch, which finds parameters A and lambda that minimize the sum of squares of the differences between the data and the exponential function A\*exp(-lambda\*t). The nested function expfun computes the sum of squares.

# **Running the Example**

To run the example, first create some random data to fit. The following commands create random data that is approximately exponential with parameters A = 40 and lambda = .5.

```
xdata = (0:.1:10)';
ydata = 40 * exp(-.5 * xdata) + randn(size(xdata));
```

To fit an exponential function to the data, enter

```
[estimates, model] = fitcurvedemo(xdata,ydata)
```

This returns estimates for the parameters A and lambda,

```
estimates =
```

40.1334 0.5025

and a function handle, model, to the function that computes the exponential function A\*exp(-lambda\*t).

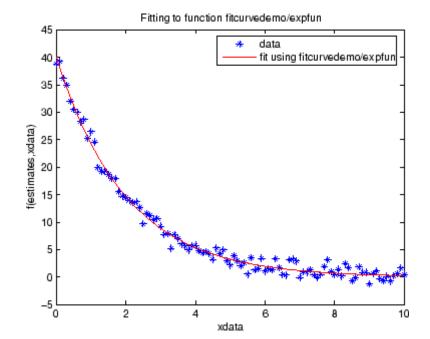
## **Plotting the Results**

To plot the fit and the data, enter the following commands.

```
plot(xdata, ydata, '*')
hold on
[sse, FittedCurve] = model(estimates);
plot(xdata, FittedCurve, 'r')
```

```
xlabel('xdata')
ylabel('f(estimates,xdata)')
title(['Fitting to function ', func2str(model)]);
legend('data', ['fit using ', func2str(model)])
hold off
```

The resulting plot displays the data points and the exponential fit.



8-12

# **Set Options**

#### In this section ...

"How to Set Options" on page 8-13

"Options Table" on page 8-13

"Tolerances and Stopping Criteria" on page 8-15

"Output Structure" on page 8-16

# 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	<ul> <li>A flag indicating whether intermediate steps appear on the screen.</li> <li>'notify' (default) displays output only if the function does not converge.</li> </ul>	fminbnd, fminsearch, fzero, lsqnonneg
	<ul> <li>'iter' displays intermediate steps (not available with lsqnonneg). See "Iterative Display" on page 8-17.</li> <li>'off' displays no intermediate steps.</li> </ul>	

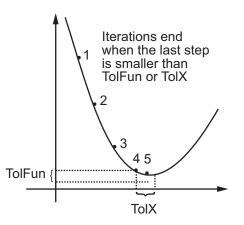
Option	Description	Solvers
	• 'final' displays just the final output.	
FunValCheck	<ul> <li>Check whether objective function values are valid.</li> <li>'on' displays an error when the objective function or constraints return a value that is complex or NaN.</li> </ul>	fminbnd, fminsearch, fzero
	• 'off' (default) displays no error.	
MaxFunEvals	The maximum number of function evaluations allowed. The default value is 500 for fminbnd and 200*length(x0) for fminsearch.	fminbnd, fminsearch
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 8-19.	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 8-27.	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 8-15.	fminsearch
TolX	The termination tolerance for $x$ . The default value is 1.e-4. See "Tolerances and Stopping Criteria" on page 8-15.	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  $|(x_i - x_{i+1})| < TolX^*(1 + |x_i|)$ , 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.

#### **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 or fminsearch with a fourth output argument, as in

```
[x,fval,exitflag,output] = fminbnd(@humps,0.3,1);
```

or

```
[x,fval,exitflag,output] = fminsearch(@three_var,v);
```

The output structure is not an option that you choose with optimset. It is an optional output for fminbnd and fminsearch.

# **Iterative Display**

You obtain details of the steps solvers take by setting the Display option to 'iter' with optimset. The displayed output contains headings and items from the following list.

Heading	Information Displayed	Solvers
Iteration	Iteration number, meaning the number of steps the algorithm has taken	fminsearch
Func-count	Cumulative number of function evaluations	fminbnd, fminsearch, fzero
x	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
	• initial simplex	fminsearch
	• expand	
	• reflect	
	• shrink	
	• contract inside	
	• contract outside	
	For details, see "fminsearch Algorithm" on page 8-7.	
	• initial (initial point)	fzero
	<ul> <li>search (search for an interval containing a zero)</li> </ul>	
	• 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 8-19
"Creating and Using an Output Function" on page 8-19
"Structure of the Output Function" on page 8-21
"Example of a Nested Output Function" on page 8-22
"Fields in optimValues" on page 8-24
"States of the Algorithm" on page 8-24
"Stop Flag" on page 8-25

# 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  ${\tt OutputFcn}$  option with the following MATLAB optimization functions:

- fminbnd
- fminsearch
- fzero

# **Creating and Using an Output Function**

The following is a simple example of an output function that plots the points generated by an optimization function.

```
function stop = outfun(x, optimValues, state)
stop = false;
hold on;
plot(x(1),x(2),'.');
```

drawnow

You can use this output function to plot the points generated by fminsearch in solving the optimization problem

$$\min_{x} f(x) = \min_{x} e^{x_1} \left( 4x_1^2 + 2x_2^2 + x_1x_2 + 2x_2 \right).$$

To do so,

- 1 Create a file containing the preceding code and save it as outfun.m in a directory on the MATLAB path.
- **2** Enter the command

options = optimset('OutputFcn', @outfun);

to set the value of the Outputfcn field of the options structure to a function handle to outfun.

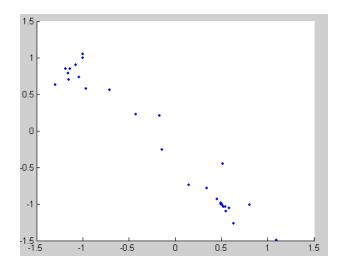
**3** Enter the following commands:

```
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 8-25.
- 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 8-24 describes the structure in detail.
- state is the current state of the algorithm. "States of the Algorithm" on page 8-24 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 8-19 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)
    z = exp(x(1))*(4*x(1)^2+2*x(2)^2+x(1)*x(2)+2*x(2));
    end
end
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

```
history(1:4,:)
```

ans =

-1.0000	1.0000
-1.0000	1.0000
-1.0750	0.9000
-1.0125	0.8500

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 optimValues are the same as at the last call to the output function, in which state is set to 'iter'.
'iter'	The algorithm is at the end of an iteration.
'done'	The algorithm is in the final state after the last iteration.

The following code illustrates how the output function might use the value of **state** to decide which tasks to perform at the current iteration.

```
switch state
    case 'init'
        % Setup for plots or guis
    case 'iter'
        % Make updates to plot or guis as needed.
    case 'interrupt'
        % Check conditions to see whether optimization
        % should quit.
    case 'done'
        % Cleanup of plots, guis, 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 GUI Input**

If you design a GUI to perform optimizations, you can make the output function stop an optimization when a user clicks a **Stop** button on the GUI. 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 8-27

"Example: Plot Function" on page 8-28

## 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 8-19.

You can use the PlotFcns option with the following MATLAB optimization functions:

- fminbnd
- fminsearch
- fzero

The predefined plot functions for these optimization functions are:

- Coptimplotx plots the current point
- @optimplotfval plots the function value
- Coptimplotfunccount 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:

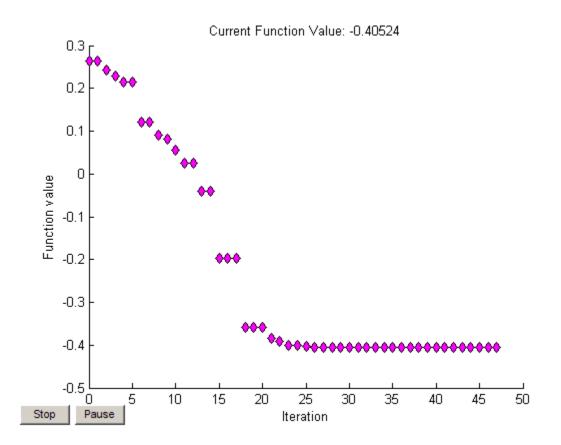
options = optimset('PlotFcns',@optimplotfval);

**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**

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.

Here is a list of typical problems and recommendations for dealing with them.

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.

# 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.

# **Function Handles**

- "Defining Functions" on page 9-2
- "Parameterizing Functions" on page 9-9

# **Defining Functions**

#### In this section ...

"Introduction" on page 9-2

"Functions In Files" on page 9-2

"Anonymous Functions" on page 9-3

"Function Plotting Function" on page 9-3

#### Introduction

MATLAB functions are written to named files or are produced at the command line as anonymous functions. In either case, a function handle is used to pass the function as an input argument to a function function.

#### **Functions In Files**

Consider the example function:

$$f(x) = \frac{1}{(x - 0.3)^2 + 0.01} + \frac{1}{(x - 0.9)^2 + 0.04} - 6.$$

A file for the function is humps.m. Its contents look like this:

function y = humps(x) y =  $1./((x - 0.3).^2 + 0.01) \dots$ +  $1./((x - 0.9).^2 + 0.04) - 6;$ 

To evaluate humps at 2.0, first use the @ symbol to obtain a function handle. Use the function handle in the same way you would use a function name to call a function:

fh = @humps; fh(2.0) ans = -4.8552

#### **Anonymous Functions**

Consider again the example function:

$$f(x) = \frac{1}{(x - 0.3)^2 + 0.01} + \frac{1}{(x - 0.9)^2 + 0.04} - 6.$$

A second way to represent the function in the MATLAB is to create an anonymous function at the command line, as follows:

fh =  $@(x)(1./((x-0.3).^2 + 0.01) ... + 1./((x-0.9).^2 + 0.04)-6);$ 

You evaluate fh at 2.0 the same way you do with a function handle for a file-defined function:

fh(2.0) ans = -4.8552

Anonymous functions can have any number of arguments. The following anonymous function has two input arguments x and y:

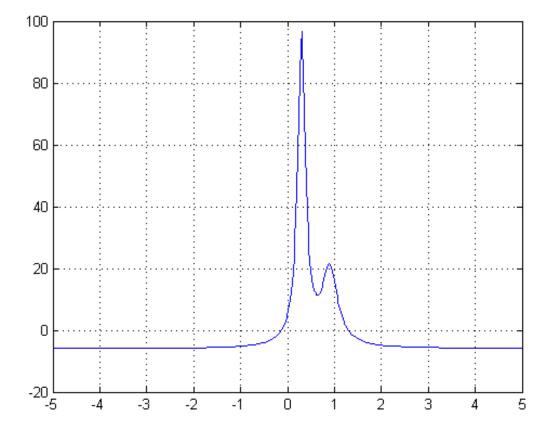
#### **Function Plotting Function**

This example shows how to use the fplot function to plot a mathematical function between a given set of axes limits.

You can control the x-axis limits only, or both the x- and y-axis limits.

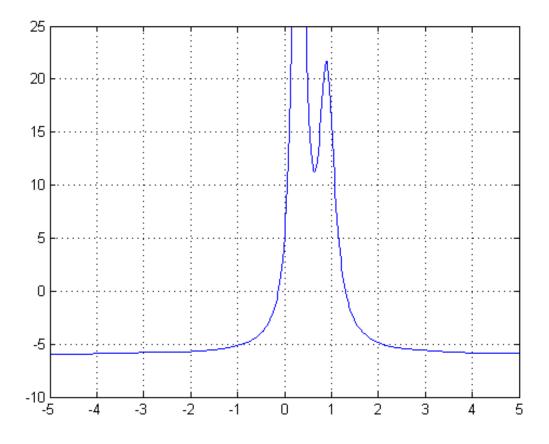
Plot the humps.m function over the x-axis range [-5 5].

```
fplot(@humps,[-5 5])
grid on
```



Zoom in on the function by selecting y-axis limits of -10 and 25.

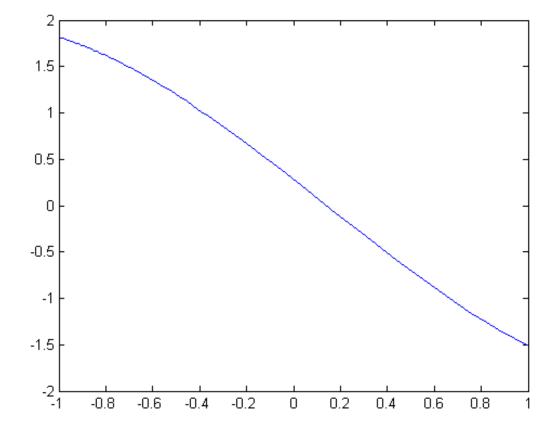
fplot(@humps,[-5 5 -10 25])
grid on



You can also pass the function handle for an anonymous function for fplot to graph.

fplot(@(x)2\*sin(x+3),[-1 1])

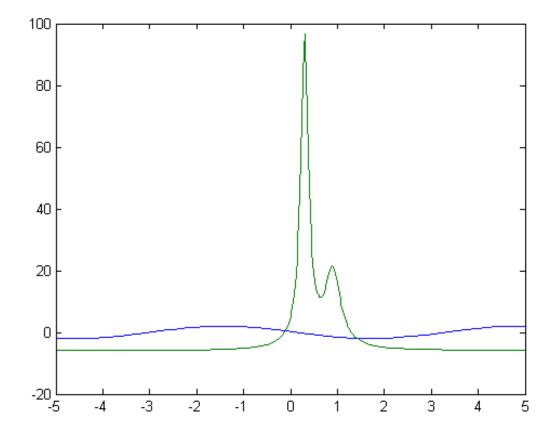
9



You can plot more than one function on the same graph with one call to fplot. If you use this with a function, then the function must take a column vector x and return a matrix where each column corresponds to each function, evaluated at each value of x.

If you pass an anonymous function consisting of several functions to fplot, the anonymous function also must return a matrix where each column corresponds to each function evaluated at each value of x

fplot(@(x)[2\*sin(x+3),humps(x)],[-5 5])



This plots the first and second functions on the same graph.

