Introduction to Scientific Computing

Differentiation Integration



Computational Calculus

•The derivative for a function y(x)

$$\left. \frac{dy}{dx} \right|_{x_0} = \lim_{\Delta x \to 0} \frac{y(x_0 + \Delta x) - y(x_0)}{\Delta x}$$

Two possible approximations

$$\left. \frac{dy}{dx} \right|_{x_0} \approx \frac{y(x_0 + \Delta x) - y(x_0)}{\Delta x}$$

$$\frac{dy}{dx}\bigg|_{x_0} \approx \frac{y(x_0 + \Delta x) - y(x_0 - \Delta x)}{2\Delta x}$$

Accuracy of approximations

Taylor series expansion

$$y(x_0 + \Delta x) = y(x_0) + y'(x_0)\Delta x + \frac{1}{2}y''(x_0)\Delta x^2 + \frac{1}{6}y'''(x_0)\Delta x^3 + \dots$$
$$y(x_0 - \Delta x) = y(x_0) - y'(x_0)\Delta x + \frac{1}{2}y''(x_0)\Delta x^2 - \frac{1}{6}y'''(x_0)\Delta x^3 + \dots$$

Two approximations

$$y'(x_0) = \frac{y(x_0 + \Delta x) - y(x_0)}{\Delta x} - \frac{1}{2}y''(x_0)\Delta x + \dots$$

$$= \frac{y(x_0 + \Delta x) - y(x_0)}{\Delta x} + O(\Delta x)$$

$$y'(x_0) = \frac{y(x_0 + \Delta x) - y(x_0 - \Delta x)}{2\Delta x} + O(\Delta x^2)$$

Choosing Δx

- •If Δx is too large the approximation will suffer.
- ·If Δx is too small we can run into numerical precision issues.

L12.m differentiate.m fn1.m

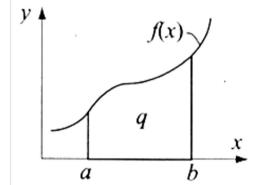
•MATLAB diff(x) function



Numerical Integration

Approximating definite integrals

$$q = \int_{a}^{b} f(x) dx = \lim_{\Delta x \to 0} \left(\sum_{x=a}^{x=b} f(x) \Delta x \right)$$



- •Function is *constant* over each interval
- Function varies linearly over each interval
- Trapezoidal Rule
- Function varies quadratically over each interval
- · Simpson's quadrature rule.
- MATLAB quad function

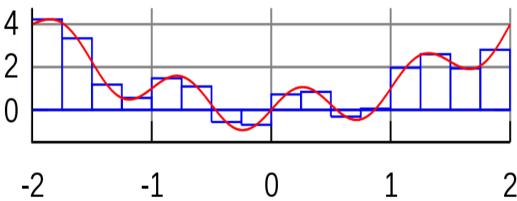
Approximating the area under the curve

•Let y be an array containing = f(x) over the interval

y = f(xmin:dx:xmax)

$$A = \int_{x_{\min}}^{x_{\max}} f(x) dx \approx y_1 \Delta x + y_2 \Delta x + y_3 \Delta x + \dots + y_{n-1} \Delta x$$

$$A \approx \Delta x \sum_{i=1}^{n-1} y_i$$



Approximating the area under the curve

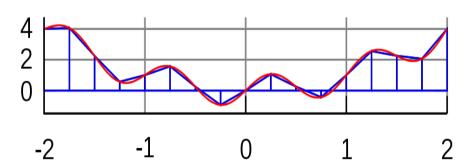
•Let y be an array containing = f(x) over the interval

y = f(xmin:dx:xmax)

Trapezoidal Approximation, integrate.m

$$A = \int_{x_{-1}}^{x_{\text{mex}}} f(x) dx \approx (y_1 + y_2) \frac{\Delta x}{2} + (y_2 + y_3) \frac{\Delta x}{2} + (y_{n-1} + y_n) \frac{\Delta x}{2}$$

$$A \approx \frac{\Delta x}{2} \left(y_1 + y_n + 2 \sum_{i=2}^{n-1} y_i \right)$$



