Part I

Matlab and Solving Equations

Lecture 1

Vectors, Functions, and Plots in MATLAB

In these notes

≫
≫

will indicate commands to be entered at the MATLAB prompt ≫ in the command window. You do not type the symbol ≫.

Entering vectors

In MATLAB, the basic objects are matrices, i.e. arrays of numbers. Vectors can be thought of as special matrices. A row vector is recorded as a $1 \times n$ matrix and a column vector is recorded as a $m \times 1$ matrix. To enter a row vector in Matlab, type the following in the command window:

≫ v = [0 1 2 3]

and press enter. MATLAB will print out the row vector. To enter a column vector type

≫ u = [9; 10; 11; 12; 13]

You can access an entry in a vector with

≫ u(2)

and change the value of that entry with

≫ u(2)=47

You can extract a *slice* out of a vector with

≫ u(2:4)

You can change a row vector into a column vector, and vice versa easily in Matlab using

≫ w = v'

(This is called *transposing* the vector and we call ' the transpose operator.) There are also useful shortcuts to make vectors such as

≫ x = -1:.1:1
≫ y = linspace(0,1,11)

Basic Formatting

To make MATLAB put fewer blank lines in its output, enter

```
≫   format compact
≫   pi
≫   x
```

To make MATLAB display more digits, enter

```
≫   format long
≫   pi
```

Note that this does not change the number of digits MATLAB is using in its calculations; it only changes what is diplayed.

Plotting Data

Consider the data in Table 1.1.[1] We can enter this data into MATLAB with the following commands entered

T (C°)	5	20	30	50	55
μ	0.08	0.015	0.009	0.006	0.0055

Table 1.1: Viscosity of a liquid as a function of temperature.

in the command window:

```
≫   x = [ 5   20   30   50   55 ]
≫   y = [ 0.08   0.015   0.009   0.006   0.0055]
```

Entering the name of the variable retrieves its current values. For instance

```
≫   x
≫   y
```

We can plot data in the form of vectors using the plot command:

```
≫   plot(x,y)
```

This will produce a graph with the data points connected by lines. If you would prefer that the data points be represented by symbols you can do so. For instance

```
≫   plot(x,y,'*')
≫   plot(x,y,'o')
≫   plot(x,y,'.')
```

---

[1]Adapted from Ayyup &McCuen 1996, p.174.

Data as a Representation of a Function

A major theme in this course is that often we are interested in a certain function $y = f(x)$, but the only information we have about this function is a discrete set of data $\{(x_i, y_i)\}$. Plotting the data, as we did above, can be thought of envisioning the function using just the data. We will find later that we can also do other things with the function, like differentiating and integrating, just using the available data. Numerical methods, the topic of this course, means doing mathematics by computer. Since a computer can only store a finite amount of information, we will almost always be working with a finite, discrete set of values of the function (data), rather than a formula for the function.

Built-in Functions

If we wish to deal with formulas for functions, MATLAB contains a number of built-in functions, including all the usual functions, such as `sin( )`, `exp( )`, etc.. The meaning of most of these is clear. The dependent variable (input) always goes in parentheses in MATLAB. For instance

```
≫  sin(pi)
```

should return the value of $\sin \pi$, which is of course 0 and

```
≫  exp(0)
```

will return e^0 which is 1. More importantly, the built-in functions can operate not only on single numbers but on vectors. For example

```
≫  x = linspace(0,2*pi,41)
≫  y = sin(x)
≫  plot(x,y)
```

will return a plot of $\sin x$ on the interval $[0, 2\pi]$

Some of the built-in functions in MATLAB include: `cos( )`, `tan( )`, `sinh( )`, `cosh( )`, `log( )` (natural logarithm), `log10( )` (log base 10), `asin( )` (inverse sine), `acos( )`, `atan( )`. To find out more about a function, use the `help` command; try

```
≫  help plot
```

User-Defined Anonymous Functions

If we wish to deal with a function that is a combination of the built-in functions, MATLAB has a couple of ways for the user to define functions. One that we will use a lot is the anonymous function, which is a way to define a function in the command window. The following is a typical anonymous function:

```
≫  f = @(x) 2*x.^2 - 3*x + 1
```

This produces the function $f(x) = 2x^2 - 3x + 1$. To obtain a single value of this function enter

```
≫  y = f(2.23572)
```

Just as for built-in functions, the function f as we defined it can operate not only on single numbers but on vectors. Try the following:

```
≫  x = -2:.2:2
≫  y = f(x)
```

This is an example of *vectorization*, i.e. putting several numbers into a vector and treating the vector all at once, rather than one component at a time, and is one of the strengths of MATLAB. The reason $f(x)$ works when x is a vector is because we represented x^2 by `x.^2`. The `.` turns the exponent operator `^` into entry-wise exponentiation, so that `[-2 -1.8 -1.6].^2` means $[(-2)^2, (-1.8)^2, (-1.6)^2]$ and yields `[4 3.24 2.56]`. In contrast, `[-2 -1.8 -1.6]^2` means the matrix product $[-2, -1.8, -1.6][-2, -1.8, -1.6]$ and yields only an error. The `.` is needed in `.^`, `.*`, and `./`. It is not needed when you `*` or `/` by a scalar or for `+`.

The results can be plotted using the `plot` command, just as for data:

```
≫  plot(x,y)
```

Notice that before plotting the function, we in effect converted it into data. Plotting on any machine always requires this step.

Exercises

1.1 Find a table of data in an engineering or science textbook or website. Input it as vectors and plot it. Use the insert icon to label the axes and add a title to your graph. Turn in the graph. Indicate what the data is and properly reference where it came from.

1.2 Find a function formula in an engineering or science textbook or website. Make an anonymous function that produces that function. Plot it on a physically relevant domain. Label the axes and add a title to your graph. Turn in the graph and include the Matlab command for the anonymous function. Indicate what the function means and properly reference where it came from.

