Lecture 3 : Solving Equations, Curve Fitting, and Numerical Techniques

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=A\b;
```

  - 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.

Worked Example: Linear Algebra

- Solve the following systems of equations:
  - System 1:

$$x + 4y = 34$$
$$-3x + y = 2$$

```
» A=[1 4;-3 1];
» b=[34;2];
» rank(A)
» x=inv(A)*b;
» x=A\b;
```

  - System 2:

$$2x - 2y = 4$$
$$-x + y = 3$$
$$3x + 4y = 2$$

```
» A=[2 -2;-1 1;3 4];
» b=[4;3;2];
» rank(A)
```

  - rectangular matrix

```
» x=A\b;
```

  - gives least squares solution

```
» error=abs(A*x1-b)
```

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; matrix invertible if det nonzero
- 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 (mostly) the same as x=inv(A)*b
- Get the condition number
  - » `c=cond(mat);` (or its reciprocal: `c = rcond(mat);`)
    - ➢ if condition number is large, when solving A*x=b, small errors in b can lead to large errors in x (optimal c==1)

Matrix Decompositions

- MATLAB has many built-in matrix decomposition methods

- The most common ones are
  - » `[V,D]=eig(X)`
    - ➢ Eigenvalue decomposition
  - » `[U,S,V]=svd(X)`
    - ➢ Singular value decomposition
  - » `[Q,R]=qr(X)`
    - ➢ QR decomposition
  - » `[L,U]=lu(X)`
    - ➢ LU decomposition
  - » `R=chol(X)`
    - ➢ Cholesky decomposition (R must be positive definite)

Exercise: Fitting Polynomials

- Find the best second-order polynomial that fits the points: (-1,0), (0,-1), (2,3).

$$a(-1)^2 + b(-1) + c = 0$$
$$a(0)^2 + b(0) + c = -1$$
$$a(2)^2 + b(2) + c = 3$$

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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

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

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 (least-squares sense) 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 = -3:.01:3;`
  - » `plot(x,polyval(p2,x), 'r--');`

Exercise: Polynomial Fitting

- Evaluate $y = x^2$ for x=-4:0.1:4.

- 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

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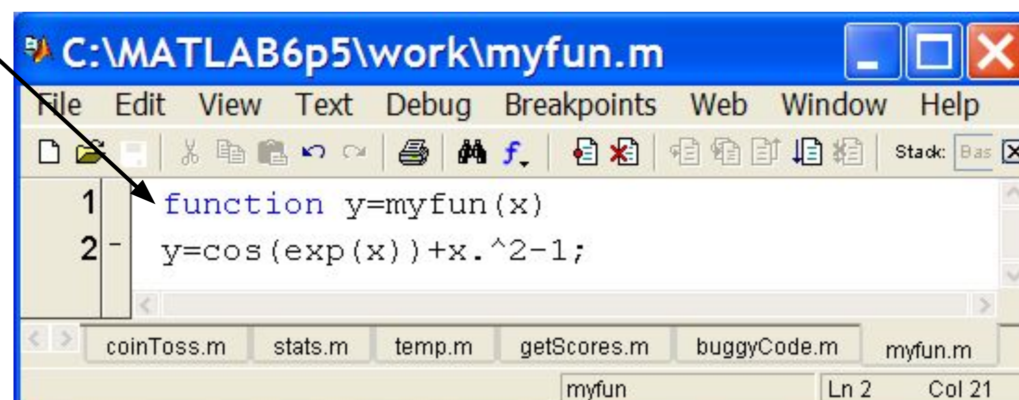
Nonlinear Root Finding

- 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 where you think the root is



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
    - ➢ myfun(x) will be the minimum of myfun for $-1 \leq x \leq 2$
- **fminsearch**: unconstrained interval
  - » `x=fminsearch('myfun',.5)`
    - ➢ finds the local minimum of myfun starting at x=0.5
- Maximize g(x) by minimizing f(x)=-g(x)
- Solutions may be local!

Anonymous Functions

- You do not have to make a separate function file
  - » `x=fzero(@myfun,1)`
    - ➢ What if myfun is really simple?

