Part 5

Chapter 19

Numerical Differentiation

School of Mechanical Engineering
Chung-Ang University

Chapter Objectives

- Understanding the application of high-accuracy numerical differentiation formulas for equispaced data.
- Knowing how to evaluate derivatives for unequally spaced data.
- Understanding how Richardson extrapolation is applied for numerical differentiation.
- Recognizing the sensitivity of numerical differentiation to data error.
- Knowing how to evaluate derivatives in MATLAB with the diff and gradient functions.
- Knowing how to generate contour plots and vector fields with MATLAB.

Introduction to Differentiation

The one dimensional forms of some constitutive laws commonly used

Law	Equation	Physical Area	Gradient	Flux	Proportional constat
Fourier's law	$q = -k\dfrac{dT}{dx}$	Heat conduction	Temperature	Heat	Thermal conductivity
Fick's law	$J = -D\dfrac{dc}{dx}$	Mass diffusion	Concentration	Mass	Diffusivity
D'Arcy' law	$q = -k\dfrac{dh}{dx}$	Flow through porous media	Head	Flow	Hydraulic conductivity
Ohm's law	$J = -\sigma\dfrac{dV}{dx}$	Current flow	Voltage	Current	Electrical conductivity
Newton's viscosity law	$\tau = -\mu\dfrac{du}{dx}$	Fluids	Velocity	Shear Stress	Dynamic Viscosity
Hooke's law	$\sigma = E\dfrac{\Delta L}{L}$	Elasticity	Deformation	Stress	Young's modulus

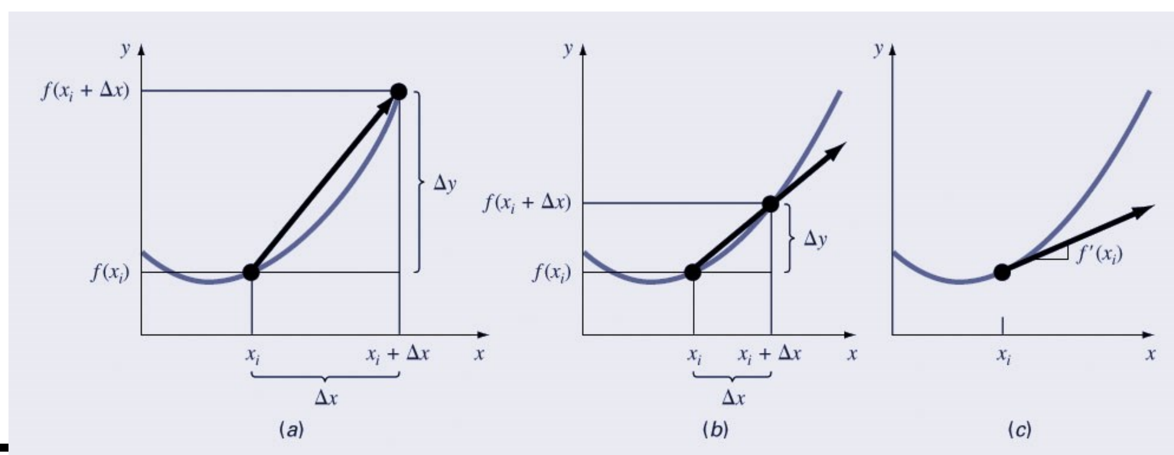
Differentiation

- The mathematical definition of a derivative begins with a difference approximation:

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

and as Δx is allowed to approach zero, the difference becomes a derivative:

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$



High-Accuracy Differentiation Formulas

- Taylor series expansion can be used to generate high-accuracy formulas for derivatives by using linear algebra to combine the expansion around several points.
- Three categories for the formula include *forward finite-difference, backward finite-difference, and centered finite-difference.*

Differentiation derived from Taylor series expansions

- There are forward difference, backward difference and centered difference approximations, depending on the points used:
- Forward:

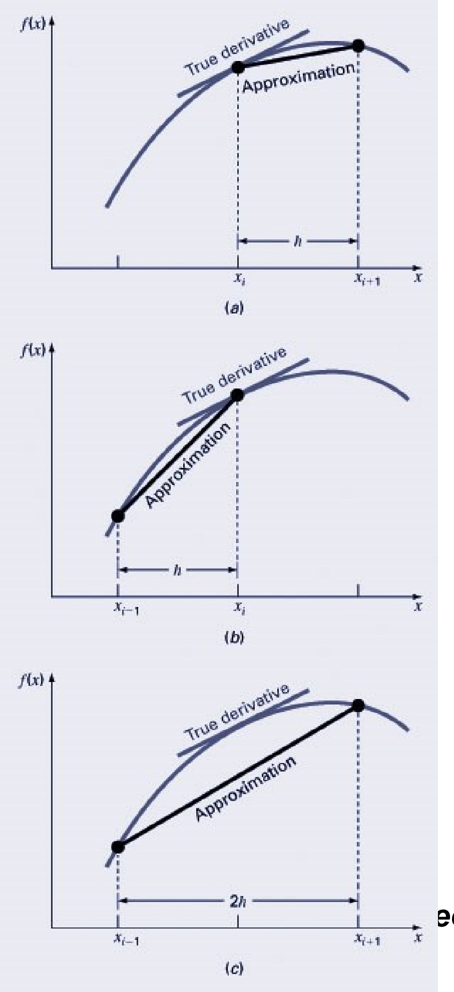
$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h)$$

- Backward:

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + O(h)$$

- Centered:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2)$$



High Accuracy Differentiation

- Forward Taylor series expansion

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \cdots$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2!}h + O(h^2)$$

- Forward-difference approximation of 1st derivative excluding the second and higher derivative term (In chapter 4)

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h)$$

- Forward-difference approximation of 2nd derivative

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h)$$

High Accuracy Differentiation

- Forward-difference approximation of 1st derivative including 2nd derivative term

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{2h^2} h + O(h^2)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2)$$

- Notice that inclusion of second-derivative term has improved the accuracy to $O(h^2)$.

Forward Finite-Difference

First Derivative	Error
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$	$O(h)$
$f''(x_i) = \dfrac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}$	$O(h^2)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3}$	$O(h)$
$f'''(x_i) = \dfrac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3}$	$O(h^2)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4}$	$O(h)$
$f''''(x_i) = \dfrac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4}$	$O(h^2)$

Backward Finite-Difference

First Derivative	Error
$f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
$f'(x_i) = \dfrac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}$	$O(h)$
$f''(x_i) = \dfrac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2}$	$O(h^2)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_i) - 3f(x_{i-1}) + 3f(x_{i-2}) - f(x_{i-3})}{h^3}$	$O(h)$
$f'''(x_i) = \dfrac{5f(x_i) - 18f(x_{i-1}) + 24f(x_{i-2}) - 14f(x_{i-3}) + 3f(x_{i-4})}{2h^3}$	$O(h^2)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_i) - 4f(x_{i-1}) + 6f(x_{i-2}) - 4f(x_{i-3}) + f(x_{i-4})}{h^4}$	$O(h)$
$f''''(x_i) = \dfrac{3f(x_i) - 14f(x_{i-1}) + 26f(x_{i-2}) - 24f(x_{i-3}) + 11f(x_{i-4}) - 2f(x_{i-5})}{h^4}$	$O(h^2)$

Centered Finite-Difference

First Derivative	Error
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h^2)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}$	$O(h^4)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}$	$O(h^2)$
$f''(x_i) = \dfrac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2}$	$O(h^4)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2h^3}$	$O(h^2)$
$f'''(x_i) = \dfrac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3}$	$O(h^4)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4}$	$O(h^2)$
$f''''(x_i) = \dfrac{-f(x_{i+3}) + 12f(x_{i+2}) + 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) + f(x_{i-3})}{6h^4}$	$O(h^4)$

Example 19.1 (1/2)

- Q. Recall that at in Ex. 4.4 we estimated the derivative of f(x) at x=0.5 using forward differences and a step size of h=0.25. The results are summarized in the table below. The exact value of f'(0.5)= -0.9125.

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

	Backward O(h)	Centered O(h²)	Forward O(h)
Estimate	-0.714	-0.934	-1.155
ε_t	21.7%	-2.4%	-26.5%

- Repeat the computation with high accuracy formulas.

