Introduction to Scientific Computing

Function vs. Scripts,
Functions as Black Boxes,
Interacting with Functions and Scripts



Functions vs. scripts

·M-file: any set of instructions stored in a MATLAB file

Function

```
function d = myFunFunction(a,b,c)
% Takes scalar values a, b, and c,
modifies and sums the values
% Modifying the input values
var1 = 2*a;
var2 = b^2;
var3 = sqrt(c);
% Calculating the output
d = var1 + var2 + var3;
```

Script

```
% Define values of scalars a, b, and c
a = 1;
b = 2;
c = 15;

% Modifying the scalar values a, b, and c
var1 = 2*a;
var2 = b^2;
var3 = sqrt(c);

% Calculating the sum of the modified scalar
values
d = var1 + var2 + var3;
```



Commonalities between functions and scripts

- ·Both stored in M-files
- ·Both modified using the "Editor" window
- Standalone pieces of code
- ·Can be called from the command window or other functions



Why use scripts?

•What is a Matlab "script"

•MATLAB M-file where all variables, constants, etc. are called within the file

•Why develop code with a "script"

- You may want to develop multiple lines of code to solve a problem
- Consistently typing that code into the command window can become laborious / doesn't "save" your code
- You can rapidly comment out and adjust syntax to debug your code



Why use functions?

•What is a function?

- ·A MATLAB M-file that starts with function
- Generally, you need to pass information into the function and the function returns one to several results

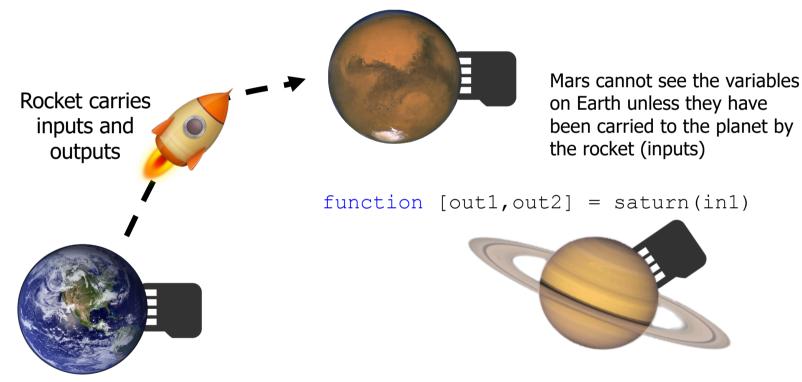
•Why use functions?

- •The function serves as a black box of code
- •Its functionality has been tested / verified and it can be called at any time without questioning the output
- ·Long, complicated computations can be broken into multiple, smaller pieces of code
- ·Enables top-down program design



Visual interpretation of scripts vs. functions

function [out1,out2,out3] = mars(in1,in2)



How to specify / use a function

·Establishing a function requires a specific syntax

•For a single output and input

```
function output = myFunc(input)
```

For multiple outputs and inputs

*Note: this would be on a single line

·Naming / saving a function

- Must start with a letter from the alphabet (a through z)
- •The name used to save the function needs to be the function name

Newton's Method

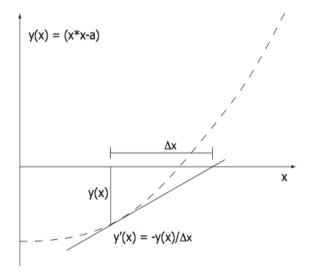
Compute the square root of a given number, a, using only +, -, *, /

Consider the function $y(x) = (x^2-a)$.

We are looking for the root of this function, that is x such that $(x^2-a)=0$

Newton's Method: At any given value of x we approximate the function by it's tangent line and compute where the line crosses the x axis. Repeat this procedure to get closer and closer to the

answer



$$y(x_i) = (x_i^2 - a); \quad y'(x_i) = 2x_i$$

$$y'(x_i) \approx \left(\frac{-y(x_i)}{\Delta x_i}\right) \Rightarrow \Delta x_i = \left(\frac{-y(x_i)}{y'(x_i)}\right)$$

$$x_{i+1} = x_i + \Delta x_i$$

$$x_{i+1} = x_i + \left(\frac{-y(x_i)}{y'(x_i)}\right) = x_i + \left(\frac{-(x_i^2 - a)}{2x_i}\right)$$
$$= (x_i + (a/x_i))/2$$