Lecture 2

MATLAB Programs

In MATLAB, programs may be written and saved in files with a suffix `.m` called *M-files*. There are two types of M-file programs: *functions* and *scripts*.

Function Programs

Begin by clicking on the new document icon in the top left of the MATLAB window (it looks like an empty sheet of paper).

In the document window type the following:

```
function y = myfunc(x)
    y = 2*x.^2 - 3*x + 1;
end
```

Save this file as: `myfunc.m` in your working directory. This file can now be used in the command window just like any predefined Matlab function; in the command window enter:

```
≫  x = -2:.1:2;      % Produces a vector of x values
≫  y = myfunc(x);    % Produces a vector of y values
≫  plot(x,y)
```

Note that the fact we used `x` and `y` in both the function program and in the command window was just a coincidence. In fact, it is the name of the file `myfunc.m` that actually mattered, not what anything in it was called. We could just as well have made the function

```
function nonsense = yourfunc(inputvector)
    nonsense = 2*inputvector.^2 - 3*inputvector + 1;
end
```

Look back at the program. All function programs are like this one, the essential elements are:

- Begin with the word `function`.
- There is an input and an output.
- The output, name of the function and the input must appear in the first line.
- The body of the program must assign a value to the output variable(s).
- The program cannot access variables in the current workspace unless they are input.

- Internal variables inside a function do not appear in the current workspace.

Functions can have multiple inputs, which are separated by commas. For example:

```
function y = myfunc2d(x,p)
    y = 2*x.^p - 3*x + 1;
end
```

Functions can have multiple outputs, which are collected into a vector. Open a new document and type:

```
function [x2 x3 x4] = mypowers(x)
    x2 = x.^2;
    x3 = x.^3;
    x4 = x.^4;
end
```

Save this file as `mypowers.m`. In the command window, we can use the results of the program to make graphs:

```
≫  x = -1:.1:1
≫  [x2 x3 x4] = mypowers(x);
≫  plot(x,x,'black',x,x2,'blue',x,x3,'green',x,x4,'red')
```

Printing, Returning, Capturing, and Printing

Notice that in the examples above, lines ending with a semicolon ";" did not print their results.

Try the following:

```
≫  myfunc(3)
≫  ans^2
```

Although `myfunc` returned a value, we did not capture it. By default MATLAB captured it as `ans` so we can use it in our next computation. However, MATLAB always uses `ans` (for answer), so the result is likely to get overwritten.

Then try:

```
≫  z = 0
≫  z = myfunc(2)
≫  z^2
```

`myfunc` returned a value that it internally called `y` and we captured the result in `z`. We can now use `z` for other calculations.

Now make a program

```
function myfuncnoreturn(x)
    y = 2*x.^2 - 3*x + 1
end
```

and try:

```
≫  myfuncnoreturn(4)
≫  ans^2
≫  y^2
```

Although the value of y was printed within the function, it was not returned, so neither the value of y nor the value of ans was changed. Thus we cannot use the result from the function.

In general, the best way to use a function is to capture the result it returns and then use or print this result. Printing within functions is bad form; however, for understanding what is happening within a function it is useful to print, so many functions in this book do print.

Script Programs

MATLAB uses a second type of program that differs from a function program in several ways, namely:

- There are no inputs and outputs.
- A script program may use, create and change variables in the current workspace (the variables used by the command window).

Below is a script program that accomplishes the same thing as the function program plus the commands in the previous section:

```
x2 = x.^2;
x3 = x.^3;
x4 = x.^4;
plot(x,x,'black',x,x2,'blue',x,x3,'green',x,x4,'red')
```

Type this program into a new document and save it as `mygraphs.m`. In the command window enter:

```
≫  x = -1:.1:1;
≫  mygraphs
```

Note that the program used the variable x in its calculations, even though x was defined in the command window, not in the program.

Many people use script programs for routine calculations that would require typing more than one command in the command window. They do this because correcting mistakes is easier in a program than in the command window.

Program Comments

For programs that have more than a couple of lines it is important to include comments. Comments allow other people to know what your program does and they also remind yourself what your program does if you set it aside and come back to it later. It is best to include comments not only at the top of a program, but also with each section. In MATLAB anything that comes in a line after a % is a comment.

For a function program, the comments should at least give the purpose, inputs, and outputs. A properly commented version of the function with which we started this section is:

```matlab
function y = myfunc(x)
    % Computes the function 2x^2 -3x +1
    % Input: x -- a number or vector;
    %               for a vector the computation is elementwise
    % Output: y -- a number or vector of the same size as x
    y = 2*x.^2 - 3*x + 1;
end
```

For a script program, there should be an initial comment stating the purpose of the script. It is also helpful to include the name of the program at the beginning. For example:

```matlab
% mygraphs
% plots the graphs of x, x^2, x^3, and x^4
% on the interval [-1,1]

% fix the domain and evaluation points
x = -1:.1:1;

% calculate powers
% x1 is just x
x2 = x.^2;
x3 = x.^3;
x4 = x.^4;

% plot each of the graphs
plot(x,x,'+-',x,x2,'x-',x,x3,'o-',x,x4,'--')
```

The MATLAB command `help` prints the first block of comments from a file. If we save the above as `mygraphs.m` and then do

≫ `help mygraphs`

it will print into the command window:

≫ `mygraphs`
≫ `plots the graphs of x, x^2, x^3, and x^4`
≫ `on the interval [-1,1]`

Exercises

2.1 Write a well-commented **function** program for the function $x^2 e^{-x^2}$, using entry-wise operations (such as `.*` and `.^`). To get e^x use `exp(x)`. Plot the function on $[-5, 5]$ using enough points to make the graph smooth. Turn in the program and the graph.