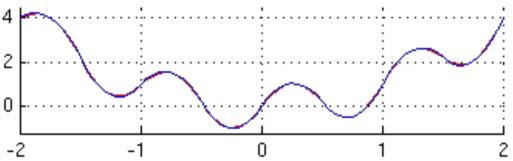
Approximating the area under the curve

•Let y be an array containing = f(x) over the interval

y = f(xmin:dx:xmax)

·Simpson's rule, simpson.m

$$A \approx \frac{h}{3} \left(y_1 + y_n + 4 \sum_{i=1}^{n-1} y_{2i} + 2 \sum_{i=1}^{n} y_{2i-1} \right), \quad h = \frac{x_{\text{max}} - x_{\text{min}}}{2n}$$



Dynamical Systems



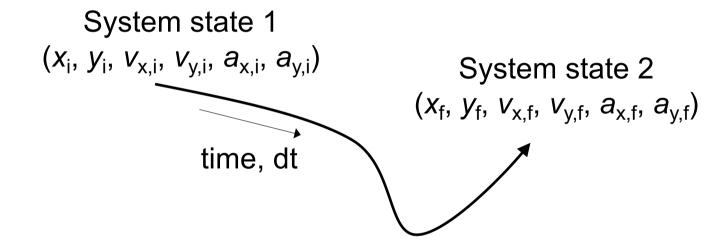
Dynamical systems

- •Dynamical systems are any systems governed by transitions from one state to another state
- •Most often, in physical systems, time (t) guides the trajectory of the system



Dynamical systems

•Discrete analysis of dynamical systems is tackled by analyzing the transition from a current state to a new state



Dynamical systems

•These systems are governed by differential equations that tell us how the state of the system changes over time

$$\frac{dx}{dt} = v_x \qquad \frac{dv_x}{dt} = a_y$$

$$\frac{dy}{dt} = v_y \qquad \frac{dv_y}{dt} = a_y$$

Baseball.m

Computational simulation of dynamical systems

In order to simulate these systems on a computer, we compute the state of the system at evenly spaced points in time

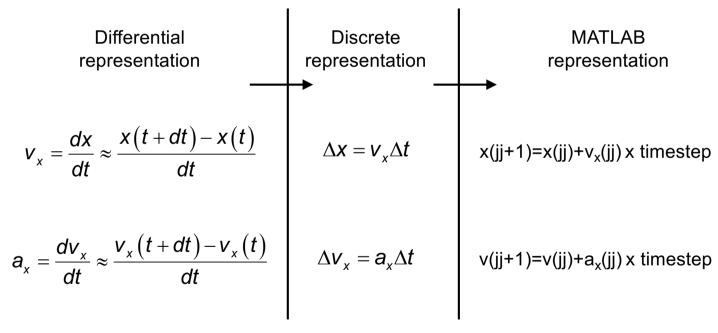
e.g. t = 0.1, 0.2, 0.3, ... seconds (aka dt = 0.1 sec)

- •The general computational method is, at each instant in time,
- Feed in the current state of the system (jj)
- Compute next state of the system (jj+1)



Computational simulation of dynamical systems

•Time is discretized by breaking up the dynamic equations into the current state and the next state often using first order approximations



Discretizing Time

•In our program the differential equations take on the form of expressions which we use to compute the next state as a function of the current state.

In our example

$$\frac{dx}{dt} \approx \frac{x(t+dt)-x(t)}{dt} = v_x \qquad x(t+dt) = x(t) + vx(t) *dt$$

$$\frac{dy}{dt} \approx \frac{y(t+dt)-y(t)}{dt} = v_y \qquad y(t+dt) = y(t) + vy(t) *dt$$

$$\frac{dv_x}{dt} \approx \frac{v_x(t+dt)-v_x(t)}{dt} = a_x = 0 \qquad vx(t+dt) = vx(t)$$

$$\frac{dv_y}{dt} \approx \frac{v_y(t+dt)-v_y(t)}{dt} = a_y = -g \qquad vy(t+dt) = vy(t) - g*dt$$

BaseballSimulator.m



Model with viscous drag

•Viscous drag adds another acceleration to the ball which is proportional to the balls velocity and acts to slow it down, *i.e.* -c*(vx, vy) where c is the viscous drag coefficient.

