Introduction to Scientific Computing

Statements

```
foo = x^2 + \sin(5*y) / \exp(67*z);
```

The semicolon at the end is optional.

Built-in MATLAB functions

```
sin(x), cos(x), exp(x), log(x), atan(x), cosh(x), sinh(x), mean(x), median(x), etc.
```

Array

```
x = [1,3,9,11,-10.2]; foo = x(3); % extracts third element in the array x(2) = 27; % reassign element in the array x = 1:15 % creates an array with the number 1 through 15 x = 4:2:28; % creates an array starting at 4 and going up by 2 until it gets to 28 x = -1.3:0.1:1.3; %creates an array starting at -1.3 and going up by 0.1 until it gets to 1.3 x = 1:2:6; % x = [1,3,5] x = [1:2:6]; % x = [1,3,5]
```

Operations on arrays

```
x = 0:0.1:10;

y = \exp(5*x).*\sin(x); % evaluate an expression on every element in the array x producing a new a plot(x,y);

x = [1,2,3,4,5];

y = [7,8,9,10,11];

z = x + y; % element-wise addition adds corresponding elements

z = x.*y; % element-wise multiplication

z = x./y; % element-wise division
```

Overflow

```
X = uint8(78); Y = uint8(190);
Z = X + Y;
% overflow - value will be clipped to 255
```

Scientific notation

Note that numbers in scientific notation have the following components

- · A sign positive or negative
- A mantissa(尾数) ex. 2.13
- An exponent ex. 17
 e.g. +2.13e17

Arrays and numerical types

When an array variable is created all of the numeric values in that array share the same numeric type. For example we can talk about an array of uint16 s or an array of doubles.

```
x = single(0:0.1:100); make an array of single precision (单精度) numbers
```

A few useful MATLAB commands

whos

Lists all of the variables currently in your workspace and shows you their types

clear

Clears all of the variables in your workspace – you can also use this to clear specific variables

clc

Just clears the command window - has no effect on the workspace

Function

```
function f = fact(n)
    f = prod(1:n);
end

function [output1,output2,output3] = myFunction(input1,input2,input3)
```

Naming a Function

Must start with a letter from the alphabet

Special Functions

```
function out1 = testFunction(in1)
% A test function
% this would report, in the help function, all of functionality of the function
% in1 = function input (units: not specified)
% out2 = function output (units : not specified)
(in the command window)
```

Search paths

The working folder at startup can be changed using the userpath function

```
userpath('C:\ATRI')
```

- Paths can also be "permanently" added to the search path using the addpath() function
- Paths can be removed using the rmpath() function

Commenting

- Highlight a selection or place your cursor on a line and press "ctrl+r" to comment a section or line of code, respectively
- "ctrl+t" uncomments the code

Anonymous Function

```
function_name = @ (arguments) expression

FtoC = @ (F) 5*(F-32)./9

% examples
FA = @ (x) exp(x^2)/sqrt(x^2+5)
FA(2)
FA = @ (x) exp(x.^2)./sqrt(x.^2+5)
FA([1 0.5 2])
```

Function Handles

```
f = @sin;
m = fminbnd(f,0,2*pi)

q = integral(@cubicPoly,0,1);
```

Vectors(Arrays)

```
% Linspace and logspace
x = linspace(1,5,5)
x = logspace(1,5,5)
x = [5, 9, 4, 1, 7, 3, 4, 8]
% Accessing vector elements
y = x(1)
y = x(1:3)
y = x(end)
y = x(end-2)
y = x([1,3,6]) \% y = [5,4,3]
% The indices start at 1, not 0.
% Overwriting
x(end) = 1;
%Add ending indices
x(end+1) = 8
x(end+1:end+2) = [6,9]
%Removing elements
x(1) = []; % Remove the first element
x(end-3,end) = [];
```

Iteration

```
for jj = 1:20
    disp(jj)
end

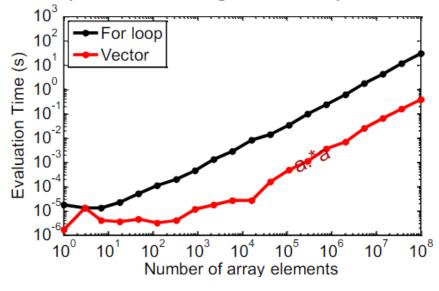
a = 1;
while a < 10
    a = a + 1;
end

% Iterate through the array
x = [1,2,3]
for element = x
    disp(element);
end</pre>
```

Array Operation vs Iteration

Array operations increase computation speed

Time to Compute a*a using a for Loop vs. Vectorization



The if statement

```
a = 1;
b = 2;
if a == 1;
    disp('a is equal to 1! Yeah');
end

elseif a == 1 && b == 2;
    disp('...')
end
```

Logical Operators

Logical Operator(Scalars)	Logical Operator(Vectors)	Function Call
&&	&	and(a,b)
	I	or(a,b)
~	~	not(a)
none	none	xor(a,b)
Attention: ~= in matlab equals to != in other languages		

Logical Vectors

```
a = [1 6 5] < 2
% a = [1,0,0]

x = [5 9 2 4 3];
v = logical([1 0 1 0 1]);
xp = x(v);
% xp = [5,2,3]</pre>
```

Creating matrices

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

A = ones(2,5);
A = zeros(2,3);
A = eye(3); % Create a identity matrix

A = \begin{bmatrix} 1 & 2 & 3;4 & 5 & 6 \end{bmatrix};
B = A' % Rows become columns and columns become rows.