Function: my_sqrt(a)

•Initial estimate for square root: x = (a/2)

```
•Repeat as abs (x^2 - a) > 1.0e-6
```

- Computer the function value at x: $y = (x^2 - a)$

- Compute the gradient at x: gradient = 2*x

- Compute the step: step = -y/gradient

- Compute the new estimate: x = x + step

·Matlab code

my_sqrt.m



Interacting with a function

·How do I "call" a function

- •Initiate function execution from the command line make sure you include the inputs! (DEMO)
- •Functions can be called from other functions (DEMO)



Function H1 line

•The first line of a function is referred to as the "H1 line" and is searchable by MATLAB using lookfor

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

```
Command Window

>> lookfor 'a test function'

testFunction - A test function

fx

- The state of the state of
```

Function help lookup

•The first contiguous block of text is returned as the help query for the function

```
Command Window

>>> help testFunction
   A test function
   This would report, in the help function, all of the functionality of the function
   in1 = function input (units: not specified)
   out2 = function output (units: not specified)

fx >>>
```

Recursive functions

•Functions can call themselves - such functions are called "recursive" functions

```
•Ex.
function recursiveAdd(nToAdd)
% Adds a number to the input up to
% a value of 25

if nToAdd<25
    nToAdd = nToAdd+1;
    disp(nToAdd)
    recursiveAdd(nToAdd);
end</pre>
```

What happens when a function is called

- 1. Arguments are *copied* to the input parameters
- 2. Function body is run in its own private work space
- it can't see or use any variables in the calling context
- 3. When the function is done the output parameters are *copied* to the output parameters so that they are available to the calling context.

4. Paths

- Matlab finds functions by searching a set of directories specified in the path
- The current directory is included (first) in that list
- It is often convenient to store the function definitions in .m files in the current directory



Search paths

- MATLAB searches through a series of folders described as the "search path" when functions or scripts are invoked
- •These paths are folders on your computer and <u>include the current working folder</u> (the folder from which your functions/scripts are currently running) and folders included during the MATLAB installation (often toolboxes)
- •The working folder at startup can be changed using the userpath function, e.g. userpath ('C:\MyMATLABwork')
- •The order in which MATLAB searches along paths can be revealed by typing path at the command line
- •Paths can also be "permanently" added to the search path using the addpath() function
- •Paths can be removed using the rmpath() function



I called a function - where did my variables go?

- ·Unless cleared, variables will persist for "scripts", but not for functions
- ·Whatever happens in a function, stays in a function
- •For instance, a variable, myVar, could be invoked in myFunction1 and resulting in myOut, which is returned to another function, say myFunction2 this function could also use myVar without retaining "memory" of myVar as invoked in myFunction1
- DEMO retention of workspace variables for a "script" but not for a function



Cleaning up your MATLAB workspace and command line

- •Variables held in memory can be cleared using the clear command or by manually by selecting and deleting variables
- •Do NOT invoke the clear command within a "function"
- •clear can be called within a "script" or from the command line
- •The command window may be cleared using the clc command



Commenting functions / scripts

- •The general rule is at least one comment for every three lines of code
- •Proper commenting helps others understand, add to, or debug your code
- Proper commenting helps the instructors grade your assignments
- Commenting / uncommenting large swaths of code
- 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



Example 1: Monthly Loan Payment

- ·Fixed rate mortgage (抵押贷款、按揭)
- Monthly payment (output) c
- amount paid monthly ensuring that the loan is paid in full with interest at the end of its term
- •Depends on (input):
- Loan amount $P_{\mathcal{O}}$ (principal)
- Interest rate *r*
- Number of monthly payments N

$$c = \left[r + \frac{r}{(1+r)^{N} - 1}\right] P_{0} = \frac{r(1+r)^{N}}{(1+r)^{N} - 1} P_{0}$$

<u>loan.m</u>

Example 2 Evaluating an Expression

$$f(x) = \frac{x^3 \sqrt{3x+5}}{(x^2+1)^2}$$

•Write a function file to evaluate allowing for x to be a vector

Calculate

- f(x) for x = 6
- f(x) for x = 1, 3, 5, 7, 9, 11

Ex10 2.m



Example 3 Converting Temperatures

- •Write a function to convert degrees Fahrenheit (° F) to degrees Celsius (° C)

 FtoC.m
- •Use it to solve the following problem:
- The change in length of an object ΔL due to temperature change ΔT is given by where

$$\Delta L = \alpha^* L^* \Delta T$$

where α is the coefficient of thermal expansion.

