NUMERICAL METHODS
BEKG2452
NUMERICAL DIFFERENTIATION
(First Derivative)

Irma Wani Jamaludin[1], Ser Lee Loh[2]
[1]irma@utem.edu.my, [2]slloh@utem.edu.my

Learning Outcomes

1. Find the first derivative of a function by using forward, backward and central differencing approximation.

2. Find the first derivative of a function by using high accuracy differentiation formula.

Numerical Differentiation
(Estimating the derivative of a function at a specific point)

Forward, Backward, Central Difference Approximation of
First Derivatives

Forward, Backward, Central Difference Approximation of
Second Derivatives

Taylor Series Expansion / Interpolation

Forward D.A. Backward D.A.	Accuracy $O(h)$:
Centered D.A. High Accuracy F.D.A. High Accuracy B.D.A.	Accuracy $O(h^2)$:
High Accuracy C.D.A.	Accuracy $O(h^4)$:

Forward D.A. Backward D.A.	Accuracy $O(h)$:
Centered D.A. High Accuracy F.D.A. High Accuracy B.D.A.	Accuracy $O(h^2)$:
High Accuracy C.D.A.	Accuracy $O(h^4)$:

5.1 Introduction

Why we need numerical differentiation?

Given a complicated function

i.e. $f(x) = \left[\cos(-9x^5 + e^{-2x})e^{x^2+4}\right]$

Evaluate $f''(-3.2)$.

Method 1

Step 1: Find the derivative of f' followed by f''.

Step 2: Evaluate $f''(-3.2)$.

Method 2

Step 1: Construct some points from $f(x)$, e.g. $f(-5)$, $f(-3)$, $f(-1)$

Step 2: Evaluate $f''(-3.2)$ by numerical differentiation.

Which one is faster and easier?

Method 2

5.1 Introduction

Taylor Series Expansion

A one-dimensional Taylor series is an expansion of a real function $f(x)$ about a point $x = a$:

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2!}(x-a)^2$$

$$+\frac{f^{(3)}(a)}{3!}(x-a)^3 + \cdots + \frac{f^{(n)}(a)}{n!}(x-a)^n + \cdots$$

It is used to approximate the first and the second derivatives.

5.1 Introduction

- The first derivative of a function/ a set of data can be obtained by using:
  - ❑ forward difference approximation
  - ❑ backward difference approximation
  - ❑ centered difference approximation
  - ❑ high-accuracy difference formulas

5.2 Finite Difference Approximations of First Derivative

Forward difference:

(use current value & future value to estimate derivative)- 2 points

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

or

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

Accuracy: $O(h) = \varepsilon_t$

5.2 Finite Difference Approximations of First Derivative

Backward difference:

(use current value & previous value to estimate derivative)

$$f'(x) = \frac{f(x) - f(x-h)}{h}$$

or

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

Accuracy: $O(h) = \varepsilon_t$

5.2 Finite Difference Approximations of First Derivative

Centered difference:

(subtract the backward from the forward Taylor series)