2.2 Write a well-commented **script** program that graphs the functions $\sin x$, $\sin 2x$, $\sin 3x$, $\sin 4x$, $\sin 5x$ and $\sin 6x$ on the interval $[0, 2\pi]$ on one plot. (π is `pi` in MATLAB.) Use a sufficiently small step size to make all the graphs smooth. Turn in the program and the graph.

Lecture 3

Newton's Method and Loops

Solving equations numerically

For the next few lectures we will focus on the problem of solving an equation:

$$f(x) = 0. \tag{3.1}$$

As you learned in calculus, the final step in many optimization problems is to solve an equation of this form where f is the derivative of a function, F, that you want to maximize or minimize. In real engineering problems the functions, f, you wish to find roots for can come from a large variety of sources, including formulas, solutions of differential equations, experiments, or simulations.

Newton iterations

We will denote an actual solution of equation (3.1) by x^*. There are three methods which you may have discussed in Calculus: the bisection method, the secant method and Newton's method. All three depend on beginning close (in some sense) to an actual solution x^*.

Recall Newton's method. You should know that the basis for Newton's method is approximation of a function by its linearization at a point, i.e.

$$f(x) \approx f(x_0) + f'(x_0)(x - x_0). \tag{3.2}$$

Since we wish to find x so that $f(x) = 0$, set the left hand side ($f(x)$) of this approximation equal to 0 and solve for x to obtain:

$$x \approx x_0 - \frac{f(x_0)}{f'(x_0)}. \tag{3.3}$$

We begin the method with the initial guess x_0, which we hope is fairly close to x^*. Then we define a sequence of points $\{x_0, x_1, x_2, x_3, \ldots\}$ from the formula:

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}, \tag{3.4}$$

which comes from (3.3). If $f(x)$ is reasonably well-behaved near x^* and x_0 is close enough to x^*, then it is a fact that the sequence will converge to x^* and will do it very quickly.

The loop: `for ... end`

In order to do Newton's method, we need to repeat the calculation in (3.4) a number of times. This is accomplished in a program using a *loop*, which means a section of a program which is repeated. The

simplest way to accomplish this is to count the number of times through. In MATLAB, a `for ... end` statement makes a loop as in the following simple function program:

```matlab
function S = mysum(n)
    % Gives the sum of the first n integers
    % Input: n
    % Output: the sum
    S = 0;               % start at zero
    % The loop:
    for i = 1:n          % do n times
        S = S + i;       % add the current integer
    end                  % end of the loop
end
```

Call this function in the command window as:

≫ `mysum(100)`

The result will be the sum of the first 100 integers. All `for ... end` loops have the same format, it begins with `for`, followed by an index (`i`) and a range of numbers (`1:n`). Then come the commands that are to be repeated. Last comes the `end` command.

Loops are one of the main ways that computers are made to do calculations that humans cannot. Any calculation that involves a repeated process is easily done by a loop.

Now let's do a program that does n steps (iterations) of Newton's method. We will need to input the function, its derivative, the initial guess, and the number of steps. The output will be the final value of x, i.e. x_n. If we are only interested in the final approximation, not the intermediate steps, which is usually the case in the real world, then we can use a single variable `x` in the program and change it at each step:

```matlab
function x = mynewton(f,f1,x0,n)
    % Solves f(x) = 0 by doing n steps of Newton's method starting at x0.
    % Inputs: f -- the function
    %         f1 -- it's derivative
    %         x0 -- starting guess, a number
    %         n -- the number of steps to do
    % Output: x -- the approximate solution
    x = x0;                      % set x equal to the initial guess x0
    for i = 1:n                  % Do n times
        x = x - f(x)/f1(x)       % Newton's formula, prints x too
    end
end
```

In the command window set to print more digits via

≫ `format long`

and to not print blank lines via

≫ `format compact`

Then define a function: $f(x) = x^3 - 5$ i.e.

```
≫   f = @(x) x^3 - 5
```

and define $f1$ to be its derivative, i.e.

```
≫   f1 = @(x) 3*x^2
```

Then run **mynewton** on this function. By trial and error, what is the lowest value of **n** for which the program converges (stops changing). By simple algebra, the true root of this function is $\sqrt[3]{5}$. How close is the program's answer to the true value?

Convergence

Newton's method converges rapidly when $f'(x^*)$ is nonzero and finite, and x_0 is close enough to x^* that the linear approximation (3.2) is valid. Let us take a look at what can go wrong.

For $f(x) = x^{1/3}$ we have $x^* = 0$ but $f'(x^*) = \infty$. If you try

```
≫   f = @(x) x^(1/3)
≫   f1 = @(x) (1/3)*x^(-2/3)
≫   x = mynewton(f,f1,0.1,10)
```

then x explodes.

For $f(x) = x^2$ we have $x^* = 0$ but $f'(x^*) = 0$. If you try

```
≫   f = @(x) x^2
≫   f1 = @(x) 2*x
≫   x = mynewton(f,f1,1,10)
```

then x does converge to 0, but not that rapidly.

If x_0 is not close enough to x^* that the linear approximation (3.2) is valid, then the iteration (3.4) gives some x_1 that may or may not be any better than x_0. If we keep iterating, then either

- x_n will eventually get close to x^* and the method will then converge (rapidly), or
- the iterations will not approach x^*.

Exercises

3.1 Enter: `format long`. Use `mynewton` on the function $f(x) = x^5 - 7$, with $x_0 = 2$. By trial and error, what is the lowest value of **n** for which the program converges (stops changing). Compute the error, which is how close the program's answer is to the true value. Compute the residual, which is the program's answer plugged into f. (See the next section for discussion.) Are the error and residual zero?