– Find the change in area of a rectangular aluminum plate 4.5 m by 2.25 m with α = 23x10⁻⁶/ $^{\circ}$ C when the temperature changes from 40 $^{\circ}$ F to 92 $^{\circ}$ F

Anonymous Function

·Good for short (one-line) calculations used frequently in a longer program.

Example: converting Fahrenheit to Celsius FtoC.m

General form

```
function_name = @ (arguments) expression

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

cube = @ (x) x^3

circle = @ (x,y) 16*x^2+9*y^2
```

Examples: Anonymous Function

$$f(x) = \frac{e^{x^2}}{\sqrt{x^2 + 5}}$$

$$FA = @ (x) \exp(x^2)/\operatorname{sqrt}(x^2+5)$$

 $FA(2)$
 $FA = @ (x) \exp(x.^2)./\operatorname{sqrt}(x.^2+5)$
 $FA([1 0.5 2])$

$$f(x,y) = 2x^2 - 4xy + y^2$$

$$HA = 0 (x,y) 2*x^2-4*x*y+y^2$$

 $HA(2,3)$

Subfunctions

- ·A function file can contain more than one user-defined function
- •First function defined, the "primary," is how the function is known to the rest of the program
- •Other functions, "subfunctions," are only known inside the function file and each has its own workspace (local variables)
- •Subfunctions are used to implement "utility" calculations for primary function



Example 4 Mean and Standard Deviation

•Write a function that calculates mean (average) and standard deviation of a list of numbers. stat.m

$$\overline{x} = \frac{x_1 + x_2 + \dots + x_n}{n}$$

$$\sigma = \sqrt{\frac{\sum_{i=1}^{i=n} (x_i - \overline{x})^2}{n-1}}$$

Function Functions

- •MATLAB built-in function fzero can find the zeros (values of x where f(x) = 0) of any function f(x). How do we describe f(x) to fzero?
- •Function functions like fzero accept functions as arguments in two ways
- Function handle
- Using the name of the function in a string



Function Handles

- •A data type holding a unique value associated with any function (user-defined, built-in, anonymous)
- Obtained by

```
@function_name
@cos
@FtoC (as function file)
FtoC (as anonymous function)
```

Example: funplot - evaluates and graphs a function over a specified range returning a matrix of values at each extreme and the midpoint.

Use user-defined function

Use anonymous function

funplot.m, Fdemo.m



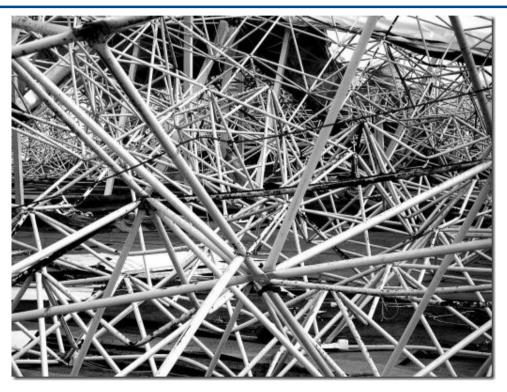
Function Names in Strings

·Older method, less efficient.

```
Pass name of function as a string
'cos'
'FtoC'

•Evaluate
var = feval('function_name', arguments)
```

Solving real problems



Start simple and build to complexity

Accessing Vector Elements, Iteration, Relational Operators



Initializing vectors in MATLAB

·You now know of several ways to input a vector into MATLAB:

Discrete method

```
x = [0.5, 1.5, 2, 3.2, 1.5, 0.4];
```

Colon operator - establishes vectors with user-defined ranges and regularly-spaced intervals

```
x = 1:1:5; or x = 1:5; x = -5:2:5;
```

• Linspace and logspace

```
x = linspace(1,5,5)

x = logspace(1,5,5)
```



Accessing vector elements

•What about accessing vector elements?