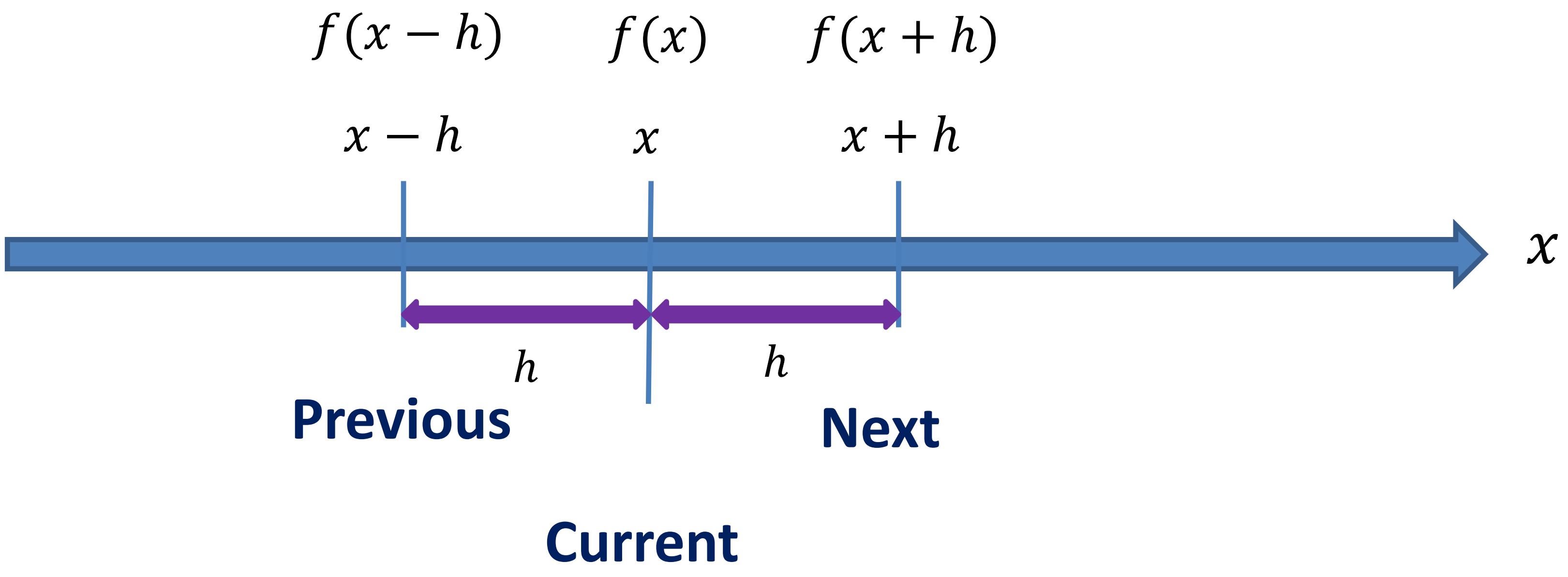
$$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