$$a_{x} = \frac{f_{x}}{m} = -c \cdot v_{x}$$

$$a_{y} = \frac{f_{y}}{m} = -c \cdot v_{y} - g$$

·We can account for drag by simply modifying our update equations:

$$x(t+dt) = x(t) + vx(t)*dt$$

 $y(t+dt) = y(t) + vy(t)*dt$
 $vx(t+dt) = vx(t) - c*vx(t)*dt$
 $vy(t+dt) = vy(t) - (g + c*vy(t))*dt$

BaseballSimulatorWithDrag.m

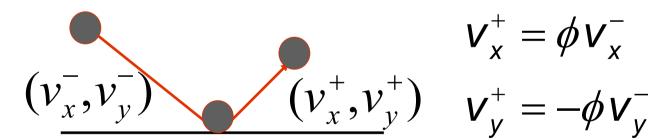


Model with Collisions

- In the real world, we would expect our ball to bounce when it hits the ground.
- In our simulation we can deal with this fact as follows:
- •Detect when the collision occurs by monitoring the height of the ball y(t) and checking when it goes negative
- Determine exactly when the collision occurs (collision time)
- Model the collision
- •Restart the simulation immediately after the collision (dt -collision time)

Modeling a collision

- ·We model a collision with the ground (or a horizontal plane) by flipping the sign of the y velocity
- ·Loss of energy is included via the coefficient of restitution, ϕ , a number between 0 and 1, which relates velocities before and after the collision

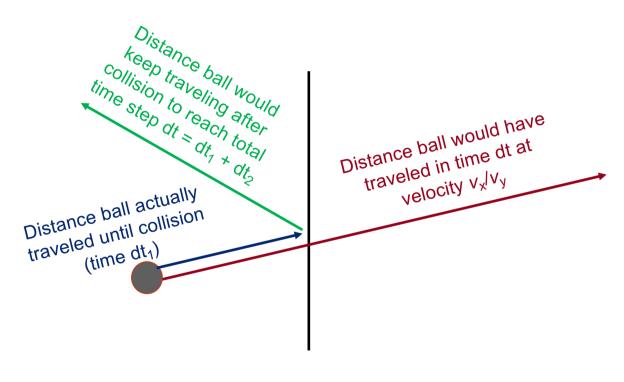


$$\mathbf{V}_{\mathsf{x}}^{\scriptscriptstyle +} = \phi \, \mathbf{V}_{\mathsf{x}}^{\scriptscriptstyle -}$$

$$V_y^+ = -\phi V_y^-$$

Modeling a collision

·How do we deal with finite time steps when modeling a collision?



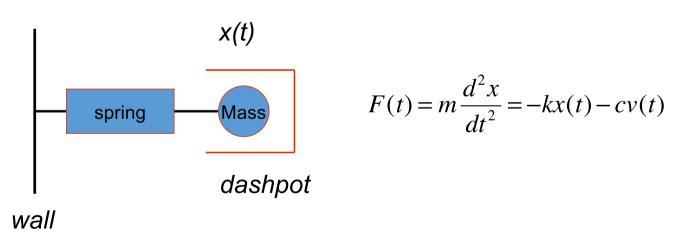
Spring Mass Dashpot System

·Consider a mass connected to a spring and a dashpot

•A classic example of a second order mechanical system used to model car suspension systems, pogo sticks, biomechanical systems etc.

SpringMassDashpot.m

•The force acting on the mass is related to its displacement, x(t), and velocity, v(t), as follows:



Other Examples

Planetary simulation

PlanetarySimulation.m

•Planets in 2D planets.m

•String Simulation
StringSimulation.m



Stochastic Systems

- •There are many situations where we are interested in simulating the behavior of a system driven by random processes.
- •A classic example is Brownian motion named after Robert Brown who studied the motion of pollen particles suspended in a liquid http://en.wikipedia.org/wiki/Brownian motion
- •We can simulate the motion of these particles by updating the position of the particles by a random step at each time instant
- •One can imagine other systems, like the stock market, where the state of the system at one instant depends probabilistically on its state at the previous instant

brownianMotion.m



Chaotic Systems

- •Most of the systems that we are interested in studying are 'well behaved' in the sense that the motions either die off over time or the system settles into a regular pattern or oscillation. However, they don't all do that.
- •Systems that display 'weird' or unpredictable behavior over time are referred to as chaotic and they occur fairly often.