•For the following assume we have defined the following vector in memory, which we reset before each operation

$$x = [5, 9, 4, 1, 7, 3, 4, 8];$$

Access the first vector index

$$y = x(1)$$

$$\rightarrow$$
 y = 5

Access a range of vector indices

$$y = x(1:3)$$

$$\rightarrow y = [5, 9, 4]$$

$$y = x(6:8)$$

$$\rightarrow y = [3, 4, 8]$$

Access the last vector index

$$y = x (end)$$

$$\rightarrow$$
 λ = 8

Accessing vector elements

Assume x = [5, 9, 4, 1, 7, 3, 4, 8];

Access an offset vector index

$$y = x(1+4)$$

$$\rightarrow$$
 y = 7

Access the antepenultimate vector index

$$y = x (end-2)$$

$$\rightarrow$$
 y = 3

Access discrete indices

$$y = x([1 \ 3 \ 6])$$

$$\rightarrow y = [5, 4, 3]$$

Overwriting / adding to vector elements

•The existing contents of a vector may be overwritten or addended

•For the following assume we have defined the following vector in memory, which we will continuously modify

$$x = [1, 2, 3];$$

•Overwrite the first index

$$x(1) = 5$$

$$\rightarrow x = [5, 2, 3];$$

•Overwrite the last index

$$x (end) = 1$$

$$\rightarrow x = [5, 2, 1];$$

Add ending indices

$$x (end+1) = 8$$

$$\rightarrow x = [5, 2, 1, 8];$$

Overwriting / adding to vector elements

•Assume x = [5, 2, 1, 8];

Add ending indices

```
x (end+1) = [6, 9];

\rightarrow assignment error (dimensions don't match)
```

Add ending indices

```
x (end+1:end+2) = [6, 9];

\rightarrow x = [5, 2, 1, 8, 6, 9];
```

Removing vector elements

·Vector elements can be removed by specifying an empty set "[]"

·Say we establish the following vector

$$x = [8, 4, 5, 9, 3, 2, 5, 6];$$

•Removing the first element of the vector

$$x(1) = [];$$
 $\rightarrow x = [4, 5, 9, 3, 2, 5, 6];$

Removing several elements from the vector

$$x (end-3:end) = [];$$

 $\rightarrow x = [8, 4, 5, 9];$

Iteration / for loops

•Formula vectorization is preferred for speed, but sometimes iteration / loops are necessary

A basic <u>for</u> loop that displays 1 through 20, by 1, at the command window

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

 for loops are preferred over while loops (shown later) when the number of iterations are known a priori / fixed

Iteration / for loops

• for loops can take in colon operators of any viable form

```
for jj = 1:3:19
     disp(jj)
end
```

for loops can also take discrete vectors

```
for jj = [1 9 5]
     disp(jj)
end
```

Note: the for loop needs a closing "end" statement to execute properly



Iteration / for loops

for loops can be nested

```
for jj = 1:10
    for kk = 1:10
        disp([jj kk])
    end
end
```

Note: each instance of the for loop requires an "end" statement

An example of a for loop

•Section 2.7.1 shows the use of a for loop for determining the square root of a number using Newton's method. Why is a for loop necessary here?

```
% Newton's method - as shown in section 2.7.1 of Essential Matlab, ed. 5,
% evaluated using for loops

clear; clc; close all

% We want to know the square root of scalar a
a = 2;

% Initial guess
x = a/2;

% For loop to converge to a solution

for jj = 1:10
    x = (x+a/x)/2;
end

disp(['The approximate square root is ',num2str(x,10),...
    ' and the actual solution is ',num2str(sqrt(a),10)])
```

Relational operators

- •Loops can also be invoked using the while command
- however, we first need to understand relational operators since while loops depend heavily on them
- ·Relational operators compare values (or vectors, matrices) and yield a true or false result

Relational operators

Relational Operator Syntax in MATLAB

Relational Operator	Meaning	
<	Less than	
<=	Less than or equal to	
==	Equal to	
~=	Not equal	
>	Larger than	
>=	Larger than or equal to	

lteration / while loops

•The while command executes a piece of code until a desired condition is satisfied

