Nonlinear Equations

ChEn 1703

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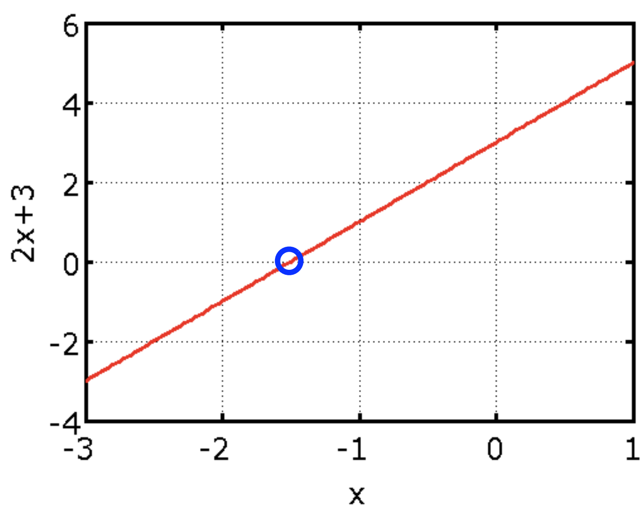
Linear vs. Nonlinear Equations

Linear Equations

$$y = ax + b$$

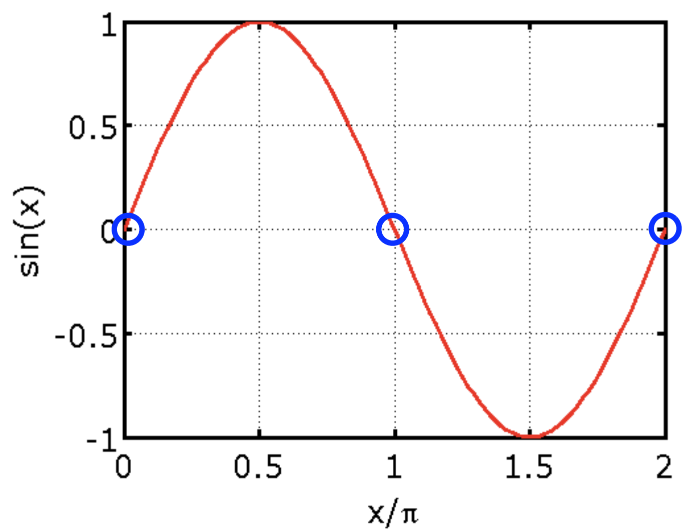
- Has a single, unique solution.
- Can be solved directly (analytically)



Nonlinear Equations

$$y = \sin(x) \qquad y = \sum_{i=1}^{n} a_i x^i$$

- May have 0...many solutions
- Sometimes cannot be solved analytically.
- Usually, numerical solutions are *iterative*, and require a *starting guess* for the solution.



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Polynomials

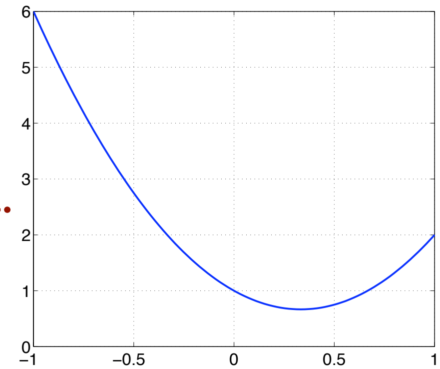
Any polynomial may be written as: $p(x) = \sum_{i=0}^{n} a_i x^i$

Example: n=3 $f(x) = \sum_{i=0}^{n} a_i x^i = a_0 + a_1 x + a_2 x^2 + a_3 x^3$

- **`roots`**`(coef)`
  - provides ALL roots of the polynomial (even imaginary ones).
- `coef` - vector of length $n+1$ containing a_i values in *descending* order
  - coefficient of highest power is first (a_n)
  - constant is last (a_0).

Example: find the roots of $y = 3x^2 - 2x + 1$
Check your answer using the quadratic formula.

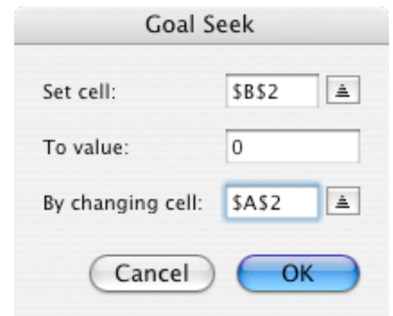
What do we expect?



