Round-Off Error Instability

(For example) three-point midpoint formula

$$f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi).$$

- every step in the computation could incur round-off error.
- division by $2h$ could magnify round-off error.

Assume round-off error model

$$f(x_0+h) = \widehat{f}(x_0+h) + e(x_0+h) \quad \text{and} \quad f(x_0-h) = \widehat{f}(x_0-h) + e(x_0-h),$$

where $|e(x_0+h)| \le \epsilon$, $|e(x_0-h)| \le \epsilon$. No other round-off errors.

It follows

$$f'(x_0) - \frac{\widehat{f}(x_0+h) - \widehat{f}(x_0-h)}{2h} \quad = \quad \frac{e(x_0+h) - e(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi)$$

It follows

$$\begin{aligned} f'(x_0) - \frac{\widehat{f}(x_0+h) - \widehat{f}(x_0-h)}{2h} &= \frac{e(x_0+h) - e(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi) \\ \left| f'(x_0) - \frac{\widehat{f}(x_0+h) - \widehat{f}(x_0-h)}{2h} \right| &\leq \left| \frac{e(x_0+h) - e(x_0-h)}{2h} \right| + \frac{h^2}{6} |f^{(3)}(\xi)|. \end{aligned}$$

Assume $|e(x_0+h)| \leq \epsilon$, $|e(x_0-h)| \leq \epsilon$ and $|f^{(3)}(\xi)| \leq M$, an upper bound on $|f^{(3)}(x)|$,

$$\left| f'(x_0) - \frac{\widehat{f}(x_0+h) - \widehat{f}(x_0-h)}{2h} \right| \leq \frac{\epsilon}{h} + \frac{M\, h^2}{6} \stackrel{def}{=} e(h).$$

Round-Off Error Instability: optimal h choice

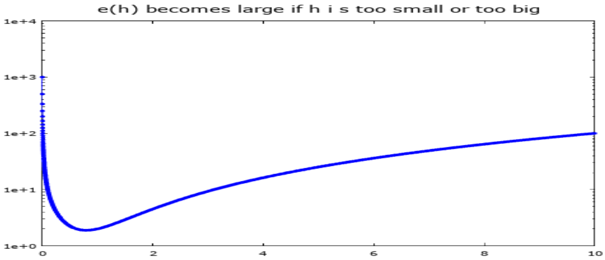
$$e(h) = \frac{\epsilon}{h} + \frac{M\,h^2}{6}$$

is smallest at

$$h_{\mathbf{min}} = \left(\frac{3\epsilon}{M}\right)^{\frac{1}{3}} = O\left(\epsilon^{\frac{1}{3}}\right),$$

with

$$e(h_{\mathbf{min}}) = \frac{1}{2}\left(\frac{9\epsilon^2}{M}\right)^{\frac{1}{3}} = O\left(\epsilon^{\frac{2}{3}}\right).$$



Richardson's Extrapolation

- **Given**: A formula $N_1(h)$ that approximates an unknown constant M for any $h \neq 0$.
- **Given**: Truncation error satisfies power series for $h \neq 0$

$$M - N_1(h) = K_1 h + K_2 h^2 + K_3 h^3 + \cdots = O(h), \qquad (1)$$

with (unknown) constants $K1, K_2, K_3, \cdots$.

Goal: Generate higher order approximations

- **Key**: Equation (1) works for *any* $h \neq 0$.

Extrapolation, Step I

$$M - N_1(h) = K_1 h + K_2 h^2 + K_3 h^3 + \cdots, \quad (2)$$

$$M - N_1(\frac{h}{2}) = K_1(\frac{h}{2}) + K_2(\frac{h}{2})^2 + K_3(\frac{h}{2})^3 + \cdots. \quad (3)$$

(3)$\times$2$-$ (2):

$$\begin{aligned} M - N_2(h) &= -\frac{K_2}{2}h^2 - \frac{3K_3}{4}h^3 - \cdots - (1 - 2^{-(t-1)})K_t h^t - \cdots, \\ &\stackrel{def}{=} \widehat{K}_2 h^2 + \widehat{K}_3 h^3 + \cdots \widehat{K}_t h^t + \cdots = O\left(h^2\right), \end{aligned} \quad (4)$$

$$\text{where} \quad N_2(h) = N_1(\frac{h}{2}) + \left(N_1(\frac{h}{2}) - N_1(h)\right).$$

Equation (4) again power series, but now 2nd order.