·A simple example

```
a = 1;
while a < 10
    a = a+1;
end</pre>
```



lteration / while loops

while loops are most appropriate when the extent (number of) iterations is **unknown** a priori

(DEMO) Newton's method using a while loop to estimate the square root of a to a finite precision



Invoking a for and while loop for n iterations

- •Say you want to evaluate some expression *n* number of times and the value of the expression is <u>not</u> known a priori
- You have two options: a for loop or a while loop
- for loops have compact syntax since they don't require a counter



Invoking a for and while loop for n iterations

•Example: Newton's Method for evaluating the square root of a for loop

```
n = 100;
a = 2;
x = a/2;
for ii = 1:n
x = (x+a/x)/2;
end
```



Invoking a for and while loop for n iterations

• while loop

```
n = 100;
a = 2;
x = a/2;
ctr = 0;
while ctr < n
    ctr = ctr+1;
    x = (x+a/x)/2;
end
```

 Neither method presents a clear time savings - what are you more comfortable with / what looks cleaner? Looping vs. Vectorization/Array Operations,

Decisions (if),

Boolean Expressions

Operations that Require while Loops,

Decisions Involving if / elseif / else,

Logical Operators

Array operations increase computation speed

·Consider the vector

a = rand(1, N) where N is the total number of array elements

Say we wish to calculate $b_i = a_i \times a_i$

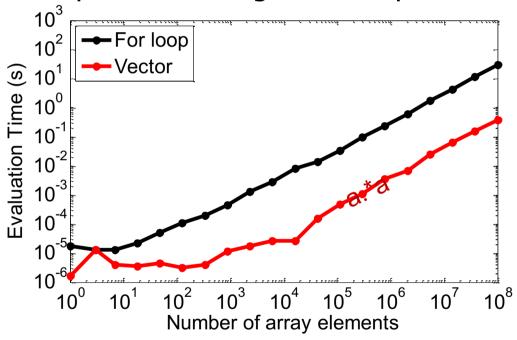
We have three options

- Array operations / vectorization
 - a.^2
 - a.*a
- LoopingUsing a for loop



Array operations increase computation speed

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



Time savings = orders of magnitude



Array operations increase computation speed

The Code Used to Generate the Previous Result (for your reference)

```
clear; clc; close all
n = round(logspace(0,8,20));
for jj = 1:length(n)
    a = rand(1,n(jj));
    clear b
    tic
    for kk = 1:length(a)
        b(kk) = a(kk)*a(kk);
    end
    t_for(jj) = toc;
    clear b
    tic
    b = a.*a;
    t_vect(jj) = toc;
end
```

continued...plotting commands

```
[ph] = plot(n,t_for,'k.-',n,t_vect,'r.-');
set(ph(1),'LineWidth',4,'MarkerSize',25)
set(ph(2),'LineWidth',4,'MarkerSize',25)
set(gca,'YTick',logspace(-10,10,21))
set(gca,'XTick',logspace(0,20,21))
set(gca,'XScale','log','YScale','log')
set(gca,'FontSize',20)
set(gca,'FontName','Arial')
lg = legend('For loop','Vector');
set(lg,'Location','NorthWest')
xlabel('Number of array elements')
ylabel('Evaluation Time (s)')
```



Decisions - the if statement

•What if you want to evaluate a variable, vector, etc. based on certain criteria?

- The if statement evaluates a condition and executes a statement or statements if that condition is met
- A simple example

```
a = 1;
if a == 1;
  disp('a is equal to 1! Yay!')
end
```

• Like a for loop, the if statement is closed with an end statement

Decisions - nested if statements

·What if several criteria need to be met?