Note that the anonymous function

fh = @(x)[2\*sin(x+3),humps(x)];

evaluates to a matrix of two columns, one for each function, when  $\boldsymbol{x}$  is a column vector.

fh([1;2;3])

	ans =	
	-1.5136 -1.9178 -0.5588	16.0000 -4.8552 -5.6383
See Also	function_han	dle
Related Examples	• "Create Fur	nctions in Files"
Concepts	• "Anonymou	s Functions"

# **Parameterizing Functions**

#### In this section...

"Overview" on page 9-9

"Parameterizing Using Nested Functions" on page 9-9

"Parameterizing Using Anonymous Functions" on page 9-10

#### **Overview**

20This 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 = \text{cubicpoly}(x,b,c)
y = x^3 + b^*x + c;
end
```

At the command line, define **b** and **c**, and then call **fzero** with an anonymous function that invokes **cubicpoly**:

```
b = 2;
c = 3.5;
x = fzero(@(x) cubicpoly(x,b,c),0)
x =
-1.0945
```

```
Note To change the values of the parameters, you must create a new anonymous function. For example:
```

b = 10; c = 25; x = fzero(@(x) x^3 + b\*x + c,0);

See Also function\_handle

Concepts

- "Nested Functions"
- "Anonymous Functions"

# 10

# Calculus

- "Ordinary Differential Equations" on page 10-2
- "Types of DDEs" on page 10-47
- "Discontinuities in DDEs" on page 10-50
- "DDE with Constant Delays" on page 10-52
- "State-Dependent Delay Problem" on page 10-55
- "Cardiovascular Model with Discontinuities" on page 10-58
- "DDE of Neutral Type" on page 10-62
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- "Boundary-Value Problems" on page 10-68
- "Partial Differential Equations" on page 10-96
- "Selected Bibliography for Differential Equations" on page 10-113
- "Integration to Find Arc Length" on page 10-114
- "Complex Line Integrals" on page 10-115
- "Singularity on Interior of Integration Domain" on page 10-118
- "Analytic Solution to Integral of Polynomial" on page 10-120
- "Integration of Numeric Data" on page 10-122

# **Ordinary Differential Equations**

#### In this section ...

"Function Summary" on page 10-2 "Initial Value Problems" on page 10-4

"Types of Solvers" on page 10-6

"Solver Syntax" on page 10-8

"Integrator Options" on page 10-9

"Examples" on page 10-10

"Troubleshooting" on page 10-39

## **Function Summary**

- "ODE Solvers" on page 10-2
- "Evaluation and Extension" on page 10-3
- "Solver Options" on page 10-3
- "Output Functions" on page 10-4

#### **ODE Solvers**

The following table lists the initial value problem solvers, the kind of problem you can solve with each solver, and the method each solver uses.

Solver	Solves These Kinds of Problems	Method
ode45	Nonstiff differential equations	Runge-Kutta
ode23	Nonstiff differential equations	Runge-Kutta
ode113	Nonstiff differential equations	Adams

Solver	Solves These Kinds of Problems	Method
ode15s	Stiff differential equations and DAEs	NDFs (BDFs)
ode23s	Stiff differential equations	Rosenbrock
ode23t	Moderately stiff differential equations and DAEs	Trapezoidal rule
ode23tb	Stiff differential equations	TR-BDF2
ode15i	Fully implicit differential equations	BDFs

#### **Evaluation and Extension**

You can use the following functions to evaluate and extend solutions to ODEs.

Function	Description
deval	Evaluate the numerical solution using the output of ODE solvers.
odextend	Extend the solution of an initial value problem for an ODE

#### **Solver Options**

An options structure contains named properties whose values are passed to ODE solvers, and which affect problem solution. Use these functions to create, alter, or access an options structure.

Function	Description
odeset	Create or alter options structure for input to ODE solver.
odeget	Extract properties from options structure created with odeset.

#### **Output Functions**

If an output function is specified, the solver calls the specified function after every successful integration step. You can use odeset to specify one of these sample functions as the OutputFcn property, or you can modify them to create your own functions.

Function	Description
odeplot	Time-series plot
odephas2	Two-dimensional phase plane plot
odephas3	Three-dimensional phase plane plot
odeprint	Print to command window

#### **Initial Value Problems**

- "First Order ODEs" on page 10-4
- "Higher Order ODEs" on page 10-5
- "Initial Values" on page 10-6

#### First Order ODEs

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 derivative of y with respect to t is denoted as y', the second derivative as y'', and so on. Often y(t) is a vector, having elements  $y_1, y_2, ..., y_n$ .

MATLAB solvers handle the following 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 matrix
- Fully implicit ODEs of the form f(t, y, y') = 0 (ode15i only)

#### **Higher Order ODEs**

MATLAB ODE solvers accept only first-order differential equations. To use the solvers with higher-order ODEs, you must rewrite each equation as an equivalent system of first-order differential equations of the form

$$y' = f(t,y)$$

You can write any ordinary differential equation

$$y^{(n)} = f(t, y, y', \dots, y^{(n-1)})$$

as a system of first-order equations by making the substitutions

$$y1 = y, y2 = y',..., yn = y^{(n-1)}$$
  
 $y_1 = y, y_2 = y', ..., y_n = y^{(n-1)}$ 

The result is an equivalent system of n first-order ODEs.

For example, you can rewrite the second-order van der Pol equation

$$y_1'' - \mu (1 - y_1^2) y_1' + y_1 = 0$$

by making the substitution

$$y'_1 = y_2$$

The resulting system of first-order ODEs is

$$y'_1 = y_2$$
  
 $y'_2 = \mu(1 - y_1^2)y_2 - y_1$ 

#### **Initial Values**

Generally there are many functions y(t) that satisfy a given ODE, and additional information is necessary to specify the solution of interest. In an *initial value problem*, the solution of interest satisfies a specific *initial condition*, that is, y is equal to  $y_0$  at a given initial time  $t_0$ . An initial value problem for an ODE is then

$$y' = f(t, y)$$
$$y(t_0) = y_0.$$

If the function f(t, y) is sufficiently smooth, this problem has one and only one solution. Generally there is no analytic expression for the solution, so it is necessary to approximate y(t) by numerical means.

#### **Types of Solvers**

- "Nonstiff Problems" on page 10-6
- "Stiff Problems" on page 10-7
- "Fully Implicit ODEs" on page 10-7

#### Nonstiff Problems

There are three solvers designed for nonstiff problems:

ode45	Based on an explicit Runge-Kutta (4,5) formula, the Dormand-Prince pair. It is a <i>one-step</i> solver – in computing $y(t_n)$ , it needs only the solution at the immediately preceding time point, $y(t_{n-1})$ . In general, ode45 is the best function to apply as a "first try" for most problems.
ode23	Based on an explicit Runge-Kutta (2,3) pair of Bogacki and Shampine. It may be more efficient than ode45 at crude tolerances and in the presence of mild stiffness. Like ode45, ode23 is a one-step solver.
ode113	Variable order Adams-Bashforth-Moulton PECE solver. It may be more efficient than ode45 at stringent tolerances and when the ODE function is particularly

expensive to evaluate. ode113 is a *multistep* solver—it normally needs the solutions at several preceding time points to compute the current solution.

#### **Stiff Problems**

Not all difficult problems are stiff, but all stiff problems are difficult for solvers not specifically designed for them. Solvers for stiff problems can be used exactly like the other solvers. However, you can often significantly improve the efficiency of these solvers by providing them with additional information about the problem. (See "Integrator Options" on page 10-9.)

There are four solvers designed for stiff problems:

ode15s	Variable-order solver based on the numerical differentiation formulas (NDFs). Optionally it uses the backward differentiation formulas, BDFs (also known as Gear's method). Like ode113, ode15s is a multistep solver. If you suspect that a problem is stiff or if ode45 failed or was very inefficient, try ode15s.
ode23s	Based on a modified Rosenbrock formula of order 2. Because it is a one-step solver, it may be more efficient than ode15s at crude tolerances. It can solve some kinds of stiff problems for which ode15s is not effective.
ode23t	An implementation of the trapezoidal rule using a "free" interpolant. Use this solver if the problem is only moderately stiff and you need a solution without numerical damping.
ode23tb	An implementation of TR-BDF2, an implicit Runge-Kutta formula with a first stage that is a trapezoidal rule step and a second stage that is a backward differentiation formula of order 2. Like ode23s, this solver may be more efficient than ode15s at crude tolerances.

#### **Fully Implicit ODEs**

The solver ode15i solves fully implicit differential equations of the form

f(t,y,y') = 0

using the variable order BDF method. The basic syntax for ode151 is

[t,y] = ode15i(odefun,tspan,y0,yp0,options)

The input arguments are

odefun	A function that evaluates the left side of the differential equation of the form $f(t,y,y') = 0$ .
tspan	A vector specifying the interval of integration, [t0,tf]. To obtain solutions at specific times (all increasing or all decreasing), use tspan = [t0,t1,,tf].
у0, ур0	Vectors of initial conditions for $y(t_0)$ and $y'(t_0)$ , respectively. The specified values must be consistent; that is, they must satisfy $f(t0,y0,yp0) = 0$ .
options	Optional integration argument created using the odeset function. See the odeset reference page for details.

The output arguments contain the solution approximated at discrete points:

t	Column vector of time points
У	Solution array. Each row in y corresponds to the solution at a time returned in the corresponding row of t.

See the ode15i reference page for more information about these arguments.

#### **Solver Syntax**

All of the ODE solver functions, except for ode15i, share a syntax that makes it easy to try any of the different numerical methods, if it is not apparent which is the most appropriate. To apply a different method to the same problem, simply change the ODE solver function name. The simplest syntax, common to all the solver functions, is

[t,y] = solver(odefun,tspan,y0,options)

where *solver* is one of the ODE solver functions listed previously.

The basic input arguments are

odefun	function handle that evaluates the system of ODEs. The function has the form
	dydt = odefun(t,y)
	where t is a scalar, and dydt and y are column vectors.
tspan	Vector specifying the interval of integration. The solver imposes the initial conditions at tspan(1), and integrates from tspan(1) to tspan(end).
у0	Vector of initial conditions for the problem
	See also "Initial Value Problems" on page 10-4.
options	Structure of optional parameters that change the default integration properties.
	"Integrator Options" on page 10-9 tells you how to create the structure and describes the properties you can specify.
The output arguments contain the solution approximated at discrete points:	
t	Column vector of time points

,	Solution array. Each row in y corresponds to the
	solution at a time returned in the corresponding row
	of t.

See the reference page for the ODE solvers for more information about these arguments.

#### **Integrator Options**

у

The default integration properties in the ODE solvers are selected to handle common problems. In some cases, you can improve ODE solver performance by overriding these defaults. You do this by supplying the solvers with an options structure that specifies one or more property values.

For example, to change the value of the relative error tolerance of the solver from the default value of 1e-3 to 1e-4,

1 Create an options structure using the function odeset by entering

options = odeset('RelTol', 1e-4);

- **2** Pass the options structure to the solver as follows:
  - For all solvers except ode15i, use the syntax

[t,y] = solver(odefun,tspan,y0,options)

• For ode15i, use the syntax

[t,y] = ode15i(odefun,tspan,y0,yp0,options)

For a complete description of the available options, see the reference page for odeset.

#### **Examples**

- "van der Pol Equation (Nonstiff)" on page 10-11
- "van der Pol Equation (Stiff)" on page 10-13
- "van der Pol Equation (Parameterizing the ODE)" on page 10-15
- "van der Pol Equation (Evaluating the Solution)" on page 10-16
- "Euler Equations (Nonstiff)" on page 10-16
- "Fully Implicit ODE" on page 10-18
- "Finite Element Discretization" on page 10-19
- "Large Stiff Sparse Problem" on page 10-23
- "Event Location" on page 10-25
- "Advanced Event Location" on page 10-28
- "Differential-Algebraic Equations" on page 10-31
- "Nonnegative Solutions" on page 10-34

• "Additional Examples" on page 10-38

#### van der Pol Equation (Nonstiff)

This example illustrates the steps for solving an initial value ODE problem:

**1 Rewrite the problem as a system of first-order ODEs.** Rewrite the van der Pol equation (second-order)

$$y_1'' - \mu \left(1 - y_1^2\right) y_1' + y_1 = 0,$$

where  $\mu > 0$  is a scalar parameter, by making the substitution  $y'_1 = y_2$ . The resulting system of first-order ODEs is

 $\begin{aligned} y_1' &= y_2 \\ y_2' &= \mu \Big( 1 - y_1^2 \Big) y_2 - y_1. \end{aligned}$ 

**2** Code the system of first-order ODEs. Once you represent the equation as a system of first-order ODEs, you can code it as a function that an ODE solver can use. The function must be of the form

dydt = odefun(t,y)

Although t and y must be the function's two arguments, the function does not need to use them. The output dydt, a column vector, is the derivative of y.

The code below represents the van der Pol system in the function, vdp1. The vdp1 function assumes that  $\mu = 1$ . The variables  $y_1$  and  $y_2$  are the entries y(1) and y(2) of a two-element vector.

function dydt = vdp1(t,y)
dydt = [y(2); (1-y(1)<sup>2</sup>)\*y(2)-y(1)];

Note that, although vdp1 must accept the arguments t and y, it does not use t in its computations.

#### **3** Apply a solver to the problem.

Decide which solver you want to use to solve the problem. Then call the solver and pass it the function you created to describe the first-order system

of ODEs, the time interval on which you want to solve the problem, and an initial condition vector.

For the van der Pol system, you can use ode45 on time interval  $[0 \ 20]$  with initial values y(1) = 2 and y(2) = 0.

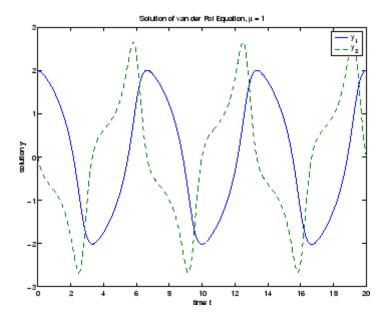
```
[t,y] = ode45(@vdp1,[0 20],[2; 0]);
```

This example uses @ to pass vdp1 as a function handle to ode45. The resulting 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  $y_2$ .

**Note** For information on function handles, see the function\_handle, func2str, and str2func reference pages.

**4** View the solver output. You can simply use the plot command to view the solver output.

```
plot(t,y(:,1),'-',t,y(:,2),'--')
title('Solution of van der Pol Equation, \mu = 1');
xlabel('time t');
ylabel('solution y');
legend('y_1','y_2')
```



As an alternative, you can use a solver output function to process the output. The solver calls the function specified in the integration property OutputFcn after each successful time step. Use odeset to set OutputFcn to the desired function. See Solver Output Properties, in the reference page for odeset, for more information about OutputFcn.

#### van der Pol Equation (Stiff)

This example presents a stiff problem. For a stiff problem, solutions can change on a time scale that is very short compared to the interval of integration, but the solution of interest changes on a much longer time scale. Methods not designed for stiff problems are ineffective on intervals where the solution changes slowly because they use time steps small enough to resolve the fastest possible change.

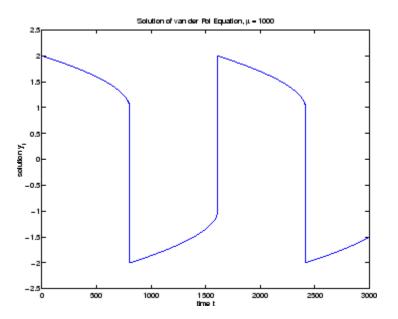
When  $\mu$  is increased to 1000, the solution to the van der Pol equation changes dramatically and exhibits oscillation on a much longer time scale. Approximating the solution of the initial value problem becomes a more difficult task. Because this particular problem is stiff, a solver intended for nonstiff problems, such as ode45, is too inefficient to be practical. A solver such as ode15s is intended for such stiff problems. The vdp1000 function evaluates the van der Pol system from the previous example, but with  $\mu = 1000$ .

```
function dydt = vdp1000(t,y)
dydt = [y(2); 1000*(1-y(1)^2)*y(2)-y(1)];
```

**Note** This example hardcodes  $\mu$  in the ODE function. The vdpode example solves the same problem, but passes a user-specified  $\mu$  as a parameter to the ODE function.

Now use the ode15s function to solve the problem with the initial condition vector of [2; 0], but a time interval of [0 3000]. For scaling reasons, plot just the first component of y(t).

