Numerical Differentiation

- **Estimate the derivatives (slope, curvature, etc.) of a function by using the function values at only a set of discrete points**
- **Ordinary differential equation (ODE)**
- **Partial differential equation (PDE)**
- **Represent the function by Taylor polynomials or Lagrange interpolation**
- **Evaluate the derivatives of the interpolation polynomial at selected (unevenly distributed) nodal points**

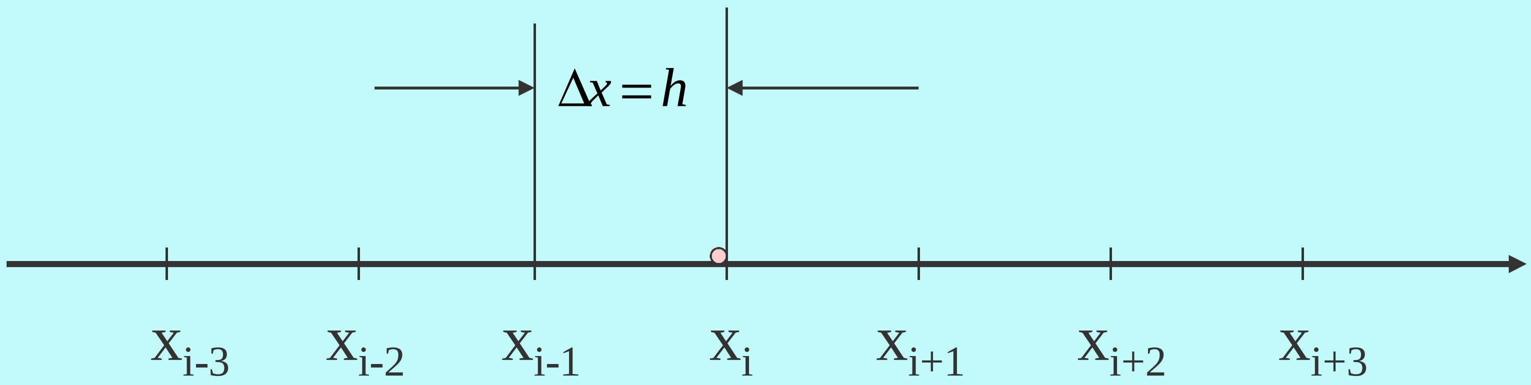
$$y = f(x)$$

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

Difference $$\frac{\Delta y}{\Delta x} = \frac{f(x+\Delta x) - f(x)}{(x+\Delta x) - x} \approx \frac{dy}{dx}$$

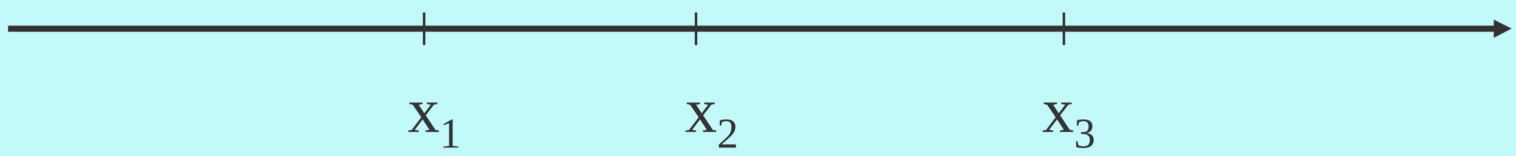
A smaller step Δx (or h) results in a smaller error

Evenly distributed points along the x-axis



Distance between two neighboring points is the same, i.e. h.

Unevenly distributed points along the x-axis



Lagrange Interpolation

- **1st-order Lagrange polynomial** *(Two-Point)*

$$f_1(x) = L_0 f(x_0) + L_1(x) f(x_1) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)$$

- **Second-o** *(Three-Point)*

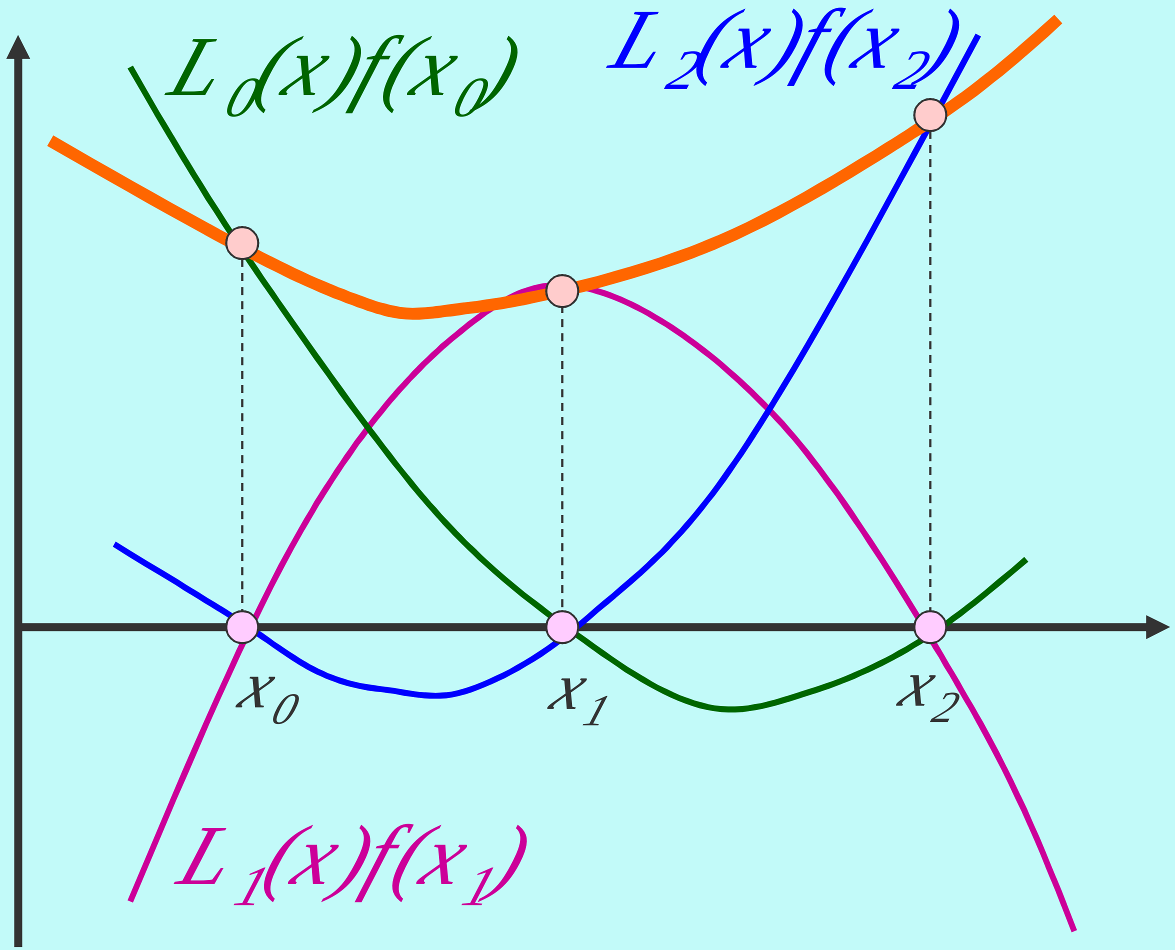
$$f_2(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

Formula

- **Lagrange interpolation polynomial for <u>unequally spaced</u> data**

$$
\begin{aligned}
f(x) &= L_{i-1}(x)\,f(x_{i-1}) + L_i(x)\,f(x_i) + L_{i+1}(x)\,f(x_{i+1}) \\
&= \frac{(x-x_i)(x-x_{i+1})}{(x_{i-1}-x_i)(x_{i-1}-x_{i+1})}\,f(x_{i-1}) \\
&\quad + \frac{(x-x_{i-1})(x-x_{i+1})}{(x_i-x_{i-1})(x_i-x_{i+1})}\,f(x_i) \\
&\quad + \frac{(x-x_{i-1})(x-x_i)}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)}\,f(x_{i+1})
\end{aligned}
$$