The if statement can be nested

Boolean expressions / logical operators

Boolean expressions can be used to circumvent nested if statements

• The Boolean statements "&&" and "||" evaluate several expressions to determine if both or any of the statements are true

Logical Operator (Vectors / Scalars)	Logical Operator (Scalars)	Meaning
&	&&	and
	II	or

Avoiding nested if statements using Boolean expressions

•The two if criteria can be combined into one if statement to clean up the code



Decisions: if, elseif, and else

•We learned about if decisions, which can be invoked to evaluate relational/logical criteria

- if statements are not limited to one set of criteria
- Multiple criteria may be evaluated using the if, else formulation
- Example
- FEM shape function



A more complete list of logical operators

Table of Logical Operators

Logical Operator (Scalars)	Logical Operator (Vectors)	Function call	Meaning
&&	&	and(a,b)	And
I		or(a,b)	Or, inclusive
		xor(a,b)	Or, exclusive
~	~	not(a)	Not / compliment

The difference between or and xor

Truth table for or and xor

statement a	statement b	or(a,b)	xor(a,b)
F	F	F	F
F	Т	Т	Т
Т	F	Т	T
Т	Т	Т	F

or = truth for both statements leads to positive output xor = truth for both statements leads to a negative output



Logical NOT

Logical Vectors



Logical NOT

- We have discussed OR and AND ad nauseam little has been said about NOT
- NOT behaves a little differently it only requires one input and returns the logical opposite

```
not(0) or ~0 returns 1
not(1) returns 0
not(3) returns 0
```

•Note: in the description of logical operators - nonzero values are treated as a truth / 1



From logical scalars to vectors

- We have covered logical scalars most often in conjunction with decisions or while loops
- A logical scalar value can be invoked by making a relational comparison between one (in the case of not / ~) or two scalar values (in the case of >, < >=. ==. ~=. etc.)
- A true result is represented by 1 while a false result is represented by 0
- •Examples of logical scalars. What would be the result of each of the following?

$$a = 3 > 2$$

$$a = 3>2$$
 $a = 2\sim=2$

$$a = 2 > 3$$

$$a = 2>3$$
 $a = 2==2$

$$a = 2 > = 2$$
 $a = ~1$

$$a = ~1$$



From logical scalars to vectors

- •Logical vectors are vectors of numbers (0 and 1) representing a true (1) or false (0) condition based on some relational expression
 - Recall, a logical scalar

$$a = 3 <= 4$$
 gives, $a = 1$

This is of a "logical" class and is 1 byte in size (compared to 8 bytes for double precision)

Logical vector

$$a = [0 \ 4 \ 9 \ 7 \ 3 \ 5] <= 4$$



How are logical vectors "made"

- Logical vectors occur as a result of a statement on a vector involving a relational operator -or- may be specified through discrete input
 - Relational operator operating on a vector

$$a = [1 6 5] < 2$$

yields $a = [1 0 0]$

Directly specifying the logical operator

$$a = [logical([1 0 0])]$$

Call to logical function required otherwise a double precision number will be created

Logical vector rules

·Say we define the following vectors in MATLAB:

```
x = [5 \ 9 \ 2 \ 4 \ 3]; <- vector of class "double"

v = logical([1 \ 0 \ 1 \ 0 \ 1]); <- logical vector

xp = x(v); <- returns elements of x corresponding to true (1) indices of the logical vector v
```

- ·Logical vector rules dictate:
 - 1) \vee may be used as a subscript for \times given that it is of class "logical"
 - 2) only the elements of x corresponding to 1's (true) in v are returned
 - 3) \times and \vee must be the same size



Examples of logical vectors

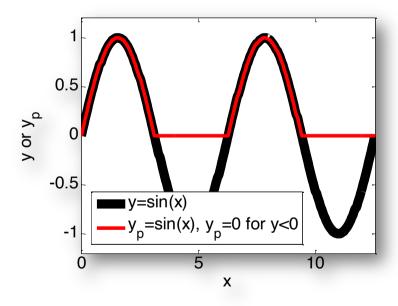
What are the results of the following?

```
x = [1 4 3 6 2 8];
v = x>3;
yields v

x = [1 4 3 6 2 8];
v = x<-3;
yields v

x = [1 4 3 6 2 8];
v = x < -3;
yields v</pre>
```

Produce the following plot:
$$y(x) = \begin{cases} \sin(x) & (\sin(x) > 0) \\ 0 & (\sin(x) \le 0) \end{cases}$$



Method 1 - for and if expressions (not logical vectors)

```
% Domain vector and sin(x)
x = 0:pi/1000:3*pi;
y = sin(x);

% For loop and if condition used to
% set negative y values to 0
for jj = 1:length(y)
    if y(jj) < 0
        y(jj) = 0;
    end
end

% Plotting the result
plot(x,y,'k.')</pre>
```



Method 2 - logical vectors

```
% Domain vector and sin(x)
x = 0:pi/1000:3*pi;
y = sin(x);
% Set all negative y values to 0
y = y.*(y>0)
% Plotting the result
plot(x,y,'k.')
```

This syntax is much more efficient!