% Expressions used to initialize arrays can include algebraic operati
a = \begin{bmatrix} 0 & 13*2 \end{bmatrix};
b = \begin{bmatrix} a(2) & 13 & a \end{bmatrix};
A = \begin{bmatrix} 1 & 5 & 9;2 & 4 & 8;3 & 6 & 7 \end{bmatrix};
c = A[3,1]; % c == 3
c = A[4]; % Matrix indices may also be accessed using a single subscr
```

Subarrays

```
% Vectors
va =[1:5]
va(:) % all elements
va(m:n) % elements m through n

% Matrix
A = [1 2 3; 4 5 6; 7 8 9];
A(:,n) % all elements in column n
A(n,:) % all elements in row n
A(:,m:n) % elements in columns m through n
A(m:n,:) % elements in rows m through n
A(m:n,p:q)

b = [1 2 3 4; 5 6 7 8; 9 10 11 12];
b(2:2:end,2:end); % [6 7 8]
```

Manipulating Matrices

Built-in function	description	
length(v)	returns length of largest array dimension	
size(A)	returns[m,n] where m and n are the size of A	
numel(A)	returns the total number of elements in the array	
reshape(A,m,n)	rearrange A to have m rows and n colomns	
diag(v)	creates square matrix with elements on the diagonal	
diag(A)	creates vector from the diagonal elements	

Resizing a Matrix

```
A(:,2) = []; % deleting rows or columns from an array A = [B \ C; \ D \ E;] % Arrays can be concatenated to form larger arrays.
```

Strings

- An array of characters typed between single quotes ('),e.g. 'Hello World'
- char built-in function My_string = char('string 1','string 2','string 3')
- Work with strings lower; isspace; isletter

Matrix Addition and Subtraction

- 1. Scalars may be added to any array, and the scalar value is added to all elements of the array
- 2. Arrays may be added and subtracted so long as they have the same dimensions

Element-by-Element Operations

- Addition(+) and subtraction (-)
- Multiplication (.*) and division (./)
- Exponentiation (.^)
- Functions applied over arrays (\sin , \log ,...)

• evaluating a function e.g. $y = x^2 - 4x$

Matrix Multiplication

- a*B Matrices may be multiplied by a scalar: Element-by-Element Multiplication
- A.*B Element-by-Element Multiplication
- A*B Matrix multiplication
- cross(X,Y) Cross product, special operation on two vectors.

Matrix division

Inverse of a matrix

- inv function or raise to -1 power
- · matrix must be square and invertible

Left Division

Solve AX = B where X and B are column vectors.

$$X = A^{-1}B$$

 $X=A \setminus B$

Right Division

Solve XC = D where X and D are column vectors.

$$X = DC^{-1}$$

X=D/C

Rotating and flipping arrays

- rot90 :Rotate counterclockwise by 90 degrees
- fliplr or flipdim(A,1): Reverse the matrix by treating a row as a whole.
- flipud or flipdim(A,2): Reverse the matrix by treating a column as a whole.

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix} \left\{ \begin{array}{c} \underbrace{\begin{array}{c} rot90(A) \\ 2 & 5 \\ 1 & 4 \end{array}} \right]$$

$$\underbrace{\begin{array}{c} fliplr(A) \ orflipdim(A,1) \\ 6 & 5 & 4 \end{array}} \right] \left\{ \begin{array}{c} 3 & 2 & 1 \\ 6 & 5 & 4 \end{array} \right]$$

$$\underbrace{\begin{array}{c} flipud(A) \ orflipdim(A,2) \\ \hline \end{array}} \left[\begin{array}{c} 4 & 5 & 6 \\ 1 & 2 & 3 \end{array} \right]$$

Actually, we use flip instead of flipdim now. And the grammer is absolutely the same. The second parameter of flip (or flipdim) is the dimension that is manipulated. It can be set to 3 or more when the dimension of array is above 2.

Built-in Matrices

- zeros(n) returns an n-by-n matrix with all the elements equal to zero
- ones(n) returns an n-by-n matrix with all the elements equal to one
- magic(n) returns an n-by-n matrix constructed from the integers 1 through n*n with equal row and column sums. The order n must be a scalar greater than or equal to 3 in order to create a valid magic square.
- eye(n) return an n-by-n identity matrix

Sparse arrays

Sparse matrices are defined by a list of elements containing non-zero elements while all other elements are assumed to be zero

```
% conventional way to create a matrix
A = zeros(1000,2000);
A(3,4) = 15;
A(100,1500) = 5;
A(1000,2000) = 9;

