Numerical Methods for Science and Engineering

Chapter Seven
Lecture one
Solutions to Linear System

Numerical Differentiation

Objective: Numerical differentiation is the process of finding derivatives numerically for a function whose values are given in data form

Numerical differentiation formulas can be derived by using the Taylor series expansion or by differentiating the interpolating polynomials.

Derivative Formula from Taylor Series

For clear idea about the different formulas and their order of errors we may use the Taylor series expansion of f(x) From Taylor series expansion for h > 0, we have

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2!}f''(x_0) + \frac{h^3}{3!}f'''(x_0) + \cdots$$
 (1)

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2!}f''(x_0) - \frac{h^3}{3!}f'''(x_0) + \cdots$$
 (2)

From the expansion of $f(x_0 + h)$, we have

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2!}f''(x_0) - \frac{h^2}{3!}f'''(x_0) - \cdots$$

which leads to the two-pont forward difference formula for $f'(x_0)$ as

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} + E$$

where the error series is

$$E = -\left[\frac{h}{2!}f''(x_0) + \frac{h^2}{3!}f'''(x_0) + \cdots\right]$$

From the expansion of $f(x_0 - h)$, we have 2-point backward difference formula

$$f'(x_0) = \frac{f(x_0) - f(x_0 - h)}{h} + E$$

So the 2 points backward difference formula become $f'(x_0) = \frac{f(x_0) - f(x_0 - h)}{h}$ o(h)

Formulas for Computing Derivatives

First Derivatives

$$f'(x_0) \approx \frac{f_1 - f_0}{h},$$

$$O(h)$$
 2-points forward difference

$$f'(x_0) \approx \frac{f_0 - f_{-1}}{h}$$
,

$$f'(x_0) \approx \frac{f_1 - f_{-1}}{2h}$$
,

$$O(h^2)$$

3-points central difference

Second Derivatives

$$f''(x_0) \approx \frac{1}{h^2} [f_{-1} - 2f_0 + f_1], \quad O(h^2)$$

$$O(h^2)$$

3-point central difference

$$f''(x_0) \approx \frac{1}{h^2} [f_0 - 2f_1 + f_2],$$
 O(h) 3-point forward difference

$$f''(x_0) \approx \frac{1}{h^2} [f_0 - 2f_{-1} + f_{-2}],$$
 O(h) 3-point backward difference

Richardson Extrapolation

If the two approximations of order $O(h^n)$ for M are $M(h_1)$ and $M(h_2)$, then the Richardson's extrapolated estimate M_R of M can be written as

$$M_R = M(h_1) + A(h_1)^n$$
 (1)

$$M_R = M(h_2) + A(h_2)^n$$
 (2)

where it is assumed that the constant multiplicative factor A is same for both cases. Subtracting (1) from (2),

$$0 = M(h_2) - M(h_1) + A(h_2^n - h_1^n)$$

or

$$A = \frac{M(h_1) - M(h_2)}{h_2^n - h_1^n}$$

Substituting in (1), we have

$$M_{R} = M(h_{1}) + \frac{h_{1}^{n} \left[M(h_{1}) - M(h_{2}) \right]}{h_{2}^{n} - h_{1}^{n}}.$$

$$M_{R} = M(h_{1}) + \frac{M(h_{1}) - M(h_{2})}{(h_{2} / h_{1})^{n} - 1}.$$

or

$$M_R = M(h_1) + \frac{M(h_1) - M(h_2)}{r^n - 1}$$

 $r = \frac{h_2}{h_1}$.

where

$$r = \frac{h_2}{h_1}.$$

This is known as the **Richardson extrapolation** formula.

Example:

The values of distance at various times are given below

| Time (t) | 4 | 6 | 8 | 10 | 12 |
|-------------|------|-------|-------|-------|-------|
| Distance(s) | 7.38 | 12.07 | 18.37 | 26.42 | 36.40 |

The speed and acceleration can be calculated by $v = \frac{ds}{dt}$ and acceleration $a = \frac{d^2s}{dt^2}$

- (a) Using three point central difference formula estimate the speeds at (i) t = 8, (ii) t = 7, and (iii) t = 9.
- (b) Using two point formulas and extrapolation estimate the speeds at (i) t = 4, and (ii) t = 12.
- (c) Use three points central difference formula and extrapolation to estimate speed at t = 8.
- (d) Use three points central or forward or backward formula to estimate the accelerations at (i) t = 8, (ii) t = 4, and (iii) t = 12.
- (e) Write down MATLAB code to estimate the speed and acceleration at time t=8 using three point central difference formulas.
- (f) Use MATAB functions "sp=spline(x,y)", "fnder(sp, dorder)" and "fnval(sp, xo)" to estimate the speed and acceleration at time t=6.5 and 10.4.