Lagrange Interpolation



Formula

- **Lagrange interpolation polynomial for unequally spaced data**

$$f(x) = L_{i-1}(x) f(x_{i-1}) + L_i(x) f(x_i) + L_{i+1}(x) f(x_{i+1})$$
$$= f(x_{i-1}) \frac{(x - x_i)(x - x_{i+1})}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} + f(x_i) \frac{(x - x_{i-1})(x - x_{i+1})}{(x_i - x_{i-1})(x_i - x_{i+1})}$$
$$+ f(x_{i+1}) \frac{(x - x_{i-1})(x - x_i)}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)}$$

- **First derivative**

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

Lagrange polynomial *(Two-Point)*

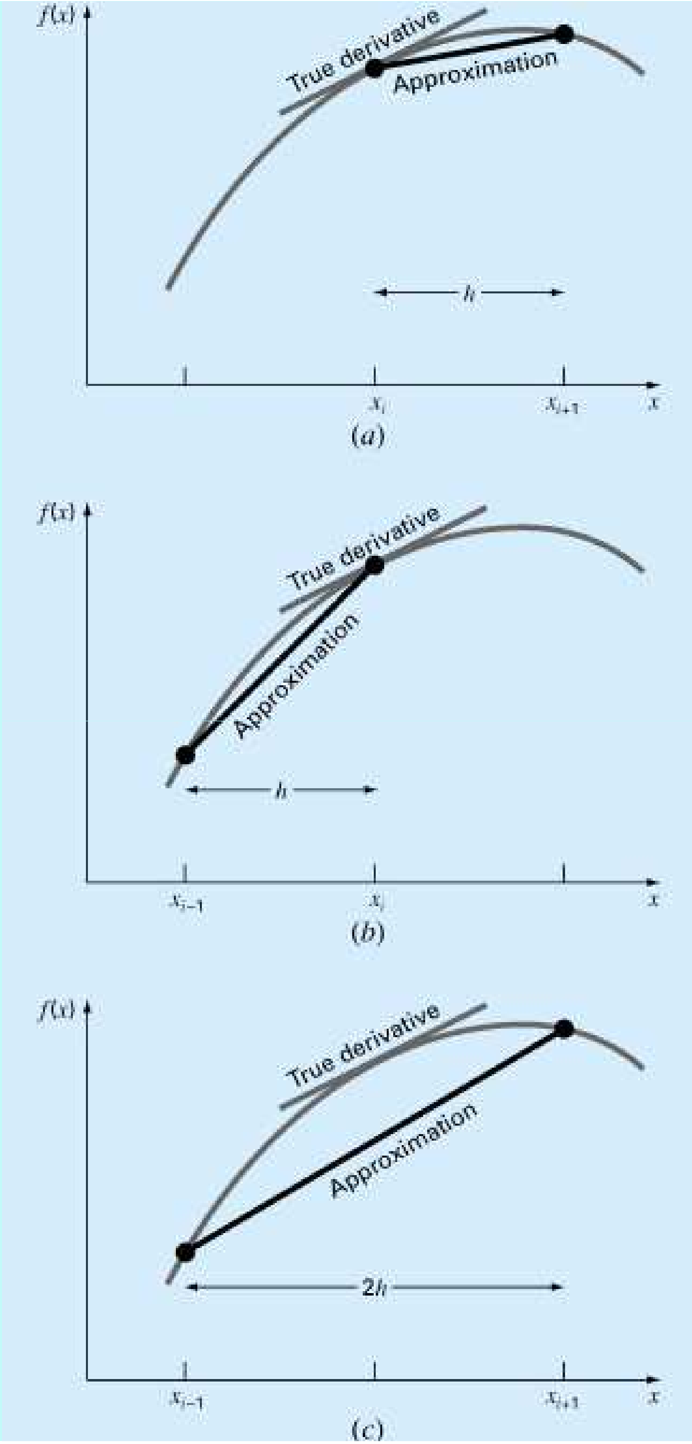
$$f_1(x) = L_0 f(x_0) + L_1(x) f(x_1) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)$$

