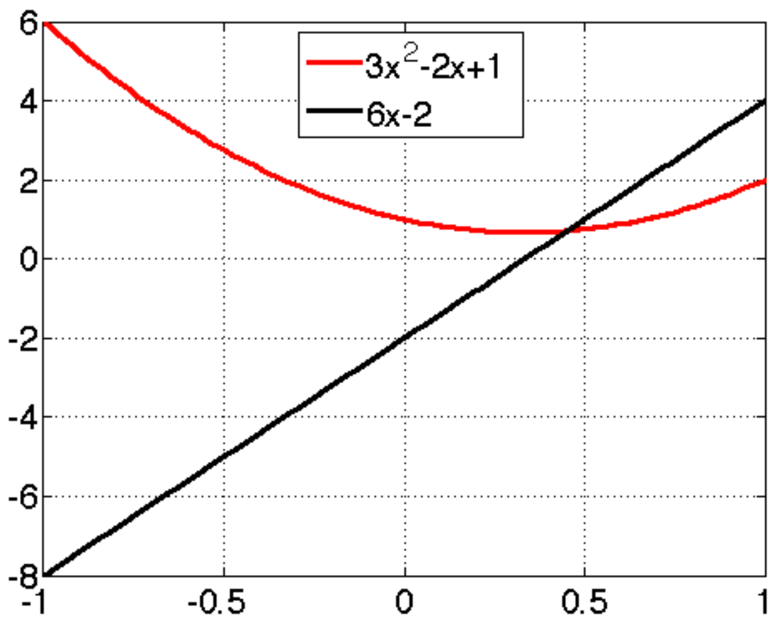
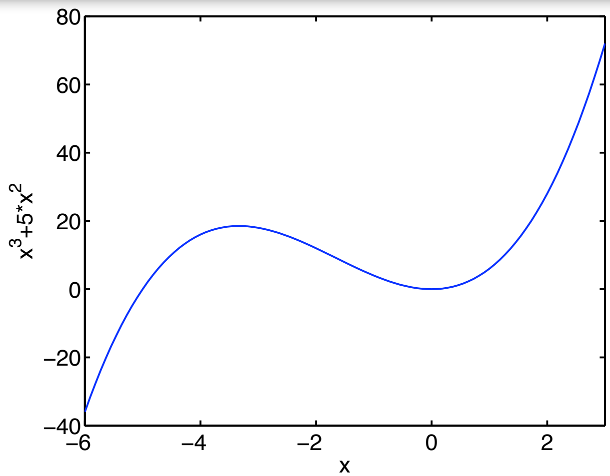
Minimizing & Maximizing Functions

Nonlinear functions may have zero to many minima and maxima.

Example: find the minimum of $y = 3x^2 - 2x + 1$



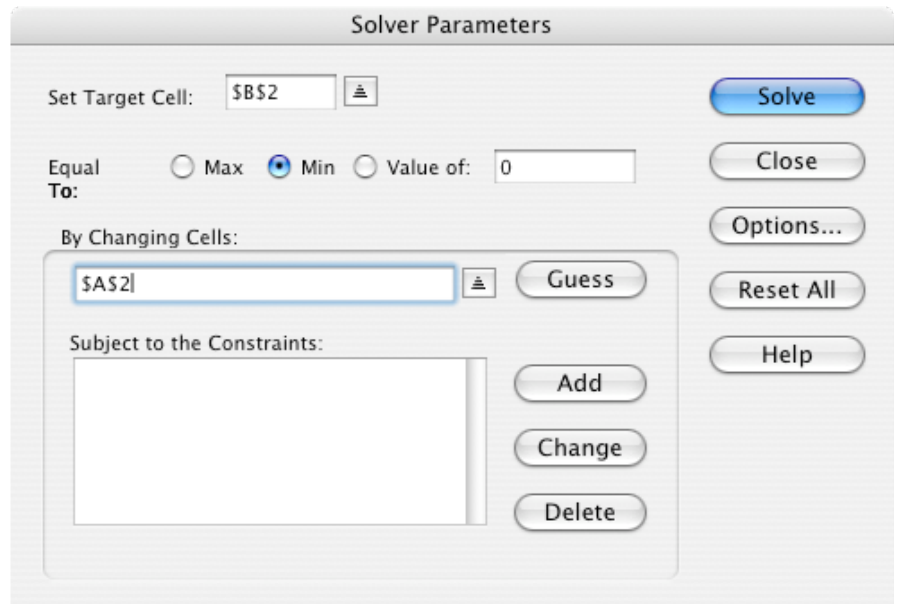
- Minima & maxima occur in functions where the *slope* changes sign (i.e. where the slope is zero).
- Local vs. Global min & max.
- Polynomials: we can find all min & max (global & local)
- General functions: iterative procedure; may only find local min/max...



