CPE 310: Numerical Analysis for Engineers

Chapter 4: Numerical Differentiation and Numerical Integration

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Numerical Differentiation

A technique used to find the derivative of a function that is given by a table

Formulas for numerical derivatives are important in solving differential equations

Derivatives from Divided Difference Tables

Derivatives from Difference Tables

Forward, Central, and Backward Difference Tables

Derivatives from Divided Difference Tables

Derivatives from Divided Difference Tables

Let $(x_i, f_i), i = 0,1,2,\cdots,n$ be a data, We can use interpolation to approximate f:

$$f(x) \approx P_n(x)$$

Let us write the polynomial $P_n(x)$ in terms of divided differences:

$$P_n(x) = f_0 + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) + \cdots + f[x_0, \cdots, x_n](x - x_0)\cdots(x - x_{n-1})$$

If $P_n(x)$ is a good approximation for $f(x)$, then $P_n'(x)$ is a good approximation for $f'(x)$

$$f'(x) \approx P'_n(x) = \frac{d}{dx}\left[f_0 + f_0^{[1]}(x - x_0) + f_0^{[2]}(x - x_0)(x - x_1) + \cdots + f_0^{[n]}(x - x_0)\cdots(x - x_{n-1})\right]$$

Recall that the derivative of a product of *n* terms is a **sum of *n* of these product terms** with one member of each term in the sum replaced by its derivative

$$\frac{d}{dx}(u * v * w) = u' * v * w + u * v' * w + u * v * w'$$

$$\frac{d}{dx}\prod_{i=0}^{n-1}(x - x_i) = \sum_{i=0}^{n-1}\frac{(x - x_0)(x - x_1)\cdots(x - x_{n-1})}{(x - x_i)}$$

$$= \sum_{i=0}^{n-1}\prod_{\substack{j=0 \\ j\neq i}}^{n-1}(x - x_j)$$

Derivatives from Divided Difference Tables

$$f'(x) \approx P'_n(x) = \frac{d}{dx}\left[f_0 + f_0^{[1]}(x-x_0) + f_0^{[2]}(x-x_0)(x-x_1) + \cdots + f_0^{[n]}(x-x_0)\cdots(x-x_{n-1})\right]$$

Differentiating the right-hand side, we obtain:

$$\frac{d}{dx}(x-x_0) = 1$$

$$\frac{d}{dx}(x-x_0)(x-x_1) = (x-x_0) + (x-x_1) = \sum_{i=0}^{1}\frac{(x-x_0)(x-x_1)}{x-x_i}$$

$$\frac{d}{dx}(x-x_0)(x-x_1)\cdots(x-x_{n-1}) = \sum_{i=0}^{n-1}\frac{(x-x_0)(x-x_1)\cdots(x-x_{n-1})}{x-x_i}$$

$$f'(x) \approx P'_n(x) = f[x_0,x_1] + f[x_0,x_1,x_2]\sum_{i=0}^{1}\frac{(x-x_0)(x-x_1)}{x-x_i} + \cdots + f[x_0,\cdots,x_n]\sum_{i=0}^{n-1}\frac{(x-x_0)(x-x_1)\cdots(x-x_{n-1})}{x-x_i}$$

Let $f(x) = x^2 - x + 1$, and tabulate for $x = 0,2,3,5,6$ (five points). Use **divided differences for approximating derivative** at $x = 4.1$ using a **cubic interpolating polynomial** starting at $x_i = 2$ to 6

x_i	f_i	$f_i^{[1]}$	$f_i^{[2]}$	$f_i^{[3]}$	$f_i^{[4]}$
0	1				
2	3	1			
3	7	**4**	1		
5	21	7	**1**	0	
6	31	10	1	**0**	0

$$f'(x) \approx P'_n(x) = f[x_0, x_1] + f[x_0, x_1, x_2] \sum_{i=0}^{1} \frac{(x - x_0)(x - x_1)}{x - x_i} + \cdots + f[x_0, \cdots, x_n] \sum_{i=0}^{n-1} \frac{(x - x_0)(x - x_1)\cdots(x - x_{n-1})}{x - x_i}$$

$$f'(x) \approx P'_n(x) = f_1^{[1]} + f_1^{[2]}[(x - x_2) + (x - x_1)] + f_1^{[3]}[(x - x_2)(x - x_3) + (x - x_1)(x - x_3) + (x - x_1)(x - x_2)]$$

$$f'(x) \approx P'_n(x) = \mathbf{4} + \mathbf{1}[(x - x_2) + (x - x_1)] + \mathbf{0}[(x - x_2)(x - x_3) + (x - x_1)(x - x_3) + (x - x_1)(x - x_2)]$$

$$f'(x) \approx P'_n(x) = \mathbf{4} + (x - 3) + (x - 2) = 2x - 1$$

$$f'(4.1) = 2(4.1) - 1 = 7.2$$

Derivatives from Difference Tables

Derivatives from Difference Tables

*When the data are **evenly spaced**, we can use a **table of function differences** to construct the interpolating polynomial*

$$P_n(s) = f_i + s\Delta f_i + \frac{s(s-1)}{2!}\Delta^2 f_i + \frac{s(s-1)(s-2)}{3!}\Delta^3 f_i + \cdots + \prod_{j=0}^{n-1}(s-j)\frac{\Delta^n f_i}{n!}$$

$$f'(x) = P_n'(s) = \frac{1}{h}\left[\Delta f_i + \sum_{j=2}^{n}\left\{\sum_{k=0}^{j-1}\prod_{\substack{l=0 \\ l\neq k}}^{j-1}(s-l)\right\}\frac{\Delta^j f_i}{j!}\right]$$

Estimate the value of $f'(3.3)$ with a **cubic polynomial** that is created if we enter the table at $i = 2$, given this difference table:

i	x_i	$f(x)$	Δf_i	$\Delta^2 f_i$	$\Delta^3 f_i$	$\Delta^4 f_i$	$\Delta^5 f_i$
0	1.30	3.669	4.017	2.479	2.041	1.672	1.386
1	1.90	6.686	5.496	4.520	3.713	3.058	2.504
2	2.50	12.182	10.016	8.233	6.771	5.562	
3	3.10	22.198	18.249	15.004	12.333		
4	3.70	40.447	33.253	27.337			
5	4.30	73.700	60.590				
6	4.90	134.290					

$$P'_n(s) = \frac{1}{h}\left[\Delta f_i + \sum_{j=2}^{n}\left\{\sum_{k=0}^{j-1}\prod_{\substack{l=0\\ l\neq k}}^{j-1}(s-l)\right\}\frac{\Delta^j f_i}{j!}\right]$$

$h = 0.6$, and we start at $x_i = 2.5 \Longrightarrow s = \frac{x-x_i}{h} = \frac{3.3-2.5}{0.6} = \frac{4}{3}$

Cubic polynomial means $n = 3$ which means the derivative is of order “2”

$$P'_3(x) = \frac{1}{h}\left[\Delta f_2 + \sum_{j=2}^{3}\left\{\sum_{k=0}^{j-1}\prod_{\substack{l=0\\ l\neq k}}^{j-1}(s-l)\right\}\frac{\Delta^j f_i}{j!}\right]$$

$$P'_3(x) = \frac{1}{h}\left[\Delta f_2 + \sum_{j=2}^{3}\left\{\sum_{k=0}^{j-1}\prod_{\substack{l=0\\l\neq k}}^{j-1}(s-l)\right\}\frac{\Delta^j f_i}{j!}\right]$$

$$P'_3(x) = \frac{1}{h}\left[\Delta f_2 + \left\{\left\{\sum_{k=0}^{1}\prod_{\substack{l=0\\l\neq k}}^{1}(s-l)\right\}\frac{\Delta^2 f_2}{2!}\right\} + \left\{\left\{\sum_{k=0}^{2}\prod_{\substack{l=0\\l\neq k}}^{2}(s-l)\right\}\frac{\Delta^3 f_2}{3!}\right\}\right]$$

$$P'_3(x) = \frac{1}{h}\left[\Delta f_2 + \left\{[(s-1)+(s-0)]\ \frac{\Delta^2 f_2}{2!}\right\} + \left\{[(s-1)(s-2)+(s-0)(s-2)+(s-0)(s-1)\ ]\frac{\Delta^3 f_2}{3!}\right\}\right]$$

$$P'_3(x) = \frac{1}{0.6}\left[10.016 + \left\{[\left(\frac{4}{3}-1\right)+(\frac{4}{3}-0)]\ \frac{8.233}{2}\right\} + \left\{[\left(\frac{4}{3}-1\right)\left(\frac{4}{3}-2\right)+\left(\frac{4}{3}-0\right)\left(\frac{4}{3}-2\right)+(\frac{4}{3}-0)(\frac{4}{3}-1)\ ]\frac{6.771}{6}\right\}\right]$$