```
[t,y] = ode15s(@vdp1000,[0 3000],[2; 0]);
plot(t,y(:,1),'-');
title('Solution of van der Pol Equation, \mu = 1000');
xlabel('time t');
ylabel('solution y_1');
```



#### van der Pol Equation (Parameterizing the ODE)

The preceding sections showed how to solve the van der Pol equation for two different values of the parameter  $\mu$ . In those examples, the values  $\mu = 1$  and  $\mu=1000$  are hard-coded in the ODE functions. If you are solving an ODE for several different parameter values, it might be more convenient to include the parameter in the ODE function and assign a value to the parameter each time you run the ODE solver. This section explains how to do this for the van der Pol equation.

One way to provide parameter values to the ODE function is to write a MATLAB file that

- Accepts the parameters as inputs.
- Contains ODE function as a nested function, internally using the input parameters.
- Calls the ODE solver.

The following code illustrates this:

```
function [t,y] = solve_vdp(mu)
tspan = [0 max(20, 3*mu)];
y0 = [2; 0];
% Call the ODE solver ode15s.
[t,y] = ode15s(@vdp,tspan,y0);
% Define the ODE function as nested function,
% using the parameter mu.
function dydt = vdp(t,y)
dydt = [y(2); mu*(1-y(1)^2)*y(2)-y(1)];
end
end
```

Because the ODE function  $\mathsf{vdp}$  is a nested function, the value of the parameter  $\mathsf{mu}$  is available to it.

To run the MATLAB file for mu = 1, enter

[t,y] = solve\_vdp(1);

To run the code for  $\mu = 1000$ , enter

[t,y] = solve\_vdp(1000);

See the vdpode code for a complete example based on these functions.

#### van der Pol Equation (Evaluating the Solution)

The numerical methods implemented in the ODE solvers produce a continuous solution over the interval of integration [a,b]. You can evaluate the approximate solution, S(x), at any point in [a,b] using the function deval and the structure sol returned by the solver. For example, if you solve the problem described in "van der Pol Equation (Nonstiff)" on page 10-11 by calling ode45 with a single output argument sol,

sol = ode45(@vdp1,[0 20],[2; 0]);

ode45 returns the solution as a structure. You can then evaluate the approximate solution at points in the vector xint = 1:5 as follows:

```
xint = 1:5;
Sxint = deval(sol,xint)
Sxint =
    1.5081    0.3235   -1.8686   -1.7407   -0.8344
    -0.7803   -1.8320   -1.0220    0.6260    1.3095
```

The deval function is vectorized. For a vector xint, the ith column of Sxint approximates the solution y(xint(i)).

#### **Euler Equations (Nonstiff)**

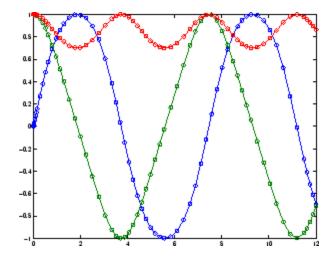
rigidode illustrates the solution of a standard test problem proposed by Krogh for solvers intended for nonstiff problems [8].

The ODEs are the Euler equations of a rigid body without external forces.

 $\begin{array}{l} y_1' = y_2 y_3 \\ y_2' = -y_1 y_3 \\ y_3' = -0.51 y_1 y_2. \end{array}$ 

For your convenience, the entire problem is defined and solved in a single MATLAB file. The differential equations are coded as the local function f. Because the example calls the ode45 solver without output arguments, the solver uses the default output function odeplot to plot the solution components.

To run this example, type rigidode at the command line.



#### **Fully Implicit ODE**

The following example shows how to use the function ode15i to solve the implicit ODE problem defined by Weissinger's equation

 $ty^{2}(y)^{3} - y^{3}(y)^{2} + t(t^{2} + 1)y' - t^{2}y = 0$ 

with the initial value  $y(1) = (3/2)^{1/2}$ . The exact solution of the ODE is

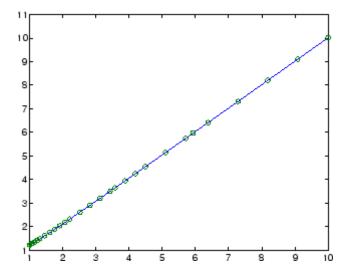
 $y(t) = (t^2 + 0.5)^{1/2}$ 

The example uses the function weissinger, which is provided with MATLAB, to compute the left-hand side of the equation.

Before calling ode15i, the example uses a helper function decic to compute a consistent initial value for  $y'(t_0)$ . In the following call, the given initial value  $y(1) = (3/2)^{1/2}$  is held fixed and a guess of 0 is specified for y'(1). See the reference page for decic for more information.

t0 = 1; y0 = sqrt(3/2); yp0 = 0; [y0,yp0] = decic(@weissinger,t0,y0,1,yp0,0); You can now call ode15i to solve the ODE and then plot the numerical solution against the analytical solution with the following commands.

```
[t,y] = ode15i(@weissinger,[1 10],y0,yp0);
ytrue = sqrt(t.^2 + 0.5);
plot(t,y,t,ytrue,'o');
```



#### **Finite Element Discretization**

fem1ode illustrates the solution of ODEs that result from a finite element discretization of a partial differential equation. The value of N in the call fem1ode(N) controls the discretization, and the resulting system consists of N equations. By default, N is 19.

This example involves a mass matrix. The system of ODEs comes from a method of lines solution of the partial differential equation

$$e^{-t}\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

with initial condition

$$u(0,x) = \sin(x)$$

and boundary conditions

$$u(t,0) = u(t,\pi) = 0.$$

An integer *N* is chosen, *h* is defined as  $\pi/(N + 1)$ , and the solution of the partial differential equation is approximated at  $x_k = kh$  for k = 0, 1, ..., N+1 by

$$u(t, x_k) = \sum_{k=1}^N c_k(t)\phi_k(x).$$

Here  $\varphi_k(x)$  is a piecewise linear function that is 1 at $x_k$  and 0 at all the other  $x_j$ . A Galerkin discretization leads to the system of ODEs

$$M(t)c' = Jc$$
, where  $c(t) = \begin{bmatrix} c_1(t) \\ \vdots \\ c_N(t) \end{bmatrix}$ 

and the tridiagonal matrices M(t) and J are given by

$$M_{i,j} = egin{cases} rac{2h}{3}e^{-t} & ext{if } i=j \ rac{h}{6}e^{-t} & ext{if } i=j\pm 1 \ 0 & ext{otherwise.} \end{cases}$$

and

$$J_{i,j} = \begin{cases} \frac{-2}{h} & \text{if } i = j \\ \frac{1}{h} & \text{if } i = j \pm 1 \\ 0 & \text{otherwise.} \end{cases}$$

The initial values c(0) are taken from the initial condition for the partial differential equation. The problem is solved on the time interval  $[0,\pi]$ .

In the fem1ode example, the properties

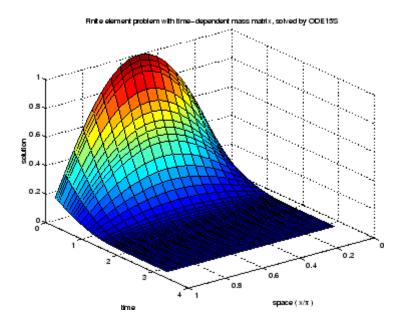
```
options = odeset('Mass',@mass,'MStateDep','none','Jacobian',J)
```

indicate that the problem is of the form M(t)y' = Jy. The nested function mass(t) evaluates the time-dependent mass matrix M(t) and J is the constant Jacobian.

To run this example, type fem1ode at the command line. From the command line, you can specify a value of N as an argument to fem1ode. The default is N = 19.

```
function fem1ode(N)
%FEM10DE Stiff problem with a time-dependent mass matrix
if nargin < 1
  N = 19;
end
h = pi/(N+1);
y0 = sin(h^{*}(1:N)');
tspan = [0; pi];
% The Jacobian is constant.
e = repmat(1/h,N,1); % e=[(1/h) ... (1/h)];
d = repmat(-2/h,N,1); % d=[(-2/h) ... (-2/h)];
% J is shared with the derivative function.
J = spdiags([e d e], -1:1, N, N);
d = repmat(h/6, N, 1);
% M is shared with the mass matrix function.
M = spdiags([d 4*d d], -1:1, N, N);
options = odeset('Mass',@mass,'MStateDep','none', ...
                 'Jacobian',J);
[t,y] = ode15s(@f,tspan,y0,options);
figure;
surf((1:N)/(N+1),t,y);
set(gca, 'ZLim',[0 1]);
view(142.5,30);
```

```
title(['Finite element problem with time-dependent mass ' ...
      'matrix, solved by ODE15S']);
xlabel('space ( x/\pi )');
ylabel('time');
zlabel('solution');
%-----
                                 function yp = f(t,y)
% Derivative function.
  yp = J*y;
             % Constant Jacobian provided by outer function
              % End nested function f
end
%-----
function Mt = mass(t)
% Mass matrix function.
  Mt = exp(-t)*M;
                    % M is provided by outer function
end
                    % End nested function mass
%----
end
```



#### Large Stiff Sparse Problem

brussode illustrates the solution of a potentially large stiff sparse problem. The problem is the classic "Brusselator" system [3] that models diffusion in a chemical reaction

$$\begin{split} &u_{i}' = 1 + u_{i}^{2} v_{i} - 4 u_{i} + \alpha \left(N + 1\right)^{2} \left(u_{i-1} - 2 u_{i} + u_{i+1}\right) \\ &v_{i}' = 3 u_{i} - u_{i}^{2} v_{i} + \alpha \left(N + 1\right)^{2} \left(v_{i-1} - 2 v_{i} + v_{i+1}\right). \end{split}$$

and is solved on the time interval [0, 10] with a = 1/50 and

$$u_i(0) = 1 + \sin(2\pi x_i)$$
  
 $v_i(0) = 3$ 

where, for i = 1,...,N,  $x_i = i/(N + 1)$ . There are 2N equations in the system, but the Jacobian is banded with a constant width 5 if the equations are ordered as  $u_1$ ,  $v_1$ ,  $u_2$ ,  $v_2$ , ...

In the call brussode(N), where N corresponds to N, the parameter  $N \ge 2$  specifies the number of grid points. The resulting system consists of 2N equations. By default, N is 20. The problem becomes increasingly stiff and the Jacobian increasingly sparse as N increases.

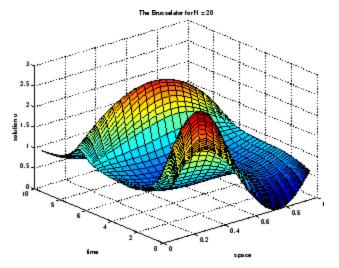
The nested function f(t,y) returns the derivatives vector for the Brusselator problem. The local function jpattern(N) returns a sparse matrix of 1s and 0s showing the locations of nonzeros in the Jacobian  $\partial f/\partial y$ . The example assigns this matrix to the property JPattern, and the solver uses the sparsity pattern 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 Brusselator problem, if the sparsity pattern is not supplied, 2N evaluations of the function are needed to compute the 2N-by-2N Jacobian matrix. If the sparsity pattern is supplied, only four evaluations are needed, regardless of the value of N.

To run this example, type brussode at the command line. From the command line, you can specify a value of N as an argument to brussode. The default is N = 20.

```
function brussode(N)
%BRUSSODE Stiff problem modeling a chemical reaction
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);
surf(x,t,u);
view(-40,30);
xlabel('space');
ylabel('time');
zlabel('solution u');
title(['The Brusselator for N = ' num2str(N)]);
% -----
function dydt = f(t,y)
c = 0.02 * (N+1)^{2};
dydt = zeros(2*N,size(y,2)); % preallocate dy/dt
% Evaluate the two 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 two 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 two 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^{(i-2,:)-2^{(i,:)+1)};
dydt(i+1,:) = 3*y(i,:) - y(i+1,:).*y(i,:).^2 + ...
              c*(y(i-1,:)-2*y(i+1,:)+3);
end
      % End nested function f
      % End function brussode
end
% -----
function S = jpattern(N)
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;
```



#### **Event Location**

**ballode** models the motion of a bouncing ball. This example illustrates the event location capabilities of the ODE solvers.

The equations for the bouncing ball are:

 $y'_1 = y_2$  $y'_2 = -9.8$ 

In this example, the event function is coded in the local functionevents

```
[value,isterminal,direction] = events(t,y)
```

which returns

- A value of the event function
- The information whether or not the integration should stop when value = 0 (isterminal = 1 or 0, respectively)
- The desired directionality of the zero crossings:

- 1	Detect zero crossings in the negative direction only
0	Detect all zero crossings
1	Detect zero crossings in the positive direction only

The length of value, isterminal, and direction is the same as the number of event functions. The ith element of each vector, corresponds to the ith event function. For an example of more advanced event location, see orbitode ("Advanced Event Location" on page 10-28).

In ballode, setting the Events property to @events causes the solver to stop the integration (isterminal = 1) when the ball hits the ground (the height y(1) is 0) during its fall (direction = -1). The example then restarts the integration with initial conditions corresponding to a ball that bounced.

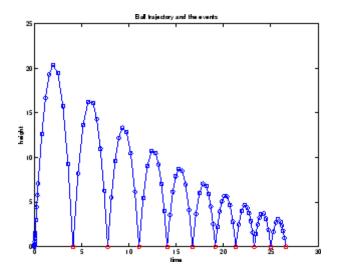
To run this example, type ballode at the command line.

```
function ballode
```

```
tstart = 0;
tfinal = 30;
y0 = [0; 20];
refine = 4;
options = odeset('Events',@events,'OutputFcn', @odeplot,...
'OutputSel',1,'Refine',refine);
```

```
set(gca, 'xlim', [0 30], 'ylim', [0 25]);
box on
hold on;
tout = tstart;
yout = y0.';
teout = [];
yeout = [];
ieout = [];
for i = 1:10
 % Solve until the first terminal event.
  [t,y,te,ye,ie] = ode23(@f,[tstart tfinal],y0,options);
  if ~ishold
    hold on
  end
 % Accumulate output.
 nt = length(t);
 tout = [tout; t(2:nt)];
 yout = [yout; y(2:nt,:)];
  teout = [teout; te];
                        % Events at tstart are never reported.
  yeout = [yeout; ye];
  ieout = [ieout; ie];
  ud = get(gcf, 'UserData');
  if ud.stop
    break;
  end
  % Set the new initial conditions, with .9 attenuation.
 y0(1) = 0;
 y0(2) = -.9*y(nt,2);
 % A good guess of a valid first time step is the length of
 % the last valid time step, so use it for faster computation.
 options = odeset(options, 'InitialStep',t(nt)-t(nt-refine),...
                            'MaxStep',t(nt)-t(1));
 tstart = t(nt);
end
```

```
plot(teout,yeout(:,1),'ro')
xlabel('time');
ylabel('height');
title('Ball trajectory and the events');
hold off
odeplot([],[],'done');
% -----
function dydt = f(t,y)
dydt = [y(2); -9.8];
8 -----
function [value,isterminal,direction] = events(t,y)
% Locate the time when height passes through zero in a
% decreasing direction and stop integration.
value = y(1);
                 % Detect height = 0
isterminal = 1; % Stop the integration
direction = -1; % Negative direction only
```



#### **Advanced Event Location**

orbitode illustrates the solution of a standard test problem for those solvers that are intended for nonstiff problems. It traces the path of a spaceship traveling around the moon and returning to the earth (Shampine and Gordon [8], p. 246).

The orbitode problem is a system of the following four equations:

$$\begin{split} y_1' &= y_3 \\ y_2' &= y_4 \\ y_3' &= 2y_4 + y_1 - \frac{\mu^* (y_1 + \mu)}{r_1^3} - \frac{\mu (y_1 - \mu^*)}{r_2^3} \\ y_4' &= -2y_3 + y_2 - \frac{\mu^* y_2}{r_1^3} - \frac{\mu y_2}{r_2^3}. \end{split}$$

where

$$\mu = \frac{1}{82.45}$$

$$\mu^* = 1 - \mu$$

$$r_1 = \sqrt{(y_1 + \mu)^2 + y_2^2}$$

$$r_2 = \sqrt{(y_1 - \mu^*)^2 + y_2^2}$$

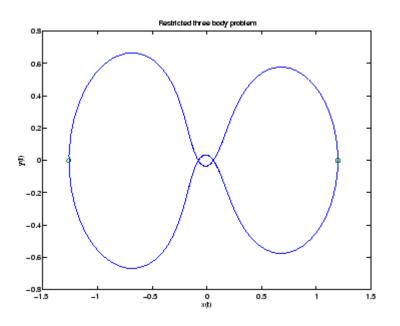
The first two solution components are coordinates of the body of infinitesimal mass, so plotting one against the other gives the orbit of the body. The initial conditions have been chosen to make the orbit periodic. The value of  $\mu$  corresponds to a spaceship traveling around the moon and the earth. Moderately stringent tolerances are necessary to reproduce the qualitative behavior of the orbit. Suitable values are 1e-5 for RelTol and 1e-4 for AbsTol.

The nested events function includes event functions that locate the point of maximum distance from the starting point and the time the spaceship returns to the starting point. Note that the events are located accurately, even though the step sizes used by the integrator are *not* determined by the location 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 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.

To run this example, type orbitode at the command line. The example uses the output function odephas2 to produce the two-dimensional phase plane plot and let you to see the progress of the integration.