- 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);`

- Can also store the function handle
  - » `func=@(x) (cos(exp(x))+x.^2-1);`
  - » `func(1:10);`

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 $f(x) = \cos(4x)\sin(10x)e^{-|x|}$ over the range −π to π. Use **fminbnd**.
- Plot the function on this range to check that this is the minimum.

Digression: Numerical Issues

- Many techniques in this lecture use floating point numbers
- **This is an approximation!**

- Examples:
  - » **`sin(pi) = ?`**
  - » **`sin(2 * pi) = ?`**
  - » **`sin(10e16 * pi) = ?`**
    - ➢ Both sin and pi are approximations!

  - » **`A = (10e13)*ones(10) + rand(10)`**
    - ➢ A is nearly singular, poorly conditioned (see **`cond(A)`**)
  - » **`inv(A)*A = ?`**

A Word of Caution

- MATLAB knows no fear!
- Give it a function, it optimizes / differentiates / integrates
  - That's great! It's so powerful!
- Numerical techniques are powerful **but** not magic
- **Beware of overtrusting the solution!**
  - You will get an answer, but it may not be what you want
- Analytical forms may give more intuition
  - Symbolic Math Toolbox

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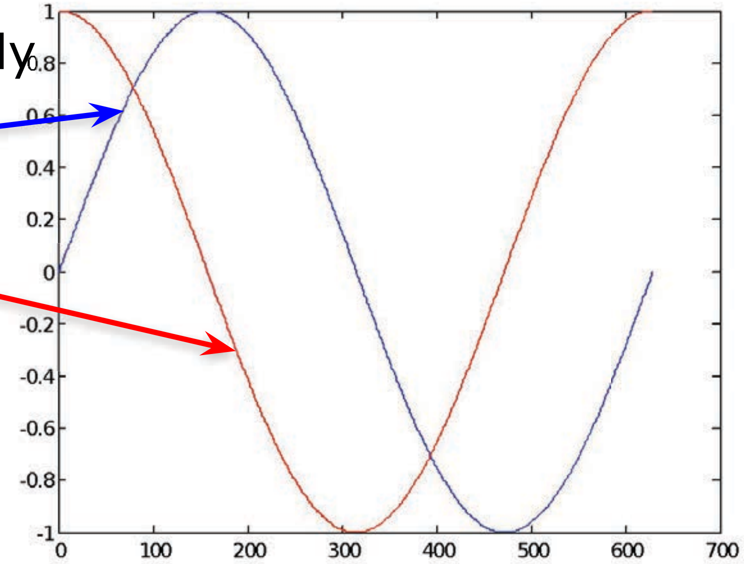
Numerical Differentiation