Single Nonlinear Equations - Excel

- Define a cell for x.
- Define a cell to calculate $f(x)$.
- Use Goal Seek (Tools→Goal Seek)
  - Choose the value you want to set the cell to (0)
  - Choose the cell that you want to change (x)

	A	B
1	x	3x^2-2x-1
2	1	0



<u>Example</u>: find the roots of $y = 3x^2 - 2x + 1$

<u>Example</u>: find the roots of $y = 3x^2 - 2x - 1$

<u>Example</u>: find the roots of $f(x) = \sin(10x^3)\exp\left(-x^2\right)$

Use starting guess of 0.1, 0.35, 0.36, 0.75

Single Nonlinear Equations - MATLAB

use for m-file functions	use for built in functions	use for anonymous functions
`fzero('fun',xo)`	`fzero(@fun,xo)`	`fzero(f,xo)`

- Looks for the root (zero) of `fun` near `xo`.
- `fun` refers to a function that takes a value `x`, returns the function value, $f(x)$.
- `xo` is the starting guess for the solver.
- Can use this for nonlinear regression (could also use for linear regression...)

Steps to Solve a Nonlinear Equation

1. Define the function you are to solve & write it in residual form $f(x)=0$.
2. Write a matlab function to calculate the value of $f(x)$ given x.
3. Choose an initial guess as best as you can.
4. Use **`fzero`** to solve the problem.

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Functions with Parameters

$y = x^a$ →

```
function y = myfun(a,x)
y = x.^a;
```

What value of x gives y=5 when a=-1.2?

1. Create an "anonymous function"
   - `tmpfun=@(x) (myfun(-1.2,x)-5)`
   - Creates a new function called "`tmpfun`" that is only a function of x. This function calls `myfun` with a=-1.2.
2. Use **`fzero`** on this new function
   - `xroot=fzero(tmpfun,1.0);`

```
clear; clc; close all;
a = -1.2;

% create an anonymous function using
% myfun with a=-1.2.  Set up for use
% with a solver to determine where it
% is equal to 5.
tmpfun = @(x) (myfun(a,x)-5);

% determine the solution
xroot = fzero(tmpfun,1.0);

% plot the results
x = logspace(-2,1);
loglog(x,myfun(a,x),'k-', ...
   xroot,myfun(a,xroot),'ro', ...
   x,x*0.0+5,'r-');

% put the value of the root on the plot
text(xroot,10,strcat('x='num2str(xroot)))
```

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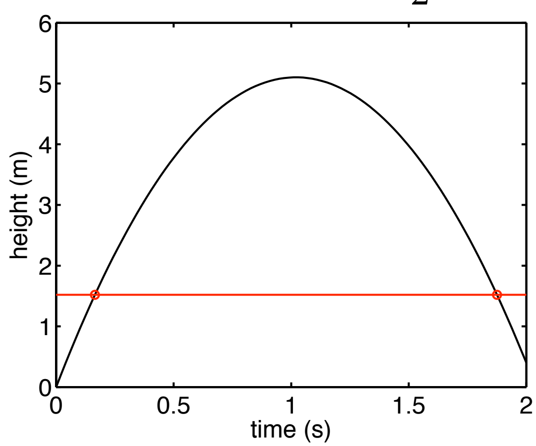
Functions with Parameters

$$h = h_0 + v_0 t + \frac{1}{2}at^2$$




```
function h = height_accelerate( ho, vo, a, t )
h = ho + vo*t + 0.5*a*t.^2;
```

General Function: find t to make $r(t)=0$.

$$r(t) = h_0 - h + v_0 t + \frac{1}{2}at^2$$

Polynomial: find t to make $p(t)=0$.

$$p(t) = h_0 - h + v_0 t + \frac{1}{2}at^2$$

```
clear; clc; close all;

ho = 0.0;  % initial height (m)
vo = 10.0; % initial velocity (m/s)
a = -9.8;  % acceleration m/s^2
h = 1.52;  % find t when we are at this h

% Create a temporary function to use with
% fsolve. We need to make a function that
% has time as its only argument.
hsolve=@(t)(height_accelerate(ho,vo,a,t)-h);

t1 = fzero(hsolve,1.0);
t2 = fzero(hsolve,3.0);

% set the polynomial coefficients and
% solve for roots of the polynomial
tt = roots( [a/2,vo,ho-h] )
```

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Functions with Parameters

$$\beta \equiv \frac{A}{LV_0}\left(1+\frac{V_0}{V_L}\right)$$

At z=0, c_A is given by $c_A = c_A^\infty + \left(c_A^\circ - c_A^\infty\right)\exp\left(-\beta D_A (t-t_\circ)\right)$

c_A	Concentration of "A" - mol/m^3
c_A°	Concentration of "A" at t=$t_\circ$
c_A^∞	Concentration of "A" at equilibrium ($t\rightarrow\infty$)
D_A	Diffusivity of "A" - m^2/s

1. Create a function to calculate c_A.
2. Given β=0.01 m^{-2}, $c_A{}^\circ$=9 mol/m^3, $c_A{}^\infty$=1 mol/m^3, and D_A=0.1 m^2/s, when will c_A=2 mol/m^3?