```
function orbitode
%ORBITODE Restricted three-body problem
mu = 1 / 82.45;
mustar = 1 - mu;
y0 = [1.2; 0; 0; -1.04935750983031990726];
tspan = [0 7];
options = odeset('RelTol',1e-5,'AbsTol',1e-4,...
                'OutputFcn',@odephas2,'Events',@events);
[t,y,te,ye,ie] = ode45(@f,tspan,y0,options);
plot(y(:,1),y(:,2),ye(:,1),ye(:,2),'o');
title ('Restricted three body problem')
ylabel ('y(t)')
xlabel ('x(t)')
% -----
                                  function dydt = f(t,y)
r13 = ((y(1) + mu)^2 + y(2)^2)^{-1.5};
r23 = ((y(1) - mustar)^2 + y(2)^2)^1.5;
dydt = [y(3)]
        y(4)
        2*y(4) + y(1) - mustar*((y(1)+mu)/r13) - ...
                       mu*((y(1)-mustar)/r23)
       -2*y(3) + y(2) - mustar*(y(2)/r13) - mu*(y(2)/r23) ];
     % End nested function f
end
% -----
                                function [value,isterminal,direction] = events(t,y)
% Locate the time when the object returns closest to the
\% initial point yO and starts to move away; stop integration.
% Also locate the time when the object is farthest from the
% initial point yO and starts to move closer.
%
% The current distance of the body is
%
```

```
%
    DSQ = (y(1) - y0(1))^{2} + (y(2) - y0(2))^{2}
%
        = \langle y(1:2) - y0(1:2), y(1:2) - y0(1:2) \rangle
%
% A local minimum of DSQ occurs when d/dt DSQ crosses zero
% heading in the positive direction. Compute d(DSQ)/dt as
%
%
  d(DSQ)/dt = 2*(y(1:2)-yO(1:2))'*dy(1:2)/dt = ...
%
                   2*(y(1:2)-y0(1:2))'*y(3:4)
%
dDSQdt = 2 * ((y(1:2)-y0(1:2))' * y(3:4));
value = [dDSQdt; dDSQdt];
isterminal = [1; 0];
                                  % Stop at local minimum
                                  % [local minimum, local maximum]
direction = [1; -1];
      % End nested function events
end
end
```



### **Differential-Algebraic Equations**

hb1dae reformulates the hb1ode example as a *differential-algebraic equation* (DAE) problem. The Robertson problem coded in hb1ode is a classic test problem for codes that solve stiff ODEs.

$$y'_{1} = -0.04y_{1} + 10^{4} y_{2} y_{3}$$
  

$$y'_{2} = 0.04y_{1} - 10^{4} y_{2} y_{3} - 3 \cdot 10^{7} y_{2}^{2}$$
  

$$y'_{3} = 3 \cdot 10^{7} y_{2}^{2}.$$

**Note** The Robertson problem appears as an example in the prolog to LSODI [4].

In hblode, the problem is solved with initial conditions  $y_1(0) = 1$ ,  $y_2(0) = 0$ ,  $y_3(0) = 0$  to steady state. These differential equations satisfy a linear conservation law that is used to reformulate the problem as the DAE

$$y'_{1} = -0.04y_{1} + 10^{4} y_{2}y_{3}$$
  

$$y'_{2} = 0.04y_{1} - 10^{4} y_{2}y_{3} - 3 \cdot 10^{7} y_{2}^{2}$$
  

$$0 = y_{1} + y_{2} + y_{3} - 1.$$

These equations do not have a solution for y(0) with components that do not sum to 1. The problem has the form of My' = f(t,y) with

$$M = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

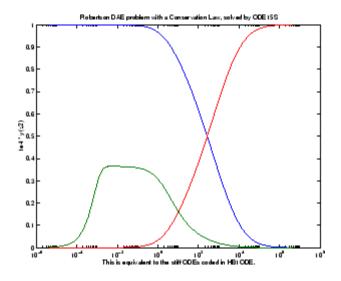
*M* is singular, but hb1dae does not inform the solver of this. The solver must recognize that the problem is a DAE, not an ODE. Similarly, although consistent initial conditions are obvious, the example uses an inconsistent value  $y_3(0) = 10^{-3}$  to illustrate computation of consistent initial conditions.

To run this example, type hbidae at the command line. Note that hbidae

• Imposes a much smaller absolute error tolerance on  $y_2$  than on the other components. This is because  $y_2$  is much smaller than the other components and its major change takes place in a relatively short time.

- Specifies additional points at which the solution is computed to more clearly show the behavior of  $y_2$ .
- Multiplies  $y_2$  by  $10^4$  to make  $y_2$  visible when plotting it with the rest of the solution.
- Uses a logarithmic scale to plot the solution on the long time interval.

```
function hb1dae
%HB1DAE Stiff differential-algebraic equation (DAE)
% A constant, singular mass matrix
M = [1 \ 0 \ 0]
    0 1 0
    0 \ 0 \ 0];
% Use inconsistent initial condition to test initialization.
v0 = [1; 0; 1e-3];
tspan = [0 \ 4*logspace(-6,6)];
% Use the LSODI example tolerances.'MassSingular' is left
% at its default 'maybe' to test the automatic detection
% of a DAE.
options = odeset('Mass',M,'RelTol',1e-4,...
                 'AbsTol',[1e-6 1e-10 1e-6],...
                 'Vectorized', 'on');
[t,y] = ode15s(@f,tspan,y0,options);
y(:,2) = 1e4*y(:,2);
semilogx(t,y);
ylabel('1e4 * y(:,2)');
title(['Robertson DAE problem with a Conservation Law, '...
       'solved by ODE15S']);
xlabel('This is equivalent to the stiff ODEs in HB10DE.');
% -----
                    function out = f(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 ];
```



#### **Nonnegative Solutions**

If certain components of the solution must be nonnegative, use **odeset** to set the NonNegative property for the indices of these components.

**Note** This option is not available for ode23s, ode15i, or for implicit solvers (ode15s, ode23t, ode23tb) applied to problems where there is a mass matrix.

Imposing nonnegativity is not always a trivial task. We suggest that you use this option only when necessary, for example in instances in which the application of a solution or integration will fail otherwise.

Consider the following initial value problem solved on the interval [0, 40]:

$$y' = -|y|, y(0) = 1$$

The solution of this problem decays to zero. If a solver produces a negative approximate solution, it begins to track the solution of the ODE through this value, the solution goes off to minus infinity, and the computation fails. Using the NonNegative property prevents this from happening.

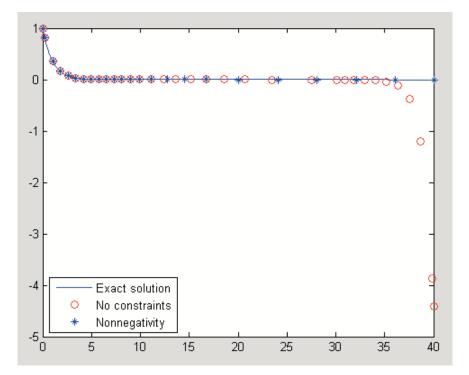
In this example, the first call to ode45 uses the defaults for the solver parameters:

ode = @(t,y) -abs(y); [t0,y0] = ode45(ode,[0, 40], 1);

The second uses options to impose nonnegativity conditions:

```
options = odeset('NonNegative',1);
[t1,y1] = ode45(ode,[0, 40], 1, options);
```

This plot compares the numerical solution to the exact solution.



Here is a more complete view of the code used to obtain this plot:

```
ode = @(t,y) -abs(y);
options = odeset('Refine',1);
```

```
[t0,y0] = ode45(ode,[0, 40], 1,options);
options = odeset(options,'NonNegative',1);
[t1,y1] = ode45(ode,[0, 40], 1, options);
t = linspace(0,40,1000);
y = exp(-t);
plot(t,y,'b-',t0,y0,'ro',t1,y1,'b*');
legend('Exact solution','No constraints','Nonnegativity', ...
'Location','SouthWest')
```

**The kneeode Example.** The kneeode example solves the "knee problem" by imposing a nonnegativity constraint on the numerical solution. The initial value problem is

 $*y' = (1-x)*y - y^2, y(0) = 1$ 

For  $0 < \epsilon < 1$ , the solution of this problem approaches null isoclines y = 1- x and y = 0 for x < 1 and x > 1, respectively. The numerical solution, when computed with default tolerances, follows the y = 1 - x isocline for the whole interval of integration. Imposing nonnegativity constraints results in the correct solution.

Here is the code that makes up the kneeode example:

```
function kneeode
%KNEEODE The "knee problem" with Nonnegativity constraints.
% Problem parameter
epsilon = 1e-6;
y0 = 1;
xspan = [0, 2];
% Solve without imposing constraints
options = [];
[x1,y1] = ode15s(@odefcn,xspan,y0,options);
% Impose nonnegativity constraint
options = odeset('NonNegative',1);
[x2,y2] = ode15s(@odefcn,xspan,y0,options);
```

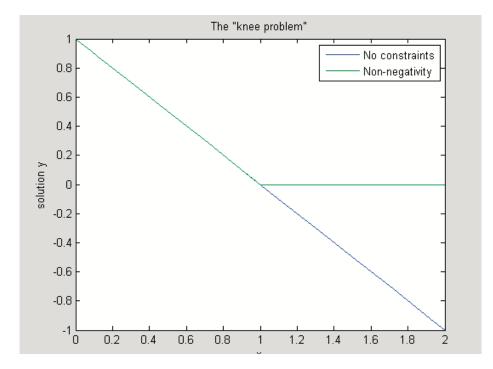
```
figure
plot(x1,y1,'b.-',x2,y2,'g-')
axis([0,2,-1,1]);
title('The "knee problem"');
legend('No constraints','nonnegativity')
xlabel('x');
ylabel('solution y')
function yp = odefcn(x,y)
    yp = ((1 - x)*y - y^2)/epsilon;
    end
end % kneeode
```

The derivative function is defined within nested function odefcn. The value of epsilon used in odefcn is obtained from the outer function:

```
function yp = odefcn(x,y)
yp = ((1 - x)*y - y^2)/epsilon;
end
```

The exmaple solves the problem using the ode15s function, first with the default options, and then by imposing a nonnegativity constraint. To run the example, type kneeode at the MATLAB command prompt.

Here is the output plot. The plot confirms correct solution behavior after imposing constraints.



### **Additional Examples**

The following additional examples are available. Type

edit examplename

to view the code and

examplename

to run the example.

Example Name	Description
amp1dae	Stiff DAE — electrical circuit
ballode	Simple event location — bouncing ball
batonode	ODE with time- and state-dependent mass matrix — motion of a baton

Example Name	Description
brussode	Stiff large problem — diffusion in a chemical reaction (the Brusselator)
burgersode	ODE with strongly state-dependent mass matrix — Burgers' equation solved using a moving mesh technique
fem1ode	Stiff problem with a time-dependent mass matrix — finite element method
fem2ode	Stiff problem with a constant mass matrix — finite element method
hb1ode	Stiff ODE problem solved on a very long interval — Robertson chemical reaction
hb1dae	Robertson problem — stiff, linearly implicit DAE from a conservation law
ihb1dae	Robertson problem — stiff, fully implicit DAE
iburgersode	Burgers' equation solved as implicit ODE system
kneeode	The "knee problem" with nonnegativity constraints
orbitode	Advanced event location — restricted three body problem
rigidode	Nonstiff problem — Euler equations of a rigid body without external forces
vdpode	Parameterizable van der Pol equation (stiff for large $\mu$ )

## Troubleshooting

- General Questions on page 10-40
- Memory and Computational Efficiency on page 10-40
- Time Steps for Integration on page 10-41
- Error Tolerance and Other Options on page 10-42

- Other Types of Equations on page 10-43
- Other Common Problems on page 10-44

#### **General Questions**

Question	Answer
How do the ODE solvers differ from integral?	integral solves problems of the form $y' = f(t)$ . The ODE solvers handle more general problems $y' = f(t,y)$ , linearly implicit problems that involve a mass matrix $M(t,y)y' = f(t,y)$ , and fully implicit problems $f(t,y,y') = 0$ .
Can I solve ODE systems in which there are more equations than unknowns, or vice versa?	No.

#### **Memory and Computational Efficiency**

Question	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 may be advantageous to use the sparse option. If the problem is nonstiff, or if you are using the sparse option, it may be possible to solve a problem with thousands of unknowns. In this case, however, storage of the result can be problematic. Try asking the solver to evaluate the solution at specific points only, or call the

Question	Answer
	solver with no output arguments and use an output function to monitor the solution.
I'm solving a very large system, but only care about a couple of the components of y. Is there any way to avoid storing all of the elements?	Yes. The user-installable output function capability is designed specifically for this purpose. When you call the solver with no output arguments, the solver does not allocate storage to hold the entire solution history. Instead, the solver calls OutputFcn(t,y,flag) at each time step. To keep the history of specific elements, write an output function that stores or plots only the elements you care about.
What is the startup cost of the integration and how can I reduce it?	The biggest startup cost occurs as the solver attempts to find a step size appropriate to the scale of the problem. If you happen to know an appropriate step size, use the InitialStep property. For example, if you repeatedly call the integrator in an event location loop, the last step that was taken before the event is probably on scale for the next integration. See ballode for an example.

### Memory and Computational Efficiency (Continued)

#### **Time Steps for Integration**

Question	Answer
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 property. The integrator tries this value, then reduces it if necessary.
Can I integrate with fixed step sizes?	No.

<b>Error Tole</b>	erance	and	Other	Options
-------------------	--------	-----	-------	---------

Question	Answer
How do I choose RelTol and AbsTol?	RelTol, the relative accuracy tolerance, controls the number of correct digits in the answer. AbsTol, the absolute error tolerance, controls the difference between the answer and the solution. At each step, the error e in component i of the solution satisfies
	<pre> e(i)  max(RelTol*abs(y(i)),AbsTol(i))</pre>
	Roughly speaking, this means that you want RelTol correct digits in all solution components except those smaller than thresholds AbsTol(i). Even if you are not interested in a component y(i) when it is small, you may have to specify AbsTol(i) 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't I 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 don't care about getting an accurate answer for one of the solution components?	You can increase the absolute error tolerance corresponding to this solution component. If the tolerance is bigger than the component, this specifies no correct digits for the component. The solver may have to get some correct digits in this component to compute other components accurately, but it generally handles this automatically.

Question	Answer
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 – the ODE solvers provide for this. Often the system is stiff. This is to be expected when the PDE is parabolic and 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 solvers: ode15s, ode23s, ode23t, ode23tb.
	If there are many equations, set the JPattern property. This might make the difference between success and failure due to the computation being too expensive. For an example that uses JPattern, see "Large Stiff Sparse Problem" on page 10-23. When the system is not stiff, or not very stiff, ode23 or ode45 is more efficient than ode15s, ode23s, ode23t, or ode23tb.
	Parabolic-elliptic partial differential equations in 1-D can be solved directly with the MATLAB PDE solver, pdepe. For more information, see "Partial Differential Equations" on page 10-96.
Can I solve differential-algebraic equation (DAE) systems?	Yes. The solvers ode15s and ode23t can solve some DAEs of the form $M(t,y)y' = f(t,y)$ where M(t,y) is singular. The DAEs must be of index 1. ode15i can solve fully implicit DAEs of index 1, $f(t,y,y') = 0$ . For examples, see amp1dae, hb1dae, or ihb1dae.

## Other Types of Equations

Question	Answer
Can I integrate a set of sampled data?	Not directly. You have to 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 like 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 this.
What do I do when I have the final and not the initial value?	All the solvers of the ODE suite allow you to solve backwards or forwards in time. The syntax for the solvers is [t,y] = ode45(odefun,[t0 tf],y0);and the syntax accepts t0 > tf.

### Other Types of Equations (Continued)

#### **Other Common Problems**

Question	Answer
The solution doesn't look like what I expected.	If you're right about its appearance, you need to reduce the error tolerances from their default values. A smaller relative error tolerance is needed to compute accurately the solution of problems integrated over "long" intervals, as well as solutions of problems that are moderately unstable. You should check whether there are solution components that stay smaller than their absolute error tolerance for some time. If so, you are not asking for any correct digits in these components. This may be acceptable for these components, but failing to compute them

Question	Answer
	accurately may degrade the accuracy of other components that depend on them.
My plots aren't smooth enough.	Increase the value of Refine from its default of 4 in ode45 and 1 in the other solvers. The bigger the value of Refine, the more output points. Execution speed is not affected much by the value of Refine.
I'm 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 isn't, the solver must take small steps to deal with this. It may help to break tspan into pieces on 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 this purpose. Switch to ode15s, ode23s, ode23t, or ode23tb.
My integration proceeds very slowly, using too many time steps.	First, check that your 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 the tspan, 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 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

### **Other Common Problems (Continued)**

Question	Answer
	the ODE function. Rather than recompute 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 t0 t tf	If you know there is a sharp change at time t, it might help to break the tspan interval into two pieces, [t0 t] and [t tf], and call the integrator twice.
but the integrator steps past without "seeing" it.	If the differential equation has periodic coefficients or solution, you might restrict the maximum step size to the length of the period so the integrator won't step over periods.

### **Other Common Problems (Continued)**

## **Types of DDEs**

#### In this section...

"Constant Delay DDEs" on page 10-47 "Time-Dependent and State-Dependent DDEs" on page 10-47 "DDEs of Neutral Type" on page 10-48 "Evaluating the Solution at Specific Points" on page 10-48 "History and Initial Values" on page 10-48 "Propagation of Discontinuities" on page 10-49

## **Constant Delay DDEs**

A system of differential equations (DDEs) with constant delays has the following form:

$$y'(t) = f(t, y(t), y(t - \tau_1), \dots, y(t - \tau_k)).$$
 (10-1)

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 10-1 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 10-1 is a special case of

$$y'(t) = f(t, y(t), y(dy_1), \dots, y(dy_p))$$
(10-2)

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 10-2 with history y(t) = S(t) for  $t < t_0$ . The ddesd function integrates with the classic four-stage, fourth-order explicit Runge-Kutta method, and it controls the size of the residual of a natural interpolant. It uses iteration to take steps that are longer than the delays.

## **DDEs of Neutral Type**

Delay differential equations of neutral type involve delays in *y* ' as well as *y*:

$$y'(t) = f(t, y(t), y(dy_1), \dots, y(dy_p), y'(dyp_1), \dots, y'(dyp_q)).$$
(10-3)

The delays in the solution must satisfy  $dy_i(t,y) \le t$ . The delays in the first derivative must satisfy  $dyp_j(t,y) < t$  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 10-2. 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 10-1 shows that  $y'(t_0)$  depends on  $y(t_0 - \tau_1), \dots, y(t_0 - \tau_k)$  for positive constants  $\tau_i$ . 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 10-1. If the delays are not constant, the propagation of discontinuities is more complicated. For neutral DDEs of the form given by Equation 10-1 or Equation 10-2, 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 10-3 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  $[t_0, t_f]$ .

## 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 $t$ 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

Nature of Discontinuity	Property	Comments
		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:

$$y_1'(t) = y_1(t-1)$$
  

$$y_2'(t) = y_1(t-1) + y_2(t-0.2)$$
  

$$y_3'(t) = y_2(t).$$

The history 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,  $\tau_1, \dots, \tau_k$  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  $[t_0, t_i]$ .

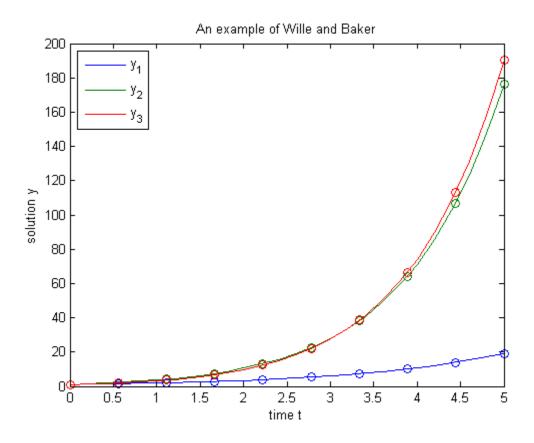
6 Plot the solution returned by dde23. Add this code to your main function.

```
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.





function\_handle

Related Examples

- "Create Functions in Files"
- "Run Functions in the Editor"

## **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:

$$y_1'(t) = y_2(t)$$
  

$$y_2'(t) = -y_2(e^{(1-y_2(t))}) \cdot y_2(t)^2 \cdot e^{(1-y_2(t))}.$$

The 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);
```

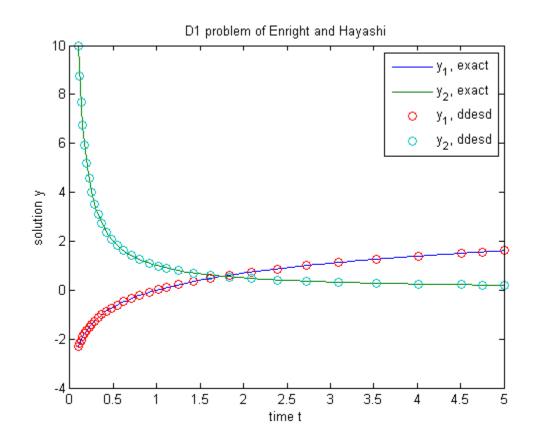
**6** Use the history function to calculate the analytical solution within the integration interval. Add this code to the main function.

```
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

 Enright, W.H. and H. Hayashi. "The Evaluation of Numerical Software for Delay Differential Equations." In *Proceedings of the IFIP TC2/WG2.5 working conference on Quality of numerical software: assessment and enhancement.* (R.F. Boisvert, ed.). London, UK: Chapman & Hall, Ltd., pp. 179-193.

See Also function\_handle

Related Examples

- "Create Functions in Files"
- "Run Functions in the Editor"

## **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;
p.R
         = 1.05;
p.r
         = 0.068;
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)) * PO;
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 .

**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')
ylabel('H(t)')
```

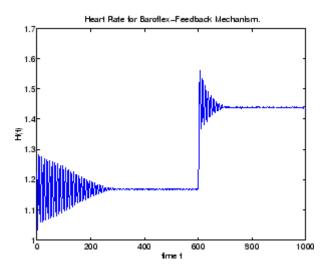
8 Define the system of DDEs as a nested function inside the main function.

```
function dydt = ddex2de(t,y,Z)
    if t <= 600
        p.R = 1.05;
    else
        p.R = 0.21 * exp(600-t) + 0.84;
    end
    ylag = Z(:,1);
    Patau = ylag(1);
    Paoft = y(1);</pre>
```

```
Pvoft = y(2);
Hoft = y(3);
dPadt = - (1 / (p.ca * p.R)) * Paoft ...
+ (1/(p.ca * p.R)) * Pvoft ...
+ (1/p.ca) * p.Vstr * Hoft;
dPvdt = (1 / (p.cv * p.R)) * Paoft...
- ( 1 / (p.cv * p.R)...
+ 1 / (p.cv * p.r) ) * Pvoft;
Ts = 1 / ( 1 + (Patau / p.alphas)^p.betas );
Tp = 1 / ( 1 + (p.alphap / Paoft)^p.betap );
dHdt = (p.alphaH * Ts) / (1 + p.gammaH * Tp) ...
- p.betaH * Tp;
dydt = [ dPadt; dPvdt; dHdt];
end
```

This function is nested so that the main function can access the 14 parameters defined in .

**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.

See Also function\_handle

• "Create F

Related Examples

- "Create Functions in Files"
- "Run Functions in the Editor"

## **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);
```

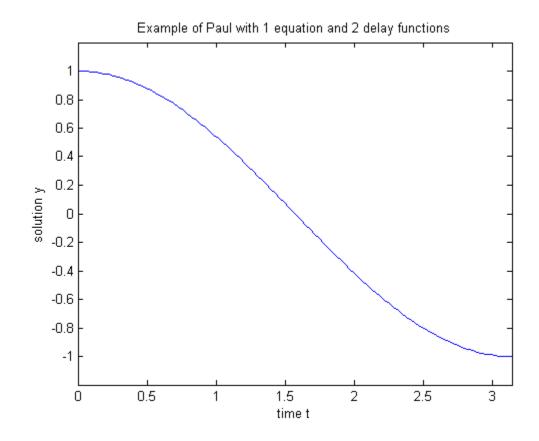
**7** Evaluate the solution at 100 equally spaced points between 0 and  $\pi$ . Add this code to the main function.

```
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.

See Also function\_handle

Related Examples

- "Create Functions in Files"
- "Run Functions in the Editor"

## 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 isy  $i(t) = 2\cos(2t) y(t/2)^{2\cos(t)} + \log(y'(t/2)) - \log(2\cos(t)) - \sin(t)$ .

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.

**4** 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);
```

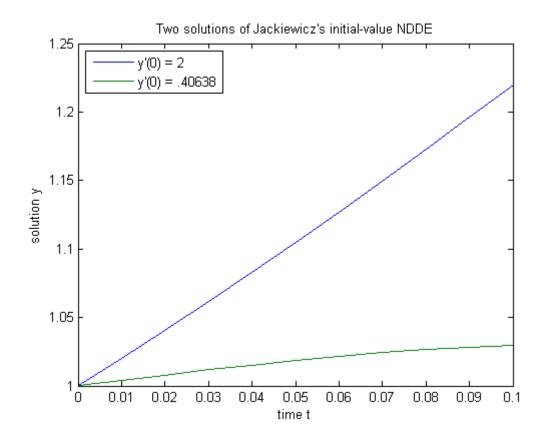
**6** Solve the equation again, this time using y'(0) = 0.4063757399599599. Add this code to the main function.

```
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.

See Also function\_handle

Related Examples

- "Create Functions in Files"
- "Run Functions in the Editor"

# **Boundary-Value Problems**

### In this section...

"Function Summary" on page 10-68

"Boundary Value Problems" on page 10-69

"BVP Solver" on page 10-70

"Integrator Options" on page 10-73

"Examples" on page 10-74

## **Function Summary**

- "BVP Solver" on page 10-68
- "BVP Helper Functions" on page 10-68
- "BVP Solver Options" on page 10-69

### **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.
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 "First Order ODEs" on page 10-4 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 10-70
- "BVP Solver Syntax" on page 10-71
- "BVP Solver Options" on page 10-73

#### 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 C<sup>1</sup>-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 I It has the b	handle that evaluates the differential equations. basic form	
	dydx = ode	efun(x,y)	
	odefun can and a varia	a scalar, and dydx and y are column vectors. also accept a vector of unknown parameters ble number of known parameters, (see "BVP ons" on page 10-73).	
bcfun		a function that evaluates the residual in the onditions. It has the basic form	
	res = bcfu	un(ya,yb)	
	y(b), and r the bounda of unknown	nd yb are column vectors representing y(a) and es is a column vector of the residual in satisfying ry conditions. bcfun can also accept a vector a parameters and a variable number of known b, (see "BVP Solver Options" on page 10-73).	
solinit	Structure with fields x and y:		
	x	Ordered nodes of the initial mesh. Boundary conditions are imposed at $a = \text{solinit.x(1)}$ and $b = \text{solinit.x(end)}$ .	
	У	Initial guess for the solution with solinit.y(:,i) a guess for the solution at the node solinit.x(i).	
	named x an an initial g solinit wi	are can have any name, but the fields must be ad y. It can also contain a vector that provides uess for unknown parameters. You can form th the helper function bypinit. See the bypinit age 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.
	<pre>sol = bvp4c(odefun,bcfun,solinit,options)</pre>
	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 bvpset 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 10-74
- "Continuation" on page 10-79
- "Singular BVPs" on page 10-86
- "Multipoint BVPs" on page 10-90
- "Additional Examples" on page 10-94

#### **Mathieu's Equation**

- "Solving the Problem" on page 10-74
- "Finding Unknown Parameters" on page 10-78
- "Evaluating the Solution" on page 10-79

**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

$$\mathbf{y}'' + (\lambda - 2 \ q \ \cos \ 2x)\mathbf{y} = 0$$

Because the unknown parameter  $\lambda$  is present, this second-order differential equation is subject to *three* boundary conditions

y(0) = 1y'(0) = 0 $y'(\pi) = 1$ 

**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.

**1** 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  $\boldsymbol{\lambda}.$  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 first-order 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:

**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.

**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).

In the call to bypinit, 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);
```

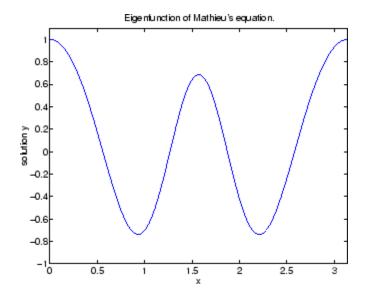
- **6** View the results. Complete the example by displaying the results:
  - **a** Print the value of the unknown parameter  $\lambda$  found by bvp4c.

```
fprintf('Fourth eigenvalue is approximately %7.3f.\n',...
sol.parameters)
```

**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<sup>1</sup>-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 10-79
- "Using Continuation to Solve a BVP" on page 10-79
- "Using Continuation to Verify Consistency" on page 10-82

**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  $\varepsilon$  is represented by  $\mathbf{e}$  and is shared with the outer function.

```
function dydx = shockODE(x,y)
pix = pi*x;
dydx = [ y(2,:)
                -x/e.*y(2,:) - pi^2*cos(pix) - pix/e.*sin(pix) ];
end % End nested function shockODE
function res = shockBC(ya,yb)
res = [ ya(1)+2
                yb(1) ];
end % End nested function shockBC
```

**2 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)

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.

```
options = bvpset('FJacobian',@shockJac,...
'BCJacobian',@shockBCJac,...
'Vectorized','on');
```

**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]);

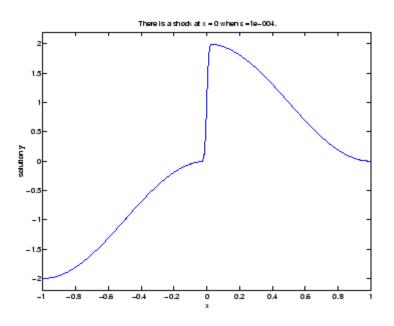
**4** Use continuation to solve the problem. To obtain the solution for the parameter  $\varepsilon = 10^{-4}$ , the example uses continuation by solving a sequence of problems for  $\varepsilon = 10^{-2}$ ,  $10^{-3}$ ,  $10^{-4}$ . The solver bvp4c does not perform continuation automatically, but the code's user interface has been designed to make continuation easy. The code uses the output sol that bvp4c produces for one value of 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

```
plot(sol.x,sol.y(1,:))
axis([-1 1 -2.2 2.2])
title(['There is a shock at x = 0 when \epsilon = '...
        sprintf('%.e',e) '.'])
xlabel('x')
ylabel('solution y')
```



**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]);
```

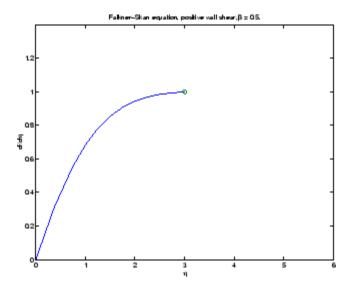
3 Solve on the initial interval. The example obtains the solution for infinity = 3. It then prints the computed value of f"(0) for comparison with the value reported by Cebeci and Keller [2]:

```
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.

