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6.094

Introduction to Programming in MATLAB®

Lecture 3: Solving Equations and Curve Fitting

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Outline

- (1) Linear Algebra
- (2) Polynomials
- (3) Optimization
- (4) Differentiation/Integration
- (5) Differential Equations

Systems of Linear Equations

MATLAB makes linear

algebra fun!

Given a system of linear equations

```
> x+2y-3z=5
> -3x-y+z=-8
> x-y+z=0
```

Construct matrices so the system is described by Ax=b

```
» A=[1 2 -3;-3 -1 1;1 -1 1];
» b=[5;-8;0];
```

And solve with a single line of code!

> x is a 3x1 vector containing the values of x, y, and z

- The \ will work with square or rectangular systems.
- Gives least squares solution for rectangular systems. Solution depends on whether the system is over or underdetermined.

More Linear Algebra

Given a matrix

```
» mat=[1 2 -3;-3 -1 1;1 -1 1];
```

- Calculate the rank of a matrix
 - » r=rank(mat);
 - > the number of linearly independent rows or columns
- Calculate the determinant
 - » d=det(mat);
 - > mat must be square
 - ➤ if determinant is nonzero, matrix is invertible
- Get the matrix inverse
 - » E=inv(mat);
 - if an equation is of the form A*x=b with A a square matrix, x=A\b is the same as x=inv(A)*b

Matrix Decompositions

- MATLAB has built-in matrix decomposition methods
- The most common ones are
 - » [V,D]=eig(X)
 - ➤ Eigenvalue decomposition
 - » [U,S,V]=svd(X)
 - Singular value decomposition
 - $\gg [Q,R]=qr(X)$
 - > QR decomposition

Exercise: Linear Algebra

- Solve the following systems of equations:
 - ➤ System 1:
 - > x + 4y = 34
 - > -3x+y=2

- ➤ System 2:
- $\geq 2x-2y=4$
- $\rightarrow -x+y=3$
- > 3x + 4y = 2

Exercise: Linear Algebra

Solve the following systems of equations:

```
➤ System 1:
 > x + 4y = 34 
> -3x + y = 2
> System 2:
 \ge 2x - 2y = 4 
\rightarrow -x+y=3
> 3x + 4y = 2
```

```
A = [1 \ 4; -3 \ 1];
b = [34;2];
» rank(A)
\gg x=inv(A)*b;
A=[2 -2;-1 1;3 4];
b=[4;3;2];
» rank(A)
   > rectangular matrix
 > x1=A b; 
   > gives least squares solution
» A*x1
```

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- (1) Linear Algebra
- (2) Polynomials
- (3) Optimization
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Polynomials

- Many functions can be well described by a high-order polynomial
- MATLAB represents a polynomials by a vector of coefficients
 if vector P describes a polynomial

$$-ax^3+bx^2+cx+d$$

 f f f f
 $P(1)$ $P(2)$ $P(3)$ $P(4)$

- $P=[1 \ 0 \ -2]$ represents the polynomial x^2-2
- $P=[2\ 0\ 0\ 0]$ represents the polynomial $2x^3$

Polynomial Operations

- P is a vector of length N+1 describing an N-th order polynomial
- To get the roots of a polynomial
 - » r=roots(P)

 > r is a vector of length N
- Can also get the polynomial from the roots
 - » P=poly(r)

 > r is a vector length N
- To evaluate a polynomial at a point
 - » y0=polyval(P,x0)
 - > x0 is a single value; y0 is a single value
- To evaluate a polynomial at many points
 - » y=polyval(P,x)
 - > x is a vector; y is a vector of the same size

Polynomial Fitting

- MATLAB makes it very easy to fit polynomials to data
- Given data vectors X=[-1 0 2] and Y=[0 -1 3]

 » p2=polyfit(X,Y,2);

 » finds the best second order polynomial that fits the points
 (-1,0),(0,-1), and (2,3)

 » see help polyfit for more information

 » plot(X,Y,'o', 'MarkerSize', 10);

 » hold on;

 » x = linspace(-2,2,1000);

 » plot(x,polyval(p2,x), 'r--');

Exercise: Polynomial Fitting

Evaluate x^2 over x=-4:0.1:4 and save it as y.

 Add random noise to these samples. Use randn. Plot the noisy signal with . markers

- fit a 2nd degree polynomial to the noisy data
- plot the fitted polynomial on the same plot, using the same x values and a red line

Exercise: Polynomial Fitting

Evaluate x^2 over x=-4:0.1:4 and save it as y.

```
» x=-4:0.1:4;
» y=x.^2;
```

 Add random noise to these samples. Use randn. Plot the noisy signal with . markers

```
» y=y+randn(size(y));
» plot(x,y,'.');
```

fit a 2nd degree polynomial to the noisy data

```
» [p]=polyfit(x,y,2);
```

 plot the fitted polynomial on the same plot, using the same x values and a red line

```
» hold on;
» plot(x,polyval(p,x),'r')
```

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Nonlinear Root Finding

- Many real-world problems require us to solve f(x)=0
- Can use fzero to calculate roots for any arbitrary function
- fzero needs a function passed to it.
- We will see this more and more as we delve into solving equations.
- Make a separate function file

```
» x=fzero('myfun',1)

» x=fzero(@myfun,1)

> 1 specifies a
    point close to
```

the root



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Minimizing a Function

- fminbnd: minimizing a function over a bounded interval
 - » x=fminbnd('myfun',-1,2);
 - > myfun takes a scalar input and returns a scalar output
 - \rightarrow myfun(x) will be the minimum of myfun for $-1 \le x \le 2$
- fminsearch: unconstrained interval
 - » x=fminsearch('myfun',.5)
 - \triangleright finds the local minimum of myfun starting at x=0.5

Anonymous Functions

- You do not have to make a separate function file
- Instead, you can make an anonymous function

```
» x=fzero(@(x)(cos(exp(x))+x^2-1), 1 );
input function to evaluate

» x=fminbnd(@(x) (cos(exp(x))+x^2-1),-1,2);
```

Optimization Toolbox

- If you are familiar with optimization methods, use the optimization toolbox
- Useful for larger, more structured optimization problems
- Sample functions (see help for more info)
 - » linprog
 - ➤ linear programming using interior point methods
 - » quadprog
 - quadratic programming solver
 - » fmincon
 - constrained nonlinear optimization

Exercise: Min-Finding

Find the minimum of the function $f(x) = \cos(4*x).*\sin(10*x).*\exp(-abs(x))$ over the range -pi to pi. Use fminbnd. Is your answer really the minimum over this range?

Exercise: Min-Finding

Find the minimum of the function $f(x) = \cos(4*x).*\sin(10*x).*\exp(-abs(x))$ over the range -pi to pi. Use fminbnd. Is your answer really the minimum over this range?

```
function y = myFun(x)
y=cos(4*x).*sin(10*x).*exp(-abs(x));
fminbnd('myFun', -pi, pi);
```

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Numerical Differentiation

```
MATLAB can 'differentiate' numerically.
 » x=0:0.01:2*pi;
                                          0.4
 y=\sin(x);
 » dydx=diff(y)./diff(x);
     > diff computes the first difference
                                          -0.4
                                          -0.6
Can also operate on matrices
                                          -0.8
 » mat=[1 3 5;4 8 6];
                                               100
                                                    200
                                                        300
                                                             400
                                                                     600
 » dm=diff(mat,1,2)
     ➤ first difference of mat along the 2<sup>nd</sup> dimension, dm=[2 2; 4 -2]
     > see help for more details
```

2D gradient

```
» [dx,dy]=gradient(mat);
```

Numerical Integration

- MATLAB contains common integration methods
- Adaptive Simpson's quadrature (input is a function)
 » q=quad('derivFun',0,10);
 » q is the integral of the function derivFun from 0 to 10
 » q2=quad(@sin,0,pi)
 » q2 is the integral of sin from 0 to pi
 Trapezoidal rule (input is a vector)
 » x=0:0.01:pi;
 » z=trapz(x,sin(x));
 » z is the integral of sin(x) from 0 to pi
 » z2=trapz(x,sqrt(exp(x))./x)

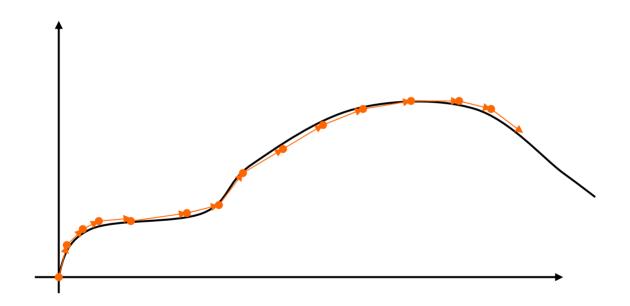
> z2 is the integral of $\sqrt{e^x/x}$ from 0 to pi

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ODE Solvers: Method

 Given a differential equation, the solution can be found by integration:



- > Evaluate the derivative at a point and approximate by straight line
- > Errors accumulate!
- Variable timestep can decrease the number of iterations

ODE Solvers: MATLAB

- MATLAB contains implementations of common ODE solvers
- Using the correct ODE solver can save you lots of time and give more accurate results

» ode23

➤ Low-order solver. Use when integrating over small intervals or when accuracy is less important than speed

» ode45

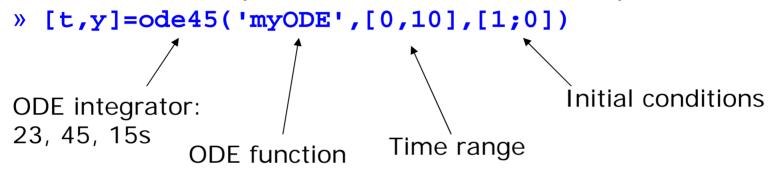
➤ High order (Runge-Kutta) solver. High accuracy and reasonable speed. Most commonly used.

» ode15s

➤ Stiff ODE solver (Gear's algorithm), use when the diff eq's have time constants that vary by orders of magnitude

ODE Solvers: Standard Syntax

To use standard options and variable time step



- Inputs:
 - ➤ ODE function name (or anonymous function). This function takes inputs (t,y), and returns dy/dt
 - ➤ Time interval: 2-element vector specifying initial and final time
 - ➤ Initial conditions: column vector with an initial condition for each ODE. This is the first input to the ODE function
- Outputs:
 - > t contains the time points
 - > y contains the corresponding values of the integrated fcn.

ODE Function

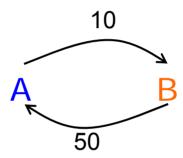
- The ODE function must return the value of the derivative at a given time and function value
- Example: chemical reaction
 - > Two equations

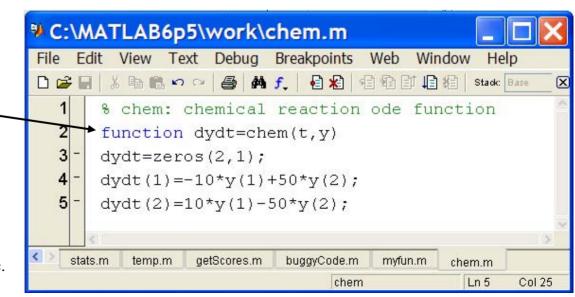
$$\frac{dA}{dt} = -10A + 50B$$

$$\frac{dB}{dt} = 10A - 50B$$

- ➤ ODE file:
 - y has [A; B]
 - dydt has
 [dA/dt;dB/dt]

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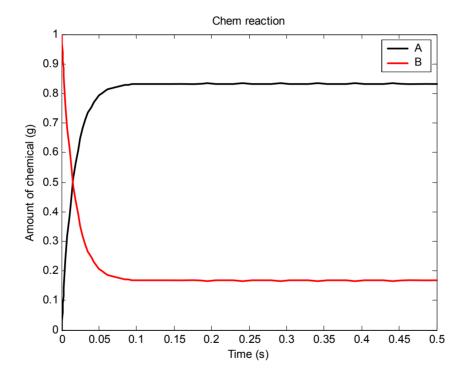


ODE Function: viewing results

To solve and plot the ODEs on the previous slide:

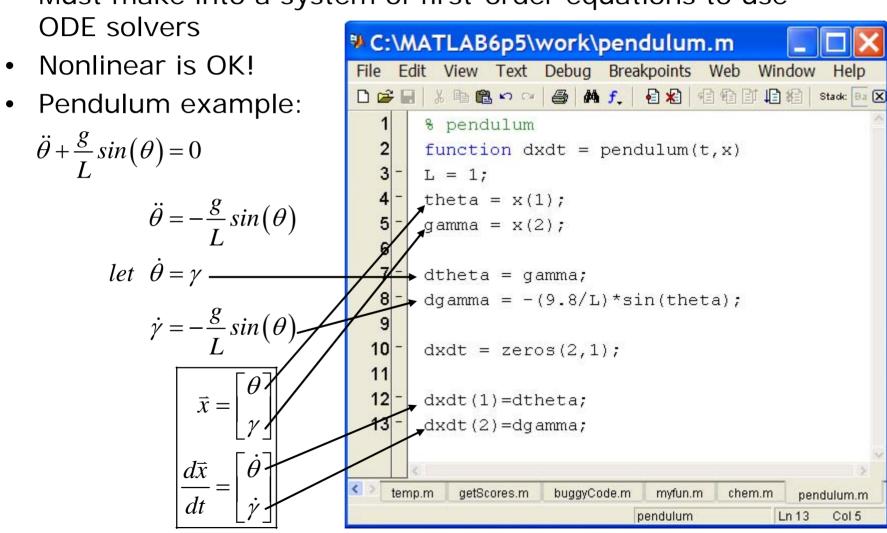
ODE Function: viewing results

The code on the previous slide produces this figure



Higher Order Equations

Must make into a system of first-order equations to use



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Plotting the Output

We can solve for the position and velocity of the pendulum:

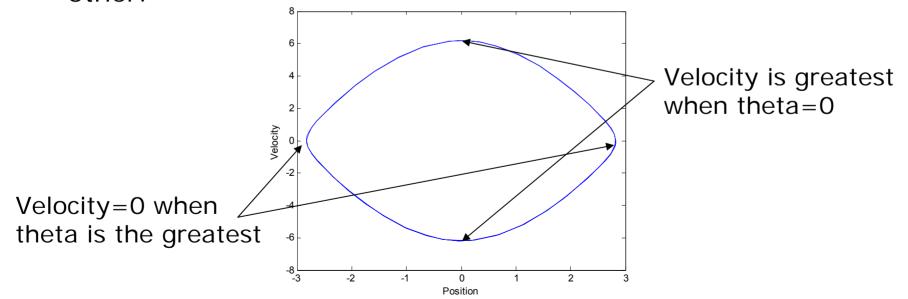
```
» [t,x]=ode45('pendulum',[0 10],[0.9*pi 0]);
         > assume pendulum is almost vertical (at top)
     » plot(t,x(:,1));
     » hold on;
     » plot(t,x(:,2),'r');
     » legend('Position','Velocity');
                                            Position
                                            Velocity
                                                        Velocity (m/s)
Position in terms of
angle (rad)
                     -2
                     -4
```

Plotting the Output

Or we can plot in the phase plane:

```
» plot(x(:,1),x(:,2));
» xlabel('Position');
» yLabel('Velocity');
```

 The phase plane is just a plot of one variable versus the other:



ODE Solvers: Custom Options

- MATLAB's ODE solvers use a variable timestep
- Sometimes a fixed timestep is desirable

```
» [t,y]=ode45('chem',[0:0.001:0.5],[0 1]);
```

- > Specify the timestep by giving a vector of times
- > The function will be evaluated at the specified points
- ➤ Fixed timestep is usually slower (if timestep is small) and possibly inaccurate (if timestep is too large)
- You can customize the error tolerances using odeset

```
» options=odeset('RelTol',1e-6,'AbsTol',1e-10);
```

- » [t,y]=ode45('chem',[0 0.5],[0 1],options);
 - ➤ This guarantees that the error at each step is less than RelTol times the value at that step, and less than AbsTol
 - ➤ Decreasing error tolerance can considerably slow the solver
 - > See doc odeset for a list of options you can customize

Exercise: ODE

 Use ODE45 to solve this differential equation on the range t=[0 10], with initial condition y(0) = 10: dy/dt=-t*y/10.
 Plot the result.

Exercise: ODE

 Use ODE45 to solve this differential equation on the range t=[0 10], with initial condition y(0) = 10: dy/dt=-t*y/10.
 Plot the result.

```
» function dydt=odefun(t,y)
» dydt=-t*y/10;

» [t,y]=ode45('odefun',[0 10],10);
» plot(t,y);
```

End of Lecture 3

- (1) Linear Algebra
- (2) Polynomials
- (3) Optimization
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We're almost done!



Issues with ODEs

- Stability and accuracy
 - ➤ if step size is too large, solutions might blow up
 - ➤ if step size is too small, requires a long time to solve
 - > use odeset to control errors
 - decrease error tolerances to get more accurate results
 - increase error tolerances to speed up computation (beware of instability!)
- Main thing to remember about ODEs
 - ➤ Pick the most appropriate solver for your problem
 - ➤ If ode45 is taking too long, try ode15s