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

Accuracy: $O(h^2) = \varepsilon_t$

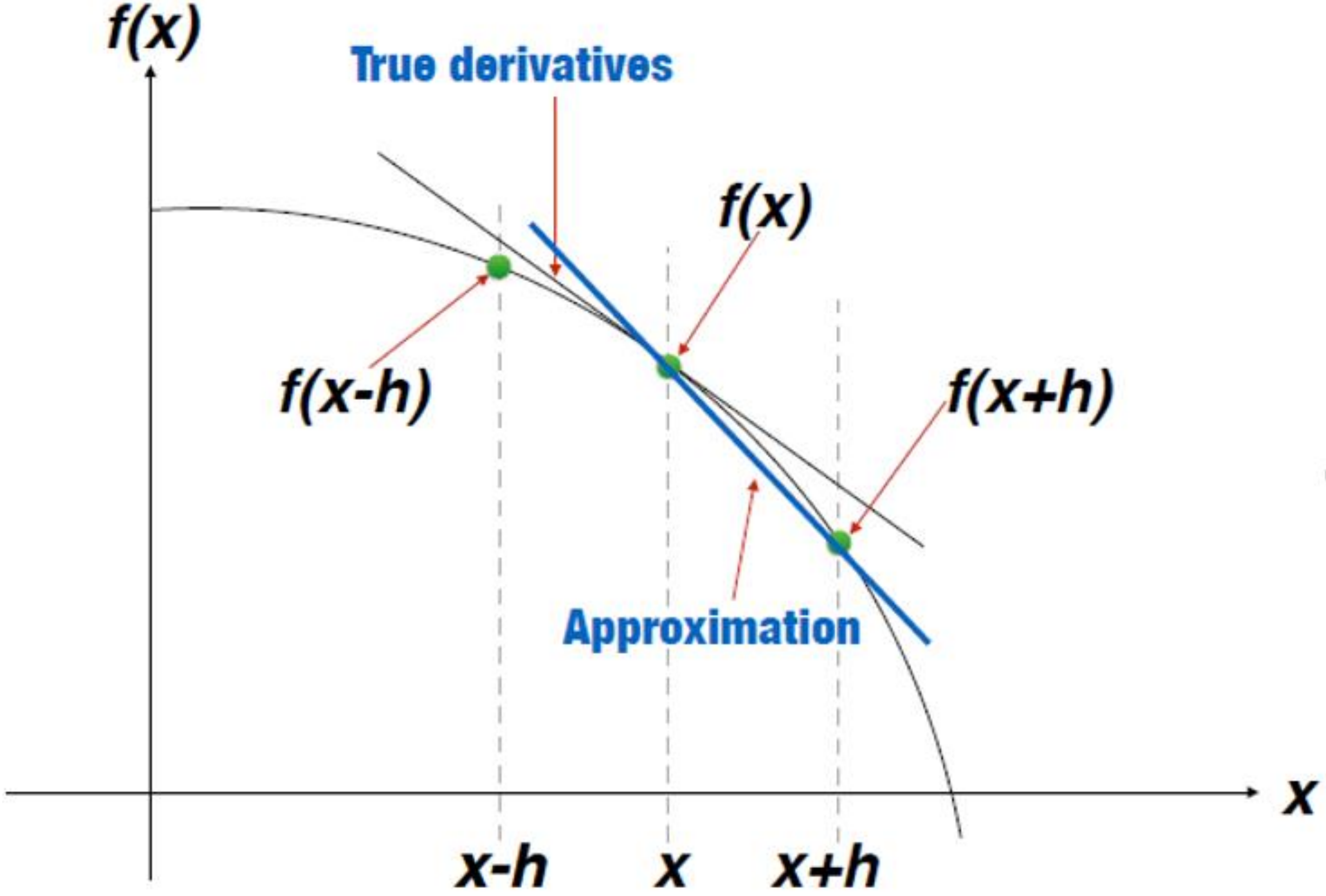
5.2 Finite Difference Approximations of First Derivative

Time Line:



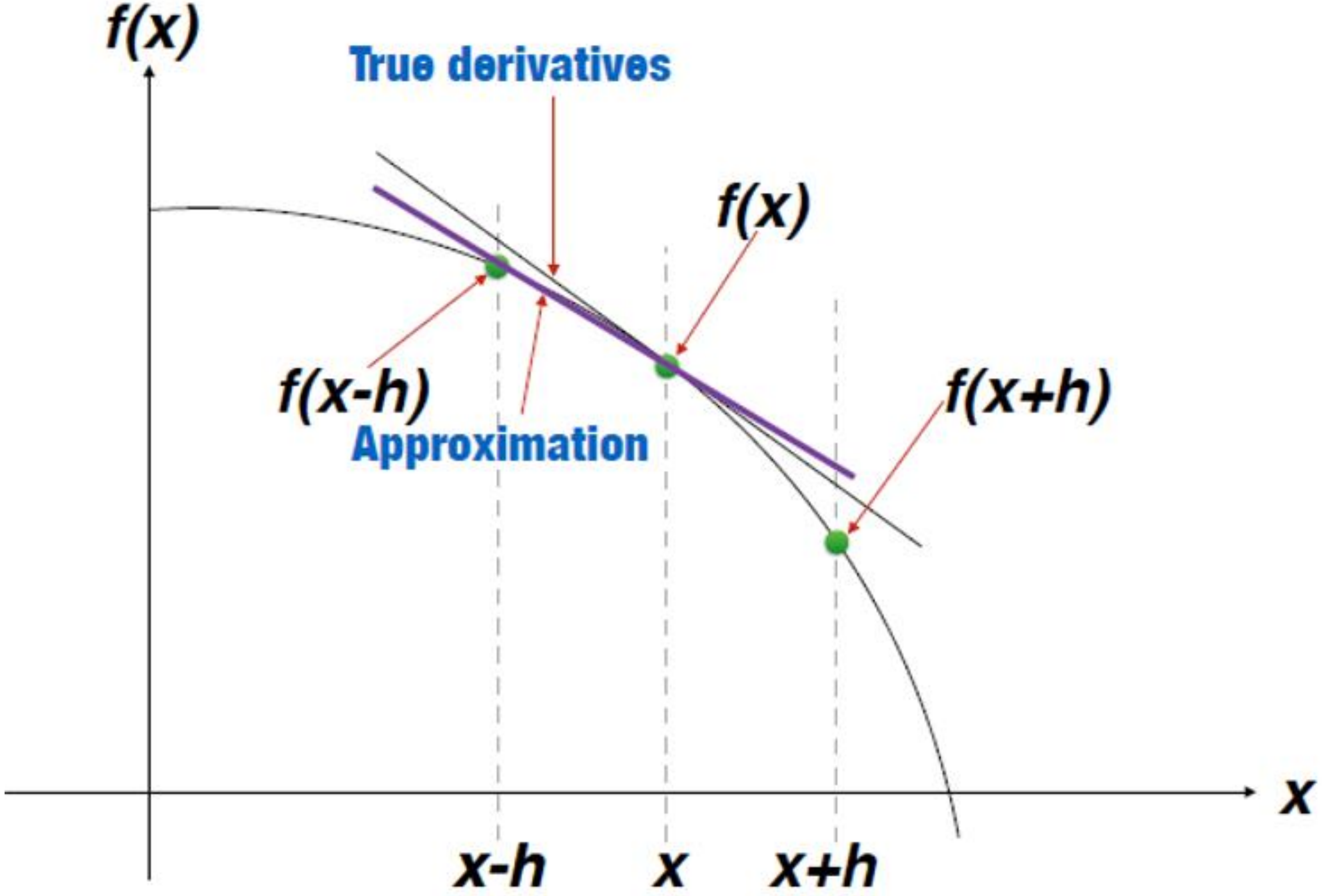
Step size: h

5.2 Finite Difference Approximations of First Derivative



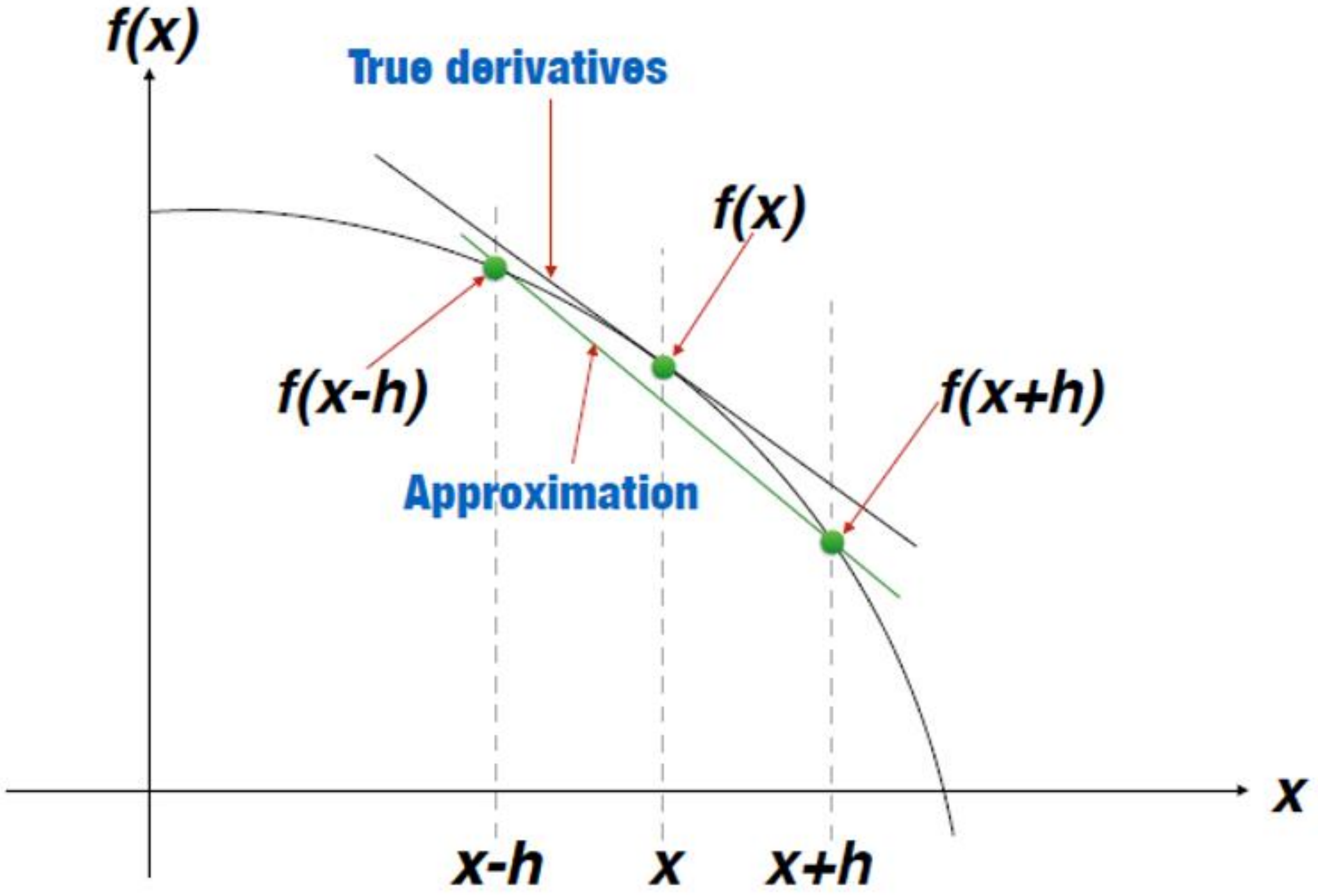
Forward Difference Approximation with accuracy of $O(h)$

5.2 Finite Difference Approximations of First Derivative



Backward Difference Approximation with accuracy of $O(h)$

5.2 Finite Difference Approximations of First Derivative



Centered Difference Approximation with accuracy of $O(h)$

5.2 Finite Difference Approximations of First Derivative

Example 1

Estimate the first derivative of a function

$$f(x) = 0.13x^5 - 0.75x^3 + 0.12x^2 - 0.5x + 1$$

at x= 0.5 with a step size of $h = 0.25$ and $h = 0.50$ using:

(a) forward and backward difference approximations of $O(h)$

(b) centered difference approximation of $O(h^2)$ to estimate the first derivative of

Note that the derivative can be calculated directly as

$$f'(x) = 0.65x^4 - 2.25x^2 + 0.24x - 0.5$$

and the true value as $f'(0.5) = -0.901875$. Hence, calculate the percent relative error for the cases above. Carry six decimal places along the computation.

Solution (a)

- For h = 0.25, the function $f(x) = 0.13x^5 - 0.75x^3 + 0.12x^2 - 0.5x + 1$ can be employed to obtain:

  $x - h = 0.25 \rightarrow f(x-h) = 0.870908$

  $x = 0.5 \rightarrow f(x) = 0.690313$

  $x + h = 0.75 \rightarrow f(x+h) = 0.406943$

- For h = 0.50, the values are:

  $x - h = 0 \rightarrow f(x-h) = 1.000000$

  $x = 0.5 \rightarrow f(x) = 0.690313$

  $x + h = 1 \rightarrow f(x+h) = 0$

- These values can be used to compute the forward, backward and centered difference approximation.