**4** Setup the figure and plot the initial solution.



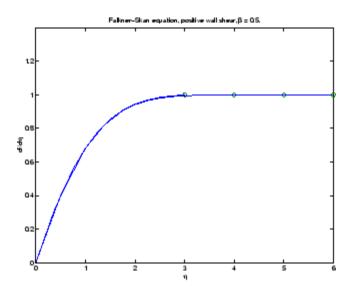
**5** Use continuation to solve the problem and plot subsequent solutions. The example then solves the problem for infinity = 4, 5, 6. It uses bypinit to extrapolate the solution sol for one value of infinity as an initial guess for the next value of infinity. For each iteration, the example prints the 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;
fprintf('Value computed using infinity = %g is %7.5f.\n', ...
Bnew,f(3,1))
plot(eta,f(2,:),eta(end),f(2,end),'o');
drawnow
end
hold off
```

The example prints

```
Value computed using infinity = 4 is 0.92774.
Value computed using infinity = 5 is 0.92770.
Value computed using infinity = 6 is 0.92770.
```

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 10-86
- "Emden's equation" on page 10-87

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)) (10-4)

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

$$y^{\prime\prime} + \frac{2}{x}y^{\prime} + y^5 = 0$$

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  $y(1) = \sqrt{3/2}$ , this BVP has the analytical solution

$$y(x) = \left(1 + \frac{x^2}{3}\right)^{-1/2}$$

**Note** The file, emdenbvp.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 emdenbvp at the command line. To run it, type emdenbvp at the command line.

1 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

$$S = \begin{bmatrix} 0 & 0 \\ 0 & -2 \end{bmatrix}$$

 $\operatorname{and}$ 

$$f(x,y) = \begin{bmatrix} y_2 \\ -y_1^5 \end{bmatrix}$$

**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.

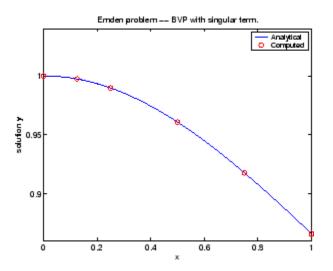
sol = bvp4c(@emdenode,@emdenbc,solinit,options);

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)/nC' = (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:

 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  $\eta$  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:

% End nested function bc

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]; % initial guess for y(x) 0 \le x \le 1
  case 2 % x in [1, \lambda]
    y = [1;1]; % initial guess for y(x), 1 \le x \le \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.

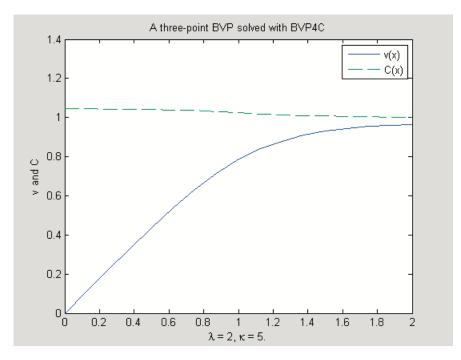
**7** View the results. Using deval, the solution can be evaluated at any point in the interval of integration.

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')
xlabel(['\lambda = ',num2str(\lambda), ...
', \kappa = ',num2str(\kappa),'.'])
ylabel('v and C')
```



## **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

 $\label{eq:stability} Additional examples are provided by ``Tutorial on Solving BVPs with BVP4C, ``available at http://www.mathworks.com/bvp_tutorial.$ 

# **Partial Differential Equations**

## In this section...

"Function Summary" on page 10-96

"Initial Value Problems" on page 10-97

"PDE Solver" on page 10-98

"Integrator Options" on page 10-101

"Examples" on page 10-102

## **Function Summary**

- "PDE Solver" on page 10-96
- "PDE Helper Function" on page 10-96

### **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

$$c\left(x,t,u,\frac{\partial u}{\partial x}\right)\frac{\partial u}{\partial t} = x^{-m}\frac{\partial}{\partial x}\left(x^{m}f\left(x,t,u,\frac{\partial u}{\partial x}\right)\right) + s\left(x,t,u,\frac{\partial u}{\partial x}\right).$$
(10-5)

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 10-5,  $f(x,t,u,\partial u/\partial x)$  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 x if they are mesh points. Discontinuities in c and/or s 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

$$u(x,t_0) = u_0(x).$$
 (10-6)

At the boundary x = a or x = b, for all *t* the solution components satisfy a boundary condition of the form

$$p(x,t,u) + q(x,t)f\left(x,t,u,\frac{\partial u}{\partial x}\right) = 0.$$
(10-7)

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 [9]. 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 10-5 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 10-97.

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 10-5.
pdefun	Function that defines the components of the PDE. It computes the terms $c$ , $f$ , and $s$ in Equation 10-5, 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 $u$ .
bcfun	Function that evaluates the terms $p$ and $q$ of the boundary conditions. It has the form
	<pre>[pl,ql,pr,qr] = bcfun(xl,ul,xr,ur,t)</pre>
	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 ql.

xmesh	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 <i>not</i> 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 $\ge 3$ .
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 $\ge 3$ .

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.

## **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. "Integrator Options" on page 10-9 tells you how to create the structure and describes the properties.

### **PDE Properties**

Properties Category	Property Name
Error control	RelTol, AbsTol, NormControl
Step-size	InitialStep, MaxStep

## **Examples**

- "Single PDE" on page 10-102
- "System of PDEs" on page 10-107
- "Additional Examples" on page 10-111

### Single PDE

- "Solving the Equation" on page 10-102
- "Evaluating the Solution" on page 10-107

**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

$$\begin{split} u(0,t) &= 0 \\ \pi e^{-t} + \frac{\partial u}{\partial x}(1,t) = 0. \end{split}$$

**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 10-98 for more information.

**1** Rewrite the PDE. Write the PDE in the form

$$c\bigg(x,t,u,\frac{\partial u}{\partial x}\bigg)\frac{\partial u}{\partial t}=x^{-m}\frac{\partial}{\partial x}\bigg(x^mf\bigg(x,t,u,\frac{\partial u}{\partial x}\bigg)\bigg)+s\bigg(x,t,u,\frac{\partial u}{\partial x}\bigg).$$

This is the form shown in Equation 10-5 and expected by pdepe. See "Initial Value Problems" on page 10-97 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 10-5) 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 pdexlic.

```
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 10-7, are

$$u(0,t) + 0 \cdot \frac{\partial u}{\partial x}(0,t) = 0 \text{ at } x = 0$$

and

$$\pi e^{-t} + 1 \cdot \frac{\partial u}{\partial x}(1,t) = 0 \text{ at } x = 1.$$

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);
qr = 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 10-98). 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).

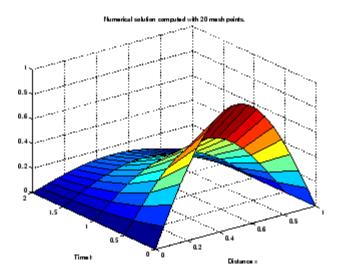
m = 0; sol = pdepe(m,@pdex1pde,@pdex1ic,@pdex1bc,x,t);

This example uses @ to pass pdex1pde, pdex1ic, and pdex1bc as function handles to pdepe.

**Note** See the function\_handle (@), func2str, and str2func reference pages, and the @ section of MATLAB Programming Fundamentals for information about function handles.

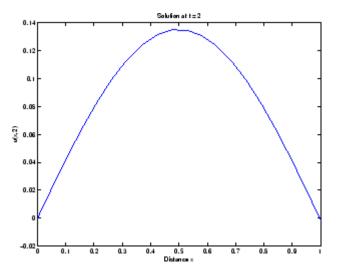
- 7 View the results. Complete the example by displaying the results:
  - **a** Extract and display the first solution component. In this example, the solution u has only one component, but for illustrative purposes, the example "extracts" it from the three-dimensional array. The surface plot shows the 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')
```



**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

$$\frac{\partial u_1}{\partial t} = 0.024 \frac{\partial^2 u_1}{\partial x^2} - F(u_1 - u_2)$$
$$\frac{\partial u_2}{\partial t} = 0.170 \frac{\partial^2 u_1}{\partial x^2} + F(u_1 - u_2)$$

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

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix} \cdot * \frac{\partial}{\partial t} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \frac{\partial}{\partial x} \begin{bmatrix} 0.024 (\partial u_1 / \partial x) \\ 0.170 (\partial u_2 / \partial x) \end{bmatrix} + \begin{bmatrix} -F(u_1 - u_2) \\ F(u_1 - u_2) \end{bmatrix}.$$

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

$$\begin{bmatrix} 0\\ u_2 \end{bmatrix} + \begin{bmatrix} 1\\ 0 \end{bmatrix} \cdot * \begin{bmatrix} 0.024(\partial u_1 / \partial x)\\ 0.170(\partial u_2 / \partial x) \end{bmatrix} = \begin{bmatrix} 0\\ 0 \end{bmatrix}$$

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

where c, f, and s correspond to the c, f, and s terms in Equation 10-5.

```
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 10-7) 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];
```

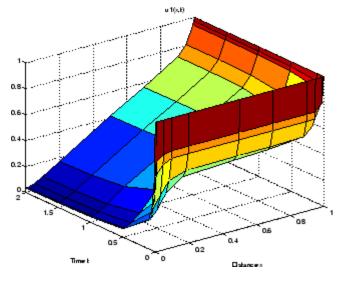
**5** Select mesh points for the solution. The solution changes rapidly for small *t*. The program selects the step size in time to resolve this sharp change, but to see this behavior in the plots, output times must be selected accordingly. There are boundary layers in the solution at both ends of [0,1], 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.

**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).

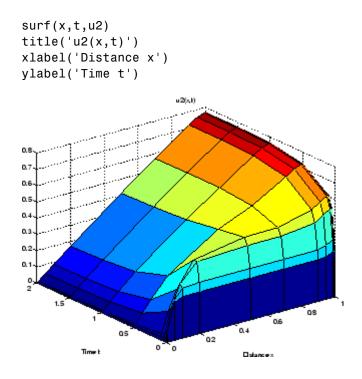
```
m = 0;
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
```

**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')
```







## **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

Example Name	Description
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 <i>t</i> .
pdex5	System of PDEs with step functions as initial conditions

# Selected Bibliography for Differential Equations

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[3] Hairer, E., and G. Wanner, *Solving Ordinary Differential Equations II*, *Stiff and Differential-Algebraic Problems*, Springer-Verlag, Berlin, 1991, pp. 5-8.

[4] Hindmarsh, A. C., "LSODE and LSODI, Two New Initial Value Ordinary Differential Equation Solvers," *SIGNUM Newsletter*, Vol. 15, 1980, pp. 10-11.

[5] Hindmarsh, A. C., and G. D. Byrne, "Applications of EPISODE: An Experimental Package for the Integration of Ordinary Differential Equations," *Numerical Methods for Differential Systems*, L. Lapidus and W. E. Schiesser eds., Academic Press, Orlando, FL, 1976, pp 147-166.

[6] Ottesen, J. T., "Modelling of the Baroflex-Feedback Mechanism with Time-Delay," J. Math. Biol., Vol. 36, 1997.

[7] Shampine, L. F., *Numerical Solution of Ordinary Differential Equations*, Chapman & Hall Mathematics, 1994.

[8] Shampine, L. F., and M. K. Gordon, *Computer Solution of Ordinary Differential Equations*, W.H. Freeman & Co., 1975.

[9] 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.

[10] W.H. Enright and H. Hayashi, "The Evaluation of Numerical Software for Delay Differential Equations," R. Boisvert (Ed.), *The Quality of Numerical Software: Assessment and Enhancement*, Chapman & Hall, London, 1997, pp. 179-192.

# **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.

 $f = @(t) sqrt(4*cos(2*t).^2 + sin(t).^2 + 1);$ 

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  $\frac{e^z}{z}$  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 =
2.7756e-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 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  $-1 \le x \le 1$ ,  $-1 \le y \le 1$ .

```
format long;
q = integral2(fun,-1,1,-1,1)
Warning: Non-finite result. The integration was unsuccessful.
Singularity likely.
q =
Inf - 3.486553786882412e+06i
```

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 =
3.771236166328260 - 3.771236166328255i
```

The integration succeeds when the singular values are on the boundary.

The exact value of this integral is  $\frac{8\sqrt{2}}{3}(1-i)$ . 8/3\*sqrt(2)\*(1-i)

ans =

3.771236166328253 - 3.771236166328253i

# **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.

k = 2; I = polyint(p,k) I = 0,6667 0 -0.5000 0 0.5000 4.0000 2.0000 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.

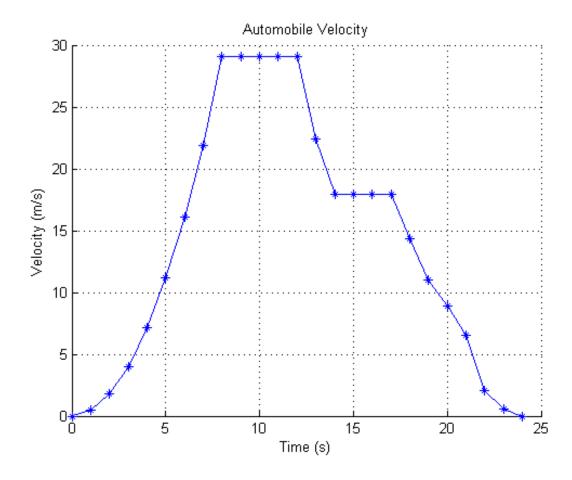
vel = [0 .45 1.79 4.02 7.15 11.18 16.09 21.90 29.05 29.05 ... 29.05 29.05 29.05 22.42 17.9 17.9 17.9 17.9 14.34 11.01 ... 8.9 6.54 2.03 0.55 0]; time = 0:24;

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;hold;
plot(time,vel,'-*');
grid on;
title('Automobile Velocity')
xlabel('Time (s)'); ylabel('Velocity (m/s)');
```

Current plot held

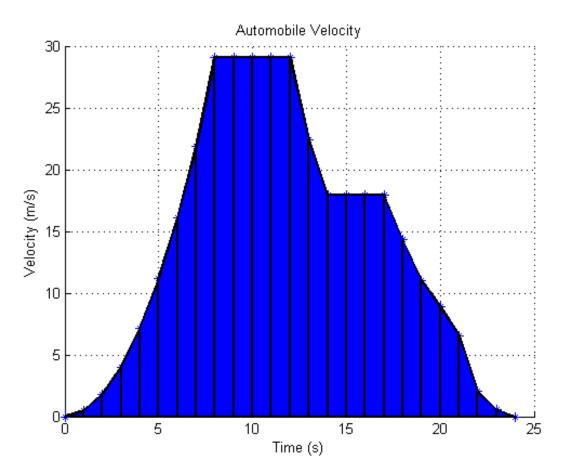


The slope is positive during periods of acceleration, zero during periods of constant velocity, and negative during periods of deceleration. At time t = 0, the vehicle is at rest with vel(1) = 0 m/s. The vehicle accelerates until reaching a maximum velocity at t = 8 s of vel(9) = 29.05 m/s and maintains this velocity for 4 s. It then decelerates to vel(14) = 17.9 m/s for 3 s and eventually back down to rest. Since this velocity curve has multiple discontinuities, a single continuous function cannot describe it.

#### **Calculate the Total Distance Traveled**

trapz performs discrete integration by using the data points to create trapezoids, so it is well suited to handling data sets with discontinuities. This method assumes linear behavior between the data points, and accuracy may be reduced when the behavior between data points is nonlinear. To illustrate, you can draw trapezoids onto the graph using the data points as vertices.