% create using a sparse matrix
A = sparse([3,100,1000],...
    [4,1500,2000],...
    [15,5,9],1000,2000);
```

%The original (full) matrix A could also be converted to a sparse matrix via the following A = sparse(A);

Matrix type	Memory(MB)	Time to compute A^2 (ms)
Full	15.2	4
Sparse	0.015	0.04

Summing array elements

Consider the following 3D array

$$A = egin{bmatrix} 1 & 1 & 1 \ 1 & 1 & 1 \end{bmatrix} egin{bmatrix} 2 & 2 & 2 \ 2 & 2 & 2 \end{bmatrix} egin{bmatrix} 3 & 3 & 3 \ 3 & 3 & 3 \end{bmatrix}$$

$$sum(A) = egin{bmatrix} 2 & 2 & 2 \end{bmatrix} egin{bmatrix} 4 & 4 & 4 \end{bmatrix} egin{bmatrix} 6 & 6 & 6 \end{bmatrix}$$

$$sum(sum(A))=[6][12][18]$$

$$sum(sum(sum(A))) = [36]$$

$$sum(A,3) = egin{bmatrix} 6 & 6 & 6 \ 6 & 6 & 6 \end{bmatrix}$$

manipulate the matrix in the same way:

- 1. treat a row as a whole
- 2. treat a column as a whole
- 3. treat the 3rd dimension a whole

Cumulative sums

- cumsum() sums cumulatively along a vector or some dimension of an array
- unless a dimension is specified, it works on the first non-singleton dimension

```
cumsum([1 2 3 4 5]);
% [1 3 6 10 15]

cumsum([1 2 3; 4 5 6]);
% ([1 2 3; 5 7 9])
```

Product

```
x(:,:,1) = [1 2 3; 4 5 6];
x(:,:,2) = [6 5 4; 3 2 1];
y = prod(x)

% y(:,:,1) == [4 10 18] and
% y(:,:,2) == [18 10 4]
```

Cumulative product

cumprod() calculates the cumulative product of array elements along the first non-singleton dimension

```
x(:,:,1) = [1; 2; 3];
x(:,:,2) = [2; 2; 2];
y = cumprod(x)

% y(:,:,1) = [1; 2; 6] and
% y(:,:,2) = [2; 4; 8]
```

Input Commands

input command

```
in1 = input('Enter data:');
% Stores input value as a numerical value or array of values of type double
in2 = input('Enter data:','s');
% Stores input value as a string (an array of characters)
```

Output Commands

disp command

```
disp(variable);
disp('text to print')
```

fprintf command

```
fprintf(format,data);
```

Formatted output placed on screen or saved to a file

Manipulate the files

save

% Save all variables in the workspace to a file

```
save('file_name');
save file_name;
% Writes file_name.mat file in binary format
% Save a few variables
save file_name var1 var2;
% Save in readable format
save -ascii file_name;
% Easy way to transfer data
```

load

```
% Load the variables in a file
load('file_name');
load file_name;
% Reads file_name.mat in binary format and restores variables
load file_name var1 var2;
% Load a few variables
load file_name var1 var2;
% Load from a text(.txt) file
load file_name.txt;
var = load('file_name.txt');
% Options
% mat, -ascii
```

Cell Arrays

```
c = {42,rand(5),'abcd'}
% c =
%     1x3 cell array
%     {[42]} {5x5 double} {['abcd']}
```

A pleasing plot

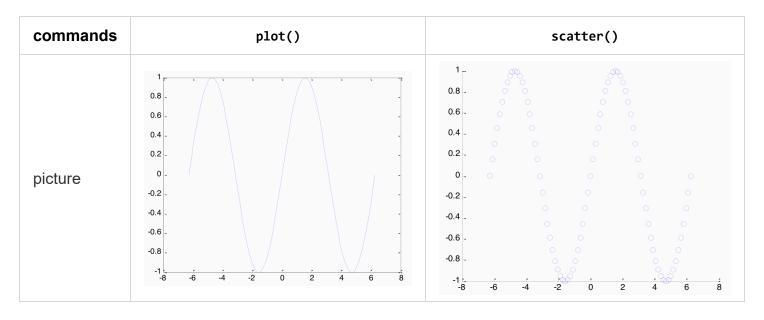
several objective measures of a good plot

- Labels with units
- Minimum amount of information to convey the objective (don't double label objects unless necessary, extraneous callouts should be avoided)
- Avoid overuse of eye candy
- Scatter plots for measured data and line plots for fits or closed form equations
- Sufficient resolution on domain to represent solution
- · Line widths, data point sizes, and text large enough to read

2D plot commands

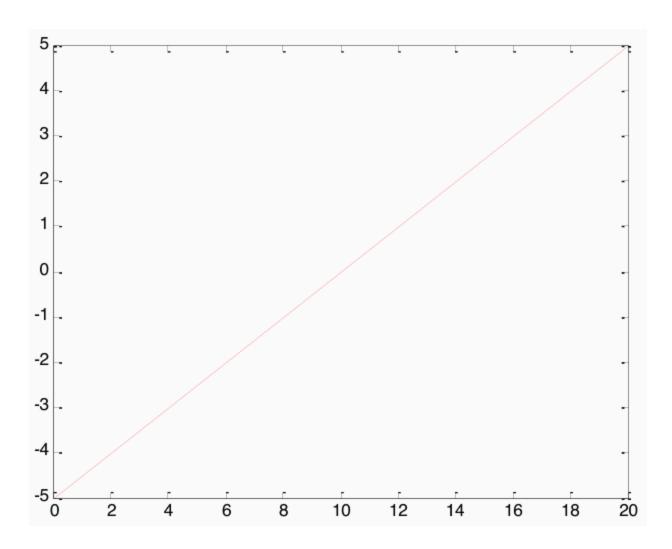
plot and scatter