- MATLAB can 'differentiate' numerically
  - » `x=0:0.01:2*pi;`
  - » `y=sin(x);`
  - » `dydx=diff(y)./diff(x);`
    - ➢ diff computes the first difference



- Can also operate on matrices
  - » `mat=[1 3 5;4 8 6];`
  - » `dm=diff(mat,1,2)`
    - ➢ first difference of mat along the 2nd dimension, dm=[2 2;4 -2]
    - ➢ The opposite of **`diff`** is the cumulative sum **`cumsum`**

- 2D gradient
  - » `[dx,dy]=gradient(mat);`

- Higher derivatives / complicated problems: Fit spline (see **help**)

Numerical Integration

- MATLAB contains common integration methods
- Adaptive Simpson's quadrature (input is a function)
  - » `q=quad('myFun',0,10)`
    - ➢ q is the integral of the function `myFun` from 0 to 10
  - » `q2=quad(@(x) sin(x).*x,0,pi)`
    - ➢ q2 is the integral of `sin(x).*x` 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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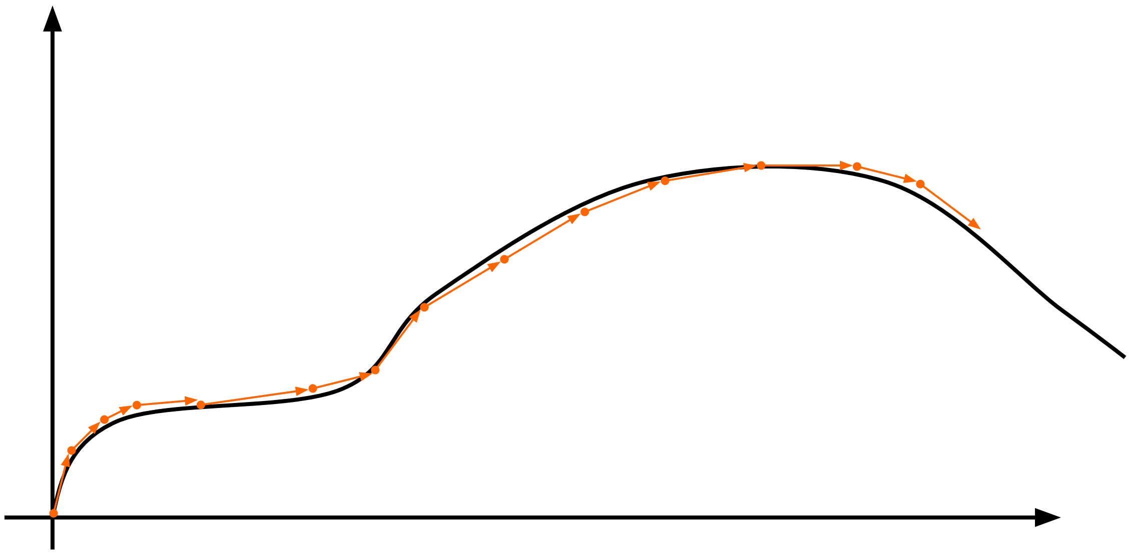
ODE Solvers: Method

- 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

```
» [t,y]=ode45('myODE',[0,10],[1;0])
```

ODE integrator:
23, 45, 15s

ODE function

Time range

Initial conditions

- Inputs:
  - ➢ ODE function name (or anonymous function). This function should take inputs (t,y), and returns dy/dt