Solution (a)

- For *h =0.25,*

Forward difference approximation:

$$f'(0.5) \approx \frac{f(x+h)-f(x)}{h}$$

$$= \frac{0.406943-0.690313}{0.25} = -1.133480$$

Backward difference approximation:

$$f'(0.5) \approx \frac{f(x)-f(x-h)}{h}$$

$$= \frac{0.690313-0.870908}{0.25} = -0.722380$$

Solution (a)

- For *h =0.5,*

Forward difference:

$$f'(0.5) \approx \frac{f(x+h) - f(x)}{h}$$

$$= \frac{0 - 0.690313}{0.5} = -1.380626$$

Backward difference:

$$f'(0.5) \approx \frac{f(x) - f(x-h)}{h}$$

$$= \frac{0.690313 - 1.000000}{0.5} = -0.619374$$

Solution (b)

- **For centered divided difference,**

When h=0.25:

$$f'(0.5) \approx \frac{f(x+h)-f(x-h)}{2h}$$

$$= \frac{0.406943-0.870908}{2(0.25)} = -0.927930$$

When h=0.5:

$$f'(0.5) \approx \frac{f(x+h)-f(x-h)}{2h}$$

$$= \frac{0-1.00000}{2(0.5)} = -1.00000$$

Solution
(percent relative error)

h	Method	Approximate value	Percent relative error
0.25	Forward	-1.133480	$\frac{\lvert -0.901875-(-1.133480)\rvert}{\lvert -0.901875\rvert}\times 100\% = \mathbf{25.680388\%}$
	Backward	-0.722380	$\frac{\lvert -0.901875-(-0.722380)\rvert}{\lvert -0.901875\rvert}\times 100\% = \mathbf{19.902426\%}$
	Centred	-0.927930	$\frac{\lvert -0.901875-(-0.927930)\rvert}{\lvert -0.901875\rvert}\times 100\% = \mathbf{2.888981\%}$
0.5	Forward	-1.380626	$\frac{\lvert -0.901875-(-1.380626)\rvert}{\lvert -0.901875\rvert}\times 100\% = \mathbf{53.083964\%}$
	Backward	-0.619374	$\frac{\lvert -0.901875-(-0.619374)\rvert}{\lvert -0.901875\rvert}\times 100\% = \mathbf{31.323742\%}$
	Centred	-1.00000	$\frac{\lvert -0.901875-(-1.000000)\rvert}{\lvert -0.901875\rvert}\times 100\% = \mathbf{10.880111\%}$

5.2 Finite Difference Approximations of First Derivative

Example 2

Use forward, backward and centered difference to estimate the first derivative of $f(t) = e^{-\sin t}$ at $t = 1$ using step size of 0.5.

Solution:

$$f'(t) = -e^{-\sin t} \cos t$$

$$f'(1) = -0.232911$$

Analytic solution

Solution

$t - h = 0.5 \rightarrow f(t-h) = 0.619139$

$t = 1.0 \rightarrow f(t) = 0.431076$

$t + h = 1.5 \rightarrow f(t+h) = 0.368802$

$f'(1) = -0.232911$

Method	Approximate value	Percent relative error
Forward	$f'(1) \approx \frac{f(t+h)-f(t)}{h} = \frac{0.368802-0.431076}{0.5}$ = -0.124548	21.6726%
Backward	$f'(1) \approx \frac{f(t)-f(t-h)}{h} = \frac{0.431076-0.619139}{0.5}$ = -0.376126	28.643%
Centred	$f'(1) \approx \frac{f(t+h)-f(t-h)}{2h} = \frac{0.368802-0.619139}{2(0.5)}$ = -0.250337	1.7426%

Error reduced

5.2 Finite Difference Approximations of First Derivative

Example 3

Given the data

x	2.5	2.6	2.7	2.8	2.9	3.0	3.1
$f(x)$	13.625	15.376	17.283	19.352	21.589	24.000	26.591

Use forward and backward difference approximations of $O(h)$ to estimate $f'(2.7)$ using the step size $h=0.2$.