$$P'_3(x) = 27.875$$

Awkward to use when we do hand computations

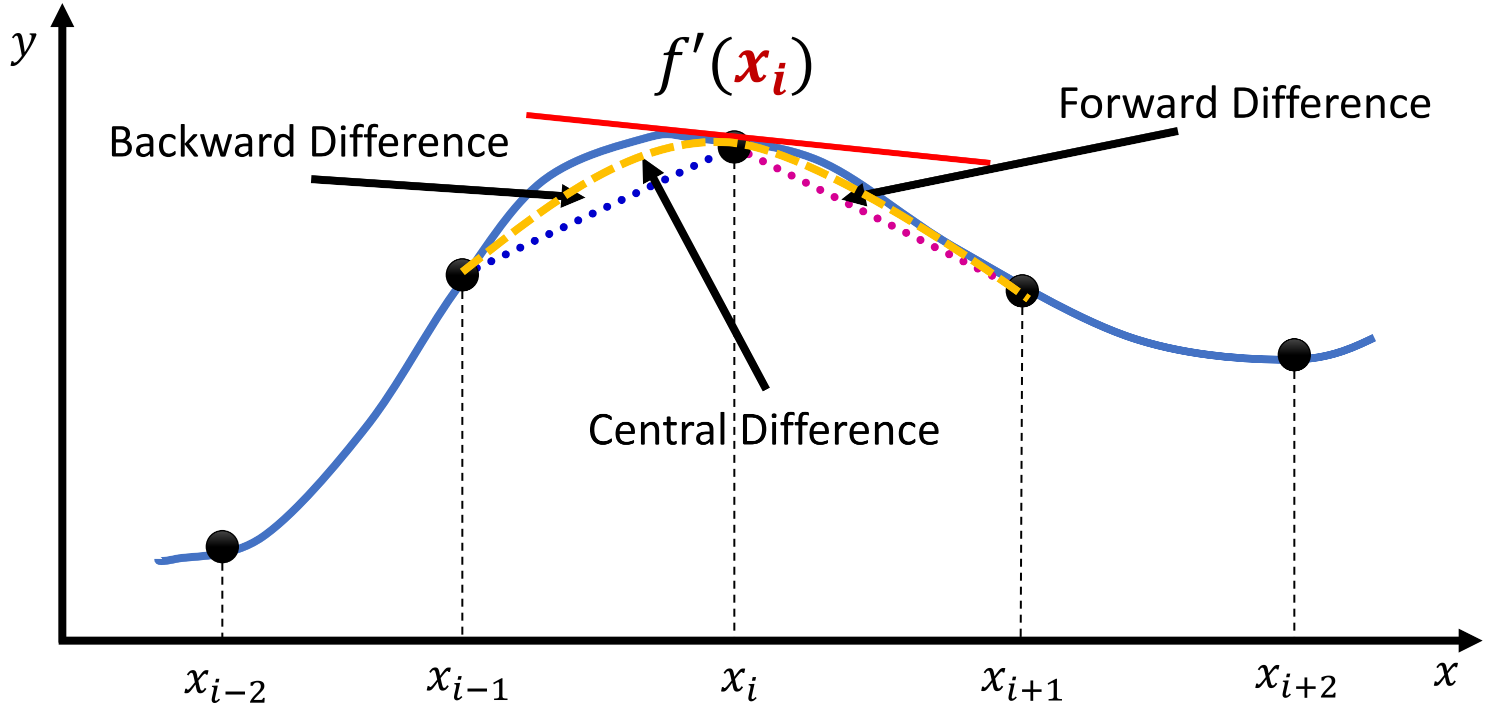
$$f'(x) = P_n'(s) = \frac{1}{h}\left[\Delta f_i + \sum_{j=2}^{n}\left\{\sum_{k=0}^{j-1}\prod_{\substack{l=0\\ l\neq k}}^{j-1}(s-l)\right\}\frac{\Delta^j f_i}{j!}\right]$$

Let us simplify it!

If we stipulate "specify" that the *x*-value must be in the **difference table**, the computation is simplified considerably.

i	x_i	$f(x)$	Δf_i	$\Delta^2 f_i$	$\Delta^3 f_i$	$\Delta^4 f_i$	$\Delta^5 f_i$
0	1.30	3.669	4.017	2.479	2.041	1.672	1.386
1	1.90	6.686	5.496	4.520	3.713	3.058	2.504
2	2.50	12.182	10.016	8.233	6.771	5.562	
3	3.10	22.198	18.249	15.004	12.333		
4	3.70	40.447	33.253	27.337			
5	4.30	73.700	60.590				
6	4.90	134.290					

First Derivative: Forward, Central, and Backward



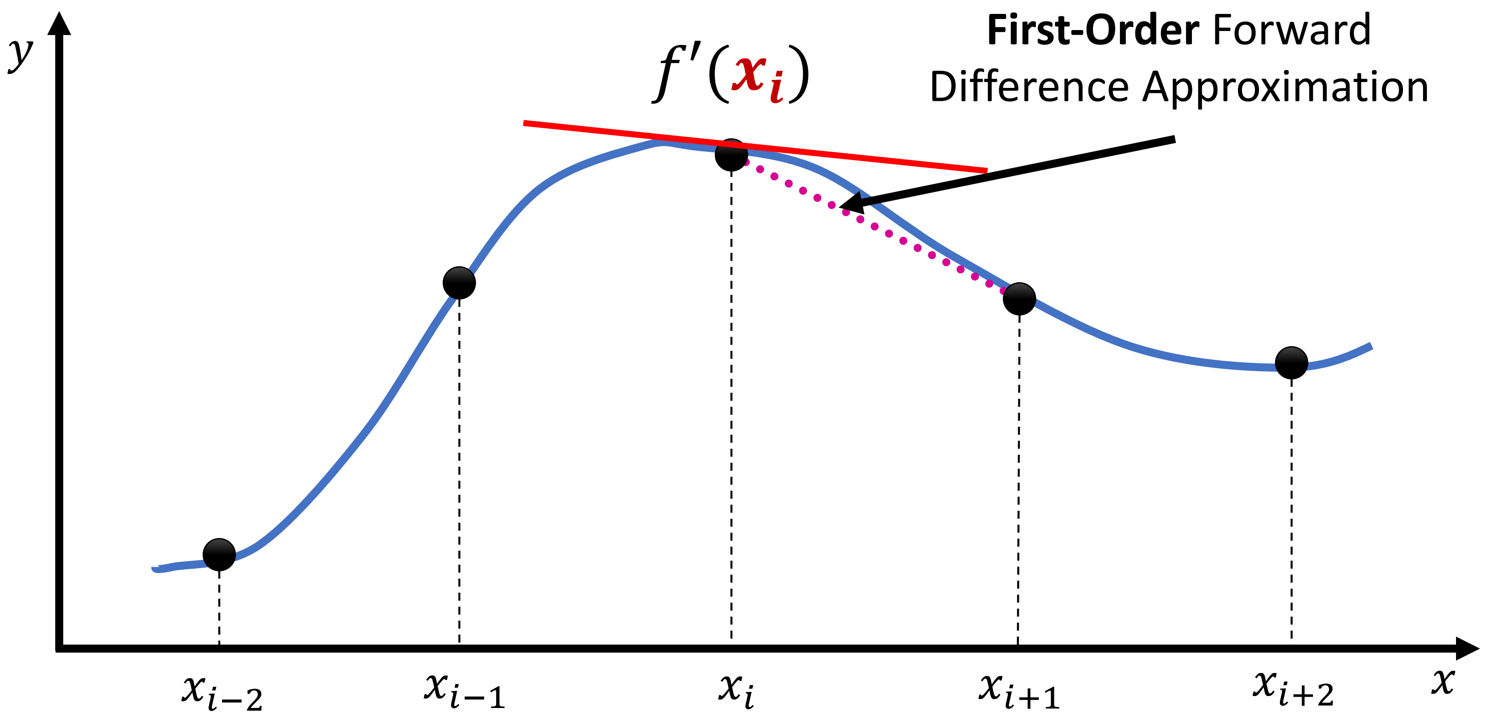
First Derivative using **Forward Difference**: $f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} = \frac{f(x_i + h) - f(x_i)}{h}$

First Derivative using **Backward Difference**: $f'(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} = \frac{f(x_i) - f(x_i - h)}{h}$

First Derivative using **Central Difference**: $f'(x_i) \approx \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}} = \frac{f(x_i + h) - f(x_i - h)}{2h}$

First Derivative: Forward Difference Approximation

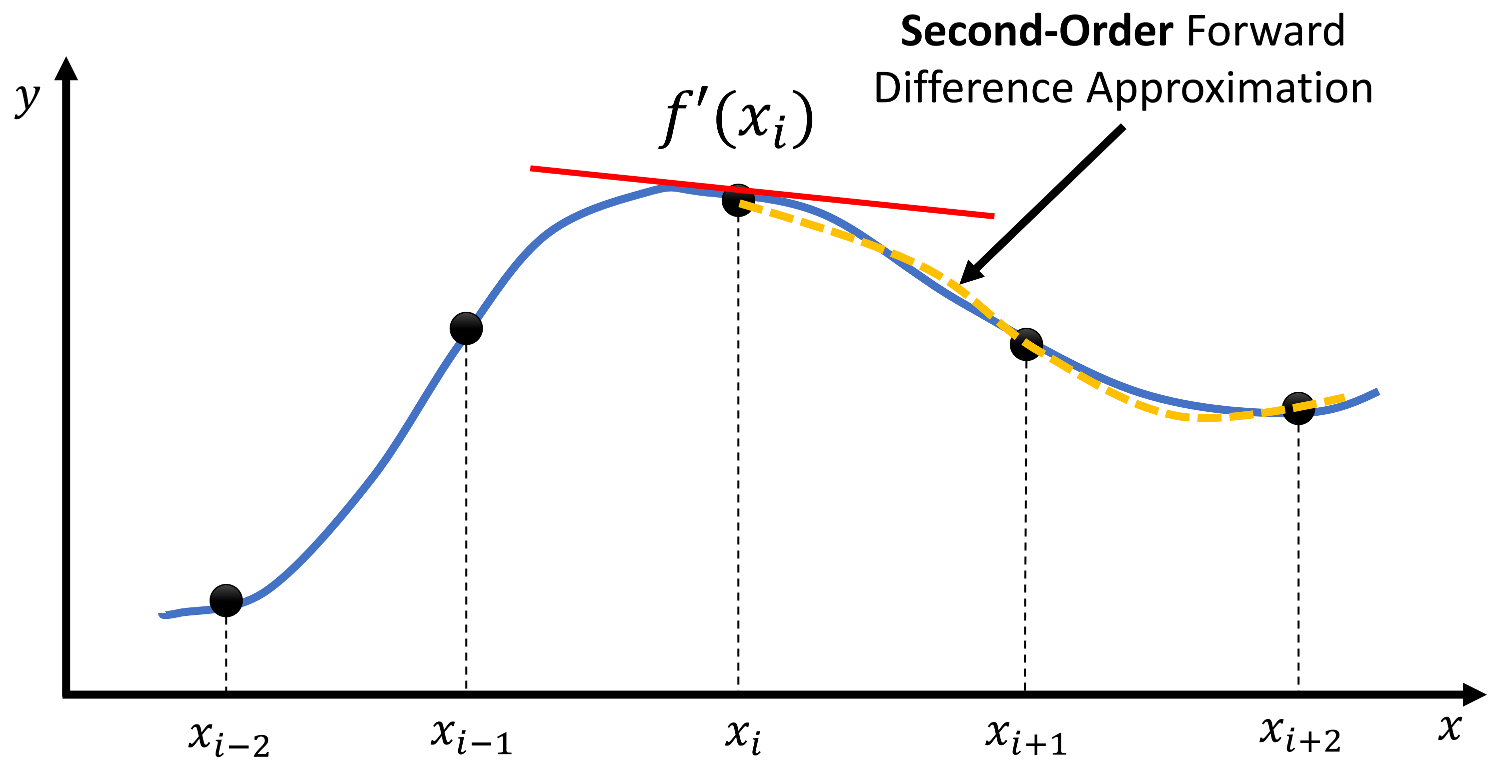
The differences all involve f-values that lie ***forward in the table*** *from* f_i