```
xverts = [time(1:end-1);time(1:end-1);time(2:end);time(2:end)];
yverts = [zeros(1,24);vel(1:end-1);vel(2:end);zeros(1,24)];
p = patch(xverts,yverts,'b','LineWidth',1.5);
```



trapz calculates the area under a set of discrete data by breaking the region into trapezoids. The function then adds the area of each trapezoid to compute the total area.

Calculate the total distance traveled by the automobile (corresponding to the shaded area) by integrating the velocity data numerically using trapz.

```
distance = trapz(time,vel)
distance =
345.2200
```

The distance traveled by the automobile in t = 24 s is about 345.22 m.

# 11

## Fourier Transforms

- "Discrete Fourier Transform (DFT)" on page 11-2
- "Fast Fourier Transform (FFT)" on page 11-8
- "Function Summary" on page 11-29

## **Discrete Fourier Transform (DFT)**

#### In this section...

"Introduction" on page 11-2

"Visualizing the DFT" on page 11-3

#### Introduction

Spectral analysis is the process of identifying component frequencies in data. For discrete data, the computational basis of spectral analysis is the *discrete Fourier transform (DFT)*. The DFT transforms time- or space-based data into frequency-based data.

The DFT of a vector x of length n is another vector y of length n:

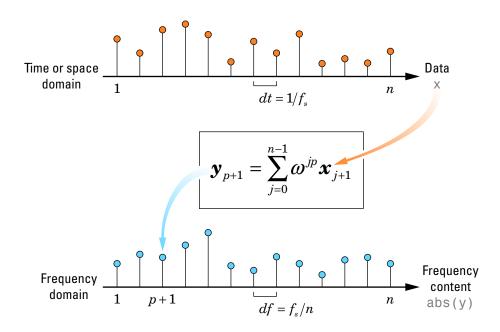
$$y_{p+1} = \sum_{j=0}^{n-1} \omega^{jp} x_{j+1}$$

where  $\omega$  is a complex *n*th root of unity:

$$\omega = e^{-2\pi i / n}$$

This notation uses *i* for the imaginary unit, and *p* and *j* for indices that run from 0 to n-1. The indices p+1 and j+1 run from 1 to *n*, corresponding to ranges associated with MATLAB vectors.

Data in the vector x are assumed to be separated by a constant interval in time or space,  $dt = 1/f_s$  or  $ds = 1/f_s$ , where  $f_s$  is the sampling frequency. The DFT y is complex-valued. The absolute value of y at index p+1 measures the amount of the frequency  $f = p(f_s / n)$  present in the data.



The first element of *y*, corresponding to zero frequency, is the sum of the data in *x*. This *DC* component is often removed from *y* so that it does not obscure the positive frequency content of the data.

## Visualizing the DFT

The documentation example function fftgui opens a graphical user interface that allows you to explore the real and imaginary parts of a data vector and its DFT. (Here fft refers to efficient computation of the DFT by the MATLAB fft function, as discussed in "Fast Fourier Transform (FFT)" on page 11-8.)

Add the examples folder to your path for access to the function fftgui.

```
addpath(fullfile(matlabroot,'/help/matlab/math/examples'))
```

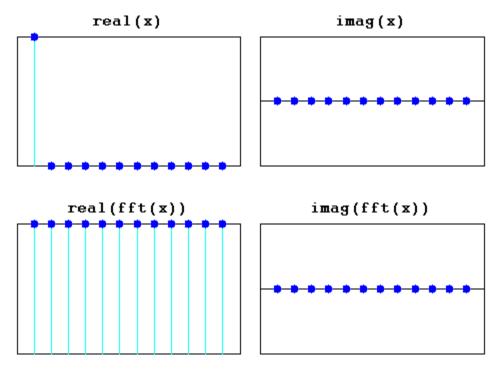
If x is a vector,

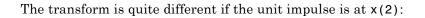
fftgui(x)

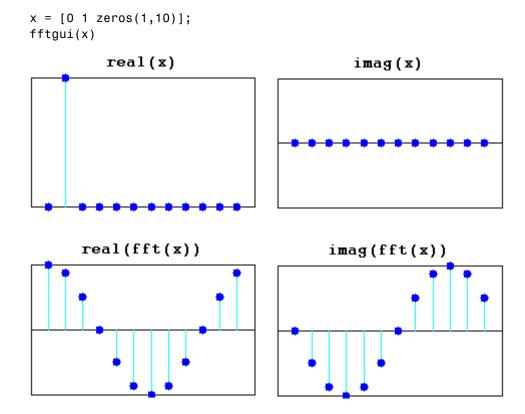
plots the real and imaginary parts of both x and its DFT (fft(x)). Use your mouse to drag points in any of the plots and the points in the other plots respond to the changes.

For example, use fftgui to display the DFT of a unit impulse at x(1):

```
x = [1 zeros(1,11)];
fftgui(x)
```

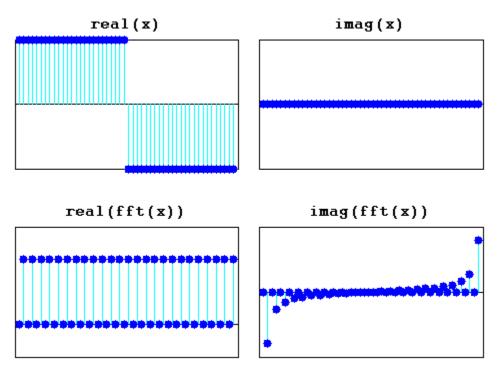


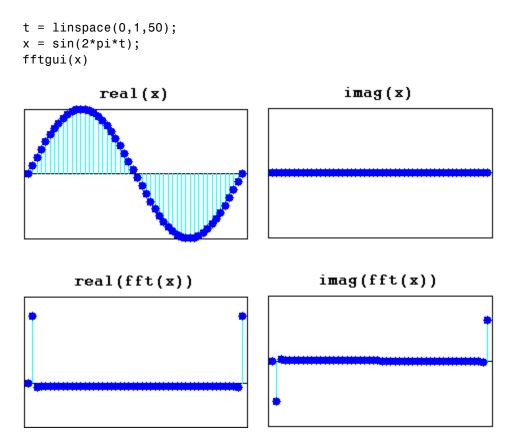




The following commands display DFTs of square and sine waves, respectively:

```
x = [ones(1,25),-ones(1,25)];
fftgui(x)
```





The midpoint of the DFT (or the point just to the right of the midpoint if the length is even), corresponding to half the sampling frequency of the data, is the *Nyquist point*. For real x, the real part of the DFT is symmetric about the Nyquist point, and the imaginary part is antisymmetric about the Nyquist point.

## Fast Fourier Transform (FFT)

#### In this section ...

"Introduction" on page 11-8

"The FFT in One Dimension" on page 11-9

"The FFT in Multiple Dimensions" on page 11-23

#### Introduction

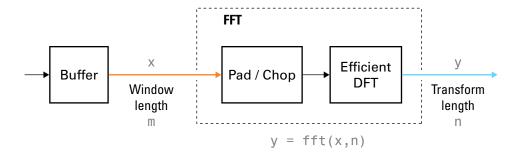
DFTs with a million points are common in many applications. Modern signal and image processing applications would be impossible without an efficient method for computing the DFT.

Direct application of the definition of the DFT (see "Discrete Fourier Transform (DFT)" on page 11-2) to a data vector of length n requires n multiplications and n additions—a total of  $2n^2$  floating-point operations. This does not include the generation of the powers of the complex nth root of unity  $\omega$ . To compute a million-point DFT, a computer capable of doing one multiplication and addition every microsecond requires a million seconds, or about 11.5 days.

Fast Fourier Transform (FFT) algorithms have computational complexity  $O(n \log n)$  instead of  $O(n^2)$ . If *n* is a power of 2, a one-dimensional FFT of length *n* requires less than  $3n \log_2 n$  floating-point operations (times a proportionality constant). For n = 220, that is a factor of almost 35,000 faster than  $2n^2$ .

The MATLAB functions fft, fft2, and fftn (and their inverses ifft, ifft2, and ifftn, respectively) all use fast Fourier transform algorithms to compute the DFT.

When using FFT algorithms, a distinction is made between the *window length* and the *transform length*. The window length is the length of the input data vector. It is determined by, for example, the size of an external buffer. The transform length is the length of the output, the computed DFT. An FFT algorithm pads or chops the input to achieve the desired transform length. The following figure illustrates the two lengths.



The execution time of an FFT algorithm depends on the transform length. It is fastest when the transform length is a power of two, and almost as fast when the transform length has only small prime factors. It is typically slower for transform lengths that are prime or have large prime factors. Time differences, however, are reduced to insignificance by modern FFT algorithms such as those used in MATLAB. Adjusting the transform length for efficiency is usually unnecessary in practice.

### The FFT in One Dimension

- "Introduction" on page 11-9
- "Basic Spectral Analysis" on page 11-10
- "Spectral Analysis of a Whale Call" on page 11-15
- "Data Interpolation Using FFT" on page 11-19

#### Introduction

The MATLAB fft function returns the DFT y of an input vector x using a fast Fourier transform algorithm:

y = fft(x);

In this call to fft, the window length m = length(x) and the transform length n = length(y) are the same.

The transform length is specified by an optional second argument:

y = fft(x,n);

In this call to fft, the transform length is n. If the length of x is less than n, x is padded with trailing zeros to increase its length to n before computing the DFT. If the length of x is greater than n, only the first n elements of x are used to compute the transform.

#### **Basic Spectral Analysis**

The FFT allows you to efficiently estimate component frequencies in data from a discrete set of values sampled at a fixed rate. Relevant quantities in a spectral analysis are listed in the following table. For space-based data, replace references to time with references to space.

Quantity	Description
х	Sampled data
<pre>m = length(x)</pre>	Window length (number of samples)
fs	Samples/unit time
dt = 1/fs	Time increment per sample
t = (0:m-1)/fs	Time range for data
y = fft(x,n)	Discrete Fourier transform (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

Consider the following data x with two component frequencies of differing amplitude and phase buried in noise.

```
fs = 100; % Sample frequency (Hz)
t = 0:1/fs:10-1/fs; % 10 sec sample
x = (1.3)*sin(2*pi*15*t) ... % 15 Hz component
+ (1.7)*sin(2*pi*40*(t-2)) ... % 40 Hz component
+ 2.5*gallery('normaldata',size(t),4); % Gaussian noise;
```

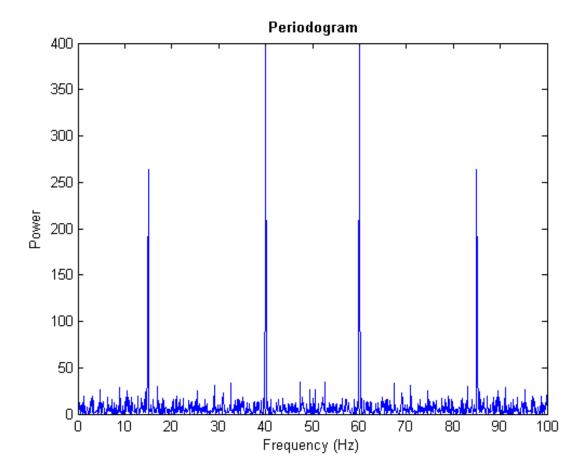
Use fft to compute the DFT y and its power.

```
m = length(x); % Window length
n = pow2(nextpow2(m)); % Transform length
y = fft(x,n); % DFT
f = (0:n-1)*(fs/n); % Frequency range
power = y.*conj(y)/n; % Power of the DFT
```

nextpow2 finds the exponent of the next power of two greater than or equal to the window length (ceil(log2(m))) and pow2 computes the power. Using a power of two for the transform length optimizes the FFT algorithm, though in practice there is usually little difference in execution time from using n = m.

To visualize the DFT, plots of abs(y), abs(y).<sup>2</sup>, and log(abs(y)) are all common. A plot of power versus frequency is called a *periodogram*.

```
plot(f,power)
xlabel('Frequency (Hz)')
ylabel('Power')
title('{\bf Periodogram}')
```



The first half of the frequency range (from 0 to the Nyquist frequency fs/2) is sufficient to identify the component frequencies in the data, since the second half is just a reflection of the first half.

In many applications it is traditional to center the periodogram at 0. The fftshift function rearranges the output from fft with a circular shift to produce a 0-centered periodogram.

y0 = fftshift(y);	% Rearrange y values
f0 = (-n/2:n/2-1)*(fs/n);	% O-centered frequency range

```
power0 = y0.*conj(y0)/n; % 0-centered power
plot(f0,power0)
xlabel('Frequency (Hz)')
ylabel('Power')
title('{\bf 0-Centered Periodogram}')
```

400 350 300 250 Power 200 150 100 50 0 ₩ -50 -30 -20 -10 10 20 30 50 Π 40 -40 Frequency (Hz)

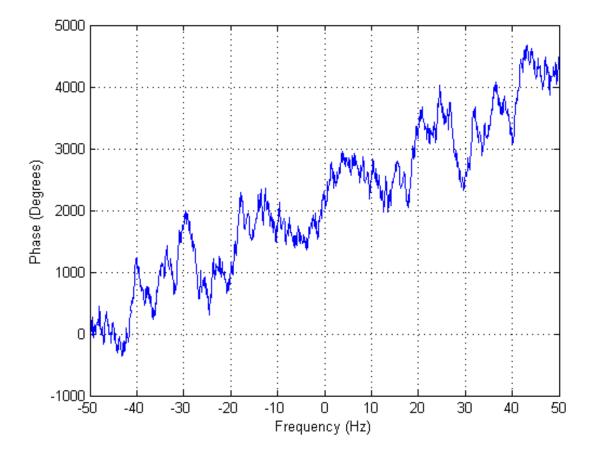
0-Centered Periodogram

The rearrangement makes use of the periodicity in the definition of the DFT.

Use the MATLAB  $\ensuremath{\mathsf{angle}}$  and  $\ensuremath{\mathsf{unwrap}}$  functions to create a phase plot of the DFT.