Solution:

| Time (t) | 4 | 6 | 8 | 10 | 12 |
|-------------|------|-------|-------|-------|-------|
| Distance(s) | 7.38 | 12.07 | 18.37 | 26.42 | 36.40 |

(a) Three-point central derivative formula for first derivative is

$$f'(x_0, h) = \frac{1}{2h} [f(x_0 + h) - f(x_0 - h)], \qquad O(h^2)$$

(i) Speed at t = 8

$$v(8,2) = \frac{1}{2 \times 2} [s(10) - s(6)] = \frac{1}{2} [26.42 - 12.07] = 3.5875.$$

(ii) Speed at t = 7. Here $h = \frac{8-6}{2} = 1$.

$$v(7,1) = \frac{1}{2 \times 1} [s(8) - s(6)] = \frac{1}{4} [18.37 - 12.07] = 3.15.$$

(iii) Speed at t = 9. Here $h = \frac{10-8}{2} = 1$.

$$v(9,1) = \frac{1}{2 \times 1} [s(10) - s(8)] = \frac{1}{2} [26.42 - 18.37] = 4.025.$$

| Time (t) | 4 | 6 | 8 | 10 | 12 |
|-------------|------|-------|-------|-------|-------|
| Distance(s) | 7.38 | 12.07 | 18.37 | 26.42 | 36.40 |

- (b) Using two point formulas and extrapolation estimate the speeds at (i) t = 4, and (ii) t = 12.
- (i) For t = 4, we have to use forward difference formula

$$f'(x_0) \approx f'(x_0, h) = \frac{1}{h} [f(x_0 + h) - f(x_0)],$$
 $O(h).$

Speed at t = 4 we need to use h = 2 and h = 4.

$$v(4,2) = \frac{1}{2}[s(6) - s(4)] = \frac{1}{2}[12.07 - 7.38] = 2.345.$$

$$v(4,4) = \frac{1}{4}[s(8) - s(4)] = \frac{1}{4}[18.37 - 7.38] = 2.7475.$$

Extrapolated value is

$$v_R(4) = v(8,2) + \frac{v(8,2) - v(8,4)}{2^1 - 1} = 2.345 + (2.345 - 2.7475) = 2.9425.$$

$$M_R = M(h_1) + \frac{M(h_1) - M(h_2)}{r^n - 1}, \qquad r = \frac{h_2}{h_1} \ (h_2 > h_1)$$

| Time (t) | 4 | 6 | 8 | 10 | 12 |
|-------------|------|-------|-------|-------|-------|
| Distance(s) | 7.38 | 12.07 | 18.37 | 26.42 | 36.40 |

- (b) Using two point formulas and extrapolation estimate the speeds at (i) t = 4, and (ii) t = 12.
- (ii) For t = 12, we have to use backward difference formula

$$f'(x_0) \approx f'(x_0, h) = \frac{1}{h} [f(x_0) - f(x_0 - h)],$$
 $O(h).$

Speed at t = 12 we need to use h = 2 and h = 4.

$$v(12,2) = \frac{1}{2}[s(12) - s(10)] = \frac{1}{2}[36.40 - 26.42] = 4.99.$$

$$v(12,4) = \frac{1}{4}[s(12) - s(8)] = \frac{1}{4}[36.42 - 18.37] = 4.5075.$$

Extrapolated value is

$$v_R(12) = v(12,2) + \frac{v(12,2) - v(12,4)}{2^1 - 1} = 4.99 + (4.99 - 4.5075) = 5.4725.$$

$$M_R = M(h_1) + \frac{M(h_1) - M(h_2)}{r^n - 1}, \qquad r = \frac{h_2}{h_1} \ (h_2 > h_1)$$

| Time (t) | 4 | 6 | 8 | 10 | 12 |
|-------------|------|-------|-------|-------|-------|
| Distance(s) | 7.38 | 12.07 | 18.37 | 26.42 | 36.40 |

(c) Use three points central difference formula and extrapolation to estimate speed at t = 8. Three points central difference formula is

$$f(x_0) \approx f'(x_0, h) = \frac{1}{2h} [f(x_0 + h) - f(x_0 - h)],$$
 $O(h^2).$

Speed at t = 8 we need to use h = 2 and h = 4.

$$v(8,2) = \frac{1}{2 \times 2} [s(10) - s(6)] = \frac{1}{4} [26.42 - 12.07] = 3.5875.$$

$$v(8,4) = \frac{1}{2 \times 4} [s(12) - s(4)] = \frac{1}{8} [36.40 - 7.38] = 3.6275.$$

Extrapolated value is

$$v_R(8) = v(8,2) + \frac{v(8,2) - v(8,4)}{2^2 - 1} = 3.5875 + \frac{3.5875 - 3.6275}{3} = 3.5742.$$

$$M_R = M(h_1) + \frac{M(h_1) - M(h_2)}{r^n - 1}, \qquad r = \frac{h_2}{h_1} \ (h_2 > h_1)$$

| Time (t) | 4 | 6 | 8 | 10 | 12 |
|-------------|------|-------|-------|-------|-------|
| Distance(s) | 7.38 | 12.07 | 18.37 | 26.42 | 36.40 |

- (d) Use three points central or forward or backward formula to estimate the accelerations at (i) t = 8, (ii) t = 4, and (iii) t = 12.
- (i) For t = 8, we have to use central difference formula (it gives better approximation).

Three point central difference formula for second derivative is

$$f''(x_0, h) = \frac{1}{h^2} (f(x_0 + h) - 2f(x_0) + f(x_0 - h)), \qquad O(h^2).$$

Acceleration at t = 8 is

$$a(8,2) = \frac{1}{2^2}[s(10) - 2s(8) + s(6)] = \frac{1}{4}[26.42 - 2(18.37) + 12.07] = 0.4375.$$

(ii) For t = 4, three point forward difference formula for second derivative is

$$f''(x_0, h) = \frac{1}{h^2} (f(x_0) - 2f(x_0 + h) + f(x_0 + 2h)).$$

Acceleration at t = 4 is

$$a(4,2) = \frac{1}{2^2}[s(4) - 2s(6) + s(8)] = \frac{1}{4}[7.38 - 2(12.07) + 18.37] = 0.4025.$$

| Time (t) | 4 | 6 | 8 | 10 | 12 |
|-------------|------|-------|-------|-------|-------|
| Distance(s) | 7.38 | 12.07 | 18.37 | 26.42 | 36.40 |

- (d) Use three points central or forward or backward formula to estimate the accelerations at (iii) t = 12.
- (iii) For t = 12, three-point backward difference formula for second derivative is

$$f''(x_0, h) = \frac{1}{h^2} (f(x_0) - 2f(x_0 - h) + f(x_0 - 2h)), \qquad O(h)$$

Acceleration at t = 12 is

$$a(12,2) = \frac{1}{2^2}[s(12) - 2s(10) + s(8)] = \frac{1}{4}[36.40 - 2(26.42) + 18.37] = 0.4825.$$

(e) Write down MATLAB code to estimate the speed and acceleration at time t=8 using three point central difference formulas.

>> clear

$$>> x=[6 \ 8 \ 10];$$

$$>> h=x(2)-x(1);$$

$$>> D1=(y(3)-y(1))/(2*h);$$

$$>> D2=(y(3)-2*y(2)+y(1))/h^2;$$

(f) Use MATLAB functions " $\mathbf{sp} = \mathbf{spline}(\mathbf{x}, \mathbf{y})$ ", " $\mathbf{fnder}(\mathbf{sp, dorder})$ " and " $\mathbf{fnval}(\mathbf{sp, xo})$ " to estimate the speed and acceleration at time t = 6.5 and 10.4.

```
>> clear
>> x=[4 6 8 10 12];
>> y=[7.38 12.07 18.37 26.42 36.40];
>> % syntax for derivative is "fnder(f, dorder)"
>> sp=spline(x,y); % generates spline function sp
>> D1sp=fnder(sp,1); % generate first derivative of spline function sp
>> ValD1=fnval(D1sp,[8.4, 11]) % gives values from D1sp
ValD1 =
  3.7501
          4.9860
>> D2sp=fnder(sp, 2); % gererates second derivative
>> ValD2=fnval(D2sp, [8.4, 11]) % gives values from D2sp
ValD2 =
 0.4445
          0.5063
```