3.2 Suppose a ball is dropped from a height of 2 meters onto a hard surface and the coefficient of restitution of the collision is .9 (see Wikipedia for an explanation). Write a well-commented **script** program to calculate the total distance the ball has traveled when it hits the surface for the **n**-th time. Enter: `format long`. By trial and error approximate how large **n** must be so that total distance stops changing. Turn in the program and a brief summary of the results.

3.3 For $f(x) = x^3 - 4$, perform 3 iterations of Newton's method with starting point $x_0 = 2$. (By hand, but use a calculator.) Calculate the solution ($x^* = 4^{1/3}$) on a calculator and find the errors and percentage errors of x_0, x_1, x_2 and x_3. Use enough digits so that you do not falsely conclude the error is zero. Put the results in a table.

Lecture 4

Controlling Error and Conditional Statements

Measuring error and the Residual

If we are trying to find a numerical solution of an equation $f(x) = 0$, then there are a few different ways we can measure the error of our approximation. The most direct way to measure the error would be as

$$\{\text{Error at step } n\} = e_n = x_n - x^*$$

where x_n is the n-th approximation and x^* is the true value. However, we usually do not know the value of x^*, or we wouldn't be trying to approximate it. This makes it impossible to know the error directly, and so we must be more clever.

One possible strategy, that often works, is to run a program until the approximation x_n stops changing. The problem with this is that it sometimes doesn't work. Just because the program stop changing does not necessarily mean that x_n is close to the true solution.

For Newton's method we have the following principle: **At each step the number of significant digits roughly doubles.** While this is an important statement about the error (since it means Newton's method converges really quickly), it is somewhat hard to use in a program.

Rather than measure how close x_n is to x^*, in this and many other situations it is much more practical to measure how close the equation is to being satisfied, in other words, how close $y_n = f(x_n)$ is to 0. We will use the quantity $r_n = f(x_n) - 0$, called the *residual*, in many different situations. Most of the time we only care about the size of r_n, so we use the absolute value of the residual as a measure of how close the solution is to solving the problem:

$$|r_n| = |f(x_n)|.$$

The `if` ... `end` statement

If we have a certain tolerance for $|r_n| = |f(x_n)|$, then we can incorporate that into our Newton method program using an `if` ... `end` statement:

```
function x = mynewton(f,f1,x0,n,tol)
    % Solves f(x) = 0 by doing n steps of Newton's method starting at x0.
    % Inputs: f -- the function
    %         f1 -- it's derivative
    %         x0 -- starting guess, a number
    %         tol -- desired tolerance, prints a warning if |f(x)|>tol
    % Output: x -- the approximate solution
    x = x0;                     % set x equal to the initial guess x0
```

```
    for i = 1:n                      % Do n times
        x = x - f(x)/f1(x)   % Newton's formula
    end
    r = abs(f(x))
    if r > tol
        warning('The desired accuracy was not attained')
    end
end
```

In this program if checks if `abs(y) > tol` is true or not. If it is true then it does everything between there and `end`. If not true, then it skips ahead to `end`.

In the command window define a function and its derivative:

≫ `f = @(x) x^3-5`
≫ `f1 = @(x) 3*x^2`

Then use the program with $n = 3$, $tol = .01$, and $x_0 = 2$. Next, change *tol* to 10^{-10} and repeat.

The loop: `while ... end`

While the previous program will tell us if it worked or not, we still have to input `n`, the number of steps to take. Even for a well-behaved problem, if we make `n` too small then the tolerance will not be attained and we will have to go back and increase it, or, if we make `n` too big, then the program will take more steps than necessary.

One way to control the number of steps taken is to iterate until the residual $|r_n| = |f(x)| = |y|$ is small enough. In MATLAB this is easily accomplished with a `while ... end` loop.

```
function x = mynewtontol(f,f1,x0,tol)
    % Solves f(x) = 0 using Newton's method until |f(x)| < tol.
    % Inputs: f -- the function
    %         f1 -- it's derivative
    %         x0 -- starting guess, a number
    %         tol -- desired tolerance, runs until |f(x)|<tol
    % Output: x -- the approximate solution
    x = x0;                          % set x equal to the initial guess x0
    y = f(x);
    while abs(y) > tol      % Do until the tolerence is reached.
        x = x - y/f1(x)     % Newton's formula
        y = f(x)
    end
end
```

The statement `while ... end` is a loop, similar to `for ... end`, but instead of going through the loop a fixed number of times it keeps going as long as the statement `abs(y) > tol` is true.

One obvious drawback of the program is that `abs(y)` might never get smaller than `tol`. If this happens, the program would continue to run over and over until we stop it. Try this by setting the tolerance to a really

small number:

≫ `tol = 10^(-100)`

then run the program again for $f(x) = x^3 - 5$. (You can use `Ctrl-c` to stop the program when it is stuck.)

One way to avoid an infinite loop is add a counter variable, say `i` and a maximum number of iterations to the programs. Using the `while` statement, this can be accomplished as:

```
function x = mynewtontol(f,f1,x0,tol)
    % Solves f(x) = 0 using Newton's method until |f(x)| < tol.
    %      Safety stop after 1000 iterations
    % Inputs: f -- the function
    %          f1 -- it's derivative
    %          x0 -- starting guess, a number
    %          tol -- desired tolerance, runs until |f(x)|<tol
    % Output: x -- the approximate solution
    x = x0;    % set x equal to the initial guess x0.
    i=0;        % set counter to zero
    y = f(x);
    while abs(y) > tol & i < 1000
        % Do until the tolerence is reached or max iter.
        x = x - y/f1(x)    % Newton's formula
        y = f(x)
        i = i+1;            % increment counter
    end
end
```

Exercises

4.1 In Calculus we learn that a geometric series has an exact sum

$$\sum_{i=0}^{\infty} r^i = \frac{1}{1-r} \, ,$$

provided that $|r| < 1$. For instance, if $r = .5$ then the sum is exactly 2. Below is a script program that lacks one line as written. Put in the missing command and then use the program to verify the result above. How many steps does it take? How close is the answer to 2?

```
% Computes a geometric series until it seems to converge
format long
format compact
r = .5;
Snew = 0;            % start sum at 0
Sold = -1;           % set Sold to trick while the first time
i = 0;               % count iterations
while Snew > Sold    % is the sum still changing?
   Sold = Snew;      % save previous value to compare to
   Snew = Snew + r^i;
   i=i+1;
Snew                 % prints the final value.
i                    % prints the # of iterations.
```

Add a line at the end of the program to compute the relative error of `Snew` versus the exact value. Run the script for $r = 0.9, 0.99, 0.999, 0.9999, 0.99999$, and 0.999999. In a table, report the number of iterations needed and the relative error for each r.