Numerical Differentiation

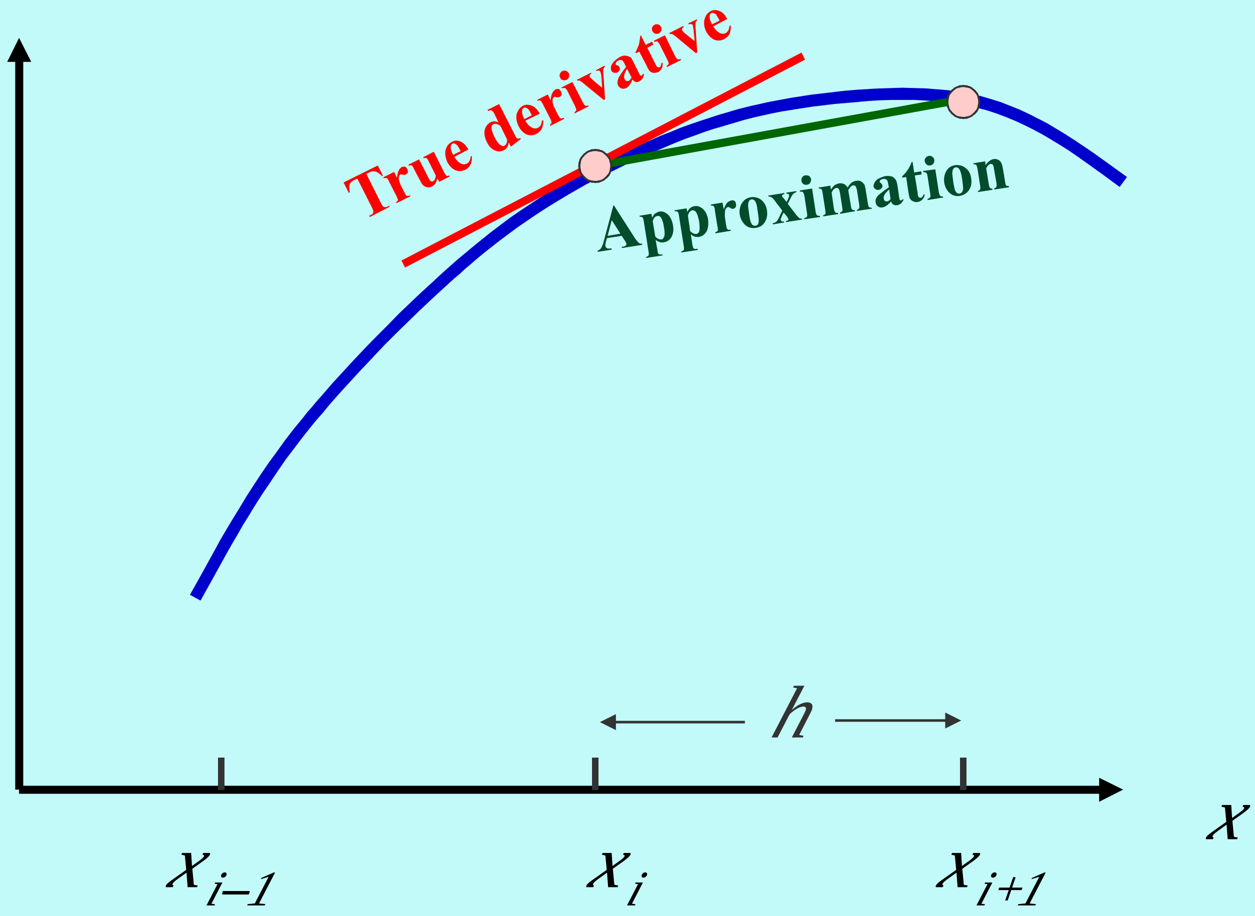
Forward difference

Backward difference

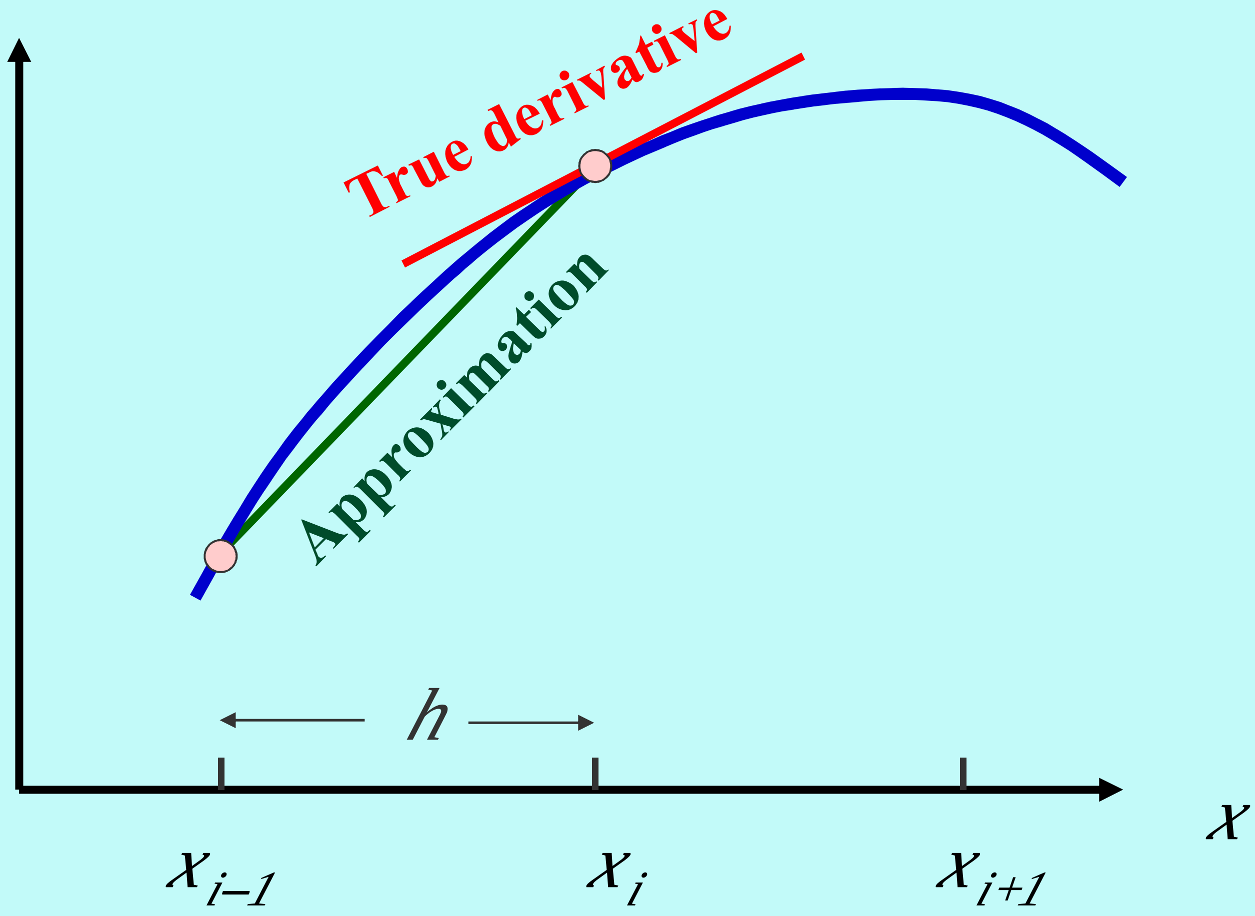
Centered difference



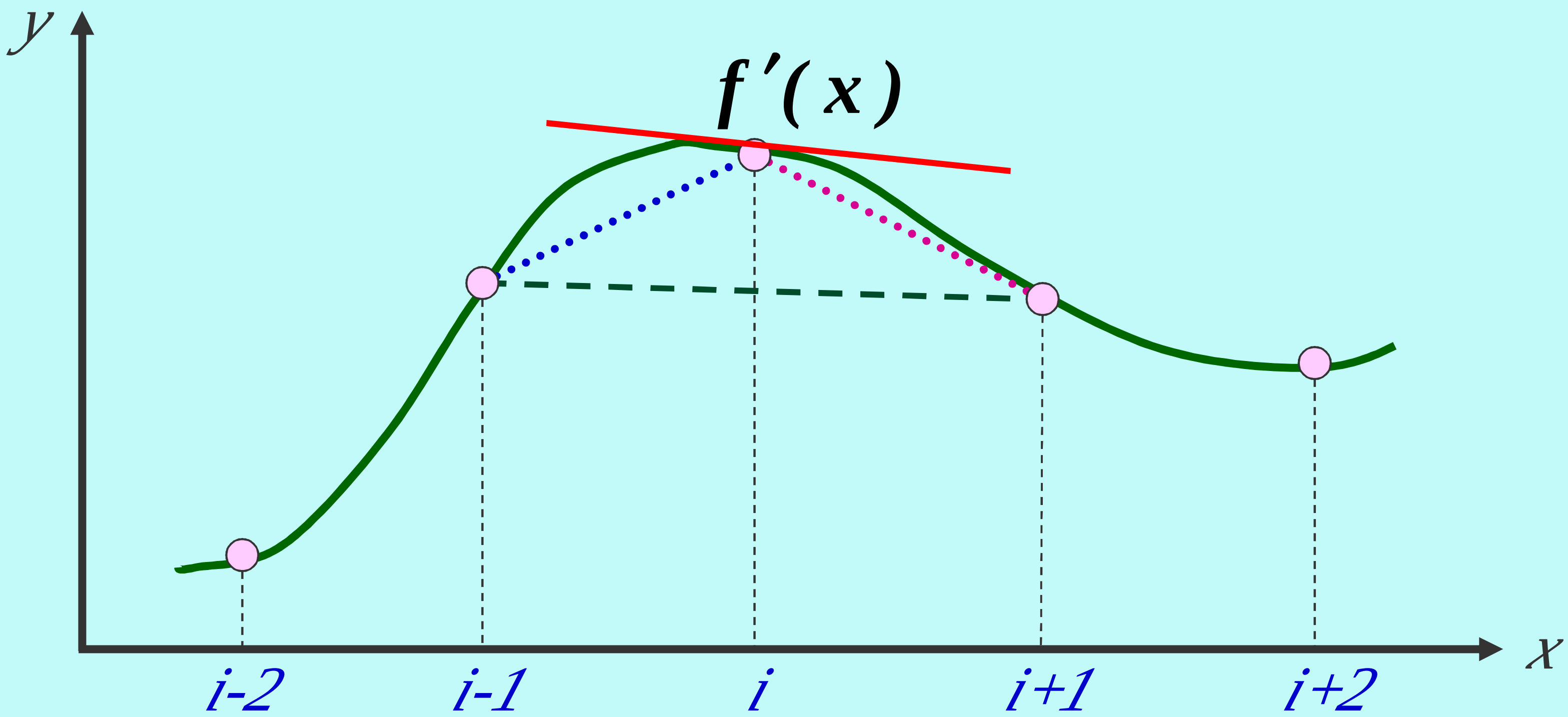
Forward difference



Backward difference

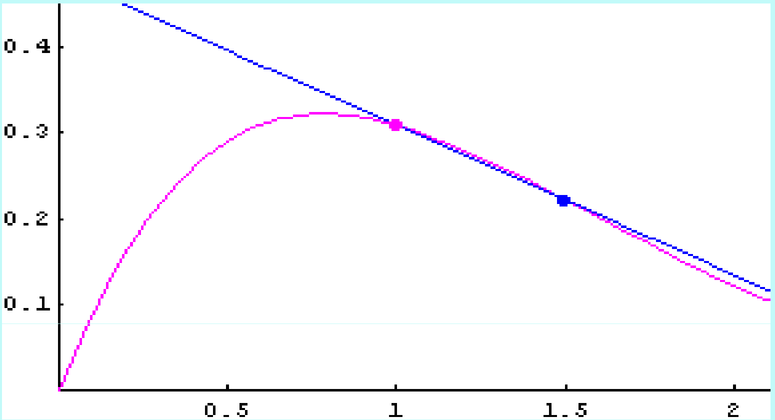


First Derivatives



- **Forward difference** $f'(x) \cong \dfrac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} = \dfrac{y_{i+1} - y_i}{x_{i+1} - x_i}$
- **Backward difference** $f'(x) \cong \dfrac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} = \dfrac{y_i - y_{i-1}}{x_i - x_{i-1}}$