The Lorenz Attractor

•A classic example of chaos theory was described by Edward Lorenz - a meteorologist at MIT

http://en.wikipedia.org/wiki/Lorenz_attractor

He was interested in simulating the behavior of a simple looking set of differential equations

$$\frac{dx}{dt} = \sigma(y - x) \qquad (\sigma, \rho, \beta)$$

$$\frac{dy}{dt} = x(\rho - z) - y$$

$$\frac{dz}{dt} = xy - \beta z$$

Lorenz Attractor

- •Prof. Lorenz observed that his simulation behaved 'weirdly' and never seemed to settle into a coherent pattern
- ·He also observed that small changes in initial conditions would lead to large changes in the final result of the system

This led him to coin the term 'The Butterfly Effect' which helps to explain why it is difficult to predict the weather

Lorenz.m, LorenzAttractor.m



N-body systems

•Another classic example of chaos in nature is due to Poincaré who pointed out that planetary systems with more than 3 bodies can demonstrate chaotic behavior.

http://en.wikipedia.org/wiki/Three-body_problem#Three-body_problem

Planets.m



ODE

Solving Single First Order ODE

$$\frac{dy}{dt} = f(y,t) \text{ for } t_0 \le t \le t_f$$
with $y = y_0$ at $t = t_0$

- Single independent variable t (time)
- Single dependent variable y
- •Solution is a function y=y(t) that satisfies the ODE
- Steps for solving with MATLAB
 - 1. Write in standard form
 - 2. Define function in MATLAB
 - 3. Select method of solution
 - 4. Solve

Numerical solutions to differential equations (Euler)

·Consider

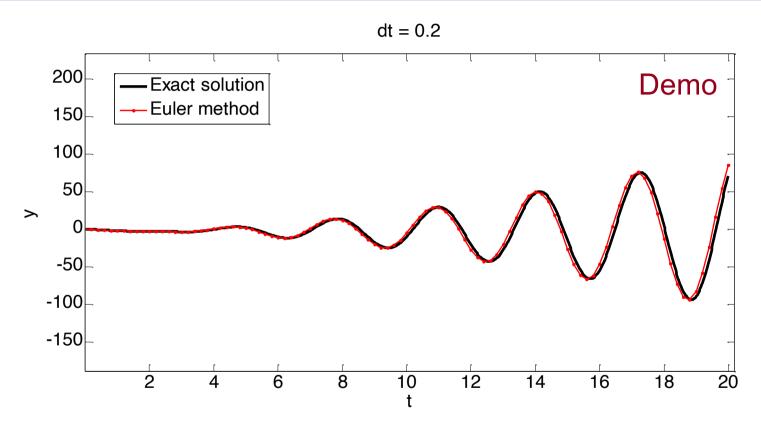
$$\frac{dx(t)}{dt} = f(t,x(t))$$

•A first order approximation for the next state of the system can be constructed using the trajectory of the system (Euler's method)

$$x(t+\Delta t) \approx x(t)+f(t,x(t))\Delta t$$

·However, this simple approximation is often very inaccurate

Visual interpretation of the Euler method



Numerical solutions to differential equations (predictor-corrector)

·Consider

$$\frac{dx(t)}{dt} = f(t, x(t))$$

•A better approximation can be constructed by considering the effective derivative over the entire interval

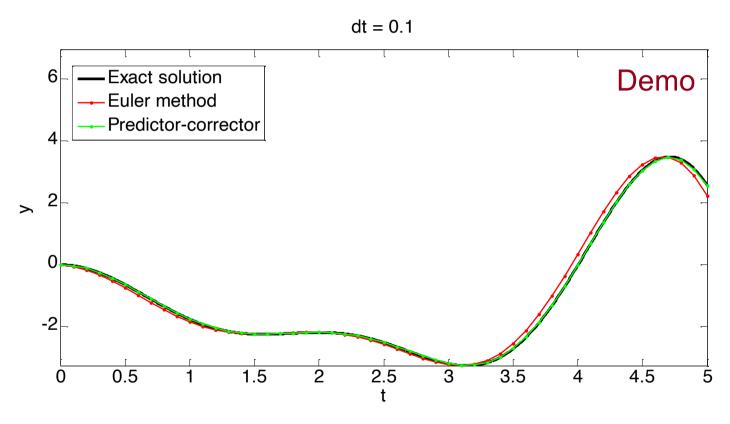
$$x(t + \Delta t) \approx x(t) + 1/2 \times (k_1 + k_2) \Delta t$$