4.2 Modify your program from exercise 3.2 to compute the total distance traveled by the ball while its bounces are at least 1 millimeter high. Use a `while` loop to decide when to stop summing; do not use a `for` loop or trial and error. Turn in your modified program and a brief summary of the results.

Lecture 5

The Bisection Method and Locating Roots

Bisecting and the `if ... else ... end` statement

Recall the bisection method. Suppose that $c = f(a) < 0$ and $d = f(b) > 0$. If f is continuous, then obviously it must be zero at some x^* between a and b. The bisection method then consists of looking half way between a and b for the zero of f, i.e. let $x = (a+b)/2$ and evaluate $y = f(x)$. Unless this is zero, then from the signs of c, d and y we can decide which new interval to subdivide. In particular, if c and y have the same sign, then $[x, b]$ should be the new interval, but if c and y have different signs, then $[a, x]$ should be the new interval. (See Figure 5.1.)
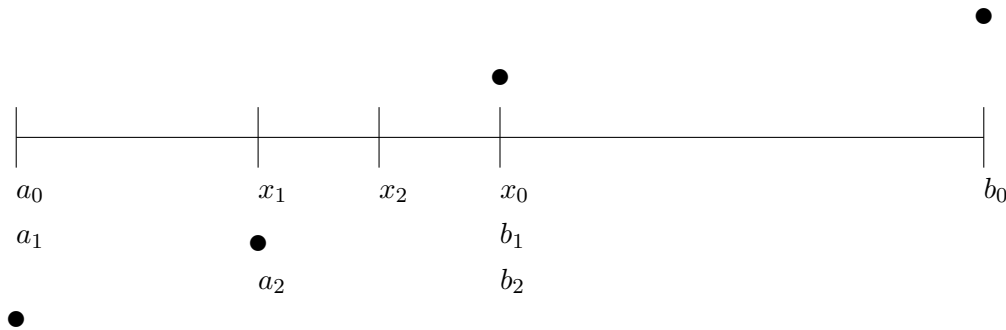

Figure 5.1: The bisection method.

Deciding to do different things in different situations in a program is called *flow control*. The most common way to do this is the `if ... else ... end` statement which is an extension of the `if ... end` statement we have used already.

Bounding the Error

One good thing about the bisection method, that we don't have with Newton's method, is that we always know that the actual solution x^* is inside the current interval $[a, b]$, since $f(a)$ and $f(b)$ have different signs. This allows us to be sure about what the maximum error can be. Precisely, the error is always less than half of the length of the current interval $[a, b]$, i.e.

$$\{\text{Absolute Error}\} = |x - x^*| < (b - a)/2,$$

where x is the center point between the current a and b.

The following function program (available to download as `mybisect.m`) does n iterations of the bisection method and returns not only the final value, but also the maximum possible error:

```
function [x e] = mybisect(f,a,b,n)
    % function [x e] = mybisect(f,a,b,n)
    % Does n iterations of the bisection method for a function f
    % Inputs: f -- a function
    %         a,b -- left and right edges of the interval
    %         n -- the number of bisections to do.
    % Outputs: x -- the estimated solution of f(x) = 0
    %          e -- an upper bound on the error

    % evaluate at the ends and make sure there is a sign change
    c = f(a); d = f(b);
    if c*d > 0.0
        error('Function has same sign at both endpoints.')
    end
    disp('          x                       y')
    for i = 1:n
        % find the middle and evaluate there
        x = (a + b)/2;
        y = f(x);
        disp([    x      y])
        if y == 0.0     % solved the equation exactly
            a = x;
            b = x;
            break       % jumps out of the for loop
        end
        % decide which half to keep, so that the signs at the ends differ
        if c*y < 0
            b=x;
        else
            a=x;
        end
    end
    % set the best estimate for x and the error bound
    x = (a + b)/2;
    e = (b-a)/2;
end
```

Another important aspect of bisection is that it always works. We saw that Newton's method can fail to converge to x^* if x_0 is not close enough to x^*. In contrast, the current interval $[a, b]$ in bisection will always get decreased by a factor of 2 at each step and so it will always eventually shrink down as small as you want it.

Locating the roots (if any)

The bisection method and Newton's method are both used to obtain closer and closer approximations of a solution, but both require starting places. The bisection method requires two points a and b that have a root between them, and Newton's method requires one point x_0 which is reasonably close to a root. How do you come up with these starting points? It depends. If you are solving an equation once, then the best thing to do first is to just graph it. From an accurate graph you can see approximately where the graph crosses zero.

There are other situations where you are not just solving an equation once, but have to solve the same equation many times, but with different coefficients. This happens often when you are developing software for a specific application. In this situation the first thing you want to take advantage of is the natural domain of the problem, i.e. on what interval is a solution physically reasonable. If that is known, then it is easy to get close to the root by simply checking the sign of the function at a fixed number of points inside the interval. Whenever the sign changes from one point to the next, there is a root between those points. The following program will look for the roots of a function f on a specified interval $[a_0, b_0]$.

```matlab
function [a,b] = myrootfind(f,a0,b0)
    % function [a,b] = myrootfind(f,a0,b0)
    % Looks for subintervals where the function changes sign
    % Inputs: f -- a function
    %          a0 -- the left edge of the domain
    %          b0 -- the right edge of the domain
    % Outputs: a -- an array, giving the left edges of subintervals
    %                on which f changes sign
    %          b -- an array, giving the right edges of the subintervals
    n = 1001;   % number of test points to use
    a = [];      % start empty array
    b = [];
    % split the interval into n-1 intervals and evaluate at the break points
    x = linspace(a0,b0,n);
    y = f(x);
    % loop through the intervals
    for i = 1:(n-1)
        if y(i)*y(i+1) < 0   % The sign changed, record it
            a = [a x(i)];
            b = [b x(i+1)];
        end
    end
    if size(a,1) == 0
        warning('no roots were found')
    end
end
```

The final situation is writing a program that will look for roots with no given information. This is a difficult problem and one that is not often encountered in engineering applications.

Once a root has been located on an interval $[a, b]$, these a and b can serve as the beginning points for the bisection and secant methods (see the next section). For Newton's method one would want to choose x_0 between a and b. One obvious choice would be to let x_0 be the bisector of a and b, i.e. $x_0 = (a + b)/2$. An

even better choice would be to use the secant method to choose x_0.

Exercises

5.1 Modify `mybisect` to solve until the absolute error is bounded by a given tolerance. Use a `while` loop to do this. Run your program on the function $f(x) = 2x^3 + 3x - 1$ with starting interval $[0, 1]$ and a tolerance of 10^{-8}. How many steps does the program use to achieve this tolerance? (You can count the step by adding 1 to a counting variable `i` in the loop of the program.) How big is the final residual $f(x)$? Turn in your program and a brief summary of the results.

5.2 Perform 3 iterations of the bisection method on the function $f(x) = x^3 - 4$, with starting interval $[1, 3]$. By hand, but use a calculator.) Calculate the errors and percentage errors of x_0, x_1, x_2, and x_3. Compare the errors with those in exercise 3.3.

Lecture 6

Secant Methods

In this lecture we introduce two additional methods to find numerical solutions of the equation $f(x) = 0$. Both of these methods are based on approximating the function by secant lines just as Newton's method was based on approximating the function by tangent lines.

The Secant Method

The secant method requires two initial approximations x_0 and x_1, preferably both reasonably close to the solution x^*. From x_0 and x_1 we can determine that the points $(x_0, y_0 = f(x_0))$ and $(x_1, y_1 = f(x_1))$ both lie on the graph of f. Connecting these points gives the (secant) line

$$y - y_1 = \frac{y_1 - y_0}{x_1 - x_0}(x - x_1).$$

Since we want $f(x) = 0$, we set $y = 0$, solve for x, and use that as our next approximation. Repeating this process gives us the iteration

$$x_{i+1} = x_i - \frac{x_i - x_{i-1}}{y_i - y_{i-1}} y_i \tag{6.1}$$

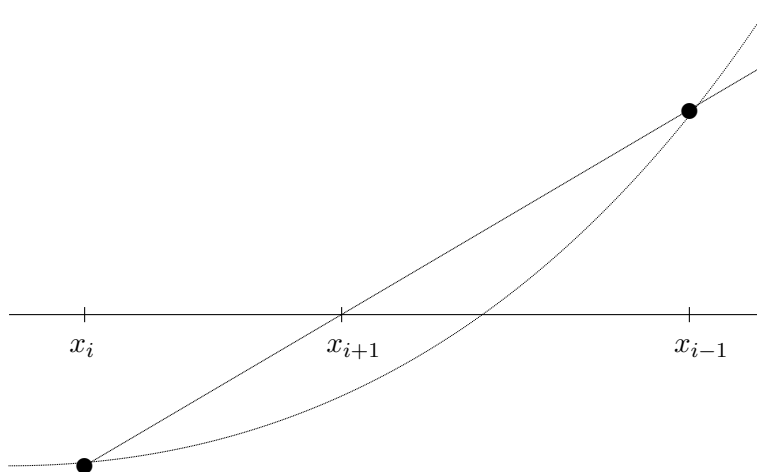with $y_i = f(x_i)$. See Figure 6.1 for an illustration.

Figure 6.1: The secant method in the case where the root is bracketed.

For example, suppose $f(x) = x^4 - 5$, which has a solution $x^* = \sqrt[4]{5} \approx 1.5$. Choose $x_0 = 1$ and $x_1 = 2$ as initial approximations. Next we have that $y_0 = f(1) = -4$ and $y_1 = f(2) = 11$. We may then calculate x_2 from the formula (6.1):

$$x_2 = 2 - \frac{2-1}{11-(-4)} 11 = \frac{19}{15} \approx 1.2666....$$

Pluggin $x_2 = 19/15$ into $f(x)$ we obtain $y_2 = f(19/15) \approx -2.425758....$ In the next step we would use $x_1 = 2$ and $x_2 = 19/15$ in the formula (6.1) to find x_3 and so on.