Min & Max of Functions - Excel

	A	B
1	x	$3x^2$-2x-1
2	0.33	-1.333333333

1. Define a cell containing the independent variable (x)
2. Define a cell containing the function value at x, $f(x)$.
3. Choose Tools→Solver
4. Select the target cell to be $f(x)$.
5. Set "By Changing Cells" to be x.
6. Choose either max or min
7. Click "solve"



NOTE: You can also use solver to *solve* a nonlinear equation (choose to set target cell to a value rather than min/max).

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Min & Max of Functions - MATLAB

Minimization

1. Define a MATLAB function to evaluate $f(x)$ given x.
2. Obtain the minimum using `fmin=fminsearch(fun,x0)`

Maximization

1. Define a MATLAB function to evaluate $-f(x)$ given x.
2. Obtain the minimum using `fmax=fminsearch(fun,x0)`

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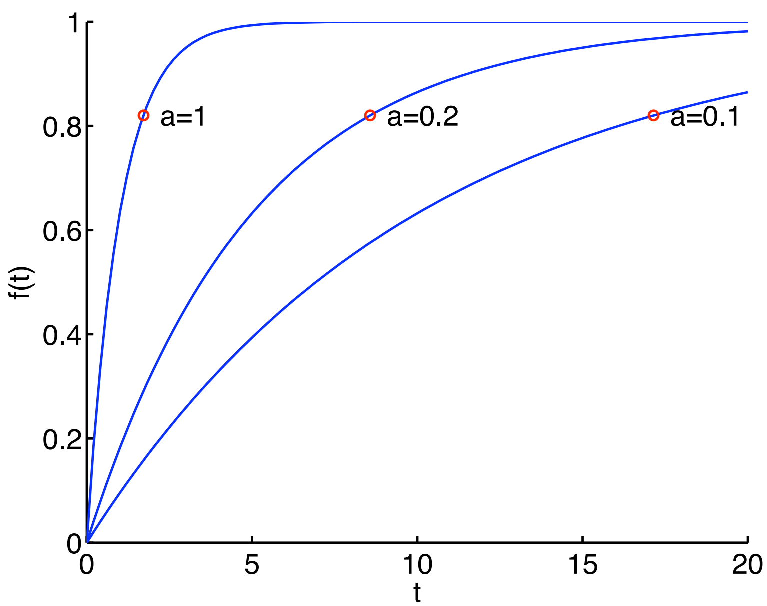
Many Nonlinear Equations (uncoupled)

$f(t) = 1 - \exp(-at)$ Find when $f(t)$=0.82 for a=[0.1 0.2 1].

```
function f = myExpFun(a,x)
f=1-exp(-a*x);
```




```
clear; clc; close all;

a = [0.1 0.2 1];
f = 0.82;
figure; hold on;

for i=1:length(a)
   res=@(t)( myExpFun(a(i),t) - f);
   tanswer = fzero(res,0.1);
   fanswer = myExpFun(a(i),tanswer);
   tt=linspace(0,20);
   plot(tt,myExpFun(a(i),tt),'b-',...
      tanswer,fanswer,'ro' );
   text( tanswer+0.5,...
         fanswer,...
         strcat('a=',num2str(a(i))) );
end

hold off;
xlabel('t'); ylabel('f(t)');
```

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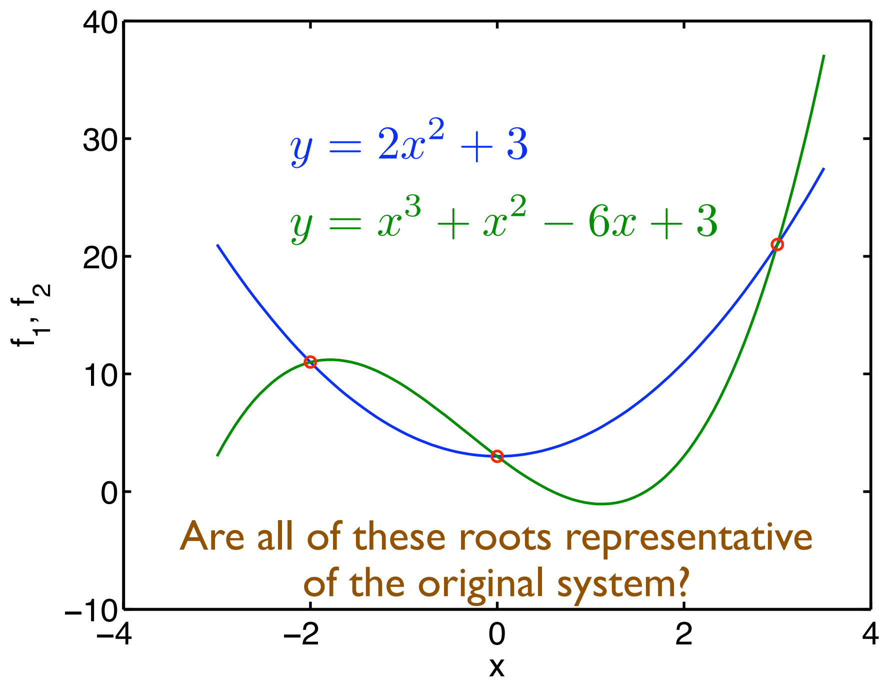
Nonlinear Systems of Equations