SAMPLE MCQ

1. Which of the following is the three point's central difference formula for first derivative?

a.
$$f'(x_0) \approx \frac{1}{2h} [3f_0 - 4f_{-1} + f_{-2}]$$

b.
$$f'(x_0) \approx \frac{1}{2h} [-3f_0 + 4f_1 - f_2]$$

c.
$$f'(x_0) \approx \frac{f_1 - f_{-1}}{2h}$$

d.
$$f'(x_0) \approx \frac{f_0 - f_{-1}}{h}$$

2. Consider the following table

| Time (t) | 4 | 6 | 8 | 10 | 12 |
|-------------|------|-------|-------|-------|-------|
| Distance(s) | 7.38 | 12.07 | 18.37 | 26.42 | 36.40 |

Which of the following is the speed at t=8 sec calculated using three points central difference formula?

- a. 3.5875 m/s
- b. 2.5 m/s
- c. 4 m/s
- d. 6 m/s

| Time (t) | 4 | 6 | 8 | 10 | 12 |
|-------------|------|-------|-------|-------|-------|
| Distance(s) | 7.38 | 12.07 | 18.37 | 26.42 | 36.40 |

3. Which of the following is the speed at t=4 sec calculated using two points forward difference formula?

- a. 3.5875 m/s b. 2.345 m/s c. 4 m/s d. 5 m/s

4. Which of the following is the acceleration at t=8 sec calculated using three points central difference formula?

- a. $0.4375 \text{ m}^2/\text{s}$ b.0 $.345 \text{ m}^2/\text{s}$ c. $0.4 \text{ m}^2/\text{s}$ d. $0.5 \text{ m}^2/\text{s}$

5. Which of the following is the speed at t=12 sec calculated using two points backward difference formula and extrapolation?

- a. 3.5875 m/s b. 5.4725 m/s c. 4.25 m/s d. 6.5 m/s

Exercise

1. The speed v (in m/s) of a rocket measured at half second intervals is

| Time t (s) | 0 | 0.5 | 1 | 1.5 | 2 |
|------------------|---|--------|--------|--------|-------|
| speed v (in m/s) | 0 | 11.860 | 26.335 | 41.075 | 59.05 |

- (a) Use central difference formula to approximate the acceleration of the rocket at times t = 1 s and t = 1.75s.
- (b) Use two-point backward difference formula and Richardson extrapolation to estimate the acceleration of the rocket at time $t=2 \ s$.
- (c) Use three-point central difference formula and extrapolation to estimate the acceleration of the rocket at time t = 1 s.
- (d) Use MATLAB to estimate the acceleration of the rocket at time t = 0.5, 1.25 and 2 using spline interpolation.

2. The distance traveled by an object is given in the table below:

| <i>t</i> (s) | 8 | 9 | 10 | 11 | 12 |
|---------------------------|--------|--------|--------|--------|--------|
| <i>s</i> (<i>t</i>) (m) | 17.453 | 21.460 | 25.752 | 30.302 | 35.084 |

The speed and acceleration can be calculated by $v = \frac{ds}{dt}$ and acceleration $a = \frac{d^2s}{dt^2}$.

- (a) Using three-point central difference formula estimate the speeds at (i) t = 9, and (ii) t = 10.5.
- (b) Using two point formulas estimate the speeds at (i) t = 8, and (ii) t = 12.
- (c) Use three points central difference formula and extrapolation to estimate speed at t = 10.
- (d) Use three points central or forward or backward difference formula to estimate the accelerations at (i) t = 10, (ii) t = 8 and (iii) t = 12.
- (e) Use MATLAB to estimate the speed and acceleration at time t= 8.5, 10.5, and 11.2 using spline interpolation.

3. The table below shows the values of f(x) at different values of x:

| X | 0.8 | 1.0 | 1.2 | 1.4 | 1.6 |
|------|-------|-------|-------|-------|-------|
| f(x) | 0.954 | 1.648 | 2.623 | 3.947 | 5.697 |

- (a) Using three point central difference formula estimate f'(1) and f'(1.3)
- (b) Using two point forward difference formula and extrapolation estimate f'(0.8).
- (c) Use three points central difference formula and extrapolation to estimate f'(1.2).
- (d) Use three points backward formula to estimate f''(1.6).
- (e) Write down MATLAB codes using "sp=spline(x,y)", "fnder(sp, dorder)" and "fnval(sp, xo)" to estimate the values of f'(x) and f''(x) at x = 0.9, 1.1 and 1.42.