$$k_1 = f(t, x(t))$$

$$k_2 = f(t + \Delta t, x(t) + k_1 \Delta t)$$

•Note that this method uses an estimate for the derivative at the beginning, k_1 , and ending, k_2 , of the interval and increases accuracy of the solution

Visual comparison of the Euler and predictor-corrector methods





Numerical solutions to differential equations (Runge-Kutta)

•Following the logic of the predictor-corrector method, the accuracy of the estimate can be improved by evaluating the derivative at its midpoint

$$x(t + \Delta t) \approx x(t) + 1/6 \times (k_1 + 2k_2 + 2k_3 + k_4) \Delta t$$

$$k_1 = f(t, x(t))$$

$$k_2 = f\left(t + \frac{\Delta t}{2}, x(t) + k_1 \frac{\Delta t}{2}\right)$$

$$k_3 = f\left(t + \frac{\Delta t}{2}, x(t) + k_2 \frac{\Delta t}{2}\right)$$

$$k_4 = f(t + \Delta t, x(t) + k_3 \Delta t)$$

where

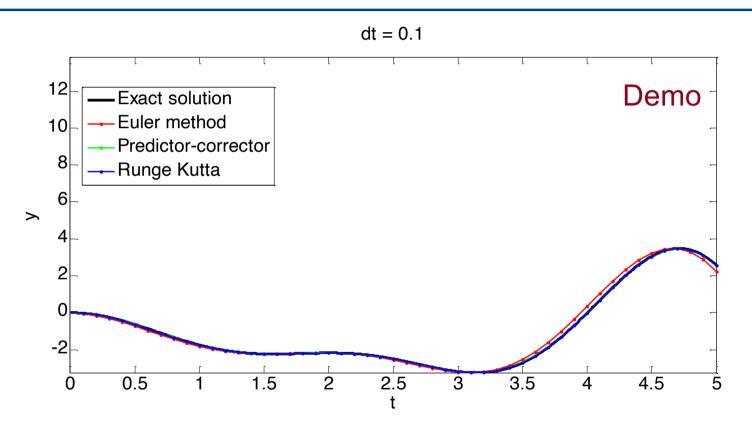
$$\frac{dx(t)}{dt} = f(t,x(t))$$

Numerical solutions to differential equations (Runge-Kutta)

- •Note that in the last slide k_1 corresponds to the derivative at the beginning of the interval, k_2 and k_3 are two estimates for the derivative at the midpoint of the interval, and k_4 is an estimate of the derivative at the end of the interval
- •The example of the last slide would be a Runge-Kutta approximation of rank 4 (RK4)
- •Runge-Kutta ODE solvers of RK23 and RK45 can be accessed with the MATLAB commands ode 23 and ode 45



Visual comparison of the Euler, predictor-corrector, and **Runge Kutta methods**



Numerical accuracy

·Essential Matlab states:

"How do we ever know when we have the 'right' numerical solution?

Well, we don't - the best we can do is increase the accuracy of the numerical method until no further wild changes occur over the interval of interest."

•DEMO of this convergence for cantilever dynamics.



Example: Solving an ODE

·Write in standard form

$$\frac{dy}{dt} = \frac{t^3 - 2y}{t} \quad \text{for } 1 \le t \le 3 \quad \text{with } y = 4.3 \quad \text{at } t = 1$$

- •Define the function in MATLAB dydt
- Select method of solution

```
ode45, ode23, ode113, ode15s, ode23s, ode23t, ode23tb
```

Solve

A simple example

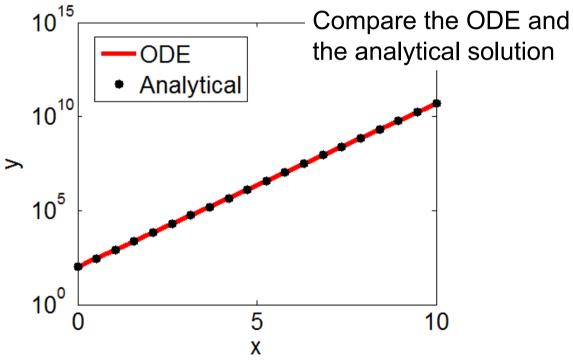
·Lets do this in MATLAB

Generalize the
$$\frac{dy}{dt} = 2y$$
 $\dot{x}_1 = 2x_1$

```
function dx = firstOrderODE(t,x)
dx = 2*x;
Define the ODE
```

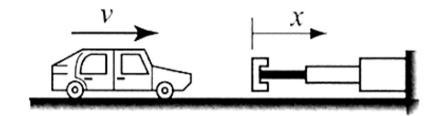
```
% Solve the ODE
[t,x] = ode45(@firstOrderODE,[0 10],[100]);
% Generate values for the analytical solution
tTest = linspace(0,10,20);
xTest = 100*exp(2*tTest);
```

A simple example



Example - Car Crash & Safety Bumper

•Force applied by bumper is a function of the velocity v and displacement x of the front edge according to



$$F = Kv^3(x+1)^3$$

where $K = 30 \text{ s-kg/m}^5$.

Car has mass m=1500kg and hits bumper at 90 km/hr (25 m/s).

Plot velocity of the car as a function of position.

Acceleration:
$$a = -Kv^3(x+1)^3/m$$

Kinematic relationship
$$a = \frac{dv}{dt} = \frac{dv}{dx}\frac{dx}{dt} = \frac{dv}{dx}v$$
 or $\frac{dv}{dx} = -\frac{Kv^2(x+1)^3}{m}$

What is a <u>state space</u> representation?

We take this...

$$\frac{d^{n}y(t)}{dt^{n}} + a_{1}\frac{d^{n-1}y(t)}{dt^{n-1}} + \dots + a_{n-1}\frac{dy(t)}{dt} + a_{n}y(t) = F$$
...and turn it into this
$$\dot{x}(t) = \underline{Ax}(t) + \underline{Bu}(t)$$

Note: this representation is only true for linear ODEs



In other words - say we have an equation of the form

$$\ddot{y} + p\ddot{y} + q\dot{y} + ry = 0$$

$$\dot{y} = something$$

This would be input into MATLAB as a series of differential equations of first order

We start by assigning generalized variables (say x) to derivatives of y of increasing order as such

$$X_1 = y$$

$$X_2 = \dot{y}$$

$$x_2 = \dot{y}$$
$$x_3 = \ddot{y}$$

Next, we rearrange the ODE to get the variable of highest order on the left side of the equation and divide out any coefficients on this variable (if they exist)

$$\ddot{y} = -p\ddot{y} - q\dot{y} - ry$$



Next, we rewrite the derivatives of the generalized variables with respect to each other and the ODE

$$\dot{x}_{1} = x_{2}$$
 $\dot{x}_{2} = x_{3}$
 $\dot{x}_{3} = -px_{3} - qx_{2} - rx_{1}$

Note that the number of linear ODEs corresponds to the order of the original equation

This equation can then be input into a function definition of the ODE for use in MATLAB

```
function xout = thirdOrderODE(t,x)

p = 2;
q = 1.5;
r = 0.1;

dx1 = x(2);
dx2 = x(3);
dx3 = -p*x(3)-q*x(2)-r*x(1);

xout = [dx1; dx2; dx3];
```

Note: time and initial condition serve as inputs

Note: the derivatives of the generalized variables are returned as a column vector



An alternate formulation of the ODE function

```
function xout = thirdOrderODE(t,x)

p = 2;
q = 1.5;
r = 0.1;

dx(1) = x(2);
dx(2) = x(3);
dx(3) = -p*x(3)-q*x(2)-r*x(1);

xout = [dx(1);dx(2);dx(3)];
```

Another alternate formulation of the ODE function

```
function dx = thirdOrderODE(t,x)

p = 2;
q = 1.5;
r = 0.1;

dx = zeros(3,1);
dx(1) = x(2);
dx(2) = x(3);
dx(3) = -p*x(3)-q*x(2)-r*x(1);
```