*The Forward difference approximation always evaluated **at the first point**:*

$$s = \frac{x_i - x_i}{h} = 0$$

x	$f(x)$	Δf
x_i	f_i	$f_{i+1} - f_i$
x_{i+1}	f_{i+1}	



*The Forward difference approximation always evaluated **at the first point**:*

$$s = \frac{x_i - x_i}{h} = 0$$

x	$f(x)$	Δf	$\Delta^2 f$
x_i	f_i	$f_{i+1} - f_i$	$f_{i+2} - 2f_{i+1} + f_i$
x_{i+1}	f_{i+1}	$f_{i+2} - f_{i+1}$	
x_{i+2}	f_{i+2}		

$$f'(x) = P_n'(s) = \frac{1}{h}\left[\Delta f_i + \sum_{j=2}^{n}\left\{\sum_{k=0}^{j-1}\prod_{\substack{l=0\\l\neq k}}^{j-1}(s-l)\right\}\frac{\Delta^j f_i}{j!}\right]$$

First-Order Forward Difference Approximation

$$s = \frac{\boldsymbol{x_i} - x_i}{h} = 0$$

$$f'(x_i) \approx \frac{1}{h}[\Delta f_i]_{n=1}$$

Second-Order Forward Difference Approximation

$$s = \frac{\boldsymbol{x_i} - x_i}{h} = 0$$

$$f'(x_i) \approx \frac{1}{h}\left[\Delta f_i - \frac{1}{2}\Delta^2 f_i\right]_{n=2}$$

First-Order Forward Difference Approximation

$$f'(x_i) \approx \frac{1}{h}[\Delta f_i]_{n=1}$$

$\boldsymbol{x}$	$\boldsymbol{f(x)}$	$\boldsymbol{\Delta f}$
$\boldsymbol{x_i}$	f_i	$f_{i+1} - f_i$
x_{i+1}	f_{i+1}	

$$f'(x_i) \approx \frac{f_{i+1} - f_i}{h}$$

Second-Order Forward Difference Approximation

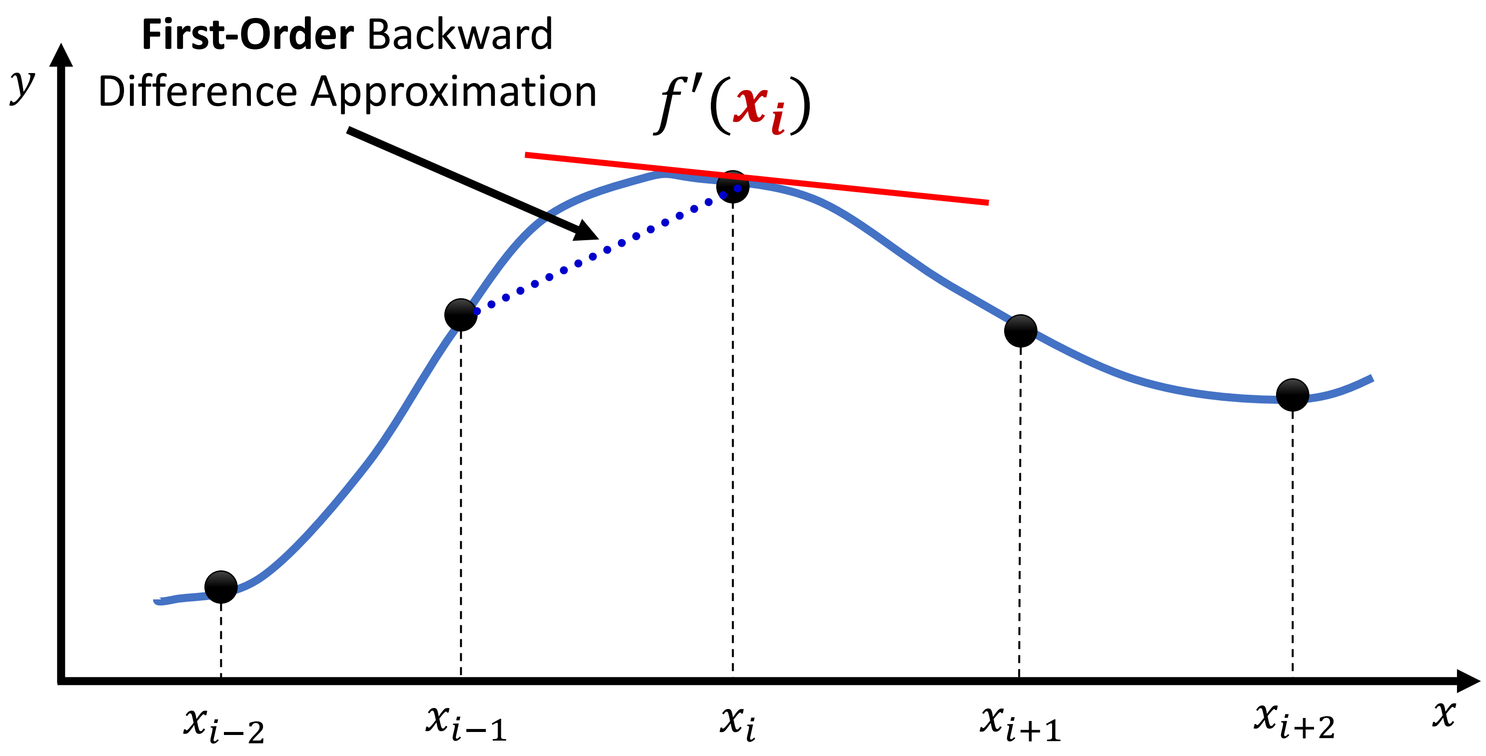
$$f'(x_i) \approx \frac{1}{h}\left[\Delta f_i - \frac{1}{2}\Delta^2 f_i\right]_{n=2}$$

$\boldsymbol{x}$	$\boldsymbol{f(x)}$	$\boldsymbol{\Delta f}$	$\boldsymbol{\Delta^2 f}$
$\boldsymbol{x_i}$	f_i	$f_{i+1} - f_i$	$f_{i+2} - 2f_{i+1} + f_i$
x_{i+1}	f_{i+1}	$f_{i+2} - f_{i+1}$	
x_{i+2}	f_{i+2}		

$$f'(x_i) \approx \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h}$$

First Derivative: Backward Difference Approximation

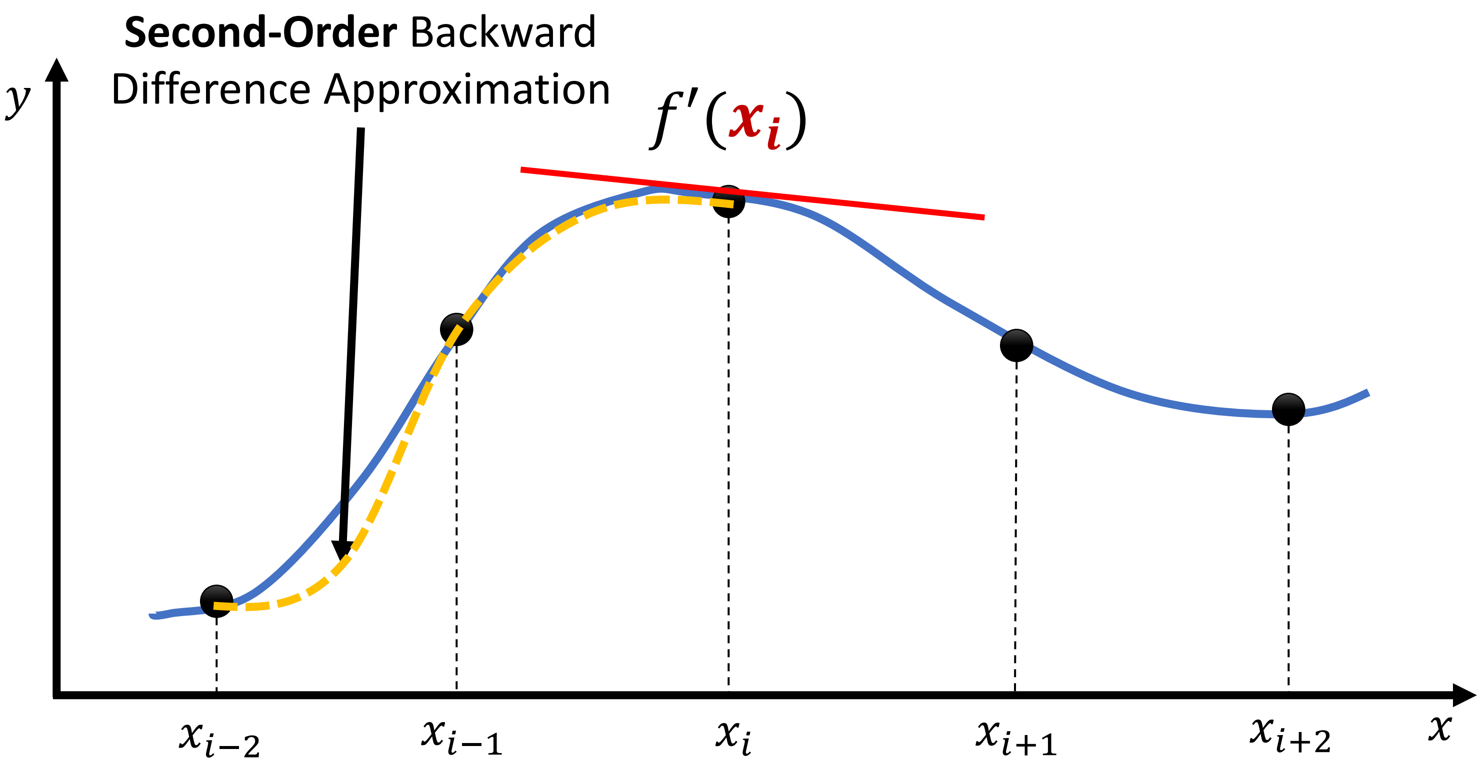
*The differences all involve f-values that lie **backward in the table** from f_i*



The First-Order Backward difference approximation is evaluated at the point which is one step ahead from the starting $\boldsymbol{x}$

$$s = \frac{\boldsymbol{x_i} - x_{i-1}}{h} = 1$$

$\boldsymbol{x}$	$\boldsymbol{f(x)}$	$\boldsymbol{\Delta f}$
x_{i-1}	f_{i-1}	$f_i - f_{i-1}$
$\boldsymbol{x_i}$	f_i	