```
x = -2*pi:pi/20:2*pi;
y = sin(x);
```



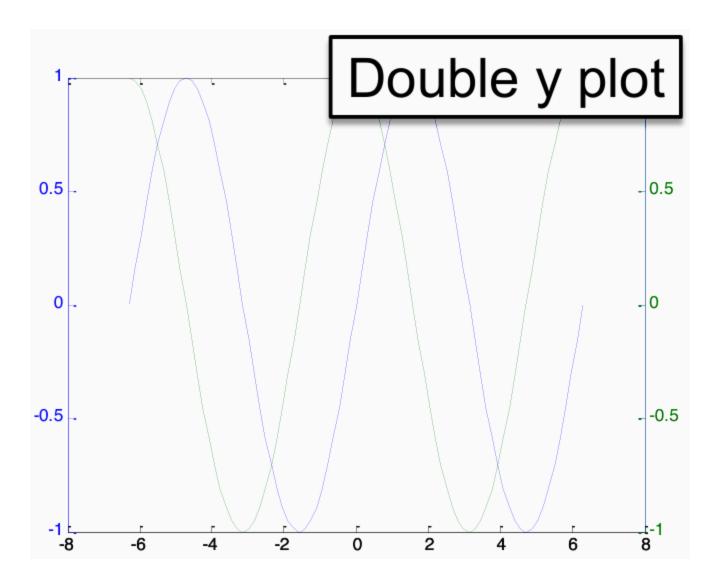
- p;ot() and scatter require vectors of equal length
- The default plot attributes are blue lines or circular blue data points, respectively
- These attributes can be modified be adjusting the line specifications of the plot linespec
- Straight lines may also be plotted by specifying the beginning and end points of the line

```
plot([0,20],[-5,5],'r-');
```



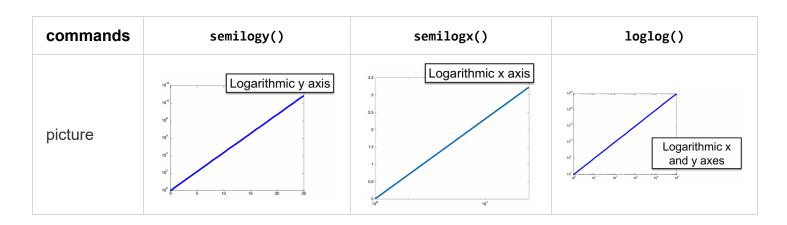
Double y plot plotyy()

```
x = -2*pi:pi/20:2*pi;
y1 = sin(x);
y2 = cos(x);
plotyy(x,y1,x,y2);
```



Logarithmic plot

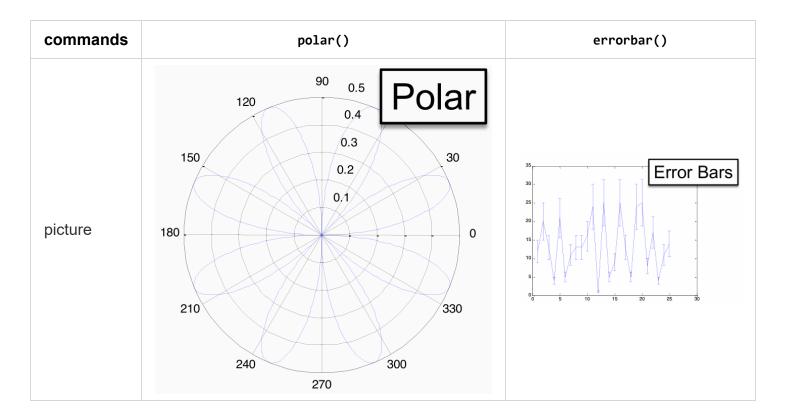
```
x = logspace(0,5,25);
y = x.^5;
loglog(x,y,'LineWidth',4)
```



polar() and Error Bars

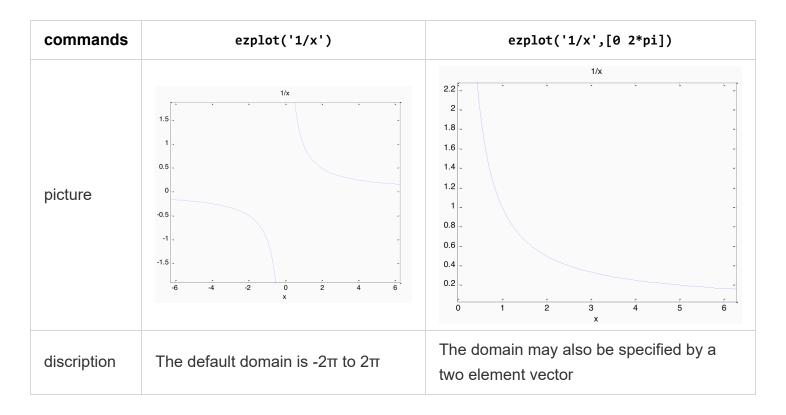
```
theta = 0:0.01:2*pi;
rho = sin(2*theta).*cos(2*theta);
polar(theta,rho)