We can then solve the function by calling the ode45 solver with respect to the ODE function

[t,x] = ode45(@thirdOrderODE,[0 10],[10 1 2])

Row vector of initial conditions x(1) = 10, x(2) = 1, etc.; the number of initial conditions equals the order of the ODE

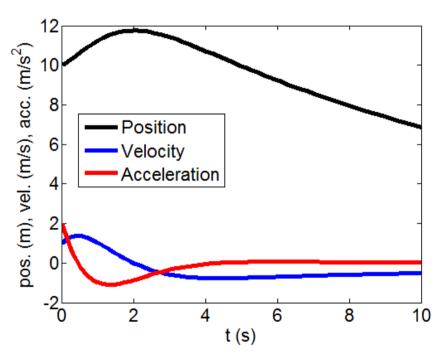
Row vector indicates the start and end time of the solution

	1		1	2	
1	0	1	10	1	
2	0.0155	2	10.0157	1.0301	
	0.0309	3	10.0318	1.0588	
	0.0464	4	10.0484	1.0859	
	0.0618	5	10.0654	1.1116	
	0.1391	6	10.1557	1.2196	
	0.2164	7	10.2531	1.2964	
	0.2937	8	10.3554	1.3458	
	0.3710	9	10.4605	1.3712	
	0.5253	10	10.6721	1.3628	
	0.6796	11	10.8774	1 2930	

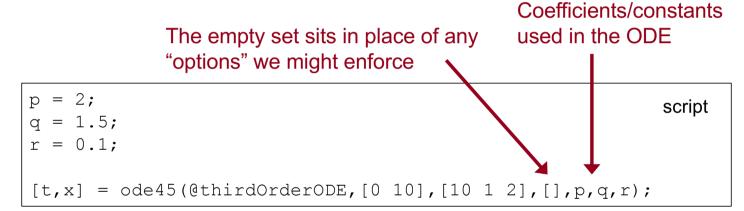
We can then plot the position, velocity, and acceleration of the system

```
p = plot(t,x(:,1),'k-',t,x(:,2),'b-',t,x(:,3),'r-');
set(p,'LineWidth',4)
set(gca,'FontSize',16)
xlabel('t (s)')
ylabel('pos. (m), vel. (m/s), acc. (m/s^2)')
legend('Position','Velocity','Acceleration')
```

The resulting plot



The values of p, q, and r were defined in the ODE function - we can also supply these values when calling the solver



```
function dx = thirdOrderODE(t, x, p, q, r)

dx = zeros(3, 1);

dx(1) = x(2);

dx(2) = x(3);

dx(3) = -p*x(3)-q*x(2)-r*x(1);
```



Systems of differential equations - Lorentz equations and chaos

Consider the following system of Lorenz equations

- This system is representative of chaotic systems in which minor changes to the input result in radically different result (butterfly effect)
- Chaos: When the present determines the future, but the approximate present does not approximately determine the future

$$\frac{dx}{dt} = -\sigma x + \sigma y$$

$$\frac{dy}{dt} = -\rho x - y - xz$$

$$\frac{dz}{dt} = -\beta z + xy$$

Systems of differential equations - Lorentz equations and chaos

How do we convert this system into a MATLAB "friendly" format

$$\frac{dx}{dt} = -\sigma x + \sigma y \qquad x_2 = y$$

$$\frac{dy}{dt} = -\rho x - y - xz$$

$$\frac{dz}{dt} = -\beta z + xy$$

$$x_1 = x$$

$$x_2 = y$$

$$x_3 = z$$

$$\dot{x}_1 = -\sigma x_1 + \sigma x_2$$

$$\dot{x}_2 = -\rho x_1 - x_2 - x_1 x_3$$

$$\dot{x}_3 = -\beta x_3 + x_1 x_2$$

Here, x_1 , x_2 , and x_3 refer to x(1), x(2), and x(3) in MATLAB

```
function dx = lorenz(t,x) function: lorenz sigma = 10; beta = 8/3; nho = 28; Note that dx(1), dx(2), and dx(3) are directly assigned to columns dx = [-sigma*x(1) + sigma*x(2); ... + rho*x(1) - x(2) - x(1) *x(3); ... + rho*x(3) + x(1) *x(2)];
```