```
phase = unwrap(angle(y0));
```

```
plot(f0,phase*180/pi)
xlabel('Frequency (Hz)')
ylabel('Phase (Degrees)')
grid on
```



Component frequencies are mostly hidden by the randomness in phase at adjacent values. The upward trend in the plot is due to the unwrap function, which in this case adds  $2\pi$  to the phase more often than it subtracts it.

#### Spectral Analysis of a Whale Call

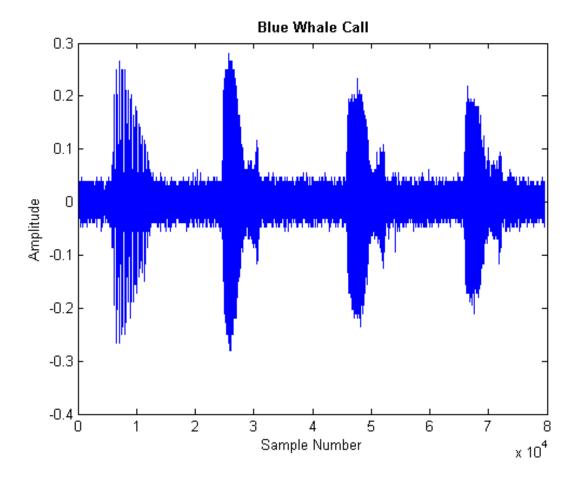
This example shows how to perform spectral analysis of audio data.

The documentation example 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. The following reads and plots the data.

```
whaleFile = fullfile(matlabroot, 'examples', 'matlab', 'bluewhale.au');
[x,fs] = audioread(whaleFile);
```

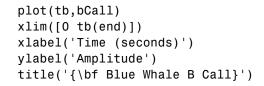
```
plot(x)
xlabel('Sample Number')
ylabel('Amplitude')
title('{\bf Blue Whale Call}')
```

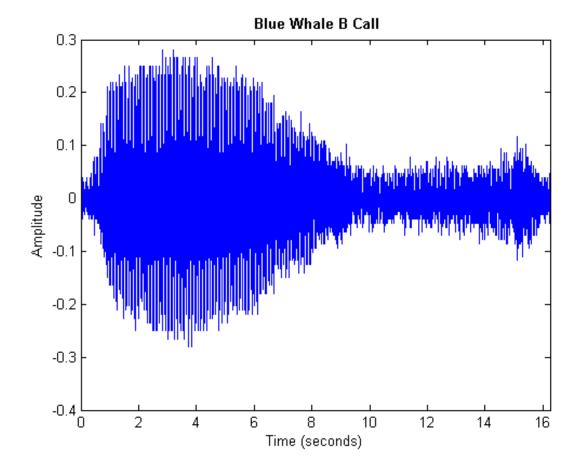


An A "trill" is followed by a series of B "moans." You can use sound(x,fs) to play the data.

The B call is simpler and easier to analyze. Use the previous plot to determine approximate indices for the beginning and end of the first B call. Correct the time base for the factor of 10 speed-up in the data.

bCall = x(2.45e4:3.10e4); tb = 10\*(0:1/fs:(length(bCall)-1)/fs); % Time base





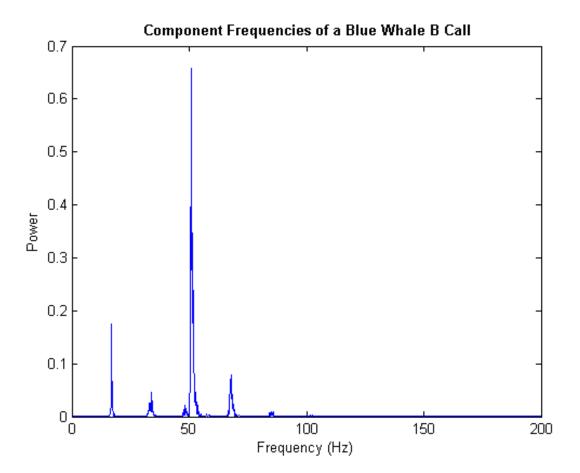
Use fft to compute the DFT of the signal. Correct the frequency range for the factor of 10 speed-up in the data.

<pre>m = length(bCall);</pre>	% Window length
<pre>n = pow2(nextpow2(m));</pre>	% Transform length

```
y = fft(bCall,n); % DFT of signal
f = (0:n-1)*(fs/n)/10; % Frequency range
p = y.*conj(y)/n; % Power of the DFT
```

Plot the first half of the periodogram, up to the Nyquist frequency.

```
plot(f(1:floor(n/2)),p(1:floor(n/2)))
xlabel('Frequency (Hz)')
ylabel('Power')
set(gca,'XTick',[0 50 100 150 200]);
title('{\bf Component Frequencies of a Blue Whale B Call}')
```



The B call is composed of a fundamental frequency around 17 Hz and a sequence of harmonics, with the second harmonic emphasized.

#### **Data Interpolation Using FFT**

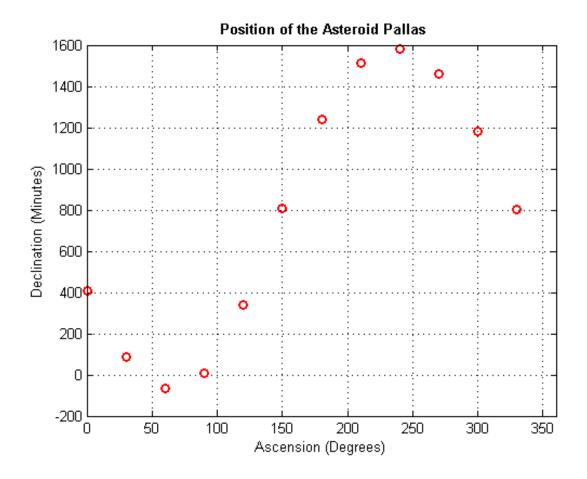
This example shows how to use FFT in a context other than spectral analysis—estimating coefficients of a trigonometric polynomial that interpolates a set of regularly-spaced data. This approach to data interpolation is described in [1].

Several people discovered fast DFT algorithms independently, and many people have contributed to their development. A 1965 paper by John Tukey and John Cooley [2] is generally credited as the starting point for modern usage of the FFT. However, a paper by Gauss published posthumously in 1866 [3] (and dated to 1805) contains indisputable use of the splitting technique that forms the basis of modern FFT algorithms.

Gauss was interested in the problem of computing accurate asteroid orbits from observations of their positions. His paper contains 12 data points on the position of the asteroid Pallas, through which he wished to interpolate a trigonometric polynomial with 12 coefficients. Instead of solving the resulting 12-by-12 system of linear equations by hand, Gauss looked for a shortcut. He discovered how to separate the equations into three subproblems that were much easier to solve, and then how to recombine the solutions to obtain the desired result. The solution is equivalent to estimating the DFT of the data with an FFT algorithm.

Here is the data that appears in Gauss' paper.

```
asc = 0:30:330;
dec = [408 89 -66 10 338 807 1238 1511 1583 1462 1183 804];
plot(asc,dec,'ro','Linewidth',2)
xlim([0 360])
xlabel('Ascension (Degrees)')
ylabel('Declination (Minutes)')
title('{\bf Position of the Asteroid Pallas}')
grid on
```



Gauss wished to interpolate a trigonometric polynomial of the form

$$y = a_0 + a_1 \cos(2\pi(x/360)) + b_1 \sin(2\pi(x/360))$$
  

$$a_2 \cos(2\pi(2x/360)) + b_2 \sin(2\pi(2x/360))$$
  

$$\dots$$
  

$$a_5 \cos(2\pi(5x/360)) + b_5 \sin(2\pi(5x/360))$$
  

$$a_6 \cos(2\pi(6x/360))$$

Use fft to perform an equivalent of Gauss' calculation.

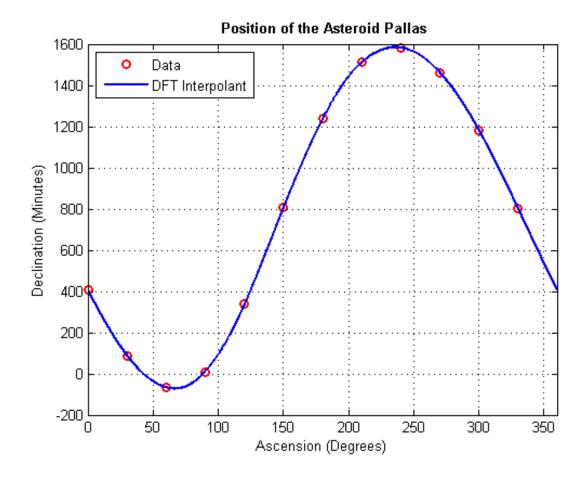
d = fft(dec); m = length(dec); M = floor((m+1)/2); a0 = d(1)/m; an = 2\*real(d(2:M))/m; a6 = d(M+1)/m; bn = -2\*imag(d(2:M))/m;

Plot the interpolant with the data.

```
hold on
```

```
x = 0:0.01:360;
n = 1:length(an);
y = a0 + an*cos(2*pi*n'*x/360) ...
+ bn*sin(2*pi*n'*x/360) ...
+ a6*cos(2*pi*6*x/360);
```

```
plot(x,y,'Linewidth',2)
legend('Data','DFT Interpolant','Location','NW')
```



#### **References.**

[1] Briggs, W. and V.E. Henson. *The DFT: An Owner's Manual for the Discrete Fourier Transform*. Philadelphia: SIAM, 1995.

[2] Cooley, J.W. and J.W. Tukey. "An Algorithm for the Machine Calculation of Complex Fourier Series." *Mathematics of Computation*. Vol. 19. 1965, pp. 297–301.

[3] Gauss, C. F. "Theoria interpolationis methodo nova tractata." *Carl Friedrich Gauss Werke*. Band 3. Göttingen: Königlichen Gesellschaft der Wissenschaften, 1866.

[4] 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.

[5] Goldstine, H. H. A History of Numerical Analysis from the 16th through the 19th Century. Berlin: Springer-Verlag, 1977.

#### The FFT in Multiple Dimensions

- "Introduction" on page 11-23
- "Diffraction Patterns" on page 11-24

#### Introduction

This section discusses generalizations of the DFT in one dimension (see "Discrete Fourier Transform (DFT)" on page 11-2).

In two dimensions, the DFT of an *m*-by-*n* array *X* is another *m*-by-*n* array *Y*:

$$Y_{p+1,q+1} = \sum_{j=0}^{m-1} \sum_{k=0}^{n-1} \omega_m^{jp} \omega_n^{kq} X_{j+1,k+1}$$

where  $\omega_m$  and  $\omega_n$  are complex roots of unity:

$$\omega_m = e^{-2\pi i/m}$$
$$\omega_n = e^{-2\pi i/n}$$

This notation uses *i* for the imaginary unit, *p* and *j* for indices that run from 0 to m-1, and *q* and *k* for indices that run from 0 to n-1. The indices p+1 and j+1 run from 1 to *m* and the indices q+1 and k+1 run from 1 to *n*, corresponding to ranges associated with MATLAB arrays.

The MATLAB function fft2 computes two-dimensional DFTs using a fast Fourier transform algorithm. Y = fft2(X) is equivalent to Y = fft(fft(X).').', that is, to computing the one-dimensional DFT of each column X followed by the one-dimensional DFT of each row of the result. The inverse transform of the two-dimensional DFT is computed by ifft2.

The MATLAB function fftn generalizes fft2 to N-dimensional arrays. Y = fftn(X) is equivalent to:

```
Y = X;
for p = 1:length(size(X))
      Y = fft(Y,[],p);
end
```

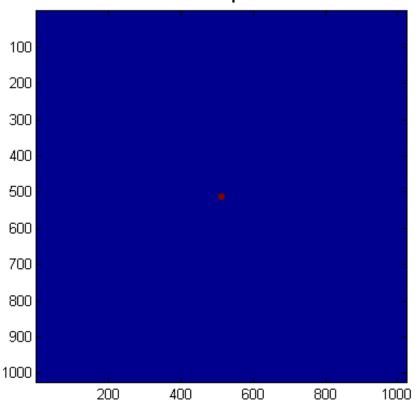
That is, to computing in place the one-dimensional DFT along each dimension of X. The inverse transform of the *N*-dimensional DFT is computed by ifftn.

#### **Diffraction Patterns**

The theory of optics predicts that the diffraction pattern produced by a plane wave incident on an optical mask with a small aperture is described, at a distance, by the Fourier transform of the mask. See, for example, [1].

Create a logical array describing an optical mask  $\boldsymbol{M}$  with a circular aperture  $\boldsymbol{A}$  of radius  $\boldsymbol{R}.$ 

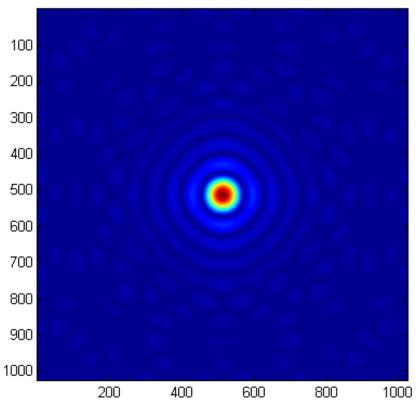
```
n = 2^10;
M = zeros(n);
I = 1:n;
x = I-n/2;
y = n/2-I;
[X,Y] = meshgrid(x,y);
R = 10;
A = (X.^2 + Y.^2 <= R^2);
M(A) = 1;
imagesc(M)
axis image
title('{\bf Circular Aperture}')
```



**Circular Aperture** 

Use fft2 to compute the two-dimensional DFT of the mask and fftshift to rearrange the output so that the zero-frequency component is at the center.

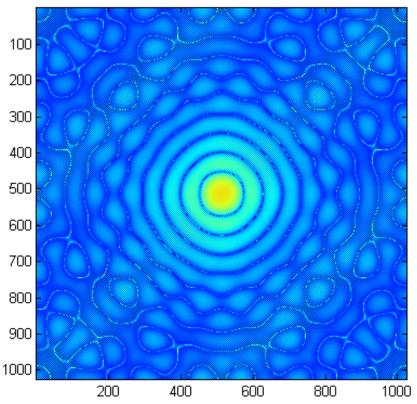
```
D1 = fft2(M);
D2 = fftshift(D1);
imagesc(abs(D2))
axis image
title('{\bf Diffraction Pattern}')
```



**Diffraction Pattern** 

The logarithm helps to bring out details of the DFT in regions where the amplitude is small.

```
D3 = log2(D2);
imagesc(abs(D3))
axis image
title('{\bf Enhanced Diffraction Pattern}')
```



**Enhanced Diffraction Pattern** 

Very small amplitudes are affected by numerical round-off. The lack of radial symmetry is an artifact of the rectangular arrangement of data.

#### **Reference.**

[1] Fowles, G. R. Introduction to Modern Optics. New York: Dover, 1989.

See Also fft | fft2 | fftn | ifft2 | ifftn | nextpow2 | pow2 | fftshift | angle | unwrap

Concepts

• "Discrete Fourier Transform (DFT)" on page 11-2

## **Function Summary**

Function	Description
fft	One-dimensional fast Fourier transform
ifft	One-dimensional inverse fast Fourier transform
fft2	Two-dimensional fast Fourier transform
ifft2	Two-dimensional inverse fast Fourier transform
fftn	N-dimensional fast Fourier transform
ifftn	N-dimensional inverse fast Fourier transform
fftshift	Rearrange DFT data to center zero-frequency component
fftw	Interface to FFTW run-time algorithm
abs	Amplitude of the DFT
angle	Phase of the DFT
unwrap	Correct phase angles with jumps greater than or equal to pi
nextpow2	Next power of two greater than or equal to a given length
pow2	Compute powers of two

MATLAB functions related to Fourier transforms include:

The MATLAB software also includes demos that use these functions in combination for Fourier analysis:

- FFT for Spectral Analysis Reviews basic spectral analysis with the FFT
- Using FFT in MATLAB Example of time series analysis with the FFT that looks for periodicity in historical data on sunspot activity