  - ➢ Time interval: 2-element vector with initial and final time
  - ➢ Initial conditions: column vector with an initial condition for each ODE. This is the first input to the ODE function
  - ➢ Make sure all inputs are in the same (variable) order
- Outputs:
  - ➢ t contains the time points
  - ➢ y contains the corresponding values of the variables

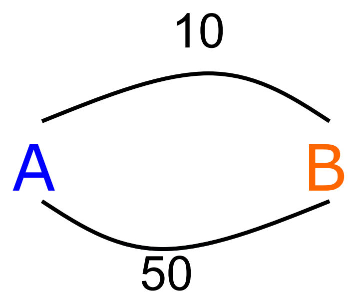
ODE Function

- The ODE function must return the value of the derivative at a given time and function value

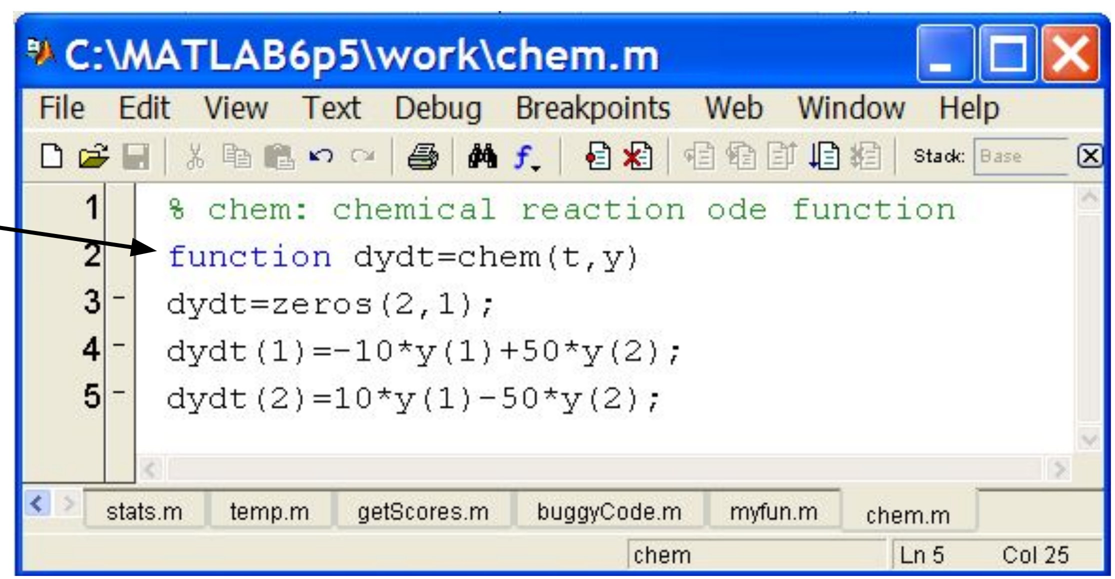
- Example: chemical reaction
  - ➢ Two equations

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

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



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



ODE Function: viewing results

- To solve and plot the ODEs on the previous slide:

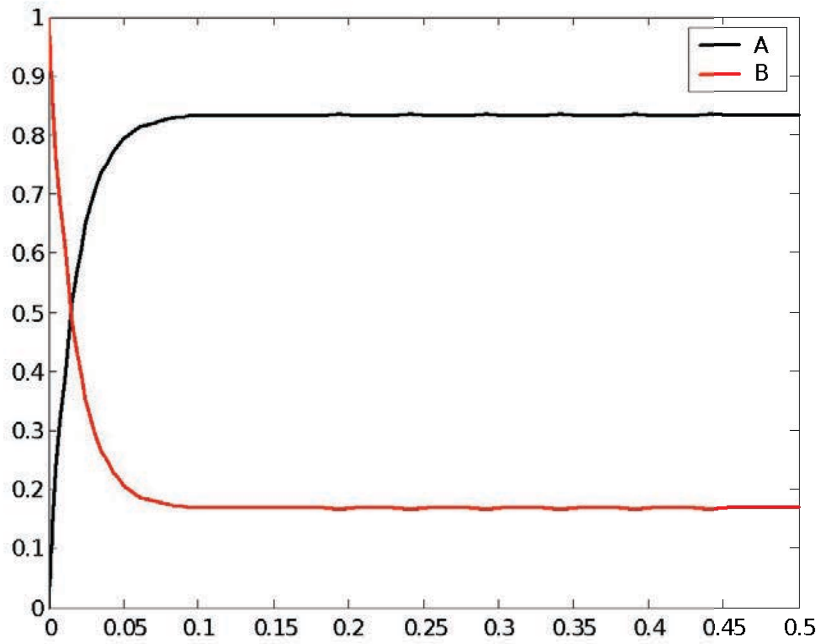
```
» [t,y]=ode45('chem',[0 0.5],[0 1]);
```

  - ➢ assumes that only chemical B exists initially

```
» plot(t,y(:,1),'k','LineWidth',1.5);
» hold on;
» plot(t,y(:,2),'r','LineWidth',1.5);
» legend('A','B');
» xlabel('Time (s)');
» ylabel('Amount of chemical (g)');
» title('Chem reaction');
```

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 ODE solvers
- Nonlinear is OK!