The Second-Order Backward difference approximation is evaluated at the point which is two steps ahead from the starting $\boldsymbol{x}$

$$s = \frac{x_i - x_{i-2}}{h} = 2$$

$\boldsymbol{x}$	$\boldsymbol{f(x)}$	$\boldsymbol{\Delta f}$	$\boldsymbol{\Delta^2 f}$
x_{i-2}	f_{i-2}	$f_{i-1} - f_{i-2}$	$f_i - 2f_{i-1} + f_{i-2}$
x_{i-1}	f_{i-1}	$f_i - f_{i-1}$	
x_i	f_i		

$$f'(x) = P_n'(s) = \frac{1}{h}\left[\Delta f_i + \sum_{j=2}^{n}\left\{\sum_{k=0}^{j-1}\prod_{\substack{l=0\\ l\neq k}}^{j-1}(s-l)\right\}\frac{\Delta^j f_i}{j!}\right]$$

First-Order Backward Difference Approximation

$$s = \frac{\boldsymbol{x_i} - x_{i-1}}{h} = 1$$

$$f'(x_i) \approx \frac{1}{h}[\Delta f_{i-1}]_{n=1}$$

Second-Order Backward Difference Approximation

$$s = \frac{\boldsymbol{x_i} - x_{i-2}}{h} = 2$$

$$f'(x_i) \approx \frac{1}{h}\left[\Delta f_{i-2} + \frac{3}{2}\Delta^2 f_{i-2}\right]_{n=2}$$

First-Order Backward Difference Approximation

$$f'(x_i) \approx \frac{1}{h}[\Delta f_{i-1}]_{n=1}$$

x	$f(x)$	Δf
x_{i-1}	f_{i-1}	$f_i - f_{i-1}$
x_i	f_i	

$$f'(x_i) \approx \frac{f_i - f_{i-1}}{h}$$

Second-Order Backward Difference Approximation

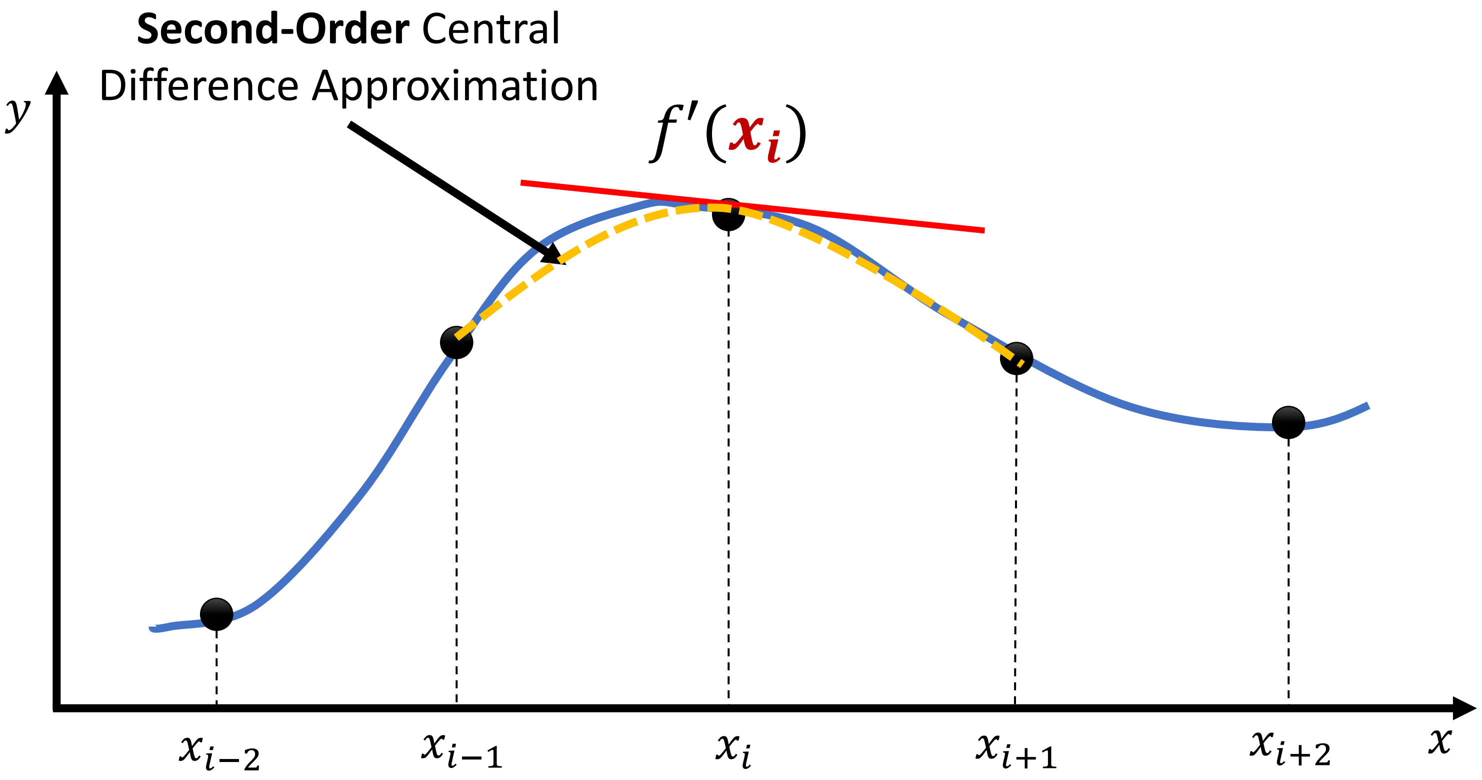
$$f'(x_i) \approx \frac{1}{h}\left[\Delta f_{i-2} + \frac{3}{2}\Delta^2 f_{i-2}\right]_{n=2}$$

x	$f(x)$	Δf	$\Delta^2 f$
x_{i-2}	f_{i-2}	$f_{i-1} - f_{i-2}$	$f_i - 2f_{i-1} + f_{i-2}$
x_{i-1}	f_{i-1}	$f_i - f_{i-1}$	
x_i	f_i		

$$f'(x_i) \approx \frac{3f_i - 4f_{i-1} + f_{i-2}}{2h}$$

First Derivative: Central Difference Approximation

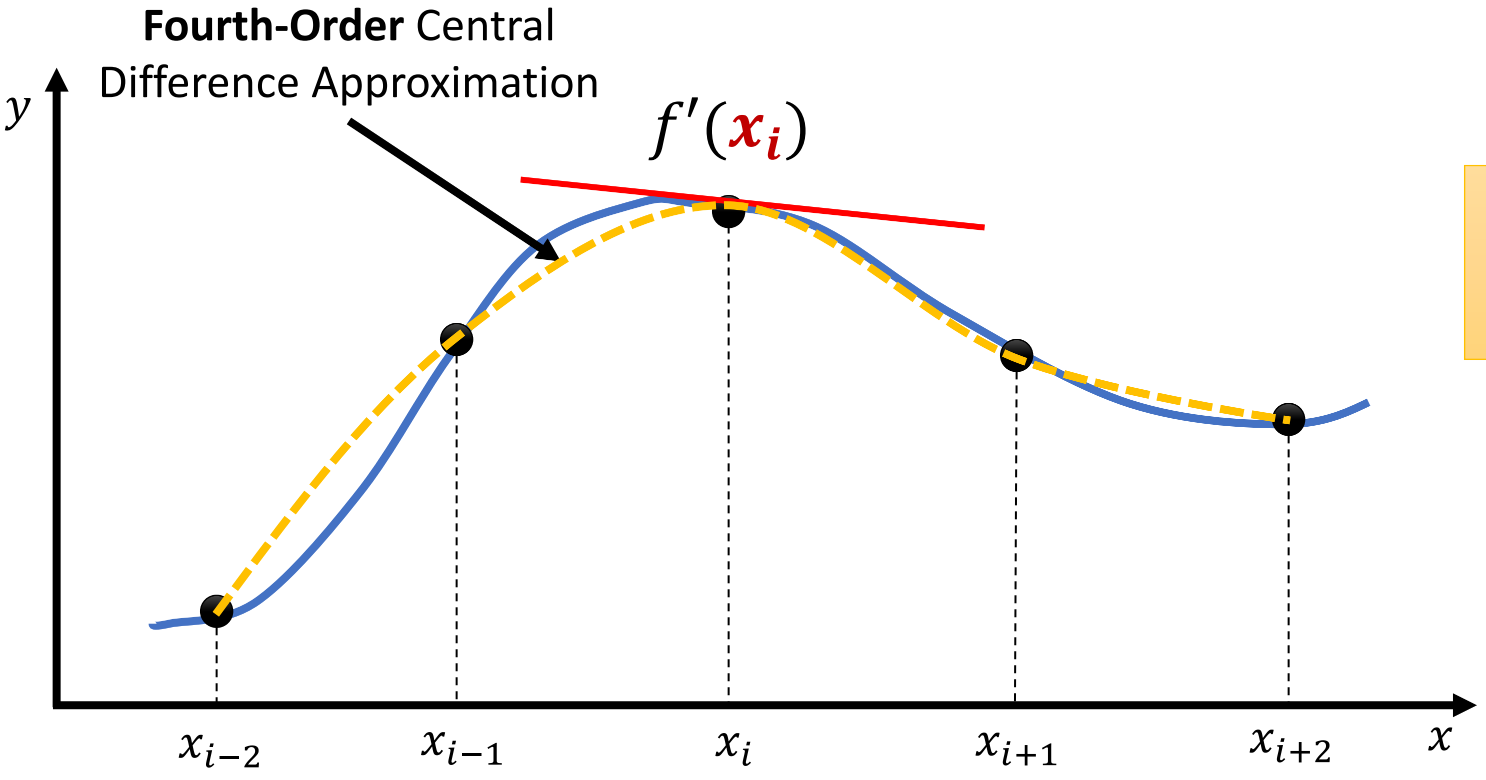
The x-value is centered within the range of x-values used in its construction



The Second-Order Central difference approximation is evaluated at the point which is one step ahead from the starting ***x***

$$s = \frac{x_i - x_{i-1}}{h} = 1$$

$\boldsymbol{x}$	$\boldsymbol{f(x)}$	$\Delta \boldsymbol{f}$	$\Delta^2 \boldsymbol{f}$
x_{i-1}	f_{i-1}	$f_i - f_{i-1}$	$f_{i+1} - 2f_i + f_{i-1}$
$\boldsymbol{x_i}$	f_i	$f_{i+1} - f_i$	
x_{i+1}	f_{i+1}		



