Numerical Methods for Science and Engineering
Lecture Note 7
Numerical Differentiation

7.1 Introduction

Numerical differentiation is the process of finding derivatives numerically for a function whose values are given in data form generated from an experiment. For evenly distributed data points and if we need the derivative at data points we may use the derivative formulas called finite differences. When the data points are not even or required derivatives are at points other than data points, we may use interpolating polynomials.
Numerical differentiation formulas can be derived by using the Taylor series expansion or by differentiating the interpolating polynomials. Here we shall consider both way of deriving the derivative formulas.

7.2 Method of Numerical Differentiation

Recall the definition of the derivative of a function

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

For finite Δx,

$$f'(x) \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

To find the derivative at $x = x_i$, we choose another point $x_{i+1} = x_i + h$ ahead of x_i . This gives two point forward difference formula

$$f'(x_i) \approx \frac{f(x_i + h) - f(x_i)}{h} = f'(x_i, h) \qquad (1)$$

If Δx is chosen as a negative number, say $\Delta x = -h$ ($h > 0$), we have

$$f'(x_i) \approx \frac{f(x_i - h) - f(x_i)}{-h} \approx \frac{f(x_i) - f(x_i - h)}{h} = f'(x_i, h) \qquad (2)$$

This is backward difference formula for first derivative.
Adding Eq.(1) and Eq.(2), we have

$$f'(x_i) \approx \frac{f(x_i + h) - f(x_i - h)}{2h} = f'(x_i, h) \qquad (3)$$

which is a-point central difference formula for first derivative.

7.3 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

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

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

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

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

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

In the two point formula the error series is of the form

$$E=a_1h+a_2h^2+a_3h^3+\cdots$$

where *a*'s does not depend on *h*.

By subtraction, we obtain

$$f(x_0+h)-f(x_0-h)=2hf(x_0)+\frac{2}{3!}h^3f'''(x_0)+\frac{2}{5!}h^5f^{(v)}(x_0)+\cdots$$

This leads to the 3-point central formula for approximating $f'(x_0)$

$$f'(x_0)=\frac{f(x_0+h)-f(x_0-h)}{2h}+E$$

With $E=-\left[\frac{1}{3!}h^2f'''(x_0)+\frac{1}{5!}h^4f^{(v)}(x_0)+\cdots\right]$

Adding the Taylor series for $f(x_0+h)$ and $f(x_0-h)$, we get

$$f(x_0+h)+f(x_0-h)=2f(x_0)+h^2f''(x_0)+\frac{2}{4!}h^4f^{(4)}(x_0)+\cdots$$

When this is rearranged, we get 3-point central difference formula for $f''(x_0)$

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

where the error series is $E=-2\left[\frac{1}{4!}h^2f^{(4)}(x_0)+\frac{1}{6!}h^4f^{(6)}(x_0)\cdots\right]$

In the three point central difference formula the error series is of the form

$$E=a_2h^2+a_4h^4+a_6h^6+\cdots$$

7.4 Formulas for Computing Derivatives

First Derivatives

$f'(x_0) \approx \dfrac{f_1 - f_0}{h}$, $O(h)$ 2-points forward difference

$f'(x_0) \approx \dfrac{f_0 - f_{-1}}{h}$, $O(h)$ 2-points backward difference

$f'(x_0) \approx \dfrac{f_1 - f_{-1}}{2h}$, $O(h^2)$ 3-points central difference

$f'(x_0) \approx \dfrac{1}{2h}\left[-3f_0 + 4f_1 - f_2\right]$, $O(h^2)$ 3-points forward difference

$f'(x_0) \approx \dfrac{1}{2h}\left[3f_0 - 4f_{-1} + f_{-2}\right]$, $O(h^2)$ 3-points backward difference

$f'(x_0) \approx \dfrac{1}{12h}\left[-f_2 + 8f_1 - 8f_{-1} + f_{-2}\right]$, $O(h^4)$ 5-points central difference

Second Derivatives

$f''(x_0) \approx \dfrac{1}{h^2}\left[f_{-1} - 2f_0 + f_1\right]$, $O(h^2)$ 3-point central difference

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

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

$f''(x_0) \approx \dfrac{1}{12h^2}\left[-f_2 + 16f_1 - 30f_0 + 16f_{-1} - f_{-2}\right]$, $O(h^2)$

5-point central difference

7.5 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

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

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

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

$$M_R = M(h_1) + \frac{h_1^n\left[M(h_1) - M(h_2)\right]}{h_2^n - h_1^n}.$$

which can be written as

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

or

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

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

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

Lower order formula and Richardson extrapolation can be used to deduce the higher order formula. For convenience we have used the notation $f'(x_0, h)$ to indicate clearly the approximation of $f'(x_0)$ with step size h and $f(x_0 + rh) = f_r$.