Example 19.1 (2/2)

- Sol)

$$
\begin{aligned}
x_{i-2} &= 0 & f(x_{i-2}) &= 1.2 \\
x_{i-1} &= 0.25 & f(x_{i-1}) &= 1.1035156 \\
x_{i} &= 0.5 & f(x_{i}) &= 0.925 \\
x_{i+1} &= 0.75 & f(x_{i+1}) &= 0.6363281 \\
x_{i+2} &= 1 & f(x_{i+2}) &= 0.2
\end{aligned}
$$

- Forward difference of $O(h^2)$ is computed as

$$f'(0.5) = \frac{-0.2 + 4(0.6363281) - 3(0.925)}{2(0.25)} = -0.859375 \qquad \varepsilon_t = 5.82\ \%$$

- Backward difference of $O(h^2)$ is computed as

$$f'(0.5) = \frac{3(0.925) - 4(1.1035156) + 1.2}{2(0.25)} = -0.878125 \qquad \varepsilon_t = 3.77\ \%$$

- Backward difference of $O(h^4)$ is computed as

$$f'(0.5) = \frac{-0.2 + 8(0.6363281) - 8(1.1035156) + 1.2}{12(0.25)} = -0.9125 \qquad \varepsilon_t = 0\ \%$$

Richardson Extrapolation

- As with integration, the Richardson extrapolation can be used to combine two lower-accuracy estimates of the derivative to produce a higher-accuracy estimate.
- For the cases where there are two $O(h^2)$ estimates and the interval is halved ($h_2=h_1/2$), an improved $O(h^4)$ estimate may be formed using:

$$D=\frac{4}{3}D(h_2)-\frac{1}{3}D(h_1)$$

- For the cases where there are two $O(h^4)$ estimates and the interval is halved ($h_2=h_1/2$), an improved $O(h^6)$ estimate may be formed using:

$$D=\frac{16}{15}D(h_2)-\frac{1}{15}D(h_1)$$

- For the cases where there are two $O(h^6)$ estimates and the interval is halved ($h_2=h_1/2$), an improved $O(h^8)$ estimate may be formed using:

$$D=\frac{64}{63}D(h_2)-\frac{1}{63}D(h_1)$$

Example 19.2

- Q. Using the same function as in Ex.19.1, estimate the first derivative at x=0.5 for a step size of h1=0.5, and h2=0.25. Use the Richardson extrapolation to compute improved estimate. The exact solution is -0.9125.

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

Sol.) The first derivative with centered difference

$$D(0.5) = \frac{0.2 - 1.2}{1} = -1.0 \qquad \varepsilon_t = -9.6\%$$

$$D(0.25) = \frac{0.6363281 - 1.103516}{0.5} = -0.934375 \quad \varepsilon_t = -2.4\%$$

$$\begin{aligned} x_{i-2} &= 0 & f(x_{i-2}) &= 1.2 \\ x_{i-1} &= 0.25 & f(x_{i-1}) &= 1.1035156 \\ x_i &= 0.5 & f(x_i) &= 0.925 \\ x_{i+1} &= 0.75 & f(x_{i+1}) &= 0.6363281 \\ x_{i+2} &= 1 & f(x_{i+2}) &= 0.2 \end{aligned}$$

Using the Richardson extrapolation, the improved Estimate is

$$D = \frac{4}{3}(-0.934375) - \frac{1}{3}(-1) = -0.9125$$

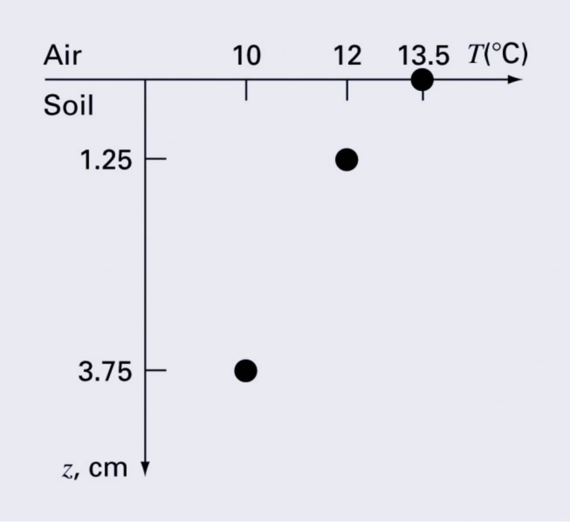
Unequally Spaced Data

- One way to calculated derivatives of unequally spaced data is to determine a polynomial fit and take its derivative at a point.
- As an example, using a second-order Lagrange polynomial to fit three points and taking its derivative yields:

$$f'(x) = f(x_0)\frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} + f(x_1)\frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} + f(x_2)\frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}$$

Example 19.3

- A temperature is measured inside the soil as shown below. Compute the heat flux into the ground at the air-soil interface.



$$q(z=0) = -k \left.\frac{dT}{dz}\right|_{z=0}$$

where q(x)=heat flux (W/m^2),
k=thermal conductivity for soil (=0.5 W/(m·K),
T=Temperature(K),
z=distance measured from the surface into the soil.

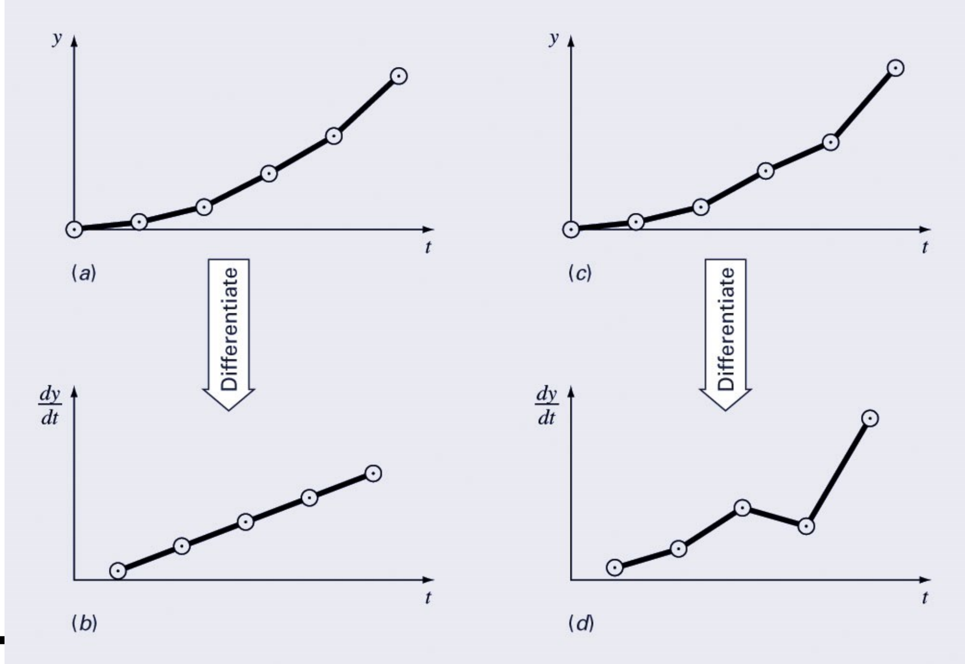
$$f'(0) = 13.5\frac{2(0)-0.0125-0.0375}{(0-0.0125)(0-0.0375)} + 12\frac{2(0)-0-0.0375}{(0.0125-0)(0.0125-0.0375)}$$

$$+10\frac{2(0)-0-0.0125}{(0.0375-0)(0.0375-0.0125)} = -1440+1440-133.333 = -133.333 \ K/m$$

$$q(z=0) = -0.5\frac{W}{m\,K}\left(-133.333\frac{W}{m}\right) = 66.667\frac{W}{m^2}$$

Derivatives and Integrals for Data with Errors

- A shortcoming of numerical differentiation is that it tends to amplify errors in data, whereas integration tends to smooth data errors.
- One approach for taking derivatives of data with errors is to fit a smooth, differentiable function to the data and take the derivative of the function.



(a) Data with no error
(b) Resulting numerical differentiation of curve (a)
(c) Data modified slightly
(d) Resulting numerical differentiation of curve (a)

→ Small data errors are amplified by numerical differentiation.

Numerical Differentiation with MATLAB

- MATLAB has two built-in functions to help take derivatives, diff and gradient:
- diff(*x*)
  - Returns the difference between adjacent elements in x

```
>> f = @(x) 0.2+25*x-200*x.^2+675*x.^3-900*x.^4+400*x.^5;
>> x = 0 : 0.1 : 0.8 ;
>> y = f(x) ;
```

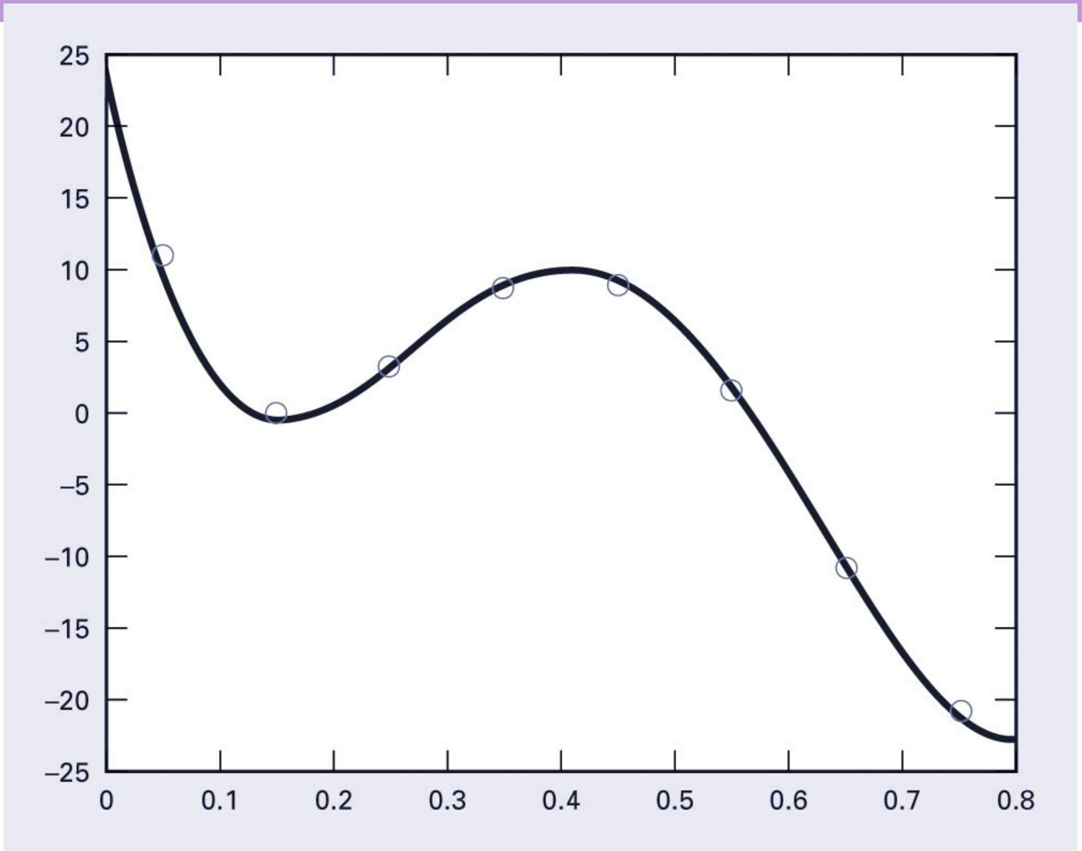
```
>> diff(x)
ans =
   Columns 1 through 5
      0.1000    0.1000   0.1000   0.1000   0.1000
   Columns 6 through 8
      0.1000   0.1000   0.1000
```

Numerical Differentiation with MATLAB

- diff(*y*)./diff(*x*)
  - Returns the difference between adjacent values in y divided by the corresponding difference in adjacent values of x

```
>> d=diff(y)./diff(x)
  Columns 1 through 5
    10.8900    -0.0100     3.1900   8.4900   8.6900
  Columns 6 through 8
     1.3900  -11.0100  -21.3100
```

```
>> n=length(x);
>> xm=(x(1:n-1)+x(2:n))./2;
   % vector d contains derivative estimates corresponding to the
   % midpoint between adjacent elements
>> xa=0:  .01 : .8 ;
>> ya=25-400*xa+3*675*xa.^2-4*900*xa.^3+5*400*xa.^4;
>> xplot(xm, d, 'o', xa, ya)
```


25
20
15
10
5
0
−5
−10
−15
−20
−25
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8

Numerical Differentiation with MATLAB

- *fx* = gradient(*f*, *h*)
  Determines the derivative of the data in f at each of the points. The program uses forward difference for the first point, backward difference for the last point, and centered difference for the interior points. h is the spacing between points; if omitted h=1.
- The major advantage of gradient over diff is gradient's result is the same size as the original data.
- Gradient can also be used to find partial derivatives for matrices:
  [*fx*, *fy*] = gradient(*f*, *h*)

```
>> dy=gradient(y, 0.1)
dy =
   Columns 1 through 5
      10.8900      5.4400     1.5900      5.8400    8.5900
   Columns 6 through 8
       5.0400    -4.8100   -16.1600   -21.3100
```

```
>> xa=0: .01 : .8 ;
>> ya=25-400*xa+3*675*xa.^2-4*900*xa.^3+5*400*xa.^4;
>> xplot(x, dy, 'o', xa, ya)
```