The Fourth-Order Central difference approximation is evaluated at the point which is two steps ahead from the starting $\boldsymbol{x}$

$$s = \frac{\boldsymbol{x_i} - x_{i-2}}{h} = 2$$

$\boldsymbol{x}$	$\boldsymbol{f(x)}$	$\Delta \boldsymbol{f}$	$\Delta^2 \boldsymbol{f}$	$\Delta^3 \boldsymbol{f}$	$\Delta^4 \boldsymbol{f}$
x_{i-2}	f_{i-2}	$f_{i-1} - f_{i-2}$	$f_i - 2f_{i-1} + f_{i-2}$	$f_{i+1} - 3f_i + 3f_{i-1} - f_{i-2}$	$f_{i+2} - 4f_{i+1} + 6f_i - 4f_{i-1} + f_{i-2}$
x_{i-1}	f_{i-1}	$f_i - f_{i-1}$	$f_{i+1} - 2f_i + f_{i-1}$	$f_{i+2} - 3f_{i+1} + 3f_i - f_{i-1}$	
$\boldsymbol{x_i}$	f_i	$f_{i+1} - f_i$	$f_{i+2} - 2f_{i+1} + f_i$		
x_{i+1}	f_{i+1}	$f_{i+2} - f_{i+1}$			
x_{i+2}	f_{i+2}				

$$f'(x) = P_n'(s) = \frac{1}{h}\left[\Delta f_i + \sum_{j=2}^{n}\left\{\sum_{k=0}^{j-1}\prod_{\substack{l=0\\l\neq k}}^{j-1}(s-l)\right\}\frac{\Delta^j f_i}{j!}\right]$$

Second-Order Central Difference Approximation

$$s = \frac{\boldsymbol{x_i} - x_{i-1}}{h} = 1$$

$$f'(x_i) \approx \frac{1}{h}\left[\Delta f_{i-1} + \frac{1}{2}\Delta^2 f_{i-1}\right]_{n=2}$$

Fourth-Order Central Difference Approximation

$$s = \frac{\boldsymbol{x_i} - x_{i-2}}{h} = 2$$

$$f'(x_i) \approx \frac{1}{h}\left[\Delta f_{i-2} + \frac{3}{2}\Delta^2 f_{i-2} + \frac{1}{3}\Delta^3 f_{i-2} - \frac{1}{12}\Delta^4 f_{i-2}\right]_{n=4}$$

Second-Order Central Difference Approximation

$$f'(x_i) \approx \frac{1}{h}\left[\Delta f_{i-1} + \frac{1}{2}\Delta^2 f_{i-1}\right]_{n=2}$$

$\boldsymbol{x}$	$\boldsymbol{f(x)}$	$\Delta \boldsymbol{f}$	$\Delta^2 \boldsymbol{f}$
x_{i-1}	f_{i-1}	$f_i - f_{i-1}$	$f_{i+1} - 2f_i + f_{i-1}$
$\boldsymbol{x_i}$	f_i	$f_{i+1} - f_i$	
x_{i+1}	f_{i+1}		

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

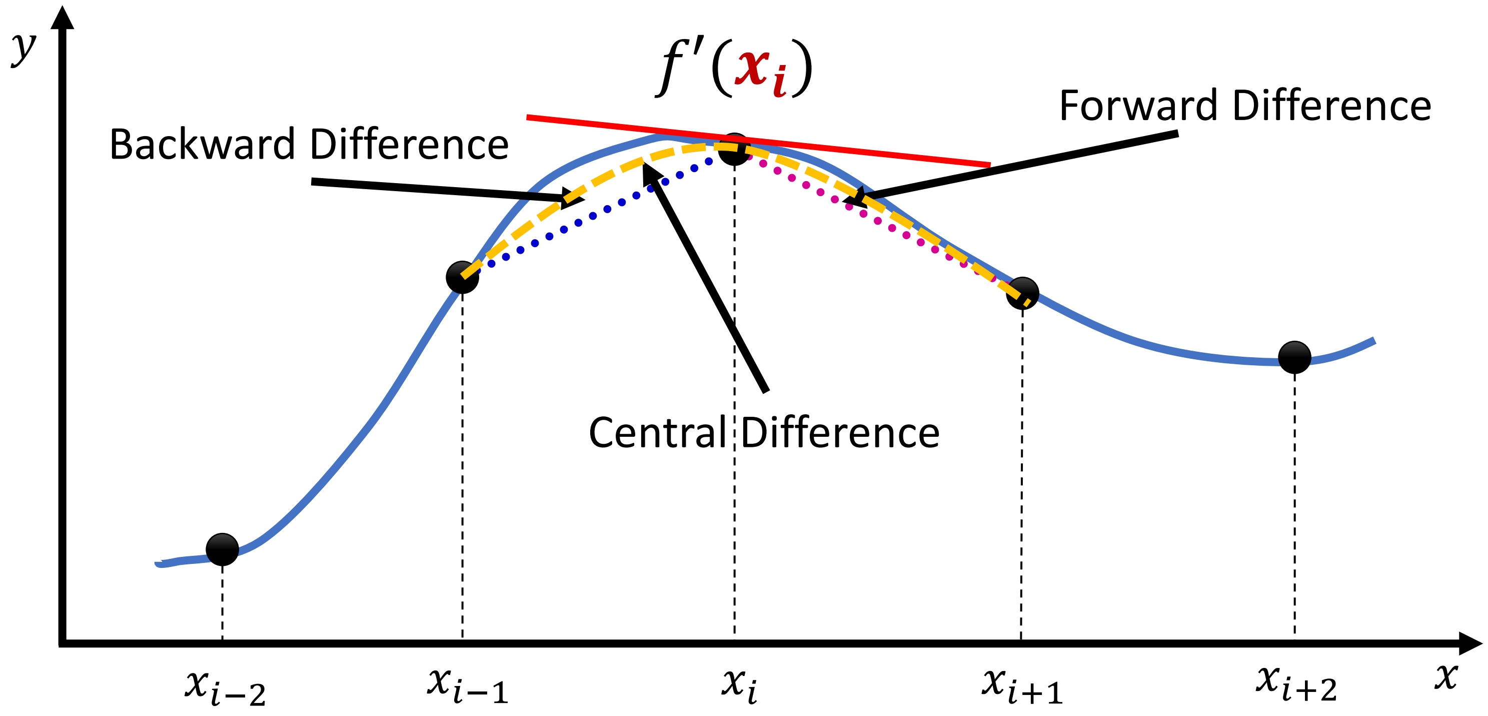
Fourth-Order Central Difference Approximation

$$f'(x_i) \approx \frac{1}{h}\left[\Delta f_{i-2} + \frac{3}{2}\Delta^2 f_{i-2} + \frac{1}{3}\Delta^3 f_{i-2} - \frac{1}{12}\Delta^4 f_{i-2}\right]_{n=4}$$

$\boldsymbol{x}$	$\boldsymbol{f}(\boldsymbol{x})$	$\Delta\boldsymbol{f}$	$\Delta^2\boldsymbol{f}$	$\Delta^3\boldsymbol{f}$	$\Delta^4\boldsymbol{f}$
x_{i-2}	f_{i-2}	$f_{i-1} - f_{i-2}$	$f_i - 2f_{i-1} + f_{i-2}$	$f_{i+1} - 3f_i + 3f_{i-1} - f_{i-2}$	$f_{i+2} - 4f_{i+1} + 6f_i - 4f_{i-1} + f_{i-2}$
x_{i-1}	f_{i-1}	$f_i - f_{i-1}$	$f_{i+1} - 2f_i + f_{i-1}$	$f_{i+2} - 3f_{i+1} + 3f_i - f_{i-1}$	
$\boldsymbol{x_i}$	f_i	$f_{i+1} - f_i$	$f_{i+2} - 2f_{i+1} + f_i$		
x_{i+1}	f_{i+1}	$f_{i+2} - f_{i+1}$			
x_{i+2}	f_{i+2}				

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

First Derivative: Forward, Central, and Backward



Forward Difference	Central Difference	Backward Difference
$f'(x_i) \approx \dfrac{f_{i+1} - f_i}{h}$	$f'(x_i) \approx \dfrac{f_{i+1} - f_{i-1}}{2h}$	$f'(x_i) \approx \dfrac{f_i - f_{i-1}}{h}$
$f'(x_i) \approx \dfrac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h}$	$f'(x_i) \approx \dfrac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12h}$	$f'(x_i) \approx \dfrac{3f_i - 4f_{i-1} + f_{i-2}}{2h}$

For $f(x) = xe^{-\frac{x}{2}}$, estimate the value of $f'(0.3)$ using $h = 0.1$ using **forward, backward** and **central** differences

$h = 0.1$

x	$f(x)$
0	0
0.1	0.095122942
0.2	0.180967484
0.3	**0.258212393**
0.4	0.327492301
0.5	0.389400392
0.6	0.444490932

$f'(x) = (1 - 0.5x)e^{-\frac{x}{2}}$

$f'(0.3) = 0.73160178$

Forward Difference

$$f'(x_i) \approx \frac{f_{i+1} - f_i}{h}$$

$$f'(0.3) \approx \frac{(0.327492301) - (0.258212393)}{0.1} = 0.692799083$$

$$f'(x_i) \approx \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h}$$

$$f'(x_i) \approx \frac{-(0.389400392) + 4(0.327492301) - 3(0.258212393)}{2(0.1)} = 0.729658173$$

Backward Difference

$$f'(x_i) \approx \frac{f_i - f_{i-1}}{h}$$

$$f'(0.3) \approx \frac{(0.258212393) - (0.180967484)}{0.1} = 0.772449093$$

$$f'(x_i) \approx \frac{3f_i - 4f_{i-1} + f_{i-2}}{2h}$$

$$f'(0.3) \approx \frac{3(0.258212393) - 4(0.180967484) + (0.095122942)}{2(0.1)} = 0.729450934$$

Central Difference

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

$$f'(0.3) \approx \frac{(0.327492301) - (0.180967484)}{2(0.1)} = 0.732624088$$

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

$$f'(0.3) \approx \frac{-(0.389400392) + 8(0.327492301) - 8(0.180967484) + (0.095122942)}{12(0.1)} = 0.73160$$