Extrapolation, Step II

$$M - N_2(h) \quad = \quad \widehat{K}_2 h^2 + \widehat{K}_3 h^3 + \cdots \widehat{K}_t h^t + \cdots, \qquad (5)$$

$$M - N_2(\frac{h}{2}) \quad = \quad \widehat{K}_2(\frac{h}{2})^2 + \widehat{K}_3(\frac{h}{2})^3 + + \cdots. \qquad (6)$$

$\dfrac{(6)\times 2^2 - (5)}{2^2 - 1}$:

$$M - N_3(h) \quad = \quad -\frac{\widehat{K}_3}{6} h^3 - \cdots - \frac{1 - 2^{-(t-2)}}{3} \widehat{K}_t h^t - \cdots,$$

$$\text{where} \quad N_3(h) \stackrel{def}{=} N_2(\frac{h}{2}) + \frac{N_2(\frac{h}{2}) - N_2(h)}{3}.$$

One more power series, but now 3rd order.

Extrapolation, Step III

- Assume

$$M - N_j(h) = \widehat{K}_j h^j + \widehat{K}_{j+1} h^{j+1} + \cdots \widehat{K}_t h^t + \cdots ,$$

- replace h by $h/2$:

$$M - N_j(\frac{h}{2}) = \widehat{K}_j(\frac{h}{2})^j + \widehat{K}_{j+1}(\frac{h}{2})^{j+1} + \cdots \widehat{K}_t(\frac{h}{2})^t + \cdots .$$

$$\frac{\text{second equation } \times 2^j - \text{ first equation}}{2^j - 1}:$$

$$M - N_{j+1}(h) \quad = \quad -\frac{\widehat{K}_{j+1}}{2(2^j - 1)} h^{j+1} - \cdots = O\left(h^{j+1}\right) ,$$

$$\text{where} \quad N_{j+1}(h) \stackrel{def}{=} N_j(\frac{h}{2}) + \frac{N_j(\frac{h}{2}) - N_j(h)}{2^j - 1}.$$

Richardson's Extrapolation Table

$O(h)$	$O(h^2)$	$O(h^3)$	$O(h^4)$
$N_1(h) \searrow$			
$\rightarrow$			
$N_1(\frac{h}{2}) \searrow$	$N_2(h) \searrow$		
$\rightarrow$	$\rightarrow$		
$N_1(\frac{h}{4}) \searrow$	$N_2(\frac{h}{2}) \searrow$	$N_3(h) \searrow$	
$N_1(\frac{h}{8}) \rightarrow$	$N_2(\frac{h}{4}) \rightarrow$	$N_3(\frac{h}{2}) \rightarrow$	$N_4(h)$

Richardson's Extrapolation: even power series

- **Given**: A formula $N_1(h)$ that approximates an unknown constant M for any $h \neq 0$.
- **Given**: Truncation error satisfies even power series for $h \neq 0$

$$M - N_1(h) = K_1 h^2 + K_2 h^4 + K_3 h^6 + \cdots = O\left(h^2\right), \qquad (7)$$

with (unknown) constants $K1, K_2, K_3, \cdots$.

Goal: Generate higher order approximations

- **Key**: Equation (7) works for *any* $h \neq 0$.

Even power extrapolation, Step I

$$M - N_1(h) = K_1 h^2 + K_2 h^4 + K_3 h^6 + \cdots, \quad (8)$$

$$M - N_1(\frac{h}{2}) = K_1(\frac{h}{2})^2 + K_2(\frac{h}{2})^4 + K_3(\frac{h}{2})^6 + \cdots. \quad (9)$$

$\dfrac{(9)\times 2^2 - (8)}{2^2 - 1}$:

$$\begin{aligned} M - N_2(h) &= -\frac{K_2}{4}h^4 - \frac{5K_3}{16}h^6 - \cdots - \frac{1 - 2^{-2(t-1)}}{3}K_t h^{2t} - \cdots, \\ &\stackrel{def}{=} \widehat{K}_2 h^4 + \widehat{K}_3 h^6 + \cdots \widehat{K}_t h^{2t} + \cdots = O\left(h^4\right), \quad (10) \end{aligned}$$

$$\text{where} \quad N_2(h) = N_1(\frac{h}{2}) + \frac{N_1(\frac{h}{2}) - N_1(h)}{3}.$$

Equation (10) again even power series, but now 4th order.

Even extrapolation, Step II

$$M - N_2(h) = \widehat{K}_2 h^4 + \widehat{K}_3 h^6 + \cdots \widehat{K}_t h^{2t} + \cdots, \qquad (11)$$

$$M - N_2(\frac{h}{2}) = \widehat{K}_2 (\frac{h}{2})^4 + \widehat{K}_3 (\frac{h}{2})^6 + \cdots. \qquad (12)$$

$\dfrac{(12)\times 2^4 - (11)}{2^4 - 1}$:

$$M - N_3(h) = -\frac{\widehat{K}_3}{20} h^6 - \cdots - \frac{1 - 2^{-2(t-2)}}{15} \widehat{K}_t h^{2t} - \cdots,$$

$$\text{where} \quad N_3(h) \stackrel{def}{=} N_2(\frac{h}{2}) + \frac{N_2(\frac{h}{2}) - N_2(h)}{15}.$$

One more even power series, but now 6-th order.

Even extrapolation, Step III

- Assume

$$M - N_j(h) = \widehat{K}_j h^{2j} + \widehat{K}_{j+1} h^{2(j+1)} + \cdots \widehat{K}_t h^{2t} + \cdots,$$

- replace h by $h/2$:

$$M - N_j(\frac{h}{2}) = \widehat{K}_j (\frac{h}{2})^{2j} + \widehat{K}_{j+1} (\frac{h}{2})^{2(j+1)} + \cdots \widehat{K}_t (\frac{h}{2})^{2t} + \cdots.$$

$\dfrac{\text{second equation } \times 4^j - \text{ first equation}}{4^j - 1}$:

$$M - N_{j+1}(h) \quad = \quad -\frac{3\widehat{K}_{j+1}}{4(4^j - 1)} h^{2(j+1)} - \cdots = O\left(h^{2(j+1)}\right),$$

$$\text{where} \quad N_{j+1}(h) \stackrel{def}{=} N_j(\frac{h}{2}) + \frac{N_j(\frac{h}{2}) - N_j(h)}{4^j - 1}.$$

Richardson's Even Extrapolation Table

$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
$N_1(h) \searrow$			
$\rightarrow$			
$N_1(\frac{h}{2}) \searrow$	$N_2(h) \searrow$		
$\rightarrow$	$\rightarrow$		
$N_1(\frac{h}{4}) \searrow$	$N_2(\frac{h}{2}) \searrow$	$N_3(h) \searrow$	
$N_1(\frac{h}{8}) \rightarrow$	$N_2(\frac{h}{4}) \rightarrow$	$N_3(\frac{h}{2}) \rightarrow$	$N_4(h)$

Even extrapolation, example

Consider Taylor expansion for a given function $f(x)$ with $h > 0$:

$$\begin{aligned} f(x+h) &= f(x) + f'(x)\,h + \frac{1}{2} f''(x)\,h^2 + \cdots + \frac{1}{n!} f^{(n)}(x)\,h^n + \cdots\,, \\ f(x-h) &= f(x) - f'(x)\,h + \frac{1}{2} f''(x)\,h^2 + \cdots + \frac{1}{n!} f^{(n)}(x)\,(-h)^n + \cdots\,. \end{aligned}$$

Take the difference:

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + \cdots + \frac{1}{(2t+1)!} f^{(2t+1)}(x)\,h^{2t} + \cdots\,.$$