Solution

Forward difference approximation:

$$f'(2.7) \approx \frac{f(x+h)-f(x)}{h} = \frac{21.589-17.283}{0.2} = 21.53$$

Backward difference approximation:

$$f'(2.7) \approx \frac{f(x)-f(x-h)}{h} = \frac{17.283-13.625}{0.2} = 18.29$$

5.2 Finite Difference Approximations of First Derivative

Exercise

Estimate the first derivative of a function

$$f(t) = 3\sin 2t$$

at t = 0.5 with a step size of $h = 0.25$ using forward and backward difference approximation of $O(h)$ and centred difference approximation of $O(h^2)$.

ANSWER:

Forward $O(h)$=1.8724, Backward $O(h)$=4.3444, Centered $O(h^2)$=3.1084

5.3 High Accuracy Differentiations Formula

- Generated from 2 Taylor series expansions.

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \cdots. \quad (1)$$

$$f(x+2h) = f(x) + 2hf'(x) + \frac{(2h)^2}{2!}f''(x) + \cdots. \quad (2)$$

(1) X 4:

$$4f(x+h) = 4f(x) + 4hf'(x) + \frac{4h^2}{2!}f''(x) + \cdots. \quad (3)$$

(3) – (2) will becomes:

$$4f(x+h) - f(x+2h) = 3f(x) + 2hf'(x)$$

5.3 High Accuracy Differentiations Formula

- Forward difference approximation: $O(h^2)$

$$f'(x) \approx \frac{1}{2h}[-f(x+2h)+4f(x+h)-3f(x)]$$

- Backward difference approximation: $O(h^2)$

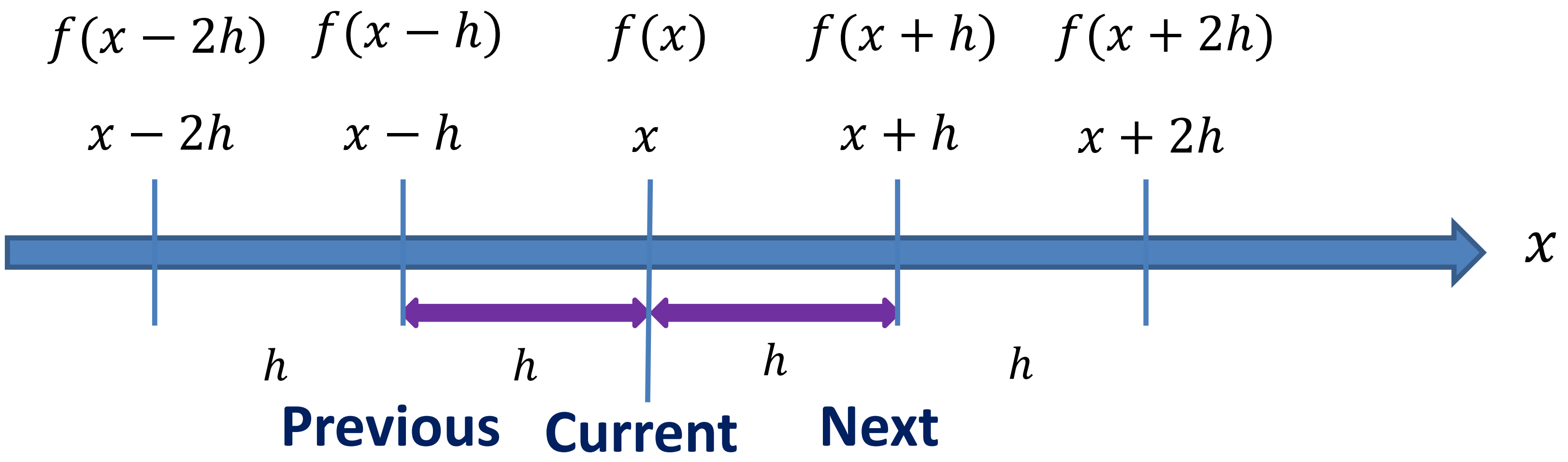
$$f'(x) \approx \frac{1}{2h}[3f(x)-4f(x-h)+f(x-2h)]$$