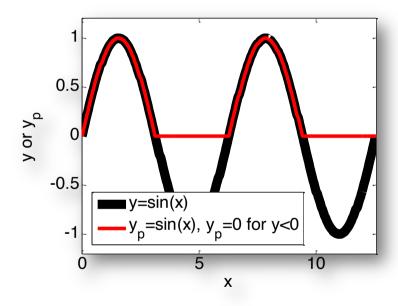


Code used for plot

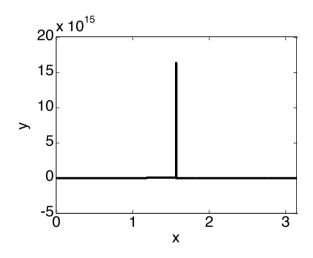
```
% Domain and y = sin(x)
x = 0:pi/100:4*pi;
y = sin(x);

% Set y<0 to 0
yp = y.*(y>0);

% Plot the result
pl = plot(x,y,'k-',x,yp,'r-');
set(gca,'FontSize',18)
set(pl(1),'LineWidth',10)
set(pl(2),'LineWidth',4)
axis([0 4*pi -1.2 1.2])
xlabel('x'), ylabel('y or y_p')
lg = legend('y=sin(x)',...
'y_p=sin(x), y_p=0 for y<0');</pre>
```



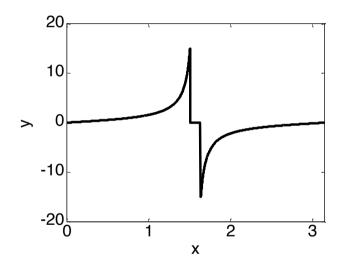
Produce the following plot: $y(x) = \tan(x)$



```
x = 0*pi:pi/10000:pi;
y = tan(x);
plot(x, y)
xlim([0 pi])
xlabel('x')
ylabel('y')
```

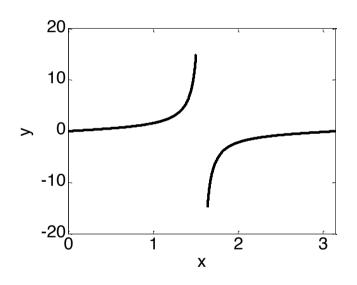
Can we use logical vectors to change the visualization of this function such that the details of y are not dominated by the asymptote?

Set large (positive and negative) values to 0



```
x = 0*pi:pi/10000:pi;
y = tan(x);
y = y.*(abs(y)<15);
plot(x,y)</pre>
```

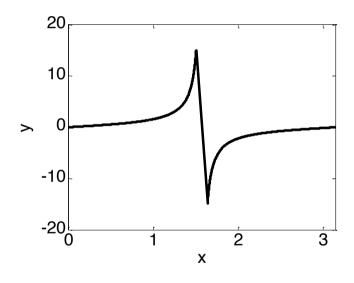
Set large (positive and negative) values to NaN



```
x = 0*pi:pi/10000:pi;
y = tan(x);
y(abs(y)>15) = NaN;
plot(x,y)
```

Note: a logical vector has been used to directly index and assign vector values

Remove large (positive and negative) values



```
x = 0*pi:pi/10000:pi;
y = tan(x);
x = x(abs(y)<15);
y = y(abs(y)<15);
plot(x,y)</pre>
```

Example Sieve of Eratosthenes

·Finds all of the primes between 1 and n

- -A prime number can be divided evenly only by 1 and itself, and it must be a whole number greater than 1.
- -An algorithm that uses logical expressions and logical indexing

·Algorithm

- 1) List the numbers from 2 to n
- 2) The first number in this list must be a prime, add it to the list of primes
- 3) Strike off all multiples of this number from the list
- 4) Repeat steps 2 through 4 until the prime being considered is greater than or equal to the square root of n
- 5) All remaining numbers in the list must also be primes