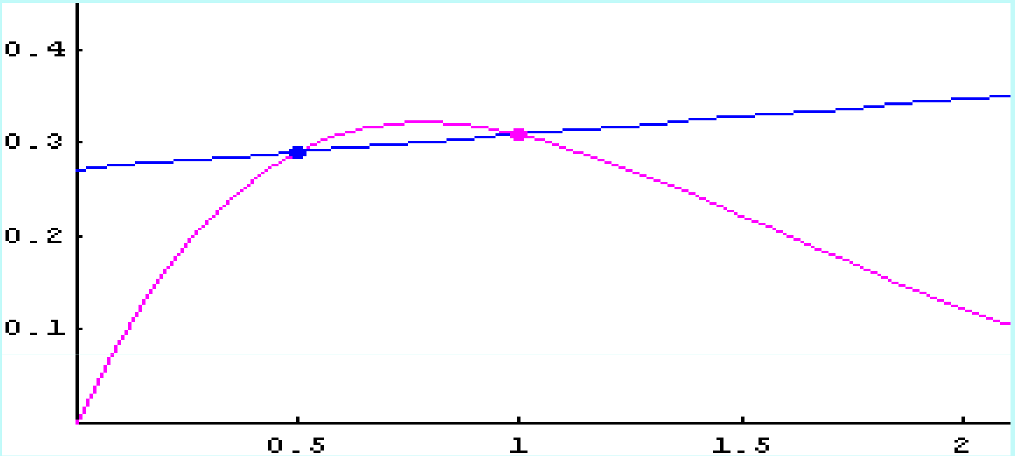
Given $f[x] = e^{-x} \operatorname{Sin}[x]$ find numerical approximations to the derivative $f'[1.0]$ using two points and the forward difference formula.



$$f[x] = e^{-x} \operatorname{Sin}[x]$$
$$f'[x] = e^{-x} \operatorname{Cos}[x] - e^{-x} \operatorname{Sin}[x]$$
$$f'[1.] = -0.110794$$
$$h = 0.5$$

$$f'[1.] \approx (f[1.+0.5] - f[1.])/(0.5) = -0.173977$$

Given $f[x] = e^{-x}\,\mathrm{Sin}[x]$ find numerical approximations to the derivative $f'[1.0]$ using two points and the backward difference formula.



$$f[x] = e^{-x}\,\mathrm{Sin}[x]$$

$$f'[x] = e^{-x}\,\mathrm{Cos}[x] - e^{-x}\,\mathrm{Sin}[x]$$

$$f'[1.] = -0.110794$$

$$h = 0.5$$

$$f'[1.] \approx (f[1.] - f[1.-0.5])/(0.5) = 0.0375472$$

Truncation Errors

- **Uniform grid spacing**

$$\begin{cases} f(x_{i+1}) = f(x_i + h) = f(x_i) + hf'(x_i) + \dfrac{h^2}{2!} f''(x_i) + \dfrac{h^3}{3!} f'''(x_i) + \cdots \\ f(x_{i-1}) = f(x_i - h) = f(x_i) - hf'(x_i) + \dfrac{h^2}{2!} f''(x_i) - \dfrac{h^3}{3!} f'''(x_i) + \cdots \end{cases}$$

$$\begin{cases} forward: \; f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h} - \dfrac{h}{2} f''(\xi_1) & O(h) \\ backward: \; f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{h} + \dfrac{h}{2} f''(\xi_2) & O(h) \\ central: \; f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h} - \dfrac{h^2}{6} f'''(\xi_3) & O(h^2) \end{cases}$$

Example: First Derivatives

- **Use forward and backward difference approximations to estimate the first derivative of**

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

at x = 0.5 with h = 0.5 and 0.25 (exact sol. = -0.9125)

- **Forward Difference**

$$\begin{cases} h = 0.5, \ \ f'(0.5) = \dfrac{f(1) - f(0.5)}{1 - 0.5} = \dfrac{0.2 - 0.925}{0.5} = -1.45, \quad |\varepsilon_t| = 58.9\% \\ h = 0.25, \ \ f'(0.5) = \dfrac{f(0.75) - f(0.5)}{0.75 - 0.5} = \dfrac{0.63632813 - 0.925}{0.25} = -1.155, \ |\varepsilon_t| = 26.5\% \end{cases}$$

- **Backward Difference**

$$\begin{cases} h = 0.5, \ \ f'(0.5) = \dfrac{f(0.5) - f(0)}{0.5 - 0} = \dfrac{0.925 - 1.2}{0.5} = -0.55, \quad |\varepsilon_t| = 39.7\% \\ h = 0.25, \ \ f'(0.5) = \dfrac{f(0.5) - f(0.25)}{0.5 - 0.25} = \dfrac{0.925 - 1.10351563}{0.25} = -0.714, \ |\varepsilon_t| = 21.7\% \end{cases}$$

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

$$f'(1.8) = \frac{f(1.8+h) - f(1.8)}{h} \quad \text{for } h > 0$$

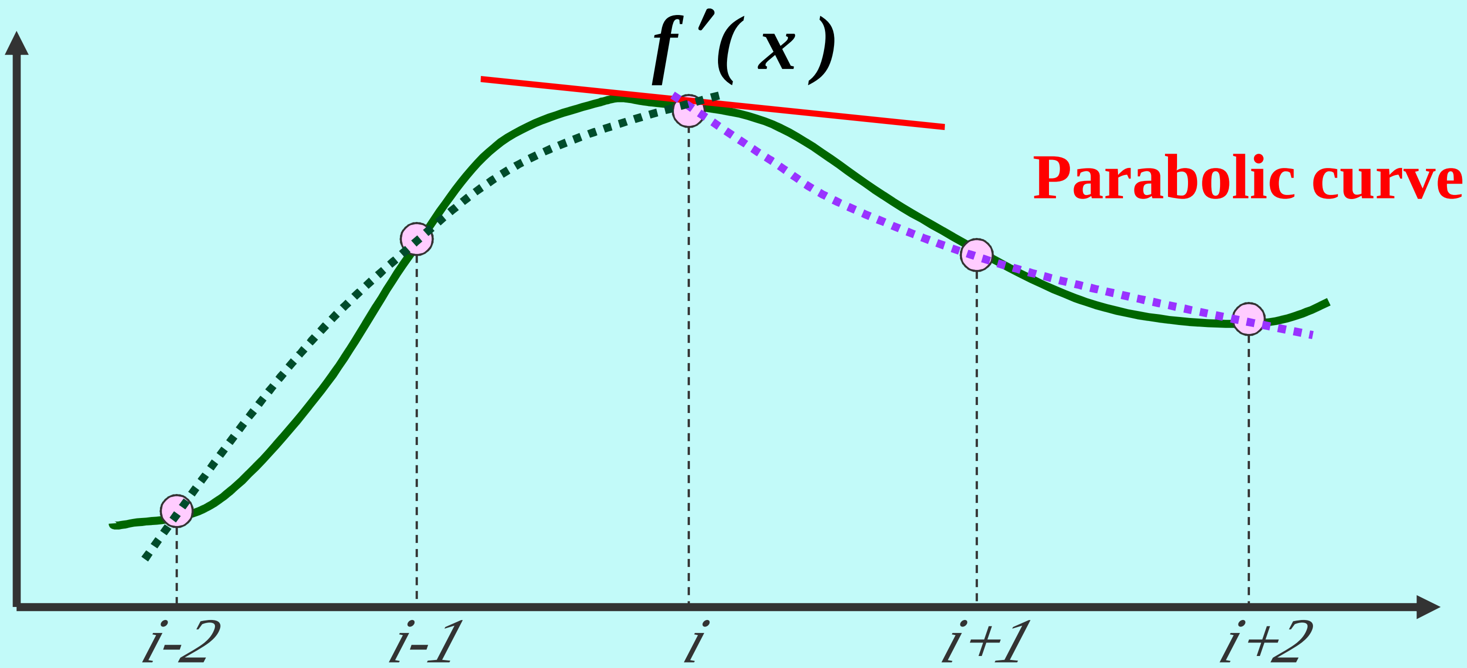
with error $\left|\frac{hf''(\xi)}{2}\right| = \frac{|h|}{2\xi^2} \le \frac{|h|}{2(1.8)^2}$

h	f'	$\frac{\lvert h\rvert}{2(1.8)^2}$
0.1	0.54067	0.01543
0.01	0.5540	0.00154
0.001	0.5554	0.00015