- Pendulum example:

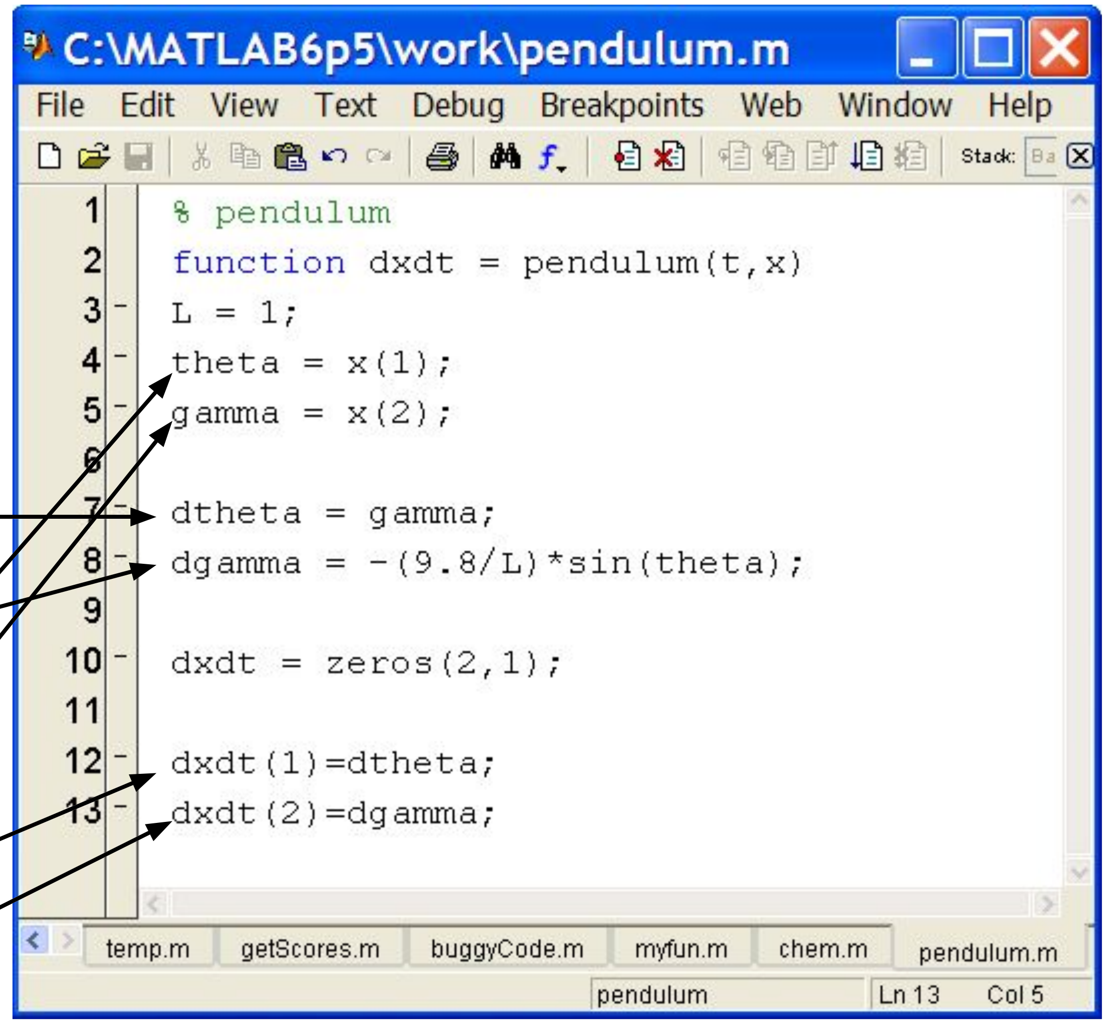
$$\ddot{\theta} + \frac{g}{L}\sin(\theta) = 0$$

$$\ddot{\theta} = -\frac{g}{L}\sin(\theta)$$

$$let \quad \dot{\theta} = \gamma$$

$$\dot{\gamma} = -\frac{g}{L}\sin(\theta)$$

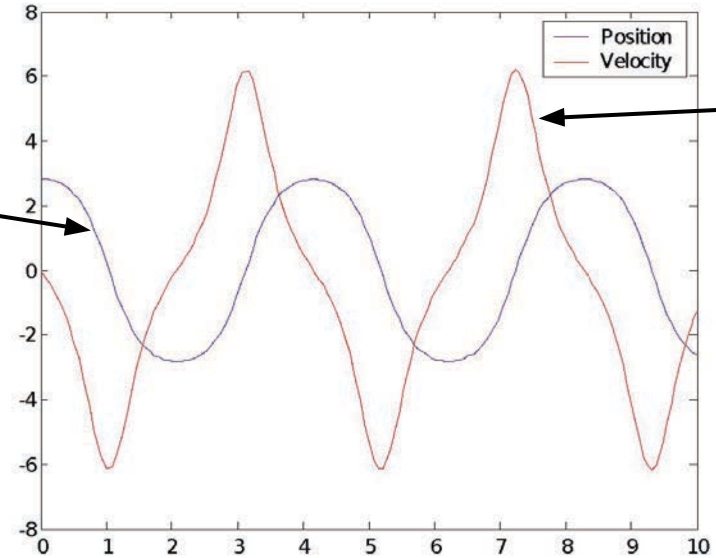
$$\boxed{\begin{array}{l} \vec{x} = \begin{bmatrix} \theta \\ \gamma \end{bmatrix} \\ \dfrac{d\vec{x}}{dt} = \begin{bmatrix} \dot{\theta} \\ \dot{\gamma} \end{bmatrix} \end{array}}$$



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 horizontal
  - » `plot(t,x(:,1));`
  - » `hold on;`
  - » `plot(t,x(:,2),'r');`
  - » `legend('Position','Velocity');`

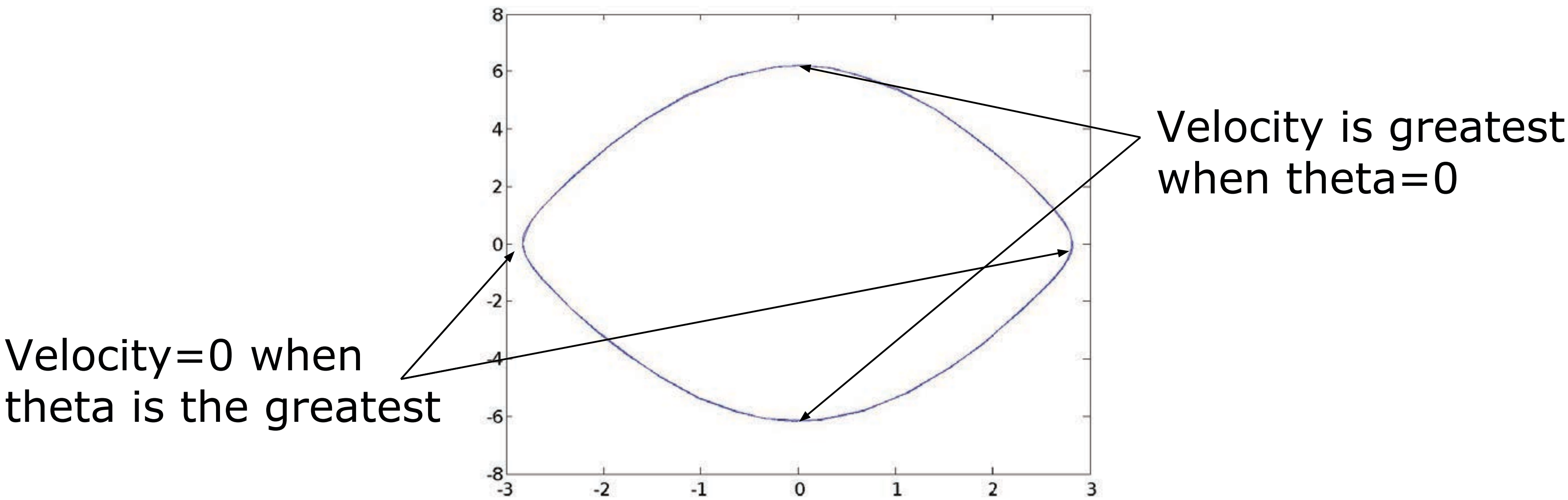
Position in terms of angle (rad)



Velocity (m/s)

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 timestep by giving a vector of (increasing) times
    - ➢ The function value will be returned at the specified points

- 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 for $y(t)$ on the range t=[0 10], with initial condition $y(0)=10$ and $dy/dt=-t\,y/10$
- Plot the result.

Exercise: ODE

- Use `ode45` to solve for $y(t)$ on the range t=[0 10], with initial condition $y(0)=10$ and $dy/dt=-t\,y/10$
- Plot the result.

- Make the following function

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

- Integrate the ODE function and plot the result

```
» [t,y]=ode45(‘odefun’,[0 10],10);
```

- Alternatively, use an anonymous function

```
» [t,y]=ode45(@(t,y) –t*y/10,[0 10],10);
```

- Plot the result

```
» plot(t,y);xlabel('Time');ylabel('y(t)');
```

Exercise: ODE

- The integrated function looks like this: