Chapter 23 Numerical Differentiation

23.1

- Remember Taylor Series :

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

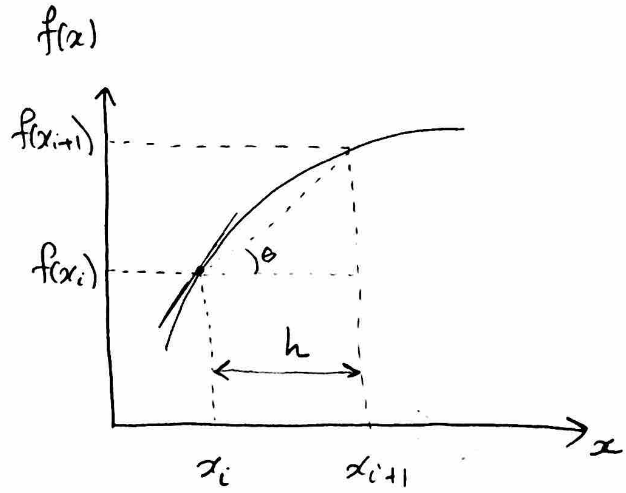
Taking first order approximation

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

→ First order approximation error order

Thus, Eq (1)

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

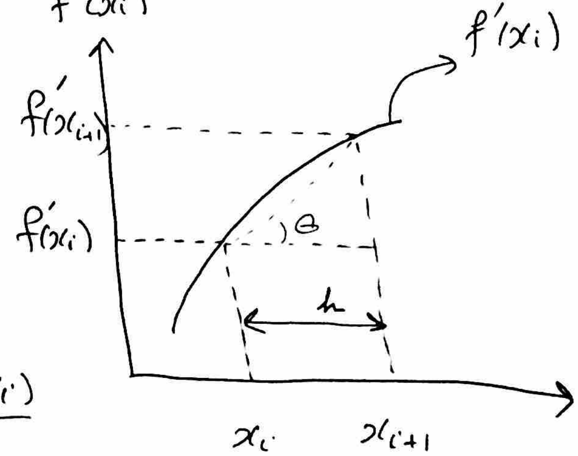


Graphically,

$f'(x_i)$ = slope

$$\text{slope} = \tan\theta = \frac{f(x_{i+1}) - f(x_i)}{h}$$

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



For 2nd derivative

$f''(x_i)$ = Slope = $\tan\theta$

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

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

Eq(2)

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

- Back to Taylor Series

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)h^2}{2} + \frac{f'''(x_i)h^3}{3!} + \dots$$

Taking 2nd order approximation:

2nd order approximation error order

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

substitute Eq(2) and re-arrange

Eq(3)

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

In a similar fashion of Eq(2), we can obtain:

Eq(4)

$$\boxed{f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}} + O(h^2)$$

The above Eq(1-4), are:

Forward Finite Divided Differences

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FIGURE 23.1
Forward finite-divided-difference formulas: two versions are presented for each derivative. The latter version incorporates more terms of the Taylor series expansion and is, consequently, more accurate.

	Error
First Derivative	
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	$O(h^2)$
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 Divided Differences (Backward F.D.D)

* Taylor series can be expanded in a backward way, thus:

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

Therefore, Backward F.D.D can be estimated as:

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

FIGURE 23.2
Backward finite-divided-difference formulas: two versions are presented for each derivative. The latter version incorporates more terms of the Taylor series expansion and is, consequently, more accurate.

* Centered Finite Divided Differences (Centered F.D.D)

Forward Taylor Series

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

Backward Taylor Series

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

Subtract Eq(b) from Eq(a) [Eq(a) − Eq(b)]

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

Thus,

Eq(5)

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

$\longrightarrow$ comes from two First orders $\Rightarrow$ 2nd order

Similarly

FIGURE 23.3
Centered finite-divided-difference formulas: two versions are presented for each derivative. The latter version incorporates more terms of the Taylor series expansion and is, consequently, more accurate.

First Derivative — Error

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

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} \qquad O(h^4)$$

Second Derivative

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

$$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2} \qquad O(h^4)$$

Third Derivative

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

$$f'''(x_i) = \frac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3} \qquad O(h^4)$$

Fourth Derivative

$$f''''(x_i) = \frac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4} \qquad O(h^2)$$

$$f''''(x_i) = \frac{-f(x_{i+3}) + 12f(x_{i+2}) - 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) - f(x_{i-3})}{6h^4} \qquad O(h^4)$$

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

find $f'(0.5)$ and let $h = 0.25$, Using

① Forward F.D.D
- $O(h)$
- $O(h^2)$

② Backward F.D.D
- $O(h)$
- $O(h^2)$

③ Centered F.D.D
- $O(h^2)$
- $O(h^4)$

Solution

① Forward F.D.D

- $O(h)$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h}, \quad x_i = 0.5, \quad x_{i+1} = x_i + h = 0.75$$

$$= \frac{f(0.75) - f(0.5)}{0.25} = -1.155$$

- $O(h^2)$

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}, \quad x_i = 0.5, \quad x_{i+1} = 0.75, \quad x_{i+2} = 1$$

$$= \frac{-f(1) + 4f(0.75) - 3f(0.5)}{(2)(0.25)} = -0.859$$

Backward F.D.D

- $O(h)$

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} = \frac{f(0.5) - f(0.25)}{0.25} = -0.714$$

$x_i = 0.5$, $x_{i-1} = x_i - h = 0.25$

- $O(h^2)$

$$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h} = \frac{3f(0.5) - 4f(0.25) + f(0)}{(2)(0.25)} = -0.878$$

$x_i = 0.5$, $x_{i-1} = 0.25$, $x_{i-2} = 0$

Centered F.D.D

- $O(h^2)$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} = \frac{f(0.75) - f(0.25)}{(2)(0.25)} = -0.934$$

- $O(h^4)$

$$f'(x_i) = \frac{-f(x_{i-2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}$$

$$= \frac{-f(1) + 8f(0.75) - 8f(0.25) + f(0)}{(12)(0.25)}$$

$$= -0.9125$$

practice If exact value of $f'(0.5)$ is -0.9125

- compute E_t of each case above and compare the accuracy

" See example 23.1 page 658 "