Lagrange polynomial *(Three-Point)*

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

First Derivatives



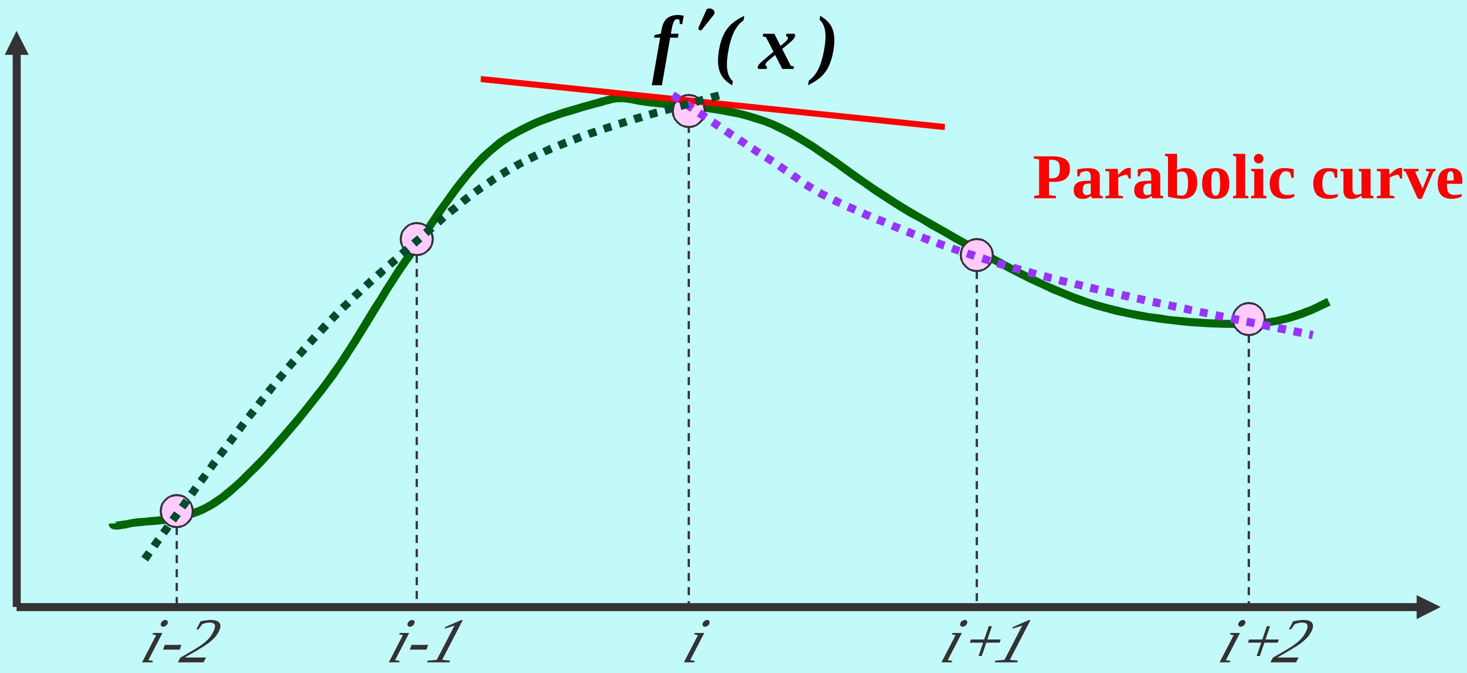
- **3 -point Forward difference**

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

- **3 -point Backward difference**

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

First Derivatives

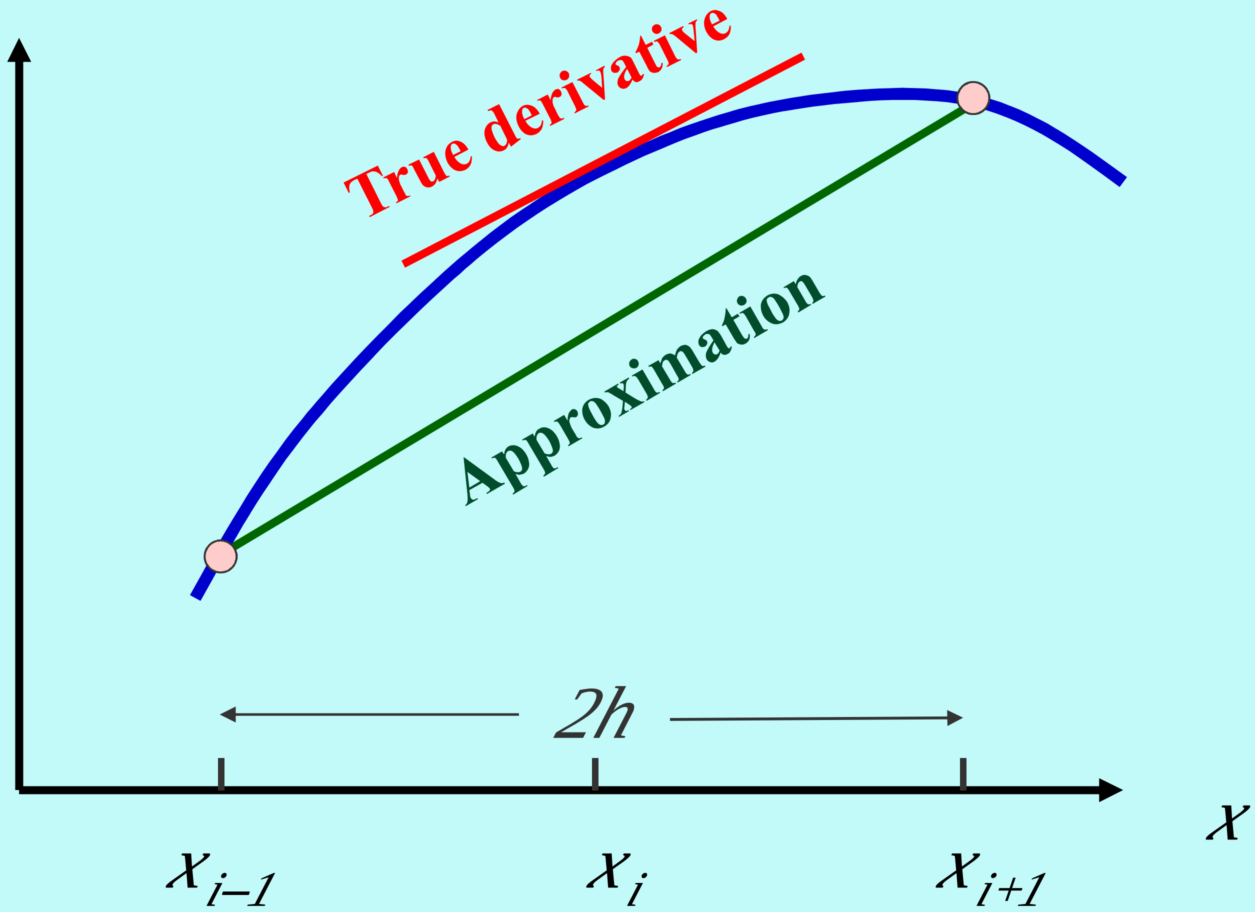


- **3 - point central difference**

$$f'(x) \cong \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}} = \frac{y_{i+1} - y_{i-1}}{x_{i+1} - x_{i-1}}$$

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

Centered difference



Example: First Derivative

- **Use central difference approximation to estimate the first derivative of**

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

at x = 0.5 with h = 0.5 and 0.25 (exact sol. = -0.9125)

- **Central Difference**

$$h = 0.5,\ \ f'(0.5) = \frac{f(1) - f(0)}{1 - 0} = \frac{0.2 - 1.2}{1} = -1.0,\quad |\varepsilon_t| = 9.6\%$$

$$h = 0.25,\ \ f'(0.5) = \frac{f(0.75) - f(0.25)}{0.75 - 0.25}$$

$$= \frac{0.63632813 - 1.10351563}{0.5} = -0.934,\ |\varepsilon_t| = 2.4\%$$

Example: First Derivatives

- **Use forward and backward difference approximations of O(h²) to estimate the first derivative of**

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

at x = 0.5 with h = 0.25 (exact sol. = -0.9125)

- **Forward Difference**

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

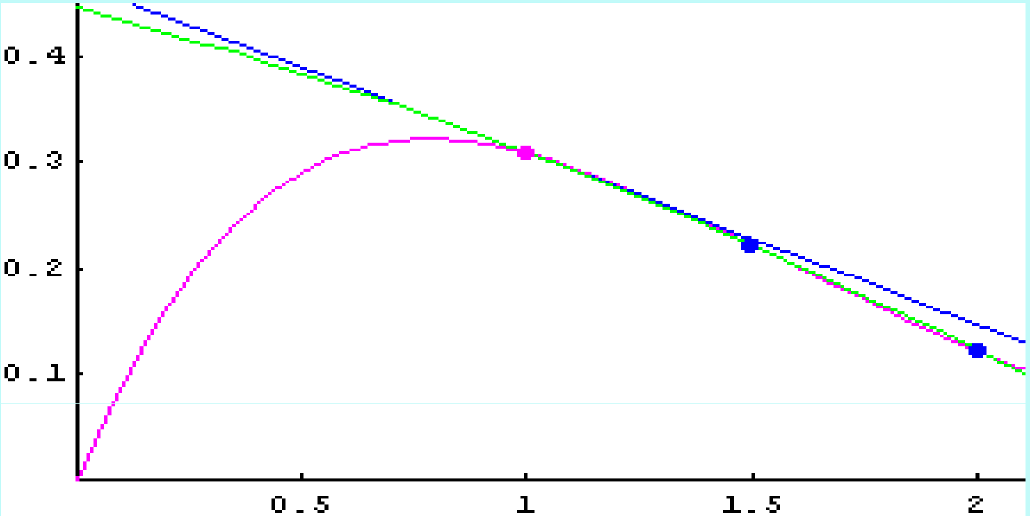
$$= \frac{-0.2 + 4(0.6363281) - 3(0.925)}{0.5} = -0.859375, \quad |\varepsilon_t| = 5.82\%$$

- **Backward Difference**

$$f'(0.5) = \frac{3f(0.5) - 4f(0.25) + f(0)}{2(0.25)}$$

$$= \frac{3(0.925) - 4(1.035156) + 1.2}{0.5} = -0.878125, \quad |\varepsilon_t| = 3.77\%$$

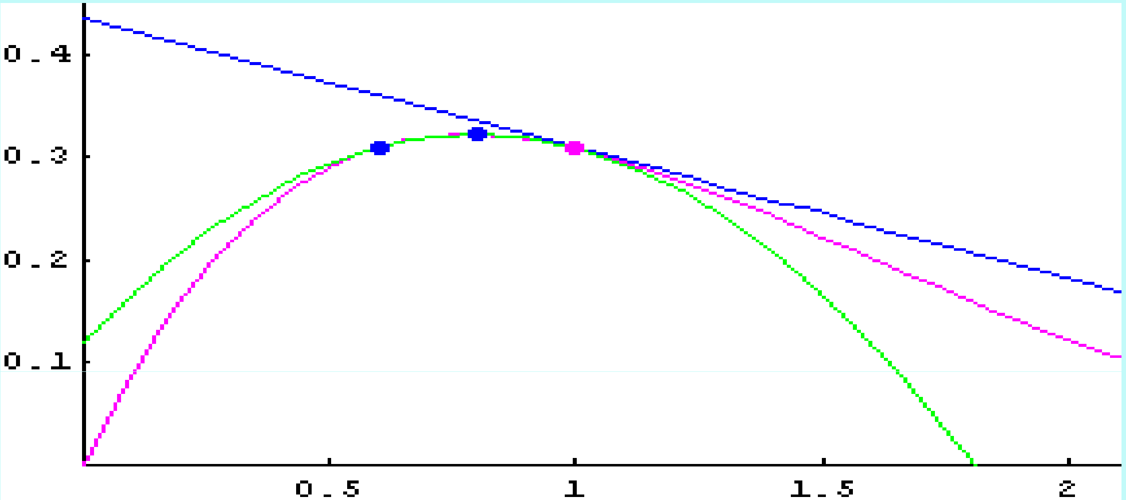
Given $f[x] = e^{-x}\,\mathrm{Sin}[x]$ find numerical approximations to the derivative $f'[1.0]$ using three points and the forward difference formula.



$$f[x] = e^{-x}\,\mathrm{Sin}[x]$$
$$f'[x] = e^{-x}\,\mathrm{Cos}[x] - e^{-x}\,\mathrm{Sin}[x]$$
$$f'[1.] = -0.110794$$
$$h = 0.5$$

$$f'[1.] \approx (-3f[1.] + 4f[1.+0.5] - f[1.+1.])/(1.) = -0.161455$$

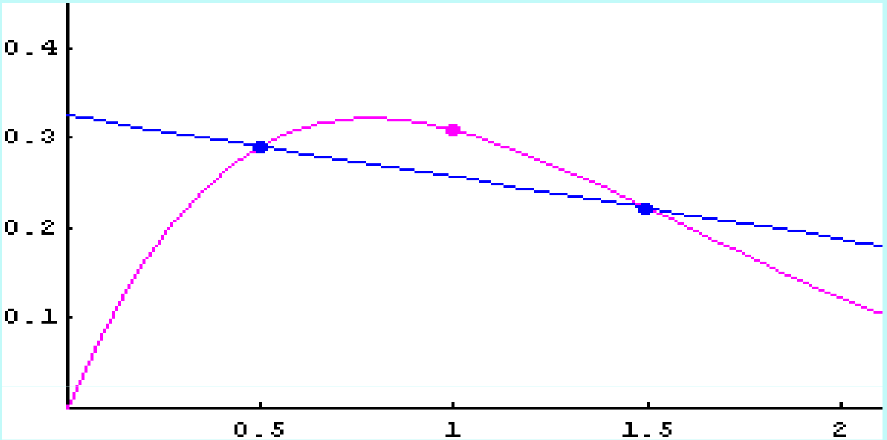
Given $f[x] = e^{-x}\,\mathrm{Sin}[x]$ find numerical approximations to the derivative $f'[1.0]$ using three points and the backward difference formula



$$f[x] = e^{-x}\,\mathrm{Sin}[x]$$
$$f'[x] = e^{-x}\,\mathrm{Cos}[x] - e^{-x}\,\mathrm{Sin}[x]$$
$$f'[1.] = -0.110794$$
$$h = 0.5$$

$$f'[1.] \approx (3f[1.] - 4f[1.-0.5] + f[1.-1.])/(1.) = -0.234466$$

Given $f[x] = e^{-x} \operatorname{Sin}[x]$ find numerical approximations to the derivative $f'[1.0]$ using three points and the central difference formula.



$$f[x] = e^{-x} \operatorname{Sin}[x]$$
$$f'[x] = e^{-x} \operatorname{Cos}[x] - e^{-x} \operatorname{Sin}[x]$$
$$f'[1.] = -0.110794$$
$$h = 0.5$$

$$f'[1.] \approx (f[1.+0.5] - f[1.-0.5])/(1.) = -0.0682151$$

Error For First Derivatives (Three-Point)

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3} f^{(3)}(\xi_0)$$

$$f'(x_0) = \frac{1}{2h}\left[-f(x_0-h) + f(x_0+h)\right] - \frac{h^2}{6} f^{(3)}(\xi_1) \leftarrow \text{equiv by letting } h = -h$$

$$f'(x_0) = \frac{1}{2h}\left[f(x_0-2h) - 4f(x_0-h) + 3f(x_0)\right] + \frac{h^2}{3} f^{(3)}(\xi_2)$$

ξ_0 lies between x_0 and $x_0 + 2h$

ξ_1 lies between $(x_0 - h)$ and $(x_0 + h)$

ξ_2 lies between x_0 and $x_0 - 2h$

Second Derivative

- **First Derivative for unequally spaced data**

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

- **Second Derivative for unequally spaced data**

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

Second-Derivatives

- **Taylor-series expansion**
- **Uniform grid spacing**

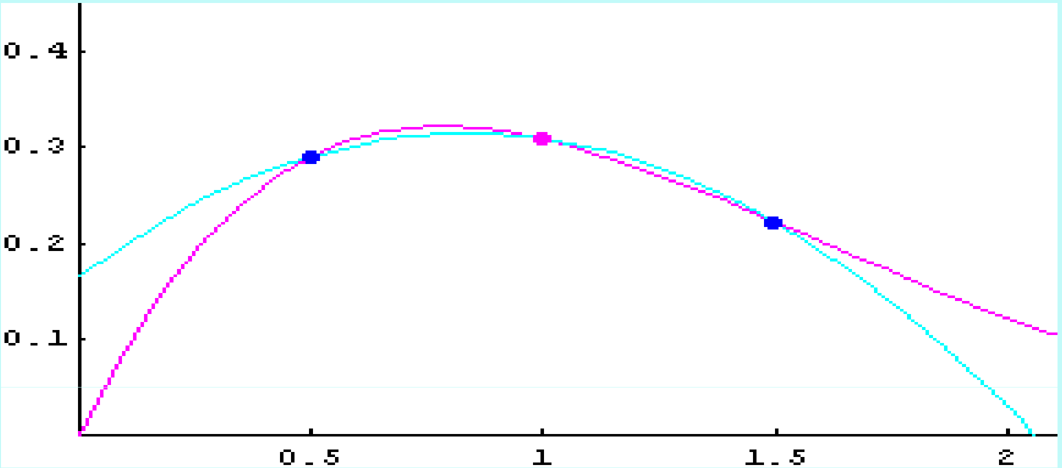
$$\begin{cases} f(x_{i+1}) = f(x_i) + hf'(x_i) + \dfrac{h^2}{2!} f''(x_i) + \dfrac{h^3}{3!} f'''(x_i) + \dfrac{h^4}{4!} f''''(x_i) + \cdots \\ f(x_{i-1}) = f(x_i) - hf'(x_i) + \dfrac{h^2}{2!} f''(x_i) - \dfrac{h^3}{3!} f'''(x_i) + \dfrac{h^4}{4!} f''''(x_i) + \cdots \end{cases}$$

$$\Rightarrow f(x_{i+1}) + f(x_{i-1}) = 2\left[f(x_i) + \frac{h^2}{2!} f''(x_i) + \frac{h^4}{4!} f''''(x_i) + \cdots \right]$$

- **Second-order accurate** *$O(h^2)$*

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

Given $f[x] = e^{-x}\,\text{Sin}[x]$ find numerical approximations to the second derivative $f''[1.0]$ using three points and the central difference formula.



$$f[x] = e^{-x}\,\text{Sin}[x]$$
$$f'[x] = e^{-x}\,\text{Cos}[x] - e^{-x}\,\text{Sin}[x]$$
$$f''[x] = -2\,e^{-x}\,\text{Cos}[x]$$
$$f''[1.] = -0.397532$$
$$h = 0.5$$

$$f''[1.] \approx (f[1.-0.5] - 2f[1.] + f[1.+0.5])/(0.25) = -0.423049$$

Centered Finite-Divided Differences

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

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

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

Forward Finite divided differences

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 differences

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

Higher Derivatives

- **All second-order accurate** *$O(h^2)$*

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

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

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

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

- **More nodal points are needed for higher derivatives**
- **Higher order formula may be derived**

Example 6.4. Let $f(x) = \cos(x)$.

(a) Use formula (6) with $h = 0.1, 0.01$, and 0.001 and find approximations to $f''(0.8)$. Carry nine decimal places in all calculations.

(b) Compare with the true value $f''(0.8) = -\cos(0.8)$.

(a) The calculation for $h = 0.01$ is

$$\begin{aligned} f''(0.8) &\approx \frac{f(0.81) - 2f(0.80) + f(0.79)}{0.0001} \\ &\approx \frac{0.689498433 - 2(0.696706709) + 0.703845316}{0.0001} \\ &\approx -0.696690000. \end{aligned}$$

(b) The error in this approximation is -0.000016709. The other calculations are summarized in Table 6.5. The error analysis will illuminate this example and show why $h = 0.01$ was best. ■

Error Analysis and Optimum Step size

the derivative of $f(t)=e^t$ at the point $t=0$.

Clearly, the exact answer is $f'(0)=1.00000$. Using a spreadheet, we get:

Forward difference formula		
h	f'	error
1.000E+00	1.718E+00	7.183E-01
1.000E-01	1.052E+00	5.171E-02
1.000E-02	1.005E+00	5.017E-03
1.000E-04	1.000E+00	5.000E-05
1.000E-05	1.000E+00	5.000E-06
1.000E-12	1.000E+00	8.890E-05
1.000E-16	0.000E+00	-1.000E+00

Error Analysis and Optimum Step size

Central difference formula		
h	f'	error
1.000E+00	1.175E+00	1.752E-01
1.000E-01	1.002E+00	1.668E-03
1.000E-02	1.000E+00	1.667E-05
1.000E-04	1.000E+00	1.667E-09
1.000E-05	1.000E+00	1.210E-11
1.000E-12	1.000E+00	3.339E-05
1.000E-16	5.551E-01	-4.449E-01

Forward difference formula		
h	f'	error
1.000E+00	1.718E+00	7.183E-01
1.000E-01	1.052E+00	5.171E-02
1.000E-02	1.005E+00	5.017E-03
1.000E-04	1.000E+00	5.000E-05
1.000E-05	1.000E+00	5.000E-06
1.000E-12	1.000E+00	8.890E-05
1.000E-16	0.000E+00	-1.000E+00

Error analysis and optimum step size

When evaluating $f'(x)$ using a computer, you find that

$$\left.\begin{aligned} f(x_0+h) &= y_+ + e_+ \\ f(x_0-h) &= y_- + e_- \end{aligned}\right\} \qquad \begin{aligned} &y_+, y_- \text{ True value} \\ &e_+, e_- \text{ Roundoff error} \end{aligned}$$

Then $f'(x_0) \approx (y_+ - y_-)/(2h)$. We have:

$$f'(x_0) = \frac{y_+ - y_-}{2h} + E(y,h) \quad \text{where} \quad E = \underbrace{\frac{e_+ - e_-}{2h}}_{\text{rounding error}} - \underbrace{\frac{h^2 f^{(3)}(c)}{6}}_{\text{truncation error}}$$

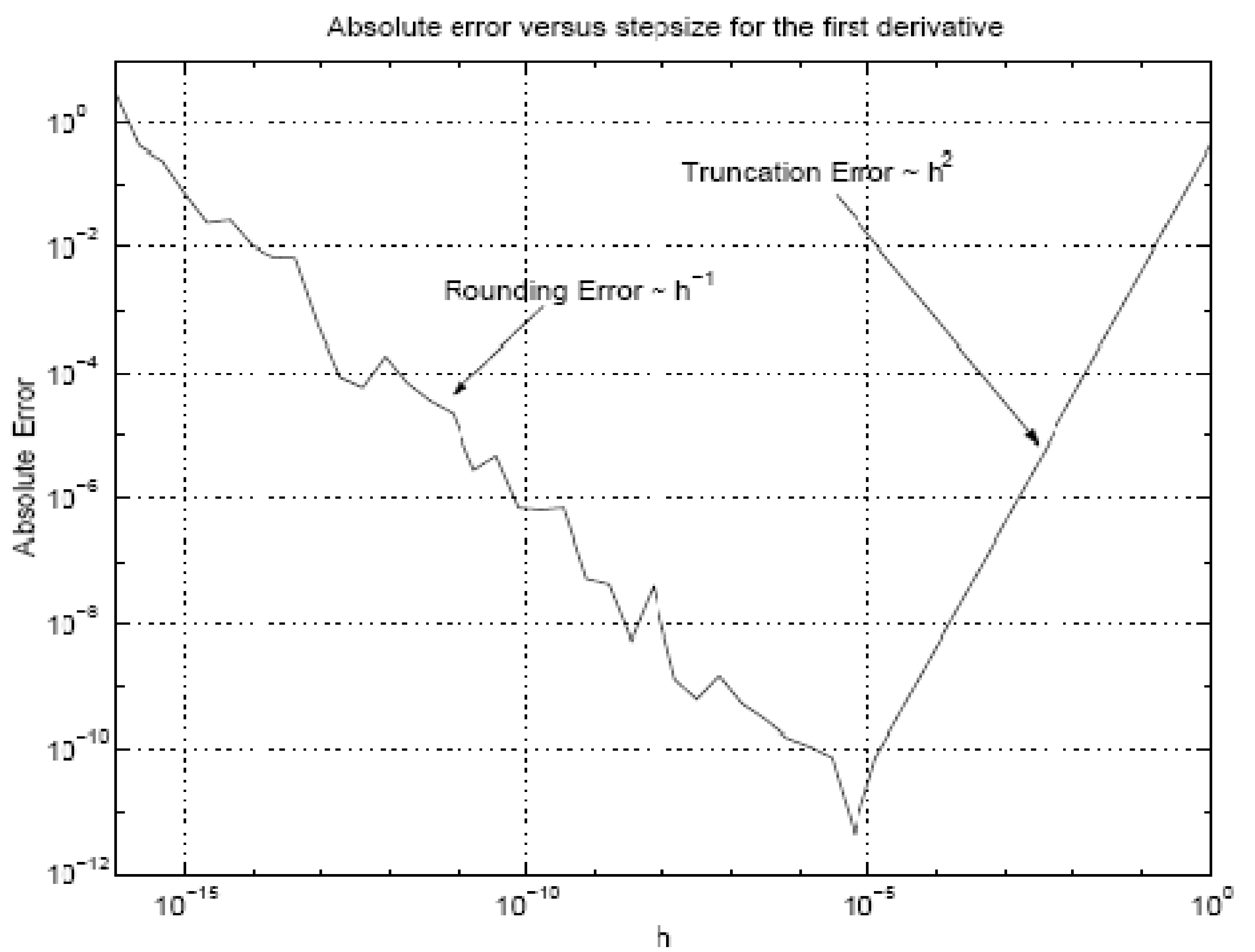
Let's assume that $|e_+| < \varepsilon$, $|e_-| < \varepsilon$ and $M = \max_{c\in[a,b]} |f^{(3)}(c)|$. Then:

$$|E| \leq \frac{\varepsilon}{h} + M\frac{h^2}{6}$$

If you want to minimize error, look for $\partial E/\partial h = 0$:

$$-\frac{\varepsilon}{h^2} + M\frac{h}{3} = 0 \quad \Rightarrow \quad \varepsilon = \frac{Mh^3}{3}$$

So that the optimal step size $h_{\text{opt}} = (3\varepsilon/M)^{1/3}$. **Note:** the error does not go to zero as $h \to 0$ on the computer due to rounding error.


Absolute error versus stepsize for the first derivative
Truncation Error ~ h^2
Rounding Error ~ h^-1
Absolute Error
h
10^0
10^-2
10^-4
10^-6
10^-8
10^-10
10^-12
10^-15
10^-10
10^-5
10^0

You can do the same analysis for the second derivative:

$$\left.\begin{array}{rcl} f(x_0+h) & = & y_+ + e_+ \\ f(x_0) & = & y+e \\ f(x_0-h) & = & y_- + e_- \end{array}\right\} \quad \begin{array}{l} y_+, y, y_- \text{ True value} \\ e_+, e, e_- \text{ Roundoff error} \end{array}$$

Then $f''(x_0) \approx (y_+ - 2y + y_-)/(h^2)$. We have:

$$f''(x_0) = \frac{y_+ - 2y + y_-}{h^2} + E(y,h) \quad \text{where} \quad E = \underbrace{\frac{e_+ - 2e + e_-}{h^2}}_{\text{rounding error}} - \underbrace{\frac{h^2 f^{(4)}(c)}{12}}_{\text{truncation error}}$$

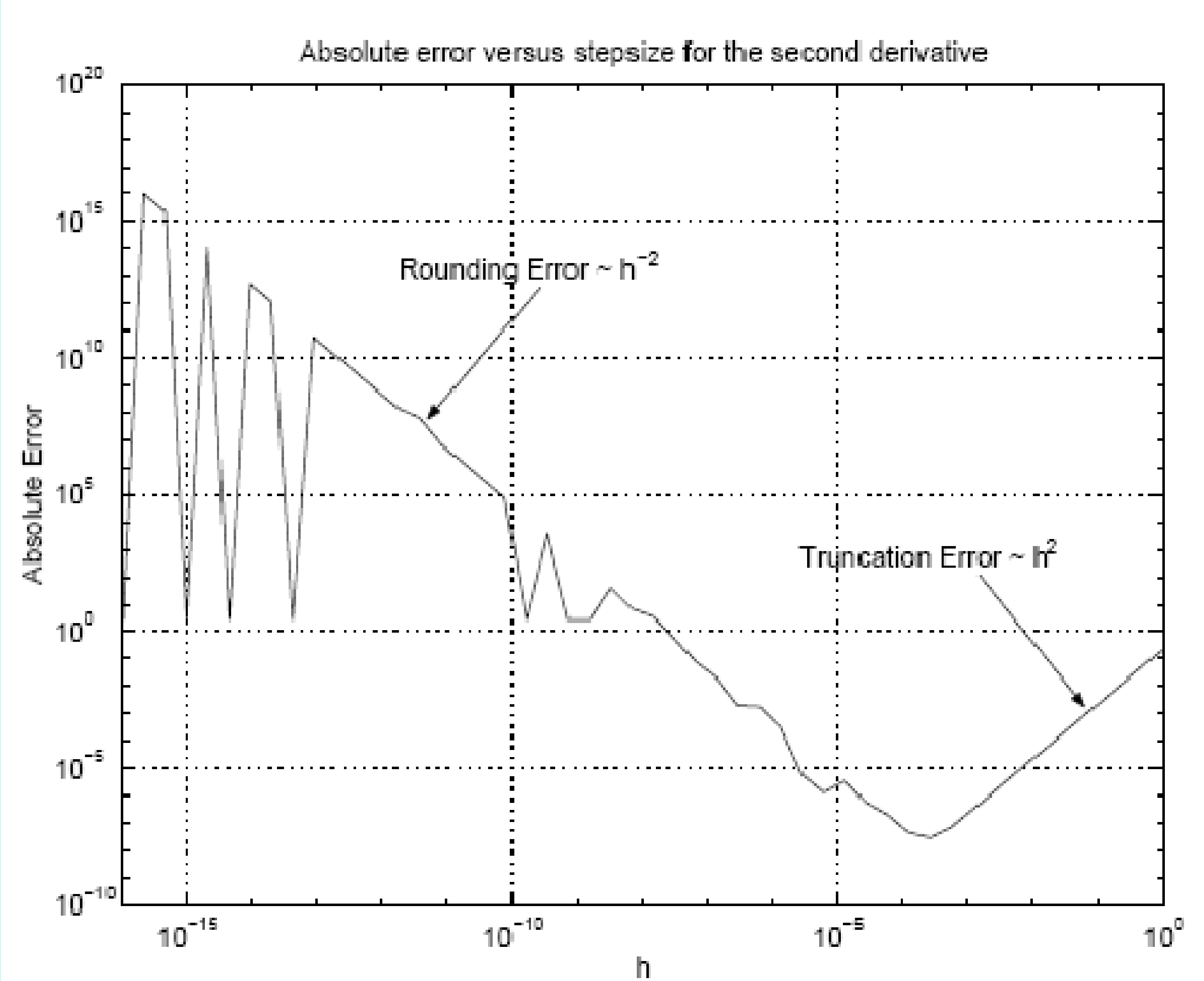
Let's assume that $|e_+| < \varepsilon$, $|e| < \varepsilon$, $|e_-| < \varepsilon$ and $M = \max_{c\in[a,b]} |f^{(4)}(c)|$. Then:

$$|E| \leq \frac{4\varepsilon}{h^2} + M\frac{h^2}{12}$$

If you want to minimize error, look for $\partial E/\partial h = 0$:

$$-\frac{8\varepsilon}{h^3} + M\frac{h}{6} = 0 \quad \Rightarrow \quad \varepsilon = \frac{Mh^4}{48}$$

So that the optimal step size $h_{\text{opt}} = (48\varepsilon/M)^{1/4}$. Again, the error does not go to zero as $h \to 0$ on the computer due to rounding error.



Absolute error versus stepsize for the second derivative
Absolute Error
h
Rounding Error ~ h^-2
Truncation Error ~ h^2
10^20
10^15
10^10
10^5
10^0
10^-5
10^-10
10^-15
10^-10
10^-5
10^0

When formula (11) is applied to Example 6.4, use the bound $|f^{(4)}(x)| \leq |\cos(x)| \leq 1 = M$ and the value $\epsilon = 0.5 \times 10^{-9}$. The optimal step size is $h = (24 \times 10^{-9}/1)^{1/4} = 0.01244666$, and we see that $h = 0.01$ was closest to the optimal value.