Alternate syntax for calling ode 45

```
% Intitial conditions (x1, x2, x3)
x0 = [-8 8 27];

% Time span
tspan = [0 40];

Function declaration as "string"

% Using the ode45 solver to numerically evaluate the ODEs
[t,x] = ode45('lorenz', tspan, x0);
```

Alternate syntax for calling for the function holding the differential equations

```
function dx = lorenz(t,x) function: lorenz sigma = 10; beta = 8/3; rho = 28; The outputs are first established as a 3x1 vector dx = zeros(3,1); dx(1) = -sigma*x(1) + sigma*x(2); dx(2) = rho*x(1) - x(2) - x(1) *x(3); dx(3) = -beta*x(3) + x(1) *x(2);
```

Alternate syntax for calling for the function holding the differential equations

```
function dout = lorenz(t,x)

sigma = 10;
beta = 8/3;
rho = 28;

dx = -sigma*x(1)+sigma*x(2);
dy = rho*x(1)-x(2)-x(1)*x(3);
dz = -beta*x(3)+x(1)*x(2);

dout = [dx;dy;dz];
function: lorenz

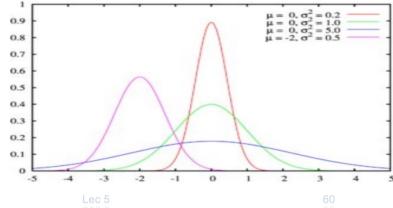
The outputs are combined at the output to a 3x1
vector
```

Random Numbers



Random Numbers

rand	Single random number between 0 and 1		
rand(1,n)	Row vector of n random numbers between 0 and 1		
rand(n)	n x n matrix of random numbers between 0 and 1		
rand(m,n)	m x n matrix of random numbers between 0 and 1		
randperm(n)	Row vector with random permutation of integers 1 through n		
randn(m,n)	m x n matrix of normally distributed random numbers with mean 0 and standard deviation 1		



Random Numbers (cont.)

·Interval (a,b)

$$(b-a)*rand + a$$

•Random integers

```
round (rand) for random 0's and 1's or use
```

round, floor, ceil on a multiple of rand

·Normal distribution mean M and standard deviation S

$$S*randn(m,n) + M$$



- ·Write a function implementing a (pseudo-)random number generator
- **Based on unpredictability of the modulus function** mod(·, ·) when applied to large numbers
- •For instance, $ni+1 = mod(8121 \ ni + 28441, 134456)$
- •Generated numbers are uniformly distributed in range [0,134456)
- For unknown parameters, predicting outcome ni+1 is hard
- ·Use above idea to produce random values in [0,1)
- •Write function that generates one or more random numbers ran in range 0≤ran<1 each time is called, based on equation

```
rani = ni / 134456
```

·Generated numbers depend on initial value n0 called seed



·Problem statement

- •write function rand0 returning an array ran of one or more numbers uniformly distributed in [0, 1)
- •input arguments are (m, n) producing an m×n array or (m) producing an m×m array
- •seed n₀ is chosen or reset by calling function seed

·Input/output

- •seed: integer input, no output
- •rand0: input is one or two integers specifying size of the array, output is the array with random values in [0,1)



·Algorithm description

•Pseudocode for rand0:

```
function ran = random(m,n)

Set n \leftarrow m if second dimension is not supplied

Create output array with "zeros" function

iseed stores the current random-looking integer n<sub>i</sub>

For every row i and every column j

iseed \leftarrow mod (8121 iseed + 28441, 134456)

ran(i,j) \leftarrow iseed/134456
```

•Pseudocode for seed:

```
function seed(new_seed)
new_seed ← round(new_seed)
iseed ← abs(new seed)
```



•Turn algorithm into MATLAB code

- Turning pseudocode to code is straightforward
- Data management issue
- Is there any data shared by the two functions?
- They both need access to the current pseudorandom number iseed
- · Variable iseed will be placed in the global memory so that it may be accessed by both function rand0 and seed

Test functions

- •By resetting seed, produced numbers should repeat
- ·Calculate the average and standard deviation of array and confirm uniform distribution