For $f(x) = xe^{-\frac{x}{2}}$, estimate the value of $f'(0.3)$ using $h = 0.05$ using **forward, backward** and **central** differences

$h = 0.05$

x	$f(x)$
0.15	0.139161523
0.2	0.180967484
0.25	0.220624226
0.3	**0.258212393**
0.35	0.293809957
0.4	0.327492301
0.45	0.359332298

$f'(x) = (1 - 0.5x)e^{-\frac{x}{2}}$

$f'(0.3) = 0.73160178$

Forward Difference

$$f'(x_i) \approx \frac{f_{i+1} - f_i}{h}$$

$$f'(0.3) \approx \frac{(0.293809957) - (0.258212393)}{0.05} = 0.711951287$$

$$f'(x_i) \approx \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h}$$

$$f'(x_i) \approx \frac{-(0.327492301) + 4(0.293809957) - 3(0.258212393)}{2(0.05)} = 0.731103491$$

Backward Difference

$$f'(x_i) \approx \frac{f_i - f_{i-1}}{h}$$

$$f'(0.3) \approx \frac{(0.258212393) - (0.220624226)}{0.05} = 0.751763346$$

$$f'(x_i) \approx \frac{3f_i - 4f_{i-1} + f_{i-2}}{2h}$$

$$f'(0.3) \approx \frac{3(0.258212393) - 4(0.220624226) + (0.180967484)}{2(0.05)} = 0.731077598$$

Central Difference

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

$$f'(0.3) \approx \frac{(0.293809957) - (0.220624226)}{2(0.05)} = 0.731857316$$

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

$$f'(0.3) \approx \frac{-(0.327492301) + 8(0.293809957) - 8(0.220624226) + (0.180967484)}{12(0.05)} = 0.7316$$

For $f(x) = xe^{-\frac{x}{2}}$, estimate the value of $f'(0.3)$ using $h = 0.025$ using **forward, backward** and **central** differences

$h = 0.025$

x	$f(x)$
0.225	0.201059403
0.25	0.220624226
0.275	0.239671946
0.3	**0.258212393**
0.325	0.276255229
0.35	0.293809957
0.375	0.310885919

$f'(x) = (1 - 0.5x)e^{-\frac{x}{2}}$

$f'(0.3) = 0.73160178$

Forward Difference

$$f'(x_i) \approx \frac{f_{i+1} - f_i}{h}$$

$$f'(0.3) \approx \frac{(0.276255229) - (0.258212393)}{0.025} = 0.721713456$$

$$f'(x_i) \approx \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h}$$

$$f'(x_i) \approx \frac{-(0.293809957) + 4(0.276255229) - 3(0.258212393)}{2(0.025)} = 0.731475625$$

Backward Difference

$$f'(x_i) \approx \frac{f_i - f_{i-1}}{h}$$

$$f'(0.3) \approx \frac{(0.258212393) - (0.239671946)}{0.025} = 0.741617867$$

$$f'(x_i) \approx \frac{3f_i - 4f_{i-1} + f_{i-2}}{2h}$$

$$f'(0.3) \approx \frac{3(0.258212393) - 4(0.239671946) + (0.220624226)}{2(0.025)} = 0.731472389$$

Central Difference

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

$$f'(0.3) \approx \frac{(0.276255229) - (0.239671946)}{2(0.025)} = 0.731665661$$

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

$$f'(0.3) \approx \frac{-(0.293809957) + 8(0.276255229) - 8(0.239671946) + (0.220624226)}{12(0.025)} = 0.7316$$

The results from the **forward-difference** formula have errors much greater than those from **central differences**

Numerical Integration

A technique used to evaluate the integral of a function that is given by a table or a function that can not be integrated analytically

Newton-Cotes Integration Formulas

Simpson's Rules

The Trapezoidal Rule A Composite Formula

Newton-Cotes Integration Formulas

The usual strategy in developing formulas for numerical integration is similar to that for numerical differentiation. We *pass a polynomial through points defined by the function*, and then integrate this **polynomial approximation** to the function.

Newton-Cotes Integration Formulas

When the values are equi-spaced "evenly spaced", our familiar **Newton-Gregory forward polynomial** is a convenient starting point, so

$$P_n(x) = f_0 + \binom{s}{1}\Delta f_0 + \binom{s}{2}\Delta^2 f_0 + \binom{s}{3}\Delta^3 f_i + \cdots + \binom{s}{n}\Delta^n f_i$$

$$\int_a^b f(x)dx = \int_a^b P_n(x_s)dx$$

The interval of integration (a, b) can match the **range of fit of the polynomial** (x_0, x_n), thus, there will be **Newton-Cotes Integration Formulas** corresponding to the varying degrees of the interpolating polynomial.

We will discuss the ones with the degree of the polynomial, 1, 2, or 3

If the degree of the polynomial is too high, errors due to round-off and local irregularities can cause a problem. This explains why it is only the **lower-degree Newton-Cotes formulas** that are often used.

Newton-Cotes Integration Formula ($n = 1$)

"Two Points"

$$\int_{x_0}^{x_1} f(x)dx \approx \int_{x_0}^{x_1} (f_0 + s\Delta f_0)dx$$

$$x \Longrightarrow s$$

$$ds = \frac{dx}{h} \Longrightarrow dx = h\, ds$$

$$s = \frac{x - x_0}{h}$$

$$\int_{x_0}^{x_1} f(x)dx \approx \int_{x_0}^{x_1} (f_0 + s\Delta f_0)dx = h \int_{s=0}^{s=1} (f_0 + s\Delta f_0)ds$$

$$\int_{x_0}^{x_1} f(x)dx \approx h f_0 s\Big]_0^1 + h\Delta f_0 \frac{s^2}{2}\Big]_0^1 = h\left(f_0 + \frac{1}{2}\Delta f_0\right)$$

$$\int_{x_0}^{x_1} f(x)dx \approx \frac{h}{2}(f_0 + f_1)$$

Newton-Cotes Integration Formula ($n = 2$)

"Three Points"

$$\int_{x_0}^{x_2} f(x)dx \approx \int_{x_0}^{x_2} \left(f_0 + s\Delta f_0 + \frac{s(s-1)}{2}\Delta^2 f_0\right) dx$$

$$x \Longrightarrow s$$

$$ds = \frac{dx}{h} \Longrightarrow dx = h\, ds$$

$$s = \frac{x - x_0}{h}$$

$$\int_{x_0}^{x_2} f(x)dx \approx h \int_{s=0}^{s=2} \left(f_0 + s\Delta f_0 + \frac{s(s-1)}{2}\Delta^2 f_0\right) ds$$

$$\int_{x_0}^{x_2} f(x)dx \approx h f_0 s]_0^2 + h\Delta f_0 \frac{s^2}{2}\Big]_0^2 + h\Delta^2 f_0 \left(\frac{s^3}{6} - \frac{s^2}{4}\right)\Big]_0^2 = h\left(2f_0 + 2\Delta f_0 + \frac{1}{3}\Delta^2 f_0\right)$$

$$\int_{x_0}^{x_2} f(x)dx \approx \frac{h}{3}(f_0 + 4f_1 + f_2)$$

Newton-Cotes Integration Formula ($n = 3$)

"Four Points"

$$\int_{x_0}^{x_3} f(x)dx \approx \int_{x_0}^{x_3} \left(f_0 + s\Delta f_0 + \frac{s(s-1)}{2}\Delta^2 f_0 + \frac{s(s-1)(s-2)}{6}\Delta^3 f_0 \right) dx$$

$$x \Longrightarrow s$$

$$ds = \frac{dx}{h} \Longrightarrow dx = h\,ds$$

$$s = \frac{x - x_0}{h}$$

$$\int_{x_0}^{x_3} f(x)dx \approx h \int_{s=0}^{s=3} \left(f_0 + s\Delta f_0 + \frac{s(s-1)}{2}\Delta^2 f_0 + \frac{s(s-1)(s-2)}{6}\Delta^3 f_0 \right) ds$$

$$\int_{x_0}^{x_3} f(x)dx \approx h f_0 s\Big]_0^3 + h\Delta f_0 \frac{s^2}{2}\Bigg]_0^3 + h\Delta^2 f_0 \left(\frac{s^3}{6} - \frac{s^2}{4} \right)\Bigg]_0^3 + h\Delta^3 f_0 \left(\frac{s^3}{24} - \frac{s^3}{6} + \frac{s^2}{6} \right)\Bigg]_0^3$$

$$\int_{x_0}^{x_3} f(x)dx \approx \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3)$$

Find the integration of $f(x) = 2x^3$ using the three Newton-Cotes Integration Formulas using $x_0 = 0$

We do **not** need the difference table?

We only need to know the value of h

$$h = 0.5$$

x	$f(x)$
0	0
0.5	0.25
1	2
1.5	6.75

2-points or ***n* = 1** Newton-Cotes Integration Formula

$$\int_0^{0.5} f(x)dx \approx \frac{h}{2}(f_0 + f_1) = \frac{0.5}{2}(0 + 0.25) = \mathbf{0.0625}$$

3-points or ***n* = 2** Newton-Cotes Integration Formula

$$\int_0^{1} f(x)dx \approx \frac{h}{3}(f_0 + 4f_1 + f_2) = \frac{0.5}{3}(0 + 4(0.25) + 2) = \mathbf{0.5}$$

4-points or ***n* = 3** Newton-Cotes Integration Formula

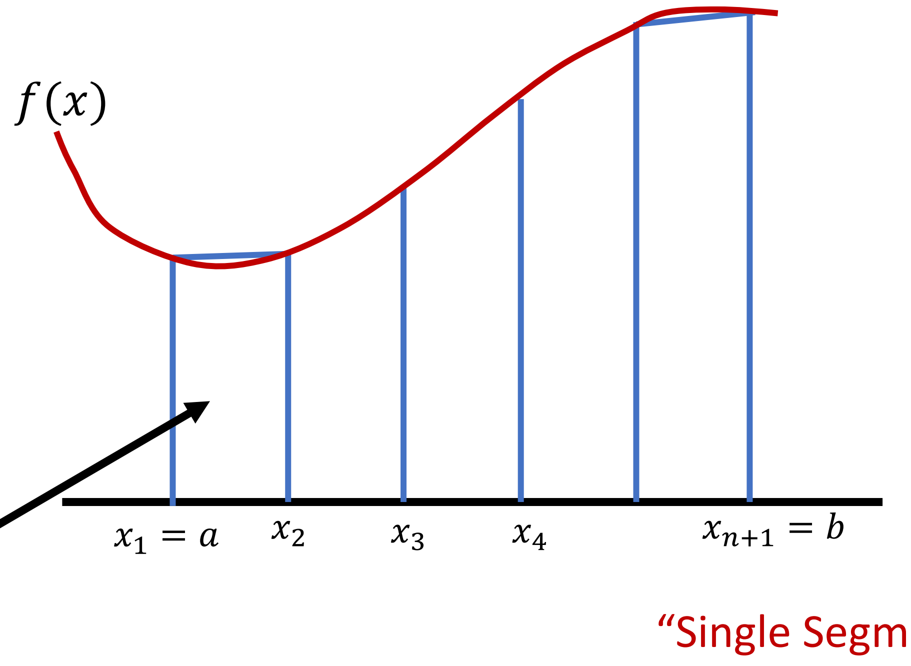
$$\int_0^{1.5} f(x)dx \approx \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) = \frac{3(0.5)}{8}(0 + 3(0.25) + 3(2) + 6.75) = \mathbf{2.5313}$$