- Centered difference approximation: $O(h^4)$

$$f'(x) \approx \frac{1}{12h}[-f(x+2h)+8f(x+h)-8f(x-h)+f(x-2h)]$$

5.3 High Accuracy Differentiations Formula

Time Line:



Step size: h

5.3 High Accuracy Differentiations Formula

Example

Use high accuracy formula to estimate the first derivative of:

$$f(x) = 0.13x^5 - 0.75x^3 + 0.12x^2 - 0.5x + 1$$

at $x = 0.5$ and step size of $h = 0.25$.

Solution

$x = 0.5 \quad \rightarrow \quad f(x) = 0.6903$

$x - h = 0.25 \quad \rightarrow \quad f(x-h) = 0.8709$

$x - 2h = 0 \quad \rightarrow \quad f(x-2h) = 1$

$x + h = 0.75 \quad \rightarrow \quad f(x+h) = 0.4069$

$x + 2h = 1 \quad \rightarrow \quad f(x+2h) = 0$

Forward difference approximation, $O(h^2)$

$$f'(0.5) \approx \frac{1}{2h}[4f(x+h) - f(x+2h) - 3f(x)]$$

$$= \frac{1}{2(0.25)}[4(0.4069) - 0 - 3(0.6903)] = -0.8866$$

Solution

$$
\begin{aligned}
x &= 0.5 && \rightarrow \quad f(x) = 0.6903 \\
x - h &= 0.25 && \rightarrow \quad f(x-h) = 0.8709 \\
x - 2h &= 0 && \rightarrow \quad f(x-2h) = 1 \\
x + h &= 0.75 && \rightarrow \quad f(x+h) = 0.4069 \\
x + 2h &= 1 && \rightarrow \quad f(x+2h) = 0
\end{aligned}
$$

Backward difference approximation, $O(h^2)$

$$f'(0.5) \approx \frac{1}{2h}\left[3f(x) - 4f(x-h) + f(x-2h)\right]$$

$$= \frac{1}{2(0.25)}\left[3(0.6903) - 4(0.8709) + 1)\right] = -0.8254$$

Solution

$x = 0.5 \quad \rightarrow \quad f(x) = 0.6903$

$x - h = 0.25 \quad \rightarrow \quad f(x-h) = 0.8709$

$x - 2h = 0 \quad \rightarrow \quad f(x-2h) = 1$

$x + h = 0.75 \quad \rightarrow \quad f(x+h) = 0.4069$

$x + 2h = 1 \quad \rightarrow \quad f(x+2h) = 0$

Centred difference approximation, $O(h^4)$

$$f'(0.5) \approx \frac{1}{12h}[-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)]$$

$$= \frac{1}{12(0.25)}[-0 + 8(0.4069) - 8(0.8709) + 1] = -0.904$$

Solution

Method	Approximate value	Percent relative error
Forward	-0.8866	1.694%
Backward	-0.8254	8.480%
Centred	-0.904	0.2356%

5.3 High Accuracy Differentiations Formula

Exercise 1

Use high accuracy formula of $O(h^2)$ and $O(h^4)$ to estimate the first derivative of

$$f(t) = e^{-\sin t}$$

at $t = 1$ using step size of 0.25.

ANSWER:

Forward $O(h^2)$ =-0.22699; Backward $O(h^2)$ =-0.22157;

Centered $O(h^4)$ =-0.23296

5.3 High Accuracy Differentiations Formula

Exercise 2

Given the following data

t	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
X	0.231	0.451	0.511	0.623	0.687	0.731	0.882	0.903	0.922	0.987

Find the first derivative using high accuracy formula of $O(h^2)$ and $O(h^4)$ at $t = 0.6$, with $h = 0.2$.

ANSWER:

Forward $O(h^2)$ =0.864; Backward $O(h^2)$ =0.304; Centered $O(h^4)$ =0.568