Thus the 3-point central difference formula for first derivative will ne written as

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

Example 7.1 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

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

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

(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 $h = \frac{10-8}{2} = 1$.

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

(b)

(i) For $t = 4$, we have to use forward difference formula

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

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

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

(ii) For $t = 12$, we have to use backward difference formula

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

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

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

(c) Three points central difference formula is

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

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

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

(d)

(i) For $t = 8$, we have to use central difference formula (it gives better approximation).

Three point central derivative formula for second derivative is

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

Acceleration at $t = 8$ is

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

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

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

Acceleration at $t = 4$ is

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

(iii) For $= 12$, three point backward difference formula for second derivative is

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

Acceleration at $t = 12$ is

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

(d)

```
>> clear
>> x=[6  8  10];
>> y=[12.07  18.37  26.42];
>> h=x(2)-x(1);
>> D1=(y(3)-y(1))/(2*h);
>> D2=(y(3)-2*y(2)+y(1))/h^2;
```

(e)
```
>> 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
```

Exercise 7

Numerical Differentiation

1. The distance s of a runner from a fixed point is measured (in metres) at intervals of half a second. The data obtained is

Time t (s)	0	0.5	1	1.5	2
Distance s (m)	0	3.65	6.8	9.9	12.15

(a) Use two points difference formulas to approximate the runner's speed at times t = 0s and t = 2s.
(b) Use three points central difference formula to approximate the runner's speed at times t = 0.5s and t = 1.25s.
(c) Use three points central difference formula to approximate the runner's acceleration at times t = 1 s.
(d) Write down MATLAB code to estimate the speed and acceleration at time at time $t = 1.5\ s$ using three point central difference formulas.

3. 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 MATAB to estimate the acceleration of the rocket at time $t = 0.5, 1.25$ and 2 using spline interpolation.

4. The voltage $E = E(t)$ in an electric circuit obeys the differential equations $E(t) = L\frac{di}{dt} + Ri$, where R is the resistance and L is the inductance. Use L =0.05, R = 2 and the value of $I(t)$ in the table'

t	1.0	1.1	1.2	1.3	1.4
$i(t)$	8.2277	7.2428	5.9908	4.5260	2.9122

(a) Find $\frac{di}{dt}(1.2)$ using three point central difference formula and extrapolation to compute $E(1.2)$
(b) Compare your result with the exact solution $I(t) = 10\exp(-t/10)\sin 2t$.
(c) Use MATAB to estimate $I'(t)$ at each value of t using spline interpolation. Write down the MATLAB commands to find the corresponding voltage $E(t)$.

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

t (s)	8	9	10	11	12
$s(t)$ (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 MATAB to estimate the speed and acceleration at time t= 8.5, 10.5, and 11.2 using spline interpolation.

6. 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 MATAB 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 .

7. A rod is rotating in a plane. The follow table gives the angle θ(in radians) through which the rod has turned for various values of time t.

Time t (s)	0	0.2	0.4	0.6	0.8
Angle θ	0	0.12	0.49	1.12	2.02

(a) Use two points difference formula to approximate the angular velocity of the rod at t = 0.6s.
(b) Use three points central difference formula to approximate the angular velocity of the rod at t = 0.6s.
(c) Use three points central difference formula to approximate the angular acceleration of the rod at t = 0.6s.
(d) Write down MATLAB code to estimate the speed and acceleration at time $t = 0.5\ s$ using three point central difference formulas.

8. The table below gives the results of an observation, θ is the observed temperature in degree celsius of a vessel of cooling water, t is the time in minutes from the beginning of observation.

Time t (min)	1	3	5	7	9
temperature θ	85.3	74.5	67.0	60.5	54.3

(a) Use two points difference formula to approximate the rate of cooling at $t = 3$ and $t = 5$

(b) Use three points central difference formula to approximate the rate of cooling at $t = 3$ and $t = 4$

(c) Write down MATLAB code to estimate the approximate rate of cooling at $t = 3$ and $t = 4$ three point central difference formulas.