x = 1:25;
y = randi(25,1,length(x));
y_err = 0.25*y;
errorbar(x,y,y_err)
```



ezplot

ezplot produces simple plots without the need for discrete input of x/y vectors

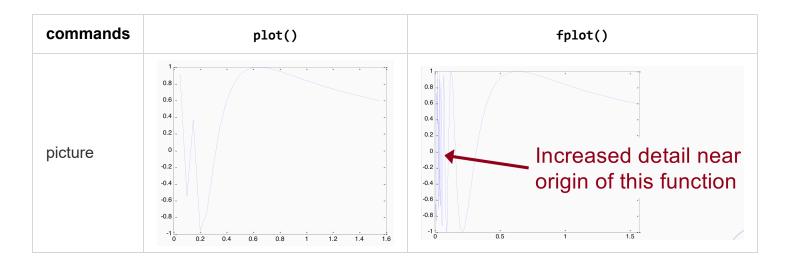


fplot

fplot intelligently selects x values based on changes to a function and may be used for rapidly changing functions

```
x = 0:.05:0.5*pi;
y = sin(1./x);
plot(x,y)

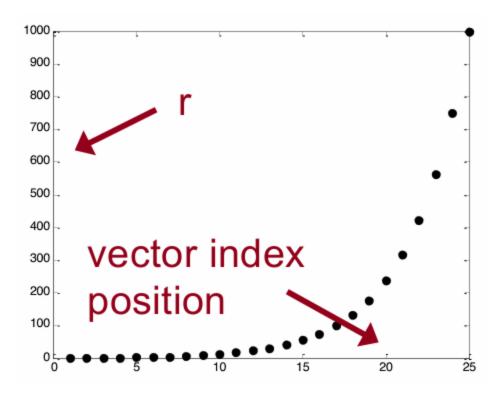
fplot('sin(1/x)',[0 0.5*pi]);
```



Plotting a vector

Most 2D plot commands can be called with a single vector, which is often useful for debugging The x values are then assigned the index location

```
r = logspace(0,3,25)
plot(r,'ko','MarkerFaceColor','k')
```



Specifying plot attributes

```
plot(x,y,'LineSpecifiers','PropertyName',PropertyValue)
```

Line specifiers include line style, line color and marker.(e.g. ro-)

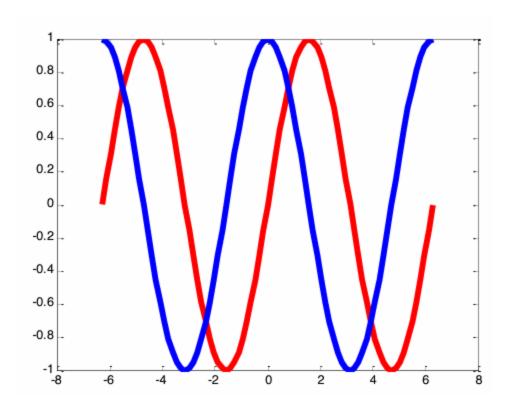
Property names include LineWidth, MarkerSize, MarkerEdgeColor, MarkerFaceColor

Overlaid plots

```
x = -2*pi:pi/20:2*pi;
y1 = sin(x);
y2 = cos(x)

% first method
plot(x,y1,'r-',x,y2,'b-','LineWidth',5)

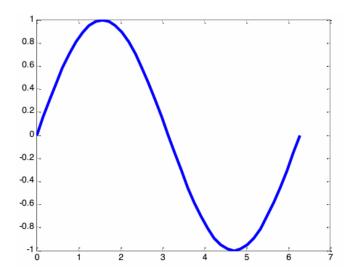
% second method
plot(x,y1,'r-','LineWidth',5)
hold on
plot(x,y2,'b-','LineWidth',5)
hold off
```

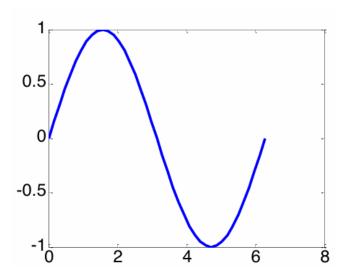


- Plot color may be specified for each vector, but line specifications such as LineWidth invoked within the plot function will be applied to all data series
- hold on is invoked after the first plot command and indicates that more data will be attributed to the existing axes;
- hold off indicates that additional plotting will overwrite the axes

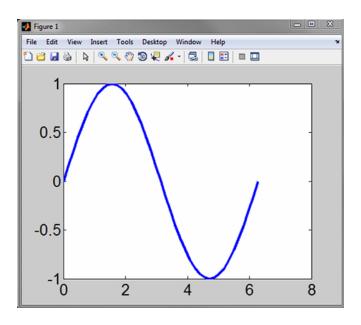
Setting axes or figure properties

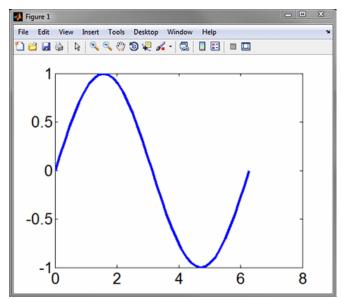
set(gca, 'Fontsize', 20)





set(gcf,'Color','w')





Plotting multiple figures

The second plot command executed (without specifying hold on) will overwrite the first plot. You need to specify a new figure establish a new parent figure window

```
x = -2*pi:pi/20:2*pi;
y1 = sin(x);
y2 = cos(x);
plot(x,y1,'k-','LineWidth',5)
figure
plot(x,y2,'k-','LineWidth',5)
```

Figures numbers may also be specified with a figure number, ex. figure(3)

Plots may then be closed using the close command

close: closes the last figure

close(n): closes figure number n

close all : closes all figures

Multiple axes on a figure

Multiple axes may be assigned to a single figure using the subplot command or by specifying the position of multiple axes

subplot(rows,columns,position)

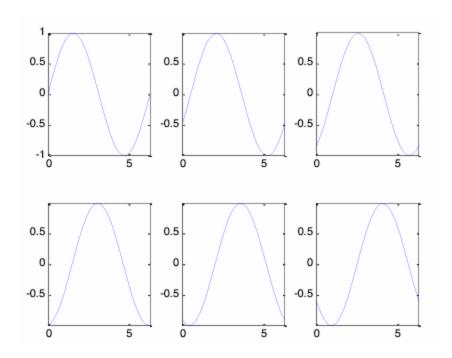
• rows: rows of axes

• columns: columns of axes

• position: position of current axes (counted along rows)

```
x = 0:pi/20:2*pi;
y1 = \sin(x-0);
y2 = \sin(x-0.5);
y3 = \sin(x-1);
y4 = sin(x-1.5);
y5 = \sin(x-2);
y6 = sin(x-2.5);
subplot(2,3,1)
plot(x,y1)
axis tight
subplot(2,3,2)
plot(x,y2)
axis tight
subplot(2,3,3)
plot(x,y3)
axis tight
subplot(2,3,4)
plot(x,y4)
axis tight
subplot(2,3,5)
plot(x,y5)
axis tight
subplot(2,3,6)
plot(x,y6)
```

axis tight

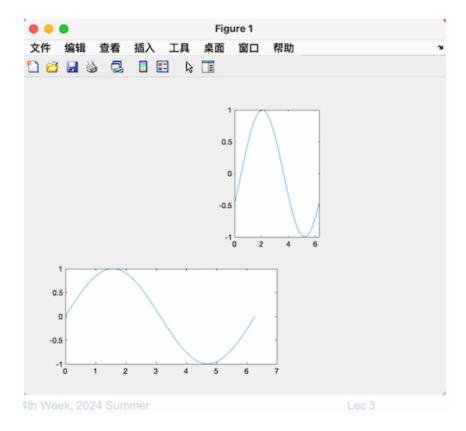


axes('Position',[x,y,w,h])

- x: lower left hand corner x coordinate
- y: lower left hand corner y coordinate
- w: width of axes
- h: height of axes

```
axes('Position',[.1 .1 .5 .3])
plot(x,y1)

axes('Position',[.5 .5 .2 .4])
plot(x,y3)
```



Specifying the domain and range

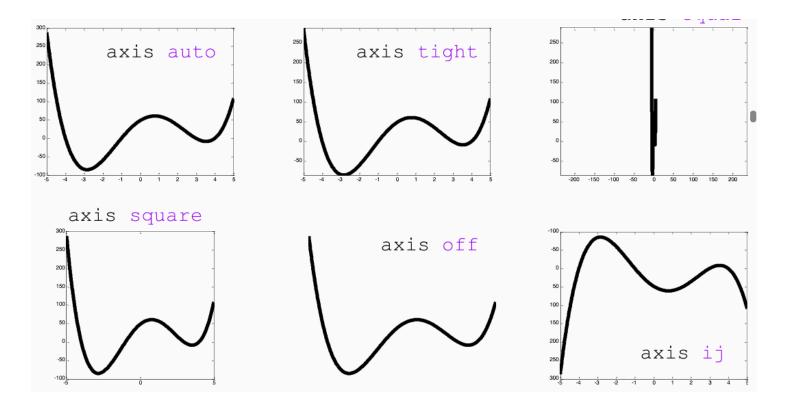
A specific domain and range may be specified using axis or xlim/ylim

```
axis([xmin xmax ymin ymax]) Or
    xlim([xmin xmax])
    ylim([ymin ymax])

e.g.