This is an even power series with 2nd order approximation

$$f'(x), \approx N_1(h) \stackrel{def}{=} \frac{f(x+h) - f(x-h)}{2h}.$$

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Take the difference:

$$\frac{f(x+h)-f(x-h)}{2h} = f'(x) + \cdots + \frac{1}{(2t+1)!}f^{(2t+1)}(x)\,h^{2t} + \cdots\,.$$

This is an even power series with 2nd order approximation

$$f'(x), \approx N_1(h) \stackrel{def}{=} \frac{f(x+h)-f(x-h)}{2h}.$$

4th order approximation

$$\begin{aligned} f'(x) &\approx N_1(h) + \frac{N_1(h)-N_1(2h)}{3} \\ &= \frac{f(x-2h)-8f(x-h)+8f(x+h)-f(x+2h)}{12h}. \end{aligned}$$

Even extrapolation, example

Approximate $f'(2.0)$ with $N_1(0.1)$ and $N_2(0.1)$ for $f(x) = xe^x$.
Solution:

$$f'(x) = (1+x)e^x, \quad \text{therefore} \quad f'(2.0) = 3e^2 \approx 22.167.$$

- $$N_1(0.1) = \frac{f(2.1) - f(1.9)}{2 \times 0.1} \approx 22.229.$$

- $$\begin{aligned} N_1(0.2) &= \frac{f(2.2) - f(1.8)}{2 \times 0.2} \approx 22.414. \\ N_2(0.1) &= N_1(h) + \frac{N_1(h) - N_1(2h)}{3} \approx 22.167. \end{aligned}$$

Numerical Integration: general idea

- **Goal**: Numerical method /quadrature for approximating $\int_a^b f(x)dx$.

Numerical Integration: general idea

- **Goal**: Numerical method /quadrature for approximating $\int_a^b f(x)dx$.
- **Approach**: Replacing $f(x)$ by a polynomial.
  - **Choose**: $n+1$ points $a \le x_0 < x_1 < \cdots < x_n \le b$.
  - **Interpolation**:

$$f(x) = P(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{j=0}^{n} (x - x_j), \quad P(x) = \sum_{j=0}^{n} f(x_j) L_j(x).$$

  - **Approximate Integration**:

$$\begin{aligned}
\int_a^b f(x)dx &= \left(\int_a^b P(x)dx\right) + \frac{1}{(n+1)!} \int_a^b f^{(n+1)}(\xi(x)) \prod_{j=0}^{n} (x - x_j)\, dx \\
&= \left(\sum_{j=0}^{n} a_j\, f(x_j)\right) + \frac{1}{(n+1)!} \int_a^b f^{(n+1)}(\xi(x)) \prod_{j=0}^{n} (x - x_j)\, dx \\
&\approx \sum_{j=0}^{n} a_j\, f(x_j),
\end{aligned}$$

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\int_a^b f(x)dx &= \left(\int_a^b P(x)dx\right) + \frac{1}{(n+1)!} \int_a^b f^{(n+1)}(\xi(x)) \prod_{j=0}^{n} (x - x_j)\, dx \\
&= \left(\sum_{j=0}^{n} a_j\, f(x_j)\right) + \frac{1}{(n+1)!} \int_a^b f^{(n+1)}(\xi(x)) \prod_{j=0}^{n} (x - x_j)\, dx \\
&\approx \sum_{j=0}^{n} a_j\, f(x_j), \quad \text{with} \quad a_j = \int_a^b L_j(x)dx = \int_a^b \prod_{k \ne j} \frac{(x - x_k)}{(x_j - x_k)} dx.
\end{aligned}$$

The Trapezoidal Rule: $n = 1$, $x_0 = a, x_1 = b, h = b - a$.