The Trapezoidal Rule-A Composite Formula

The first of the Newton-Cotes formulas, based on approximating $f(x)$ on (x_0, x_1) by a straight line, is also called the ***trapezoidal rule***

The Trapezoidal Rule-A Composite Formula

To evaluate *f(x) integral over a and b,* we subdivide the interval from *a* to *b* into *n* subintervals and approximated by the sum of all the trapezoidal areas



*There is **no necessity** to make the subintervals equal in width, but our formula is simpler if this is done*

$\Delta x = \mathrm{h}$

The area under the curve in each subinterval is approximated by the trapezoid formed by **replacing the curve by its secant line** drawn between the endpoints of the curve

"Single Segment Trapezoidal Rule"

$$\int_{x_i}^{x_{i+1}} f(x)dx \approx \frac{f(x_i) + f(x_{i+1})}{2}(\Delta x) = \frac{h}{2}(f_i + f_{i+1})$$

The Trapezoidal Rule-A Composite Formula

To evaluate the integral $\int_a^b f(x)dx$ by **trapezoidal rule**, we divide the interval $[a, b]$ into n subintervals

$$[a, b] \Longrightarrow [x_1, x_2], [x_2, x_3], \cdots, [x_n, x_{n+1}]$$

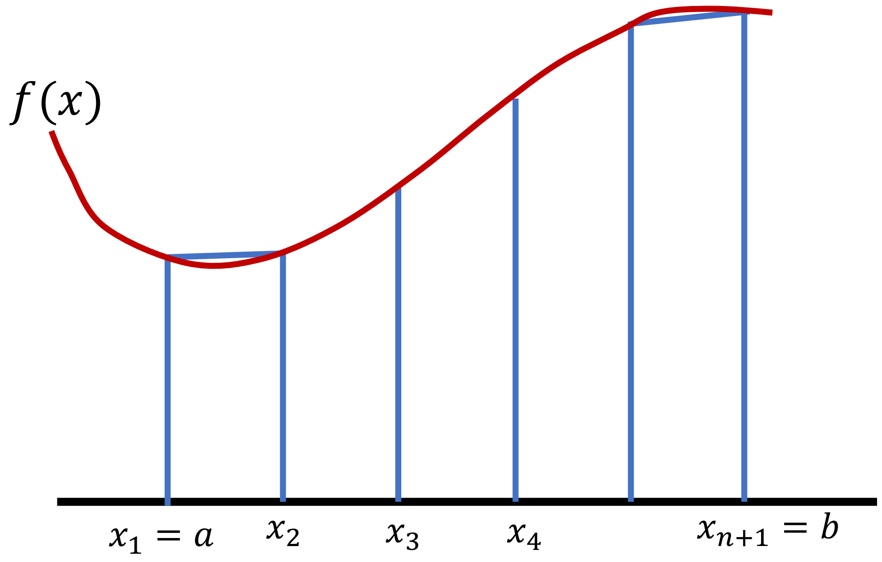
$$a = x_0, \qquad b = x_{n+1}, \qquad h = x_{i+1} - x_i$$

"Composite Trapezoidal Rule"

$$\int_a^b f(x)dx \approx \frac{h}{2}\sum_{i=1}^{n}[f_i + f_{i+1}]$$

$$\int_a^b f(x)dx \approx \frac{h}{2}(f_1 + 2f_2 + 2f_3 + \cdots + 2f_n + f_{n+1})$$

The Trapezoidal Rule-A Composite Formula



It is obvious from the Figure that the method is **subject to large errors** unless the subintervals are **small**, for replacing a curve by a straight line is hardly accurate

Integrate the function tabulated in the Table over the interval from $x = 1.8$ to $x = 3.4$

$$\int_a^b f(x)dx \approx \frac{h}{2}\sum_{i=1}^{n}[f_i + f_{i+1}]$$

1	2	3	4	5	6	7	8

1.8 2.0 2.2 2.4 2.6 2.8 3.0 3.2 3.4

x	$f(x)$
1.6	4.953
1.8	**6.050**
2.0	7.389
2.2	9.025
2.4	11.023
2.6	13.464
2.8	16.445
3.0	20.086
3.2	24.533
3.4	**29.964**
3.6	36.598
3.8	44.701

$$\int_{1.8}^{3.4} f(x)dx \approx \frac{(0.2)}{2}\sum_{i=1}^{8}(f_i + f_{i+1})$$

$$\approx \frac{(0.2)}{2}(f_1 + 2f_2 + 2f_3 + 2f_4 + 2f_5 + 2f_6 + 2f_7 + 2f_8 + f_9)$$

$$\approx \frac{(0.2)}{2}(6.050 + 2(7.389) + 2(9.025) + 2(11.023) + 2(13.464)$$
$$+2(16.445) + 2(20.086) + 2(24.533) + 29.964)$$

$$\int_{1.8}^{3.4} f(x)dx \approx 23.9944$$

Simpson’s Rules

The composite Newton-Cotes formulas based on quadratic and cubic interpolating polynomials are known as ***Simpson's rules***

The **quadratic** Newton-Cotes formula is known as ***Simpson's* 1/3 *rule***
and the **cubic** Newton-Cotes formula is known as ***Simpson's* 3/8 *rule***

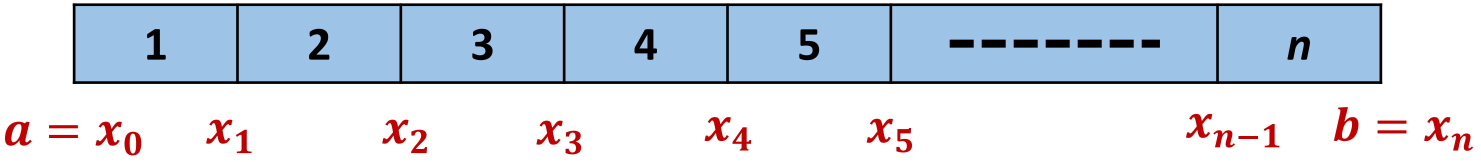
Simpson's $\frac{1}{3}$ Rule

$$\int_a^b f(x)dx \approx \frac{h}{3}\left(f(a) + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots + 4f_{n-1} + f(b)\right)$$

We build upon **3-Point Newton-Cotes formula** to get a **composite rule** that is applied to a subdivision of the interval of integration into *n* panels (***n* must be even**)

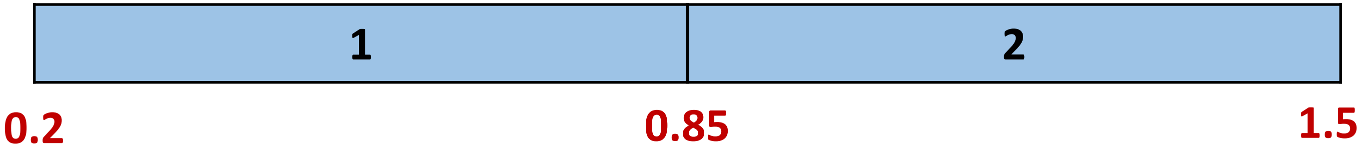
$$\int_{x_0}^{x_2} f(x)dx \approx \frac{h}{3}(f_0 + 4f_1 + f_2)$$

3-Points or ***n* = 2** Newton-Cotes Integration Formula



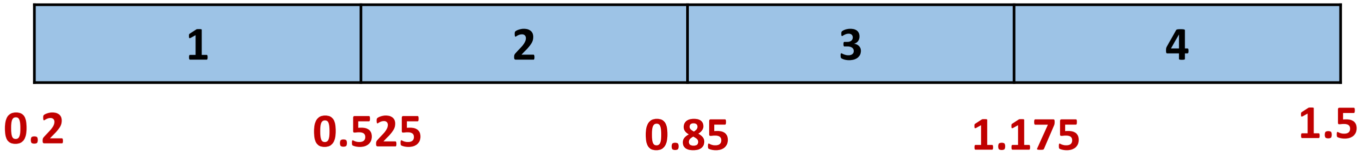
Use Simpson's $\frac{1}{3}$ rule to evaluate the integral of e^{-x^2} over the interval 0.2 to 1.5, using 2, 4, and 8 subdivisions

$$\int_a^b f(x)dx \approx \frac{h}{3}\left(f(a) + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots + 4f_{n-1} + f(b)\right)$$



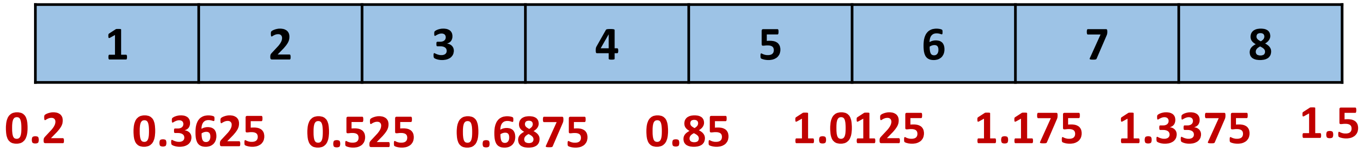
$$h = \frac{1.5 - 0.2}{2} = 0.65$$

$$\int_{0.2}^{1.5} f(x)dx \approx \frac{h}{3}\left(f(0.2) + 4f(0.85) + f(1.5)\right) = \frac{0.65}{3}(0.9608 + 4(0.4855) + 0.1054) = 0.65181$$



$$h = \frac{1.5 - 0.2}{4} = 0.325$$

$$\int_{0.2}^{1.5} f(x)dx \approx \frac{h}{3}(f(0.2) + 4f(0.525) + 2f(0.85) + 4f(1.175) + f(1.5)) = 0.65860$$



$$h = \frac{1.5 - 0.2}{8} = 0.1625$$

$$\int_{0.2}^{1.5} f(x)dx \approx \frac{h}{3}\left(f(0.2) + 4f(0.3625) + 2f(0.525) + 4f(0.6875) + 2f(0.85) + 4f(1.0125) + 2f(1.175) + 4f(1.3375) + f(1.5)\right) = 0.65878$$

What if we have a function given via tabulated values?