Below is a program for the secant method (available to download as `mysecant.m`). Notice that it requires two input guesses x_0 and x_1, but it does not require the derivative to be input.

```
function x = mysecant(f,x0,x1,n)
    % Solves f(x) = 0 by doing n steps of the secant method
    %    starting with x0 and x1.
    % Inputs: f -- the function
    %         x0 -- starting guess, a number
    %         x1 -- second starting guess
    %         n -- the number of steps to do
    % Output: x -- the approximate solution
    y0 = f(x0);
    y1 = f(x1);
    for i = 1:n                    % Do n times
        x = x1 - (x1-x0)*y1/(y1-y0)    % secant formula.
        y=f(x)                % y value at the new approximate solution.
        % Move numbers to get ready for the next step
        x0=x1;
        y0=y1;
        x1=x;
        y1=y;
    end
end
```

The *Regula Falsi* (False Position) Method

The *Regula Falsi* method is a combination of the secant method and bisection method. As in the bisection method, we have to start with two approximations a and b for which $f(a)$ and $f(b)$ have different signs. As in the secant method, we follow the secant line to get a new approximation, which gives a formula similar to (6.1),

$$x = b - \frac{b-a}{f(b) - f(a)} f(b) \,.$$

Then, as in the bisection method, we check the sign of $f(x)$; if it is the same as the sign of $f(a)$ then x becomes the new a and otherwise let x becomes the new b. Note that in general either $a \to x^*$ or $b \to x^*$ but not both, so $b - a \not\to 0$. For example, for the function in Figure 6.1, $a \to x^*$ but b would never move.

Convergence

If we can begin with a good choice x_0, then Newton's method will converge to x^* rapidly. The secant method is a little slower than Newton's method and the *Regula Falsi* method is slightly slower than that. However, both are still much faster than the bisection method.

If we do not have a good starting point or interval, then the secant method, just like Newton's method, can fail altogether. The *Regula Falsi* method, just like the bisection method, always works because it keeps the solution inside a definite interval.

Simulations and Experiments

Although Newton's method converges faster than any other method, there are contexts when it is not convenient, or even impossible. One obvious situation is when it is difficult to calculate a formula for $f'(x)$ even though one knows the formula for $f(x)$. This is often the case when $f(x)$ is not defined explicitly, but implicitly. There are other situations, which are very common in engineering and science, where even a formula for $f(x)$ is not known. This happens when $f(x)$ is the result of experiment or simulation rather than a formula. In such situations, the secant method is usually the best choice.

Exercises

6.1 Perform 3 iterations of the secant method on the function $f(x) = x^3 - 4$, with starting points $x_{-1} = 1$ and $x_0 = 3$. (By hand, but use a calculator.) Calculate the errors and percentage errors of x_1, x_2, and x_3. Compare the errors with those in exercise 3.3 and 5.2.

6.2 Perform 3 iterations of the *Regula Falsi* method on the function $f(x) = x^3 - 4$, with starting interval $[1, 3]$. (By hand, but use a calculator.) Calculate the errors and percentage errors of x_1, x_2, and x_3. Compare the errors with those in exercises 3.3 and 5.2.

6.3 Modify the program `mysecant.m` to iterate until the absolute value of the residual is less than a given tolerance. (Let `tol` be an input instead of `n`.) Modify the comments appropriately. Test program on the function in the exercises above and then turn in the program.

Lecture 7

Symbolic Computations

The focus of this course is on numerical computations, i.e. calculations, usually approximations, with floating point numbers. However, MATLAB can also do *symbolic* computations, which means exact calculations using symbols as in Algebra or Calculus.

Note: To do symbolic computations in MATLAB one must have the Symbolic Toolbox.

Defining functions and basic operations

Before doing any symbolic computation, one must declare the variables used to be symbolic:

≫   `syms x y`

A function is defined by simply typing the formula:

≫   `f = cos(x) + 3*x^2`

Note that coefficients must be multiplied using *. To find specific values, you must use the command `subs`:

≫   `subs(f,pi)`

This command stands for *substitute*, it substitutes π for x in the formula for f. If we define another function:

≫   `g = exp(-y^2)`

then we can compose the functions:

≫   `h = compose(g,f)`

i.e. $h(x) = g(f(x))$. Since f and g are functions of different variables, their product must be a function of two variables:

≫   `k = f*g`
≫   `subs(k,[x,y],[0,1])`

We can do simple calculus operations, like differentiation:

≫   `f1 = diff(f)`
≫   `k1x = diff(k,x)`

indefinite integrals (antiderivatives):

```
≫  F = int(f)
```

and definite integrals:

```
≫  int(f,0,2*pi)
```

To change a symbolic answer into a numerical answer, use the `double` command which stands for *double precision*, (not times 2):

```
≫  double(ans)
```

Note that some antiderivatives cannot be found in terms of elementary functions; for some of these the antiderivative can be expressed in terms of special functions:

```
≫  G = int(g)
```

and for others MATLAB does the best it can:

```
≫  int(h)
```

For definite integrals that cannot be evaluated exactly, MATLAB does nothing and prints a warning:

```
≫  int(h,0,1)
```

We will see later that even functions that don't have an antiderivative can be integrated numerically. You can change the last answer to a numerical answer using:

```
≫  double(ans)
```

Plotting a symbolic function can be done as follows:

```
≫  ezplot(f)
```

or the domain can be specified:

```
≫  ezplot(g,-10,10)
≫  ezplot(g,-2,2)
```

To plot a symbolic function of two variables use:

```
≫  ezsurf(k)
```

It is important to keep in mind that even though we have defined our variables to be symbolic variables, plotting can only plot a finite set of points. For intance:

```
≫  ezplot(cos(x^5))
```

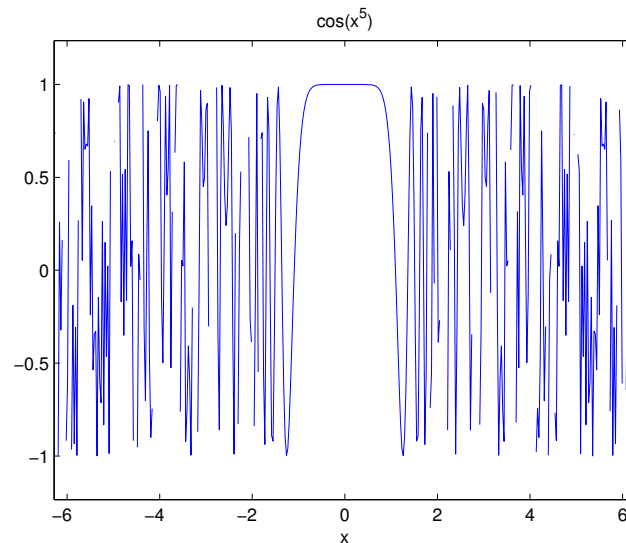will produce the plot in Figure 7.1, which is clearly wrong, because it does not plot enough points.