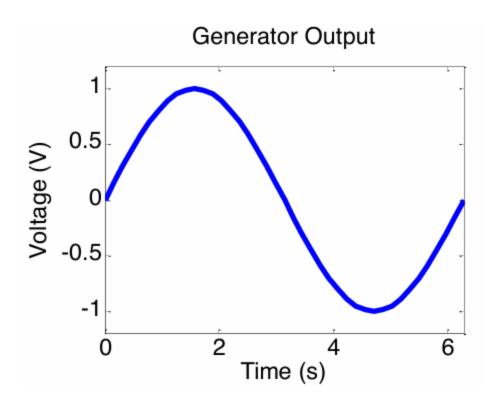
plot(x,y1,'LineWidth',5)
    axis([0 1.5*pi 0 1.5])
    set(gca,'FontSize',20)
```

The axis command offers many predefined axis scaling/sizing operations.



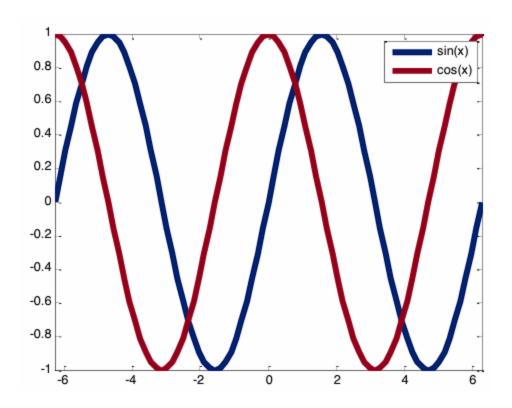
Labeling and titling axes

```
plot(x,y1,'LineWidth',5)
set(gca,'FontSize',20)
xlabel('Time (s)')
ylabel('Voltage (V)')
title('Generator Output')
axis([0 2*pi -1.2 1.2])
```



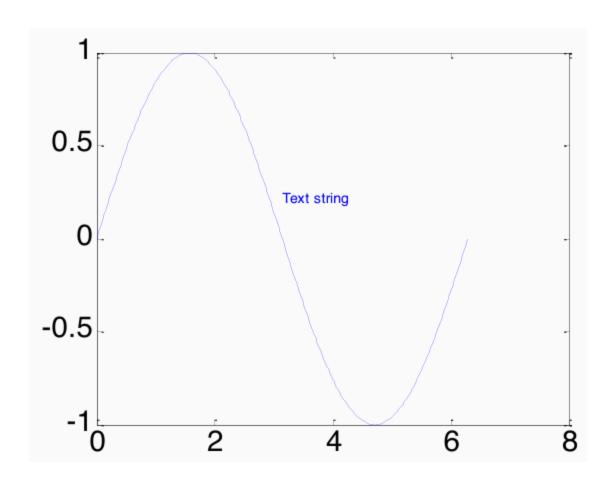
Adding a legend

legend('sin(x)','cos(x)','Location','NorthEast')



Placing text on a plot

text(pi,0.2,'Text string','Color','b')



3D plot

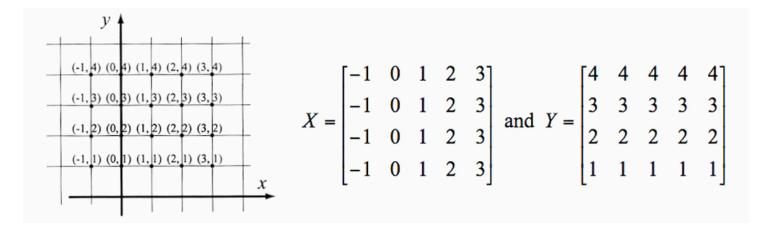
Three steps

- 1. Make a grid in the x-y plane
- 2. Find the value of z for each point of the grid
- 3. Draw the mesh or surface plot

```
plot3(x, y, z, 'line specifiers', 'PropertyName', PropertyValue)
```

meshgrid

```
[X, Y] = meshgrid(x, y)
```



- X, Y: matrices of x and y coordinates, respectively
- x, y: vectors that define the domain of the grid

Mesh and surface plots

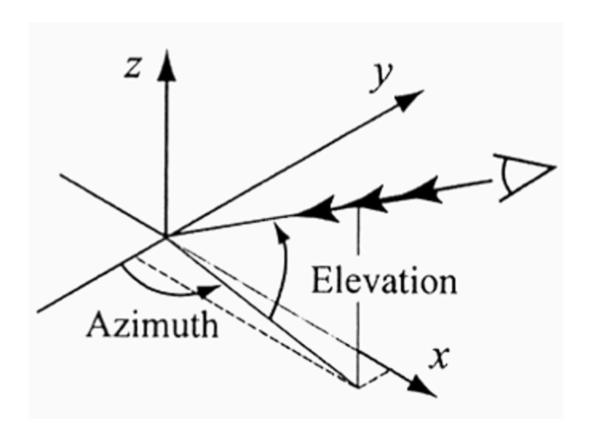
- mesh(X,Y,Z) lines connecting the points
- surf(X,Y,Z) areas colored

Other 3D Plots

- Sphere
- Cylinder
- 3D bar
- 3D stem
- 3D scatter
- 3D pie

Controlling the View in 3D

```
view(az, el) or view([az, el])
az : azimuth relative to negative y-axis (default is -37.5°)
el : elevation from x-y plane (default is 30°)
```



Graphics handles

Figures, axes, and plots can all be assigned handles

These handles look a lot like "variables" and serve as a pointer to the object

```
myHandle1 = plot(x,y);
myFig = figure;
h = axes;

set

set(<handle>,<property>,<propertyValue>)
e.g.

pl1 = plot(x,y);
set(pl1,'LineWidth',2)

get
```

get(<handle>,,,

e.g.