- **Linear Interpolation**:

$$
\begin{aligned}
P_1(x) &= \frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1), \\
f(x) &= P_1(x) + \frac{1}{2} f''(\xi(x))(x - x_0)(x - x_1).
\end{aligned}
$$

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- **Linear Interpolation**:

$$\begin{aligned} P_1(x) &= \frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1), \\ f(x) &= P_1(x) + \frac{1}{2} f''(\xi(x))(x - x_0)(x - x_1). \end{aligned}$$

- **Quadrature**:

$$\begin{aligned} \int_a^b P_1(x) dx &= \int_a^b \left(\frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1) \right) dx \\ &= \frac{1}{2} \left(\frac{(x - x_1)^2}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)^2}{(x_1 - x_0)} f(x_1) \right)_{x_0}^{x_1} = \frac{h}{2} \left(f(x_0) + f(x_1) \right). \end{aligned}$$

The Trapezoidal Rule: $n = 1$, $x_0 = a, x_1 = b, h = b - a$.

- **Linear Interpolation**:

$$\begin{aligned} P_1(x) &= \frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1), \\ f(x) &= P_1(x) + \frac{1}{2} f''(\xi(x))(x - x_0)(x - x_1). \end{aligned}$$

- **Quadrature**:

$$\int_a^b P_1(x)dx = \int_a^b \left(\frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1) \right) dx$$

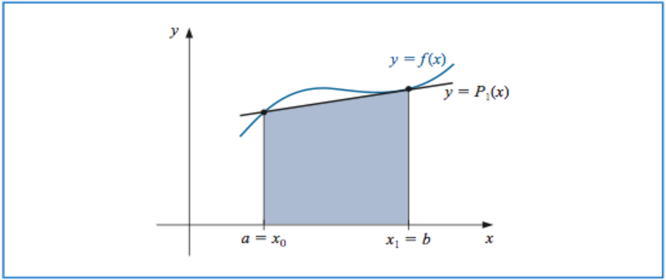
$$= \frac{1}{2} \left(\frac{(x - x_1)^2}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)^2}{(x_1 - x_0)} f(x_1) \right)_{x_0}^{x_1} = \frac{h}{2} \left(f(x_0) + f(x_1) \right).$$

- **Error**:

$$\begin{aligned} \int_a^b \frac{1}{2} f''(\xi(x))(x - x_0)(x - x_1)dx &= \frac{f''(\xi)}{2} \int_a^b (x - x_0)(x - x_1)dx \\ &= -\frac{f''(\xi)}{12} (b - a)^3. \end{aligned}$$

Trapezoidal Rule, $n = 1$, $x_0 = a, x_1 = b$, $h = b - a$

$$\int_a^b f(x)dx = \frac{h}{2}(f(x_0) + f(x_1)) - \frac{h^3}{12} f''(\xi).$$



Simpson's Rule: $n = 2,\ x_0 = a, x_1 = \frac{a+b}{2}, x_2 = b,\ h = \frac{b-a}{2}$.

- **Quadratic Interpolation**:

$$P_2(x_j) = f(x_j), \quad j = 0, 1, 2.$$

$$\begin{aligned} P_2(x) &= \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_1)(x-x_0)}{(x_2-x_1)(x_2-x_0)} f(x_2) \\ &\quad + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1). \end{aligned}$$

Simpson's Rule: $n = 2,\ x_0 = a, x_1 = \frac{a+b}{2}, x_2 = b,\ h = \frac{b-a}{2}.$

- **Quadrature Rule**

$$\int_a^b P_2(x)dx = f(x_0)\int_a^b \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}\,dx + f(x_2)\int_a^b \frac{(x-x_1)(x-x_0)}{(x_2-x_1)(x_2-x_0)}\,dx$$

$$+f(x_1)\int_a^b \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}\,dx.$$

Simpson's Rule:

$$f(x) = P_2(x) + \frac{1}{3!} f^{(3)}(\xi(x))(x - x_0)(x - x_1)(x - x_2).$$

- **Quadrature Error**:

$$\frac{1}{3!}\int_a^b f^{(3)}(\xi(x))(x - x_0)(x - x_1)(x - x_2)\,dx$$
$$= \frac{f^{(3)}(\xi)}{6}\int_a^b (x - x_0)(x - x_1)(x - x_2)\,dx$$
$$\overset{??}{=} 0.$$

Error estimate wrong. Need better approach.

Simpson's Rule: $n = 3$, $x_0 = a, x_1 = \frac{a+b}{2}, x_2 = b$, $h = \frac{b-a}{2}$.