Example:
find the solution of the equations:

$$x = \sqrt{\frac{y-3}{2}}$$
$$y = x^3 + x^2 - 6x + 3$$

- Solve analytically...
- What condition(s) are we looking for, and how do we express these mathematically?
- Solve this using Excel
- Solve this using MATLAB



$$r_1 = x - \sqrt{\frac{y-3}{2}}$$
$$r_2 = y - x^3 - x^2 + 6x - 3$$

Nonlinear Systems - MATLAB

`x=fsolve(fun,xo)`

- Solves for zero of `fun` near `xo`.
- `x` and `xo` are vectors; `fun` takes a vector and returns the residual vector.
- if `fun` takes a scalar (vector of length 1) then this behaves like **`fzero`**...
- Requires the "optimization" toolbox - included in the student version...

```
function res = nonlinSysDemo(X)
% x=sqrt((y-3)/2)
% y=x^3+x^2-6x+3
%
% X(1) is x
% X(2) is y

if ( max(size(X)) ~= 2 )
   error('Invalid use of function nonlinSysDemo');
end

x = X(1);
y = X(2);
res = [ x-sqrt((y-3)/2); y-(x^3+x^2-6*x+3) ];
```

```
xyguess = [1 10];
xy = fsolve('nonlinSysDemo',xyguess);
```

```
>> fsolve('nonlinSysDemo',[0,0])
Maximum number of function evaluations reached:
 increase options.MaxFunEvals.

ans =

   0.0000 - 0.0000i   3.0000 - 0.0000i
```

```
>> fsolve('nonlinSysDemo',[10,30])
Optimization terminated: first-order optimality is less than options.TolFun.

ans =

    3.0000   21.0000
```

```
>> fsolve('nonlinSysDemo',[-10,3])
Optimizer appears to be converging to a point which is not a root.
 Norm of relative change in X is less than max(options.TolX^2,eps) but
 sum-of-squares of function values is greater than or equal to sqrt(options.TolFun)
 Try again with a new starting guess.

ans =

  -3.0393 + 0.0043i   2.2033 + 0.0000i
```

Regression Revisited

Linear Least-Squares Regression:

- solve a system of linear equations for the parameters.

Can also formulate this as a optimization problem:

- pick the best value of the parameters to maximize R^2 value.
- pick best value of the parameters to minimize sum of squared errors.
- works for problems where parameters enter linearly or nonlinearly.

$\hat{\phi}_i$ Value predicted by the function.

ϕ_i Observed value (data).

$\bar{\phi} = \frac{1}{n}\sum_{i=1}^{n}\phi_i$ Average value of φ

$$R^2 = 1 - \frac{\sum_{i=1}^{n}\left(\phi_i - \hat{\phi}_i\right)^2}{\sum_{i=1}^{n}\left(\phi_i - \bar{\phi}\right)^2}$$

$$\varepsilon = \sum_{i=1}^{n}\left(\phi_i - \hat{\phi}\right)^2$$ sum of squared errors.

Maximize R^2 or minimize ε by changing parameters.

NOTE: These two options are entirely equivalent!

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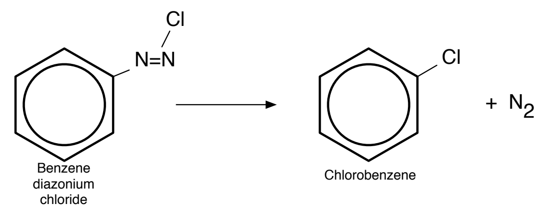
Example - Reaction Rate Constant

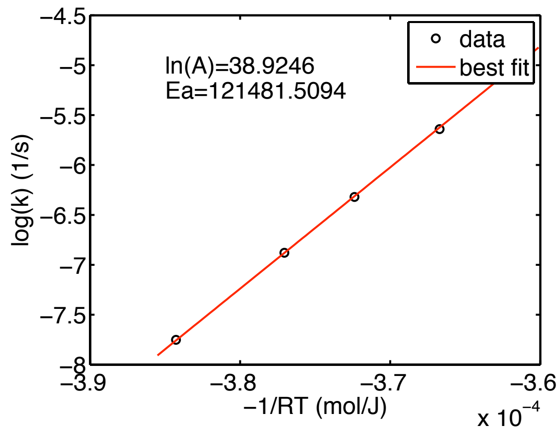
$$k = A \exp\left(\frac{-E_a}{RT}\right)$$

Pre-exponential factor; Activation energy; rate "constant"; Gas constant R=8.314 J/mol-K; Temperature



We rearranged this equation to get the parameters appearing linearly and solved it using the normal equations...

$$\ln(k) = \ln(A) - \frac{E_a}{RT}$$



T (K)	k (1/s)
313	0.00043
319	0.00103
323	0.00180
328	0.00355
333	0.00717

Let's solve this problem as a minimization problem for both the nonlinear and linear forms...

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