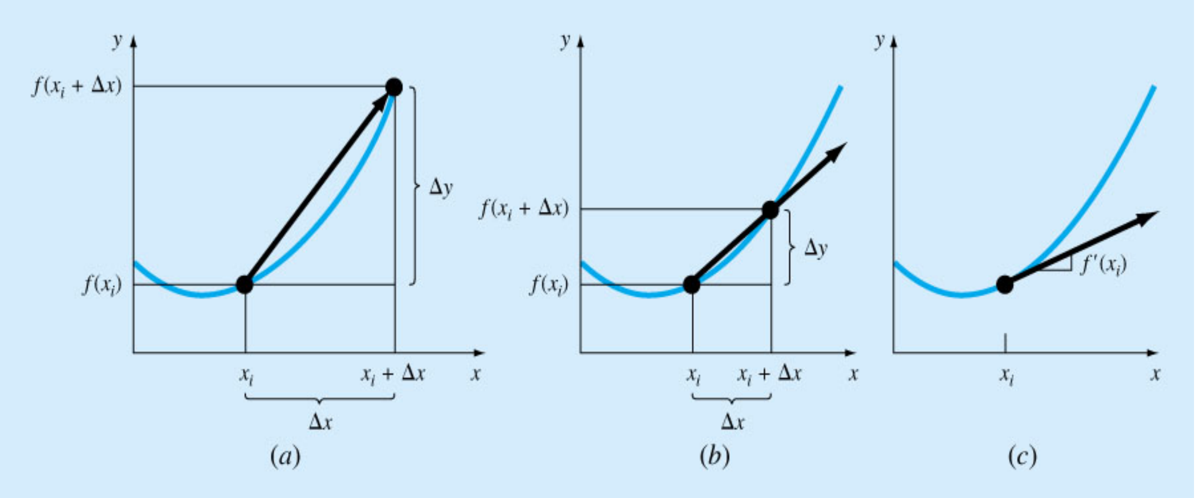
Numerical Differentiation and Integration

What are Differentiation and Integration?

Differentiation:

rate of change of a dependent variable with respect to an independent variable.

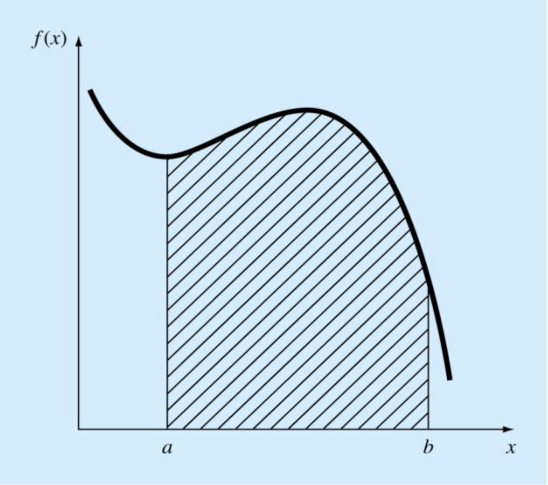
$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$



Integration:

the integral of the function *f*(*x*) with respect to the independent variable *x*, evaluated between the limits *x* = *a* to *x* = *b*.

$$I = \int_a^b f(x)\,dx$$



Numerical Differentiation and Integration

Differentiation and Integration in numerical computing

$$\frac{d^k f(x)}{dx^k} \approx w_0 f(x_0) + w_1 f(x_1) + \ldots + w_n f(x_n) = \sum_{i=0}^{n} w_i f(x_i)$$

$$\int_a^b f(x)dx \approx w_0 f(x_0) + w_1 f(x_1) + \ldots + w_n f(x_n) = \sum_{i=0}^{n} w_i f(x_i)$$

Polynomial Exactness Theorem: For any given n+1 samples x_i , the the following n+1 point approximation formulas have at least n.

$$\frac{d^k f(x)}{dx^k} \approx P_{0,n}^{(k)}(x) = \underbrace{L_0^{(k)}(x)}_{W_0} \cdot f(x_0) + \ldots + \underbrace{L_n^{(k)}(x)}_{W_n} \cdot f(x_n)$$

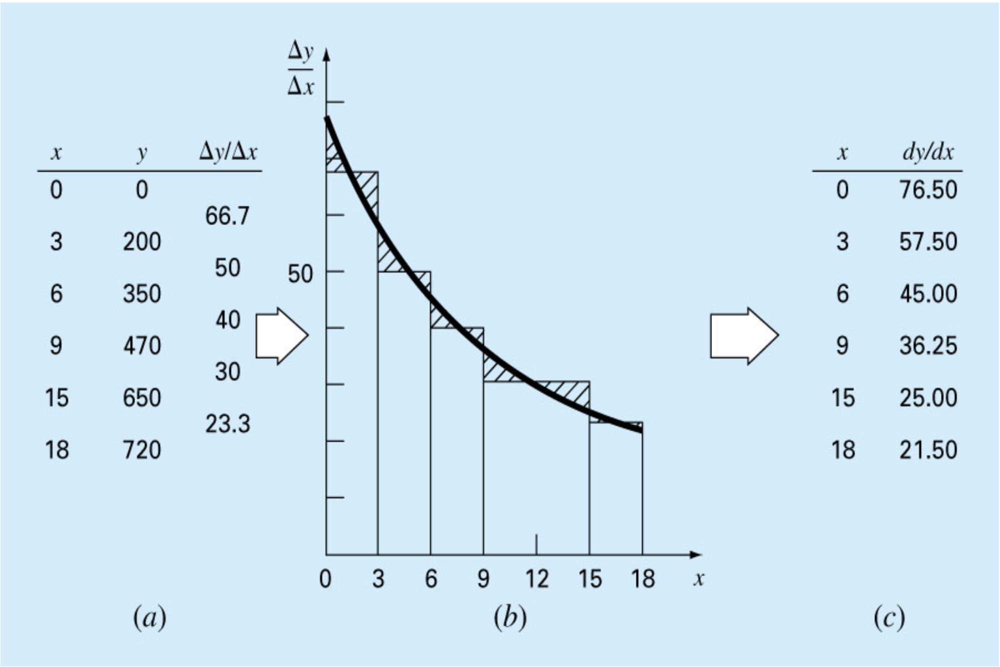
$$\int_a^b f(x)dx \approx \int_a^b P_{0,n}(x)dx = \underbrace{\int_a^b L_0(x)dx}_{W_0} \cdot f(x_0) + \ldots + \underbrace{\int_a^b L_n(x)dx}_{W_n} \cdot f(x_n)$$

where

$$\frac{d^k 1}{dx^k} = w_0 + w_1 + \ldots + w_n = 0$$ - For differentiation

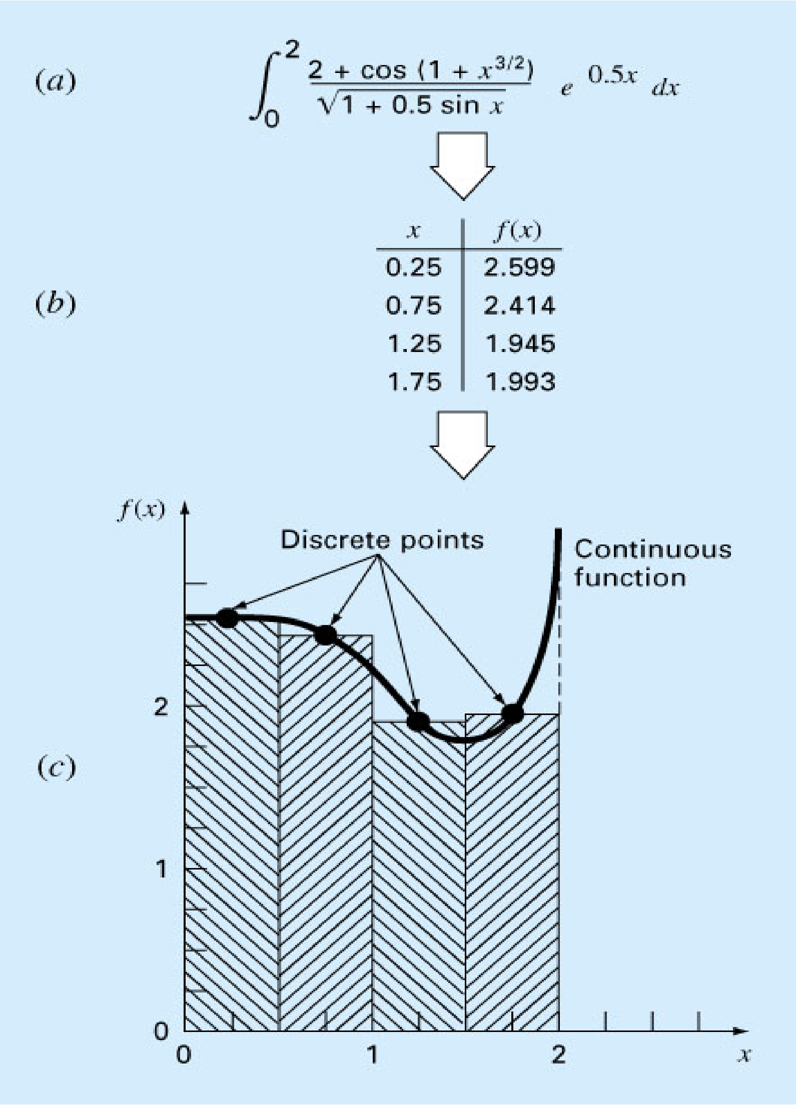
$$\int_a^b 1\, dx = w_0 + w_1 + \ldots + w_n = b - a$$ - For Integration

Examples of Numerical Differentiation and Integration



Differentiation

There exists much more efficient and accurate numerical methods than these two! They are the ones we are to learn!



Integration

Differentiation and Integration

The function to be differentiated or integrated will typically be in one of the following three forms:

- A simple continuous function such as polynomial, an exponential, or a trigonometric function.
- A complicated continuous function that is difficult or impossible to differentiate or integrate directly.
- A tabulated function where values of x and f(x) are given at a number of discrete points, as is often the case with experimental or field data.

Derivatives of equally space

Forward Difference Approximation

The derivative of $f(x)$ at x_0 is:

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

For a finite $h = \Delta x$ for small values of *h.*

An approximation to this is:

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

From Taylor series

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

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

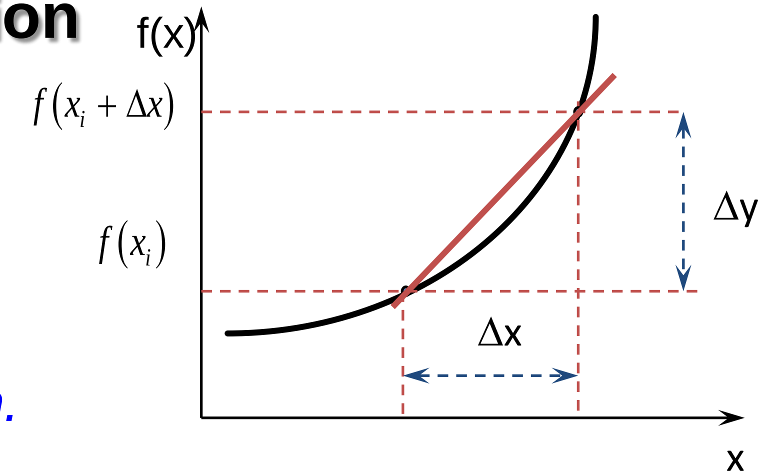


Figure 1 Graphical Representation of forward difference approximation of first derivative.

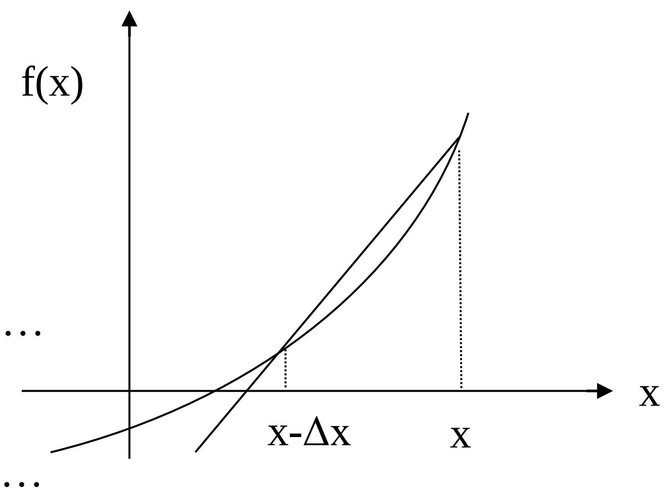


Figure 2 Graphical Representation of backward difference approximation of first derivative

The **forward difference** approximation of the first derivative uses (1) for 2 terms.

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

$$\Rightarrow \Delta x = x_{i+1} - x_i$$

The **backward difference** approximation of the first derivative uses (2) for 2 terms.

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

$$\Rightarrow \Delta x = x_i - x_{i-1}$$

The **Central difference** approximation of the first derivative uses subtraction of equation (2) from equation (1).

$$f(x_{i+1}) - f(x_{i-1}) = f'(x_i)(2\Delta x) + \frac{2f'''(x_i)}{3!}(\Delta x)^3 + \ldots$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} - \frac{f'''(x_i)}{3!}(\Delta x)^2 + \ldots$$

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

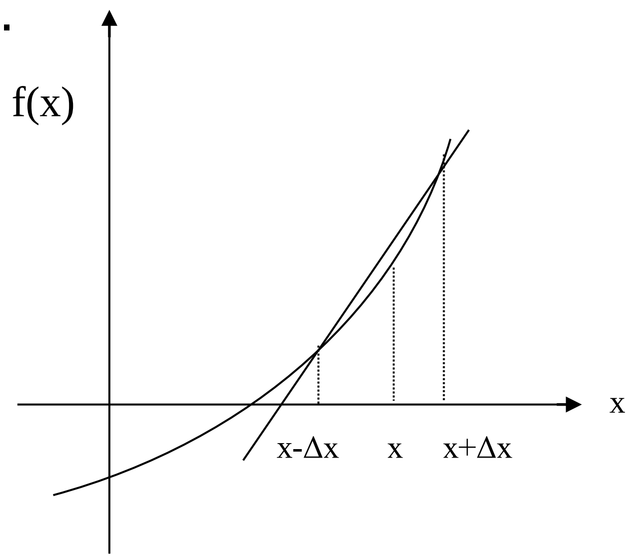
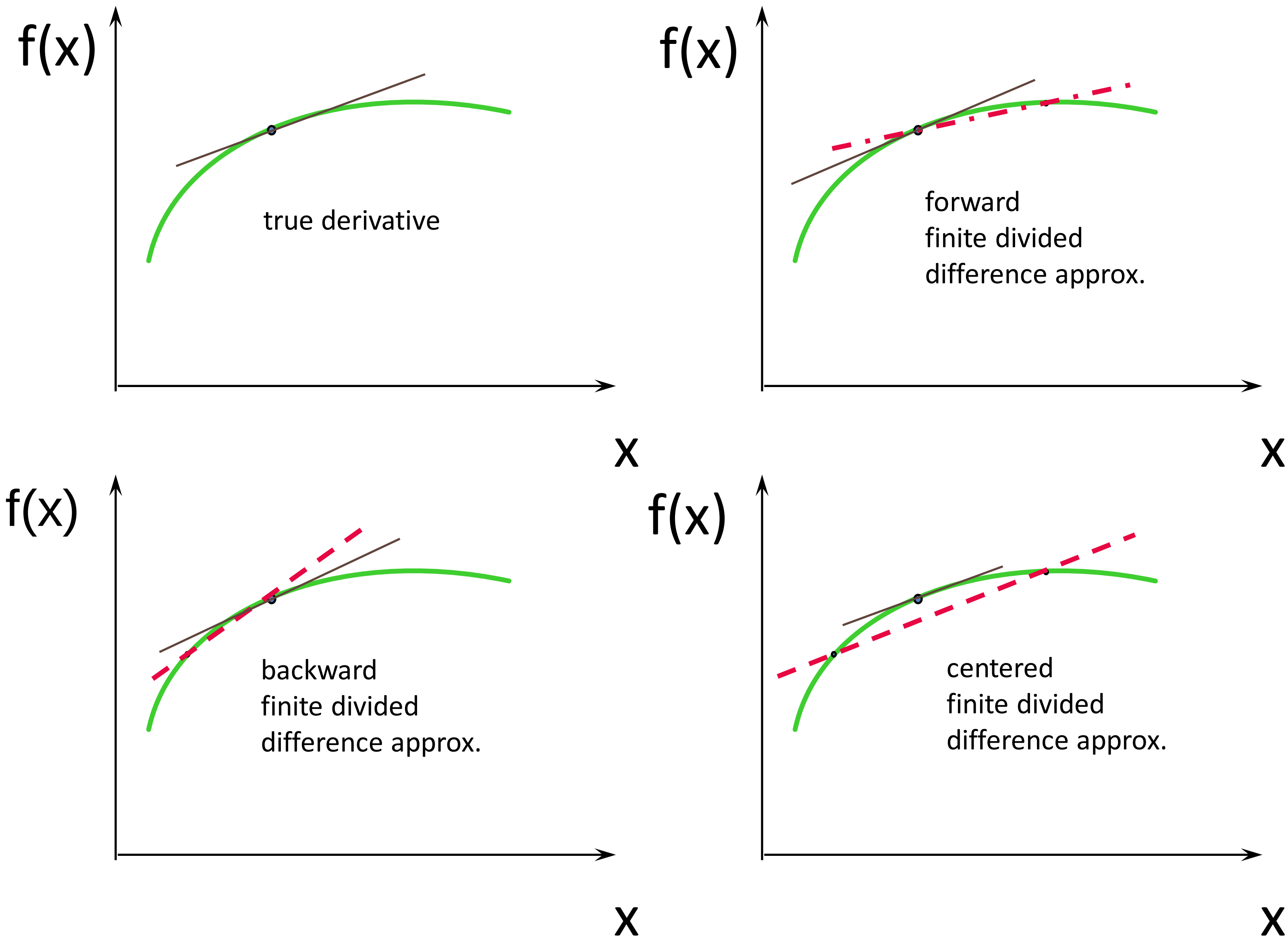


Figure 3 Graphical Representation of central difference approximation of first derivative



f(x)
x
true derivative
f(x)
x
forward
finite divided
difference approx.
f(x)
x
backward
finite divided
difference approx.
f(x)
x
centered
finite divided
difference approx.

High Accuracy Differentiation Formulas

High-accuracy divided-difference formulas can be generated by including additional terms from the Taylor series expansion.

Forward finite-divided-difference formulas

	First Derivative	Second Derivative
2 points	$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$	$f''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$
3 points	$f'(x_i) = \dfrac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	$f''(x_i) = \dfrac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}$

Forward finite-divided-difference formulas

First Derivative | Error

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

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

Second Derivative

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

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

Third Derivative

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

$$f'''(x_i) = \frac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3} \qquad O(h^2)$$

Fourth Derivative

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

$$f''''(x_i) = \frac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4} \qquad O(h^2)$$

Backward finite-divided difference formulas

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

Centered finite-divided difference formulas

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

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

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

Summary of Errors

Error term of 2 points Forward Difference

$$\frac{f(x+h)-f(x)}{h}=f'(x)+O(h) \quad \Rightarrow \quad O(h)=\frac{h}{2}f^{(2)}(x)+\frac{h^2}{3!}f^{(3)}(x)+\cdots$$

Error term of 3 points Forward Difference

$$\frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}=f'(x)+O(h^2)$$

$$O(h^2)=-\frac{2h^2}{3!}f^{(3)}(x)-\frac{6h^3}{4!}f^{(4)}(x)-\cdots$$

Error term of 3 points Central Difference

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

$$O(h^2)=-\frac{h^2}{3!}f^{(3)}(x)-\frac{h^5}{6!}f^{(6)}(x)-\cdots$$

Example: $f(x) = xe^x$

Find the approximate value of $f'(2)$ with $h = 0.1$

x	$f(x)$
1.9	**12.703199**
2.0	**14.778112**
2.1	**17.148957**
2.2	**19.855030**

Using the Forward Difference formula:

$$f'(x_0) \approx \frac{1}{h}\{f(x_0+h) - f(x_0)\}$$

$$f'(2) \approx \frac{1}{0.1}\{f(2.1) - f(2)\}$$

$$= \frac{1}{0.1}\{17.148957 - 14.778112\}$$

$$= 23.708450$$

Using the 1st Three-point formula:

$$f'(x_0) \approx \frac{1}{2h}\{-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\}$$

$$f'(2) \approx \frac{1}{2\times 0.1}[-3f(2) + 4f(2.1) - f(2.2)]$$

$$= \frac{1}{0.2}[-3\times 14.778112 + 4\times 17.148957 - 19.855030] = 22.032310$$

Using the 2nd Three-point formula:

$$\boldsymbol{f'(x_0) \approx \frac{1}{2h}\{f(x_0+h) - f(x_0-h)\}}$$

$$f'(2) \approx \frac{1}{2\times 0.1}[f(2.1) - f(1.9)]$$

$$= \frac{1}{0.2}[17.148957 - 12.703199] = 22.228790$$

The exact value of $f'(2)$ is : 22.167168

Comparison of the results with *h* = 0.1

The exact value of $f'(2)$ is 22.167168

Formula	$f'(2)$	Error
Forward Difference	23.708450	1.541282
1st Three-point	22.032310	0.134858
2nd Three-point	22.228790	0.061622

Example: The velocity of a rocket is given by

$$v(t) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100t}\right] - 9.8t \quad , \quad 0 \le t \le 30$$

where 'v' is given in m/s and 't' is given in seconds.

a) Use **forward** difference approximation of the first derivative of $v(t)$ to calculate the acceleration at $t = 16s$. Use a step size of $\Delta t = 2s$.

b) Find the exact value of the acceleration of the rocket.

c) Calculate the absolute relative true error for part (b).

Solution: $$a(t_i) \cong \frac{v(t_{i+1}) - v(t_i)}{\Delta t} \qquad t_i = 16$$

$$\Delta t = 2 \;; \quad t_{i+1} = t_i + \Delta t = 18$$

$$v(18) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100(18)}\right] - 9.8(18) \;= 453.02 \quad \text{m/s}$$

$$v(16) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100(16)}\right] - 9.8(16) \;= 392.07 \quad \text{m/s}$$

Hence $$a(16) = \frac{v(18) - v(16)}{2} = 453.02 - 392.07 = 30.475 \quad \text{m/s}^2$$

The exact value of $a(16)$ can be calculated by differentiating

$$v(t) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100t}\right] - 9.8t \quad \Rightarrow \quad a(t) = \frac{d}{dt}[v(t)] = \frac{-4040 - 29.4t}{-200 + 3t}$$

$$a(16) = 29.674 \quad \text{m/s}^2$$

The absolute relative true error is

$$|\varepsilon_t| = \left|\frac{True Value - Approximate Value}{True Value}\right| \times 100 = \left|\frac{29.674 - 30.475}{29.674}\right| \times 100 = 2.6993\%$$

a) Use **backward** difference approximation of the first derivative of $v(t)$ to calculate the acceleration at $t = 16\,\text{s}$. Use a step size of $\Delta t = 2s$.

b) Find the absolute relative true error for part (a).

Solution: $a(t) \approx \frac{v(t_i) - v(t_{i-1})}{\Delta t}$ $\quad t_i = 16 \quad \Delta t = 2 \quad t_{i-1} = t_i - \Delta t = 14$

$$v(16) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100(16)}\right] - 9.8(16) \;= 392.07 \;\; \text{m/s}$$

$$v(14) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100(14)}\right] - 9.8(14) \;= 334.24 \;\; \text{m/s}$$

$$a(16) \approx \frac{v(16)-v(14)}{2} = \frac{392.07-334.24}{2} \approx 28.915 \quad \text{m/s}^2$$

The exact value of the acceleration at $t = 16\,\text{s}$ is $a(16) = 29.674 \quad \text{m/s}^2$

The absolute relative true error is

$$|\varepsilon_t| = \left|\frac{TrueValue - ApproximateValue}{TrueValue}\right| \times 100 = \left|\frac{29.674-28.915}{29.674}\right| \times 100 = 2.5584\%$$

(a) Use **central** divided difference approximation of the first derivative of $v(t)$ to calculate the acceleration at $t = 16s$. Use a step size of $\Delta t = 2s$.

(a) Find the absolute relative true error for part (a).

Solution: $a(t_i) \approx \frac{v(t_{i+1})-v(t_{i-1})}{2\Delta t}$ $\Delta t = 2$ $t_{i+1} = t_i + \Delta t = 16+2 = 18$

$t_{i-1} = t_i - \Delta t = 16-2 = 14$ $\Rightarrow$ $a(16) = \frac{v(18)-v(14)}{2(2)} = \frac{v(18)-v(14)}{4}$

$$v(18) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100(18)}\right] - 9.8(18) = 453.02 \quad \text{m/s}$$

$$v(14) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100(14)}\right] - 9.8(14) = 334.24 \quad \text{m/s}$$

Hence $a(16) = \dfrac{v(18) - v(14)}{4} = 453.02 - 334.24 = 29.695 m/s^2$

The exact value of $a(16)$ can be calculated by differentiating $a(16) = 29.674 \ \ \text{m/s}^2$

The absolute relative true error is

$$|\varepsilon_t| = \left| \frac{TrueValue - ApproximateValue}{TrueValue} \right| \times 100 = \left| \frac{29.674 - 29.695}{29.674} \right| \times 100 = 0.070769\%$$

Comparison of FDD, BDD, CDD

The results from the three difference approximations are given in Table 1.

Type of Difference Approximation	$a(16)$ (m/s^2)	$\lvert \in_t \rvert \%$
Forward	30.475	2.6967
Backward	28.915	2.5584
Central	29.695	0.069157

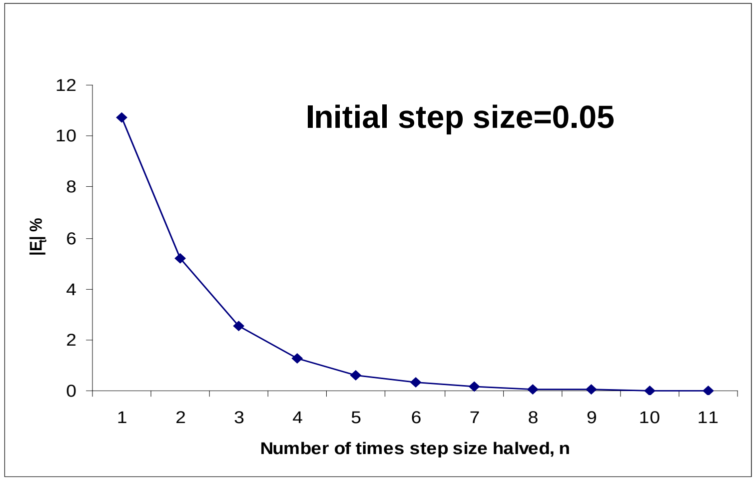
Table 1 Summary of *a* (16) using different divided difference approximations

Effect Of Step Size in forward difference method.

$f(x) = 9e^{4x}$ Value of $f'(0.2)$ using forward difference method.

h	$f'(0.2)$	E_a	$\lvert\varepsilon_a\rvert\%$	Significant digits	E_t	$\lvert\varepsilon_t\rvert\%$
0.05	88.69336				-8.57389	10.70138
0.025	84.26239	-4.430976	5.258546	0	-4.14291	5.170918
0.0125	82.15626	-2.106121	2.563555	1	-2.03679	2.542193
0.00625	81.12937	-1.0269	1.265756	1	-1.00989	1.260482
0.003125	80.62231	-0.507052	0.628923	1	-0.50284	0.627612
0.001563	80.37037	-0.251944	0.313479	2	-0.25090	0.313152
0.000781	80.24479	-0.125579	0.156494	2	-0.12532	0.156413
0.000391	80.18210	-0.062691	0.078186	2	-0.06263	0.078166
0.000195	80.15078	-0.031321	0.039078	3	-0.03130	0.039073
9.77E-05	80.13512	-0.015654	0.019535	3	-0.01565	0.019534
4.88E-05	80.12730	-0.007826	0.009767	3	-0.00782	0.009766

Absolute Relative True Error

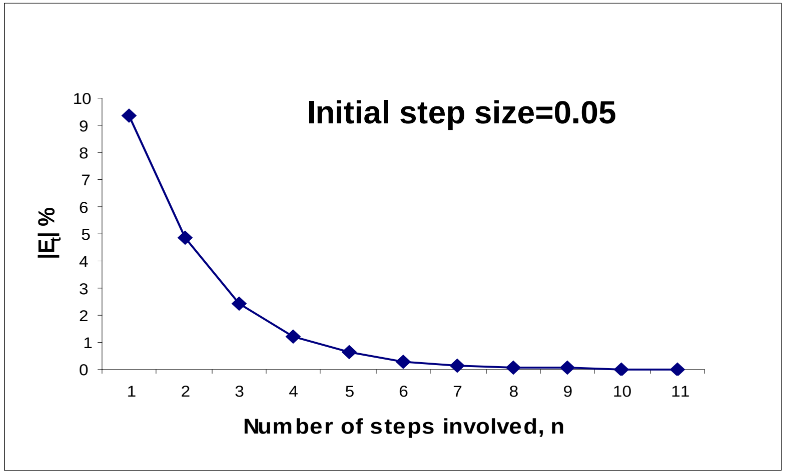


Effect Of Step Size in backward difference method.

$f(x) = 9e^{4x}$ Value of $f'(0.2)$ using backward difference method.

h	$f'(0.2)$	E_a	$\lvert\varepsilon_a\rvert\%$	Significant digits	E_t	$\lvert\varepsilon_t\rvert\%$
0.05	72.61598				7.50349	9.365377
0.025	76.24376	3.627777	4.758129	1	3.87571	4.837418
0.0125	78.14946	1.905697	2.438529	1	1.97002	2.458849
0.00625	79.12627	0.976817	1.234504	1	0.99320	1.239648
0.003125	79.62081	0.494533	0.62111	1	0.49867	0.622404
0.001563	79.86962	0.248814	0.311525	2	0.24985	0.31185
0.000781	79.99442	0.124796	0.156006	2	0.12506	0.156087
0.000391	80.05691	0.062496	0.078064	2	0.06256	0.078084
0.000195	80.08818	0.031272	0.039047	3	0.03129	0.039052
9.77E-05	80.10383	0.015642	0.019527	3	0.01565	0.019529
4.88E-05	80.11165	0.007823	0.009765	3	0.00782	0.009765

Absolute Relative True Error

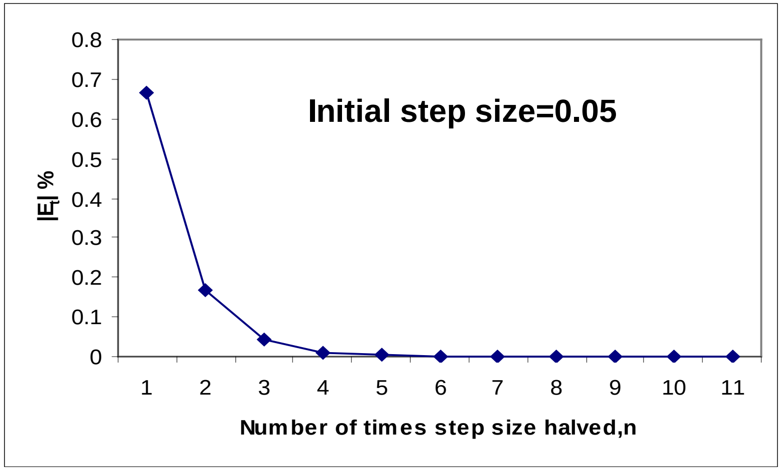


Effect Of Step Size in central difference method.

$f(x) = 9e^{4x}$ Value of $f'(0.2)$ using central difference method.

h	$f'(0.2)$	E_a	$\lvert\varepsilon_a\rvert\%$	Significant digits	E_t	$\lvert\varepsilon_t\rvert\%$
0.05	80.65467				-0.53520	0.668001
0.025	80.25307	-0.4016	0.500417	1	-0.13360	0.16675
0.0125	80.15286	-0.100212	0.125026	2	-0.03339	0.041672
0.00625	80.12782	-0.025041	0.031252	3	-0.00835	0.010417
0.003125	80.12156	-0.00626	0.007813	3	-0.00209	0.002604
0.001563	80.12000	-0.001565	0.001953	4	-0.00052	0.000651
0.000781	80.11960	-0.000391	0.000488	5	-0.00013	0.000163
0.000391	80.11951	-9.78E-05	0.000122	5	-0.00003	4.07E-05
0.000195	80.11948	-2.45E-05	3.05E-05	6	-0.00001	1.02E-05
9.77E-05	80.11948	-6.11E-06	7.63E-06	6	0.00000	2.54E-06
4.88E-05	80.11947	-1.53E-06	1.91E-06	7	0.00000	6.36E-07

Absolute Relative True Error



Newton's Forward Difference Formula

$$\frac{dy}{dp}=\frac{1}{h}\left\{\Delta y_0+\left[\frac{2p-1}{1\cdot 2}\right](\Delta^2 y_0)+\left[\frac{(3p^2-6p+2)}{1\cdot 2\cdot 3}\right](\Delta^3 y_0)+\left[\frac{(4p^3-18p^2+22p-6)}{1\cdot 2\cdot 3\cdot 4}\right](\Delta^4 y_0)+\ldots\right\}$$

$$\frac{d^2y}{dp^2}=\frac{1}{h^2}\left\{\Delta^2 y_0+(p-1)(\Delta^3 y_0)+\left[\frac{(6p^2-18p+11)}{12}\right](\Delta^4 y_0)+\ldots\right\}$$

$$\frac{d^3y}{dp^3}=\frac{1}{h^3}\left\{\Delta^3 y_0+\left[\frac{(12p-18)}{12}\right](\Delta^4 y_0)+\ldots\right\}$$

at $x = x_0$, $p = 0$

$$\left(\frac{dy}{dx}\right)_{x=x_0}=\frac{1}{h}\left[\Delta y_0-\frac{1}{2}\Delta^2 y_0+\frac{1}{3}\Delta^3 y_0-\ldots\right]$$

$$\left(\frac{d^2y}{dx^2}\right)_{x=x_0}=\frac{1}{h^2}\left[\Delta^2 y_0-\Delta^3 y_0+\frac{11}{12}\Delta^4 y_0-\ldots\right]$$

$$\left(\frac{d^3y}{dx^3}\right)_{x=x_0}=\frac{1}{h^3}\left[\Delta^3 y_0-\frac{3}{2}\Delta^4 y_0+\frac{7}{4}\Delta^5 y_0-\ldots\right]$$

Newton's Backward Difference Formula

$$\frac{dy}{dp} = \frac{1}{h}\left\{\nabla y_n + \left[\frac{(2p+1)}{1\cdot 2}\right](\nabla^2 y_n) + \left[\frac{(3p^2+6p+2)}{1\cdot 2\cdot 3}\right](\nabla^3 y_n) + \left[\frac{(4p^3+18p^2+22p+6)}{1\cdot 2\cdot 3\cdot 4}\right](\nabla^4 y_n) + \ldots\right\}$$

$$\frac{d^2y}{dp^2} = \frac{1}{h^2}\left\{\nabla^2 y_n + (p+1)(\nabla^3 y_n) + \left[\frac{(6p^2+18p+11)}{12}\right]\cdot(\nabla^4 y_n) + \ldots\right\}$$

$$\frac{d^3y}{dp^3} = \frac{1}{h^3}\left\{\nabla^3 y_n + \left[\frac{(12p+18)}{12}\right](\nabla^4 y_n) + \ldots\right\}$$

at $\boxed{x = x_n, p = 0}$

$$\left(\frac{dy}{dx}\right)_{x=x_n} = \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \ldots\right]$$

$$\left(\frac{d^2y}{dx^2}\right)_{x=x_n} = \frac{1}{h^2}\left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \ldots\right]$$

$$\left(\frac{d^3y}{dx^3}\right)_{x=x_n} = \frac{1}{h^3}\left[\nabla^3 y_n + \frac{3}{2}\nabla^4 y_n + \frac{7}{4}\nabla^5 y_n + \ldots\right]$$

Find Maxima and Minima of a Tabulated Function

$$\frac{dy}{dp} = \Delta y_0 + \left[\frac{2p-1}{2}\right](\Delta^2 y_0) + \left[\frac{3p^2-6p+2}{6}\right](\Delta^3 y_0) + \ldots$$ For maxima or minima, $\boxed{\frac{dy}{dp} = 0}$

EXAMPLE Find the first and second derivatives of $f(x)$, at $x = 1.5$, if

x	1.5	2.0	2.5	3.0	3.5	4.0
$f(x)$	3.375	7.000	13.625	24.000	38.875	59.000

Solution

Since $x = 1.5$ is in the first half of the table, we will use Newton's forward difference formula.

Taking $x_0 = 1.5$, we have

$$y_0 = 3.375$$
$$\Delta y_0 = 3.625$$
$$\Delta^2 y_0 = 3$$
$$\Delta^3 y_0 = 0.75$$
$$\Delta^4 y_0 = 0$$
$$h = 0.5$$

The forward difference table is as follows

x	$f(x)$	Δ	Δ^2	Δ^3	Δ^4	Δ^5
1.5	3.375					
		3.625				
2.0	7.000		3			
		6.625		0.75		
2.5	13.625		3.75		0	
		10.375		0.75		0
3.0	24.000		4.5		0	
		14.875		0.75		
3.5	38.875		5.25			
		20.125				
4.5	59.000					

Newton's forward difference formula is given by

$$\left(\frac{dy}{dx}\right)_{x=x_0} = \frac{1}{h}\left(\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \ldots\right)$$

$$= \frac{1}{0.5}\left(3.625 - \frac{1}{2}\times 3 + \frac{1}{3}\times 0.75 - \frac{1}{4}\times 0\right)$$

$$= \frac{1}{0.5}(3.625 - 1.5 + 0.25 + 0) = \frac{1}{0.5}(3.875 - 1.5)$$

$$= \frac{1}{0.5}\times 2.375 = 4.75$$

$$\left(\frac{d^2y}{dx^2}\right)_{x=x_0} = \frac{1}{h^2}\left(\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 - \frac{5}{6}\Delta^5 y_0 + \dots\right)$$

$$= \frac{1}{(0.5)^2}\left(3 - 0.75 + \frac{11}{12}\times 0 - \frac{5}{6}\times 0\right)$$

$$= \frac{1}{(0.5)^2}(3-0.75) = \frac{1}{0.25}(2.25) = 9$$

EXAMPLE From the table given below, for what values x and y is minimum? Also find this value of y.

x	3	4	5	6	7	8
y	0.205	0.240	0.259	0.262	0.250	0.224

Solution The difference table is

x	y	Δ	Δ^2	Δ^3
3	0.205			
		0.035		
4	0.240		– 0.016	
		0.019		0.000
5	0.259		– 0.016	
		0.003		0.001
6	0.262		– 0.015	
		– 0.012		0.001
7	0.250		– 0.014	
		– 0.026		
8	0.224			

$x_0 = 3$, we have
$$y_0 = 0.205$$
$$\Delta y_0 = 0.035$$
$$\Delta^2 y_0 = -0.016$$
$$\Delta^3 y_0 = 0$$

Newton's forward difference formula gives

$$y = 0.205 + p(0.035) + \left[\frac{p(p-1)}{2}\right](-0.016) \qquad \text{(i)}$$

$$\frac{dy}{dp} = 0.035 + \left[\frac{2p-1}{2}\right](-0.016)$$

For y to be minimum $\qquad \dfrac{dy}{dp} = 0$

$$0.035 + (-0.008)(2p-1) = 0$$

which gives $p = 2.6875$

$\therefore \qquad x = x_0 + ph = 3 + 2.6875 \times 1$

$$= 5.6875$$

Hence, y is minimum, when $x = 5.6875$.

Putting $p = 2.6875$ in (i), the minimum value of y is

$$= 0.205 + 2.6875 \times 0.035 + \frac{1}{2}(2.6875 \times 1.6875)(-0.016)$$

$$= 0.2628$$

Derivatives of Unequally Spaced

Lagrange Polynomial

$$f_n(x) = \sum_{i=0}^{n} L_i(x) f(x_i)$$

$$L_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

For example, the second order Lagrange polynomial passing through $(x_0, y_0), (x_1, y_1), (x_2, y_2)$ is

$$f_2(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

$$f_2{}'(x) = \frac{2x - (x_1 + x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{2x - (x_0 + x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{2x - (x_0 + x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

$$f_2''(x) = \frac{2}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{2}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{2}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

Example: The upward velocity of a rocket is given as a function of time in Table

t (s)	**v(t)** m/s
0	0
10	227.04
15	362.78
20	517.35
22.5	602.97
30	901.67

Table Velocity as a function of time

Determine the value of the acceleration at $t = 16\ \mathrm{s}$ using the second order Lagrangian polynomial interpolation for velocity.

Solution:

$$v(t) = \left(\frac{t - t_1}{t_0 - t_1}\right)\left(\frac{t - t_2}{t_0 - t_2}\right)v(t_0) + \left(\frac{t - t_0}{t_1 - t_0}\right)\left(\frac{t - t_2}{t_1 - t_2}\right)v(t_1) + \left(\frac{t - t_0}{t_2 - t_0}\right)\left(\frac{t - t_1}{t_2 - t_1}\right)v(t_2)$$

$$a(t) = \frac{2t - (t_1 + t_2)}{(t_0 - t_1)(t_0 - t_2)}v(t_0) + \frac{2t - (t_0 + t_2)}{(t_1 - t_0)(t_1 - t_2)}v(t_1) + \frac{2t - (t_0 + t_1)}{(t_2 - t_0)(t_2 - t_1)}v(t_2)$$

$$a(16) = \frac{2(16)-(15+20)}{(10-15)(10-20)}(227.04) + \frac{2(16)-(10+20)}{(15-10)(15-20)}(362.78) + \frac{2(16)-(10+15)}{(20-10)(20-15)}(517.35)$$

$$= -0.06(227.04) - 0.08(362.78) + 0.14(517.35) = 29.784 \quad \text{m/s}^2$$

Example: Let $f(x) = \ln x$ and $x_0 = 1.8$

Find an approximate value for $f'(1.8)$

h	$f(1.8)$	$f(1.8+h)$	$\frac{f(1.8+h)-f(1.8)}{h}$
0.1	**0.5877867**	**0.6418539**	**0.5406720**
0.01	**0.5877867**	**0.5933268**	**0.5540100**
0.001	**0.5877867**	**0.5883421**	**0.5554000**

The exact value of $f'(1.8) = 0.55\overline{5}$