- **Cubic Interpolation**, x_1 is double node:

$$P_3(x_j) = f(x_j), \quad j = 0, 1, 2; \quad P_3'(x_1) = f'(x_1).$$

$$\begin{aligned} P_3(x) \quad = \quad & \frac{(x - x_1)^2(x - x_2)}{(x_0 - x_1)^2(x_0 - x_2)} f(x_0) + \frac{(x - x_1)^2(x - x_0)}{(x_2 - x_1)^2(x_2 - x_0)} f(x_2) \\ & + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} \left(1 - \frac{(x - x_1)(2x_1 - x_0 - x_2)}{(x_1 - x_0)(x_1 - x_2)}\right) f(x_1) \\ & + \frac{(x - x_0)(x - x_1)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f'(x_1). \end{aligned}$$

Simpson's Rule: $n = 3,\ x_0 = a, x_1 = \frac{a+b}{2}, x_2 = b,\ h = \frac{b-a}{2}.$

- **Quadrature Rule**

$$\int_a^b P_3(x)dx = f(x_0)\int_a^b \frac{(x-x_1)^2(x-x_2)}{(x_0-x_1)^2(x_0-x_2)}\,dx + f(x_2)\int_a^b \frac{(x-x_1)^2(x-x_0)}{(x_2-x_1)^2(x_2-x_0)}\,dx$$

$$+f(x_1)\int_a^b \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}\left(1 - \frac{(x-x_1)(2x_1-x_0-x_2)}{(x_1-x_0)(x_1-x_2)}\right)\,dx$$

$$+f'(x_1)\int_a^b \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_1-x_0)(x_1-x_2)}\,dx$$

Simpson's Rule: $n = 3$, $x_0 = a, x_1 = \frac{a+b}{2}, x_2 = b$, $h = \frac{b-a}{2}$.

- **Quadrature Rule**

$$\int_a^b P_3(x)dx = f(x_0)\int_a^b \frac{(x-x_1)^2(x-x_2)}{(x_0-x_1)^2(x_0-x_2)}\,dx + f(x_2)\int_a^b \frac{(x-x_1)^2(x-x_0)}{(x_2-x_1)^2(x_2-x_0)}\,dx$$

$$+f(x_1)\int_a^b \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}\left(1-\frac{(x-x_1)(2x_1-x_0-x_2)}{(x_1-x_0)(x_1-x_2)}\right)\,dx$$

$$+f'(x_1)\int_a^b \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_1-x_0)(x_1-x_2)}\,dx$$

$$= \frac{h}{3}\left(f(x_0) + 4f(x_1) + f(x_2)\right).$$

Stroke of luck: $f'(x_1)$ does not appear in quadrature

Simpson's Rule:

$$f(x) = P_3(x) + \frac{1}{4!} f^{(4)}(\xi(x))(x - x_0)(x - x_1)^2(x - x_2).$$

- **Quadrature Rule**:

$$\begin{aligned}\int_a^b f(x)\,dx &= \int_a^b P_3(x)\,dx + \frac{1}{4!}\int_a^b f^{(4)}(\xi(x))(x-x_0)(x-x_1)^2(x-x_2)\,dx \\ &= \frac{h}{3}\left(f(x_0) + 4f(x_1) + f(x_2)\right) \\ &\quad + \frac{1}{4!}\int_a^b f^{(4)}(\xi(x))(x-x_0)(x-x_1)^2(x-x_2)\,dx \\ &\approx \frac{h}{3}\left(f(x_0) + 4f(x_1) + f(x_2)\right).\end{aligned}$$

- **Quadrature Error**:

$$\begin{aligned}&\frac{1}{4!}\int_a^b f^{(4)}(\xi(x))(x-x_0)(x-x_1)^2(x-x_2)\,dx \\ &= \frac{f^{(4)}(\xi)}{24}\int_a^b (x-x_0)(x-x_1)^2(x-x_2)\,dx = -\frac{f^{(4)}(\xi)}{90}\,h^5.\end{aligned}$$