```
fig1 = figure
pl1 = plot(x,y);
get(fig1, 'Position')
```

ODE

say we have an equation of the form

$$\ddot{y} + p\ddot{y} + q\dot{y} + ry = 0$$

We start by assigning generalized variables (say x) to derivatives of y of increasing order as such

$$x_1=y, x_2=\dot{y}, x_3=\ddot{y}$$

Next, we rearrange the ODE to get the variable of highest order on the left side of the equation and divide out any coefficients on this variable

$$\ddot{y} = -p\ddot{y} - q\dot{y} - ry$$

Next, we rewrite the derivatives of the generalized variables with respect to each other and the ODE

$$\dot{x_1} = x_2, \dot{x_2} = x_3, \dot{x_3} = -px_3 - qx_2 - rx_1$$

```
function xout = thirdOrderODE(t,x)
% time and initial condition serve as inputs
p = 2;
q = 1.5;
r = 0.1;

dx1 = x(2);
dx2 = x(3);
dx3 = -p*x(3)-q*x(2)-r*x(1);

xout = [dx1; dx2; dx3];
% the derivatives of the generalized variables are returned as a column vector end

[t,x] = ode45(@thirdOrderODE,[0 10],[10 1 2]);
% [0 10] indicates the start and end time of the solution
% [10 1 2] indicates initial conditions. x(1) = 10, x(2) = 1, etc.
```

Polynimials

MATLAB represents polynomials as a vector

```
p = [8 5] \% 8x+5

p = [5 0 0 6 -7 0] \% 5x^5+6x^2-7x
```

Value of a polynomial

```
v = polyval(p,x)
% p is vector of coefficients
% x is the point to evaluate, it can be scalar, vector or matrix
```

Polynomial Functions

· Roots of a polynomial

```
r = roots(p)
```

Polynomial from its roots

```
p = poly(r)
```

Polynomial multiplication(convolution)

```
c = conv(a,b)
```

• Polynomial division (deconvolution)

$$[q, r] = deconv(a,b)$$

Derivatives of polynomials

Curve Fitting

The Method of Least Square

Minimize sum of squares of residuals at all data points

p = polyfit(x, y, n)

x, y: vectors of data coordinates

n :degree of polynomial

p :vector of coefficients for polynomial fit

Fitting with other than Polynomials

Fitting Methods	relationship	linear form	code
Power	$y=bx^m$	$\ln y = m \ln x + \ln b$	p=polyfit(log(x),log(y),1)
Exponential	$y=be^{mx} \ y=b10^{mx}$	$\ln y = mx + \ln b \ \log y = mx + \log b$	<pre>p=polyfit(x,log(y),1) p=polyfit(x,log10(y),1)</pre>
Logarithmic	$y = m \ln x + b$ $y = m \log x + b$		<pre>p=polyfit(log(x),y,1) p=polyfit(log10(x),y,1</pre>
Reciprocal	$rac{1}{mx+b}$	$rac{1}{y}=mx+b$	p=polyfit(x,1./y,1)

Interpolation

yi = interp1(x, y, xi, 'method')

x, y: vectors of data coordinates

xi: horizontal coordinate of interpolation point

method: method to use for interpolation

methods

nearest value of data point nearest

linear linear spline

spline cubic spline interpolation

pchip piecewise cubic Hermite interpolation

Probability and Statistics

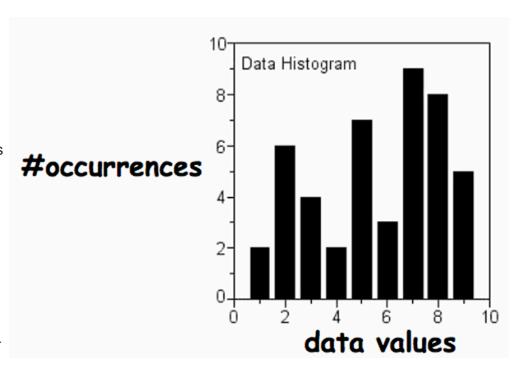
The basics

avg = mean(x)
med = median(x)

Histograms

Histograms plot the frequency of occurrence of the data values not the data themselves hist(y) Data divided into 10 bins hist(y,n) Data divided into n (scalar) bins hist(y,x) Vector x specifies bin centers

n = hist(y) Vector of number
of points in each bin



Error Function

$$erf(x)=rac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt$$

*高斯函数是正态分布的密度函数

Random Numbers

```
v=rand random value in [0,1]
rand(n) an n x n matrix with random values
rand(r,c) an r x c matrix with random values
X = rand(s,___) s: randstreams
```

Root Finding

```
x = fzero(fun,x_0)
fun: function to be solved
x0: initial guess at solution
x: solution
```

Function can be specified as

- a mathematical expression as a string with no predefined variables
- function handle
- name of an anonymous function

sort

1D

```
[y,I] = sort(x)
x = input
y = sorted array
I = permutation index
```

2D

```
y = sort(x,dim,mode)
dim: selects a dimension along which to sort
mode: 'ascend', 'descend'
```

Vocabulary

- Scalars 标量
- portions 部分
- extraneous 无关的

- eye candy 视觉上具吸引力,但没什么实质内容的东西
- resolution 分辨率
- domain 范围,领域
- consecutive 连续的
- convolution 卷积
- interpolate 插值
- combinatorial 组合的