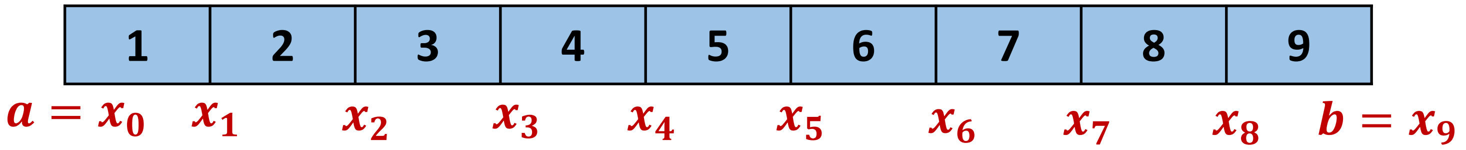
We can apply Simpson's $\frac{1}{3}$ rule to a table of evenly spaced function values in an obvious way if the **number of intervals is even**

Simpson's $\frac{1}{3}$ Rule

What if the number of intervals from the tabulated values is **not** even?

Subinterval *at one end with the* ***trapezoidal rule*** *and the rest with* ***Simpson's*** $\boldsymbol{\frac{1}{3}}$ ***rule***

> "Select the **end subinterval** for applying the trapezoidal rule where the function is *more nearly linear*"



OPTION I: $\int_a^b f(x)dx$ = **Simpson's $\frac{1}{3}$ Rule** $\int_{x_0}^{x_8} f(x)dx$ + **Trapezoidal Rule** $\int_{x_8}^{x_9} f(x)dx$

OPTION II: $\int_a^b f(x)dx$ = **Trapezoidal Rule** $\int_{x_0}^{x_1} f(x)dx$ + **Simpson's $\frac{1}{3}$ Rule** $\int_{x_1}^{x_9} f(x)dx$

Apply **Simpson's $\frac{1}{3}$ rule** to the data in the table. What is the difference results if we apply **trapezoidal rule** at the left end rather than the right end?

$$\int_{0.7}^{2.1} f(x)dx = \int_{0.7}^{1.9} f(x)dx + \int_{1.9}^{2.1} f(x)dx$$

$$\int_{0.7}^{1.9} f(x)dx \approx \frac{0.2}{3}(f(0.7) + 4f(0.9) + 2f(1.1) + 4f(1.3) + 2f(1.5) + 4f(1.7) + f(1.9))$$

$$\int_{0.7}^{1.9} f(x)dx \approx 1.51938$$

$$\int_{0.7}^{2.1} f(x)dx \approx 1.81678$$

$$\int_{1.9}^{2.1} f(x)dx \approx \frac{0.2}{2}\big(f(1.9) + f(2.1)\big) = 0.29740$$

x	$f(x)$
0.7	0.64835
0.9	0.91360
1.1	1.16092
1.3	1.36178
1.5	1.49500
1.7	1.55007
1.9	1.52882
2.1	1.44513

$$\int_{0.7}^{2.1} f(x)dx = \int_{0.7}^{0.9} f(x)dx + \int_{0.9}^{2.1} f(x)dx$$

$$\int_{0.7}^{0.9} f(x)dx \approx \frac{0.2}{2}\big(f(0.7) + f(0.9)\big) = 0.15620$$

$$\int_{0.7}^{2.1} f(x)dx \approx 1.81762$$

$$\int_{0.7}^{1.9} f(x)dx \approx \frac{0.2}{3}\big(f(0.9) + 4f(1.1) + 2f(1.3) + 4f(1.5) + 2f(1.7) + 4f(1.9) + f(2.1)\big) = 1.66142$$

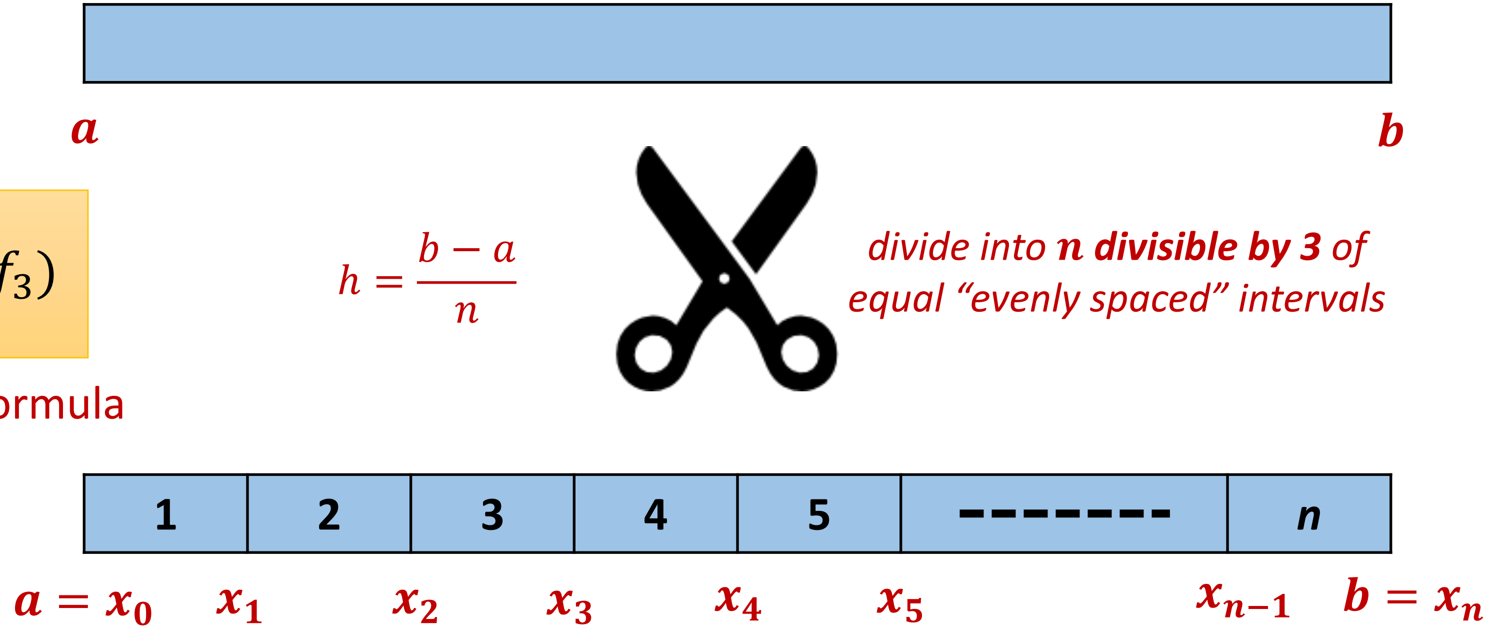
Simpson's $\frac{3}{8}$ Rule

$$\int_a^b f(x)dx \approx \frac{3h}{8}[f(a) + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + 2f_6 + \cdots + 2f_{n-3} + 3f_{n-2} + 3f_{n-1} + f(b)]$$

We build upon **4-Point Newton-Cotes formula** to get a **composite rule** that is applied to a subdivision of the interval of integration into *n* panels (***n* must be divisible by 3**)

$$\int_{x_0}^{x_3} f(x)dx \approx \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3)$$

4-Points or ***n* = 3** Newton-Cotes Integration Formula



Use Simpson's $\frac{3}{8}$ rule to evaluate the integral of e^{-x^2} over the interval 0.2 to 1.5, using 3 and 6 subdivisions

$$\int_a^b f(x)dx \approx \frac{3h}{8}[f(a) + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + 2f_6 + \cdots + 2f_{n-3} + 3f_{n-2} + 3f_{n-1} + f(b)]$$

$$h = \frac{1.5 - 0.2}{3} = 0.4333$$

1	2	3

0.2 **0.6333** **1.0666** **1.5**

$$\int_{0.2}^{1.5} f(x)dx \approx \frac{3h}{8}[f(0.2) + 3f(0.6333) + 3(1.0666) + f(1.5)] = 0.65593$$

$$h = \frac{1.5 - 0.2}{6} = 0.2167$$

1	2	3	4	5	6

0.2 **0.4167** **0.6334** **0.8501** **1.0668** **1.2835** **1.5**

$$\int_{0.2}^{1.5} f(x)dx \approx \frac{3h}{8}[f(0.2) + 3f(0.4167) + 3f(0.6334) + 2f(0.8501) + 3f(1.0668) + 3f(1.2835) + f(1.5)] = 0.65872$$

Simpson's $\frac{3}{8}$ Rule

What if the number of intervals from the tabulated values is **not** divisible by 3?

1	2	3	4	5	6	7	8	9	10	11

$a = x_0$ x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8 x_9 x_{10} $b = x_{11}$

OPTION I: $\int_a^b f(x)dx$ = **Simpson's $\frac{3}{8}$ Rule** $\int_{x_0}^{x_3} f(x)dx +$ **Simpson's $\frac{1}{3}$ Rule** $\int_{x_3}^{x_{11}} f(x)dx$

OPTION II: $\int_a^b f(x)dx$ = **Simpson's $\frac{1}{3}$ Rule** $\int_{x_0}^{x_8} f(x)dx +$ **Simpson's $\frac{3}{8}$ Rule** $\int_{x_8}^{x_{11}} f(x)dx$

OPTION III: $\int_a^b f(x)dx$ = **Simpson's $\frac{3}{8}$ Rule** $\int_{x_0}^{x_9} f(x)dx +$ **Trapezoidal Rule** $\int_{x_9}^{x_{11}} f(x)dx$

OPTION IV: $\int_a^b f(x)dx$ = **Trapezoidal Rule** $\int_{x_0}^{x_2} f(x)dx +$ **Simpson's $\frac{3}{8}$ Rule** $\int_{x_2}^{x_{11}} f(x)dx$