Figure 7.1: Graph of $\cos(x^5)$ produced by the ezplot command. It is wrong because $\cos u$ should oscillate smoothly between -1 and 1. The problem with the plot is that $\cos(x^5)$ oscillates extremely rapidly, and the plot did not consider enough points.

Other useful symbolic operations

MATLAB allows you to do simple algebra. For instance:

```
≫ poly = (x - 3)^5
≫ polyex = expand(poly)
≫ polysi = simplify(polyex)
```

To find the symbolic solutions of an equation, $f(x) = 0$, use:

```
≫ solve(f)
≫ solve(g)
≫ solve(polyex)
```

Another useful property of symbolic functions is that you can substitute numerical vectors for the variables:

```
≫ X = 2:0.1:4;
≫ Y = subs(polyex,X);
≫ plot(X,Y)
```

Exercises

7.1 Starting from `mynewton` write a well-commented **function** program `mysymnewton` that takes as its input a symbolic function f and the ordinary variables x_0 and n. Let the program take the symbolic derivative f', and then use `subs` to proceed with Newton's method. Test it on $f(x) = x^3 - 4$ starting with $x_0 = 2$. Turn in the program and a brief summary of the results.

7.2 Find a *complicated* function in an engineering or science textbook or website. Make a well-commented **script** program that defines a symbolic version of this function and takes its derivative and indefinite integral symbolically. Plot the function, its derivative and antiderivative on the same plot for the relevant domain of the function. In the comments of the script describe what the function is and properly reference where you got it. Turn in your script and the plot.

Review of Part I

Methods and Formulas

Solving equations numerically:

$f(x) = 0$ — an equation we wish to solve.

x^* — a true solution.

x_0 — starting approximation.

x_n — approximation after n steps.

$e_n = x_n - x^*$ — error of n-th step.

$r_n = y_n = f(x_n)$ — residual at step n. Often $|r_n|$ is sufficient.

Newton's method:

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

Bisection method:

$f(a)$ and $f(b)$ must have different signs.
$x = (a + b)/2$
Choose $a = x$ or $b = x$, depending on signs.
x^* is always inside $[a, b]$.
$e < (b - a)/2$, current maximum error.

Secant method:

$$x_{i+1} = x_i - \frac{x_i - x_{i-1}}{y_i - y_{i-1}} y_i$$

Regula Falsi

- a hybrid between secant and bisection methods.

$$x = b - \frac{b - a}{f(b) - f(a)} f(b)$$

Choose $a = x$ or $b = x$, depending on signs.

Convergence:

Bisection is very slow.
Newton is very fast.
Secant methods are intermediate in speed.
Bisection and Regula Falsi never fail to converge.
Newton and Secant can fail if x_0 is not close to x^*.

Locating roots:

Use knowledge of the problem to begin with a reasonable domain.
Systematically search for sign changes of $f(x)$.
Choose x_0 between sign changes using bisection or secant.

Usage:

For Newton's method one must have formulas for $f(x)$ and $f'(x)$.
Secant methods are better for experiments and simulations.
Bisection and *Regula Falsi* are slower, but keep the root within the current bounds.

Matlab

Commands:

```
v = [0 1 2 3]
```
....Make a row vector.
```
u = [0; 1; 2; 3]
```
....Make a column vector.
```
w = v'
```
.... Transpose: row vector $\leftrightarrow$ column vector
```
x = linspace(0,1,11)
```
......................................Make an evenly spaced vector of length 11.
```
x = -1:.1:1
```
.... Make an evenly spaced vector, with increments 0.1.
```
y = x.^2
```
....Square all entries.
```
plot(x,y)
```
.... plot y vs. x.
```
f = @(x) 2*x.^2 - 3*x + 1
```
....Make an anonymous function.
```
y = f(x)
```
....A function can act on a vector.
```
plot(x,y,'*','red')
```
....A plot with options.
```
Control-c
```
.... Stops a computation.

Program structures:

`for ... end` example:

```
for i=1:20
    S = S + i;
end
```

if ... end example:

```
if y == 0
    disp('An exact solution has been found')
end
```

while ... end example:

```
while i <= 20
    S = S + i;
    i = i + 1;
end
```

if ... else ... end example:

```
if c*y>0
    a = x;
else
    b = x;
end
```

Function Programs:

- Begin with the word `function`.

- There are inputs and outputs.

- The outputs, name of the function and the inputs must appear in the first line.
  i.e. `function x = mynewton(f,x0,n)`

- The body of the program must assign values to the outputs.

- Internal variables are not visible outside the function.

- A function program may use variables in the current workspace unless they are inputs.

Script Programs:

- There are no inputs and outputs.

- A script program may use, create and change variables in the current workspace.

Symbolic:

```
syms x y
f = 2*x^2 - sqrt(3*x)
subs(f,sym(pi))
double(ans)
g = log(abs(y)) ............................................. MATLAB uses log for natural logarithm.
```

```
h(x) = compose(g,f)
k(x,y) = f*g
ezplot(f)
ezplot(g,-10,10)
ezsurf(k)
f1 = diff(f,'x')
F = int(f,'x') ................................................... indefinite integral (antiderivative)
int(f,0,2*pi) ............................................................... definite integral
poly = x*(x - 3)*(x-2)*(x-1)*(x+1)
polyex = expand(poly)
polysi = simple(polyex)
solve(f)
solve(g)
solve(polyex)
```