

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 $h \neq 0$

$$M - N_1(h) = K_1h + K_2h^2 + K_3h^3 + \dots = O(h), \quad (1)$$

with (unknown) constants K_1, K_2, K_3, \dots .

Goal: Generate higher order approximations

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

Extrapolation, Step I

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

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

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

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

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

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

Extrapolation, Step II

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

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

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

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

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

One more power series, but now 3rd order.

Extrapolation, Step III

- ▶ Assume

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

- ▶ replace h by $h/2$:

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

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

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

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

Richardson's Extrapolation Table

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

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 $h \neq 0$

$$M - N_1(h) = K_1 h^2 + K_2 h^4 + K_3 h^6 + \dots = O(h^2), \quad (7)$$

with (unknown) constants K_1, K_2, K_3, \dots .

Goal: Generate higher order approximations

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

Even power extrapolation, Step I

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

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

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

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

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

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

Evan extrapolation, Step II

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

$$M - N_2\left(\frac{h}{2}\right) = \widehat{K}_2 \left(\frac{h}{2}\right)^4 + \widehat{K}_3 \left(\frac{h}{2}\right)^6 + \dots. \quad (12)$$

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

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

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

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

Evan extrapolation, Step III

- ▶ Assume

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

- ▶ replace h by $h/2$:

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

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

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

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

Richardson's Evan Extrapolation Table

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

Evan extrapolation, example

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

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

Take the difference:

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

This is an even power series with 2nd order approximation

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

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$$f(x-h) = f(x) - f'(x)h + \frac{1}{2}f''(x)h^2 + \dots + \frac{1}{n!}f^{(n)}(x)(-h)^n + \dots.$$

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

4th order approximation

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

Evan extrapolation, example

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

Solution:

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



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



$$N_1(0.2) = \frac{f(2.2) - f(1.8)}{2 \times 0.2} \approx 22.414.$$

$$N_2(0.1) = N_1(h) + \frac{N_1(h) - N_1(2h)}{3} \approx 22.167.$$

Numerical Integration: general idea

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- ▶ **Approach:** Replacing $f(x)$ by a polynomial.
 - ▶ **Choose:** $n + 1$ points $a \leq x_0 < x_1 < \dots < x_n \leq b$.
 - ▶ **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:**

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

Numerical Integration: general idea

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

► **Linear Interpolation:**

$$P_1(x) = \frac{(x - x_1)}{(x_0 - x_1)}f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)}f(x_1),$$

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

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

► **Quadrature:**

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

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► Linear Interpolation:

$$P_1(x) = \frac{(x - x_1)}{(x_0 - x_1)}f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)}f(x_1),$$

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► Quadrature:

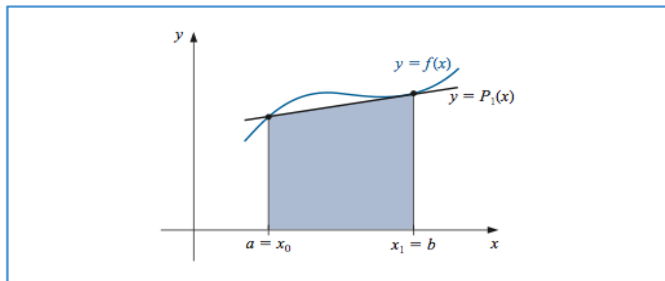
$$\begin{aligned}\int_a^b P_1(x)dx &= \int_a^b \left(\frac{(x - x_1)}{(x_0 - x_1)}f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)}f(x_1) \right) dx \\ &= \frac{1}{2} \left(\frac{(x - x_1)^2}{(x_0 - x_1)}f(x_0) + \frac{(x - x_0)^2}{(x_1 - x_0)}f(x_1) \right)_{x_0}^{x_1} = \frac{1}{2} (f(x_0) + f(x_1)).\end{aligned}$$

► 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:**

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

$$P_2(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_1)(x - x_0)}{(x_2 - x_1)(x_2 - x_0)} f(x_2) \\ + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1).$$

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:**

$$\begin{aligned} & \frac{1}{3!} \int_a^b f^{(3)}(\xi(x))(x - x_0)(x - x_1)(x - x_2) dx \\ &= \frac{f^{(3)}(\xi)}{6} \int_a^b (x - x_0)(x - x_1)(x - x_2) dx \\ &\stackrel{??}{=} 0. \end{aligned}$$

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:

$$P_3(x_j) = f(x_j), \quad j = 0, 1, 2; \quad P'_3(x_1) = f'(x_1).$$

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

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

► Quadrature Rule

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

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

► **Quadrature Rule**

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

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:

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

► Quadrature Error:

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

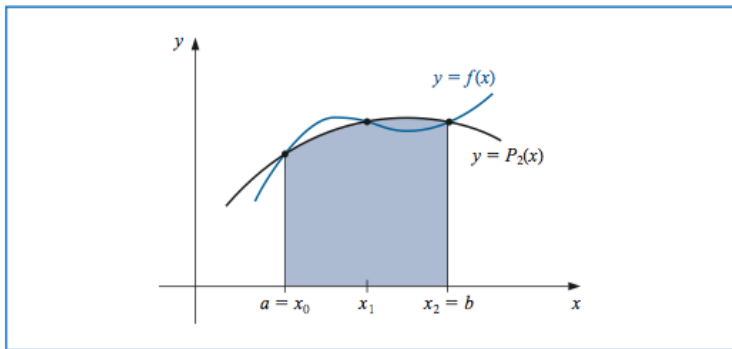
Simpson's Rule: $n = 3$, $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$, $h = \frac{b-a}{2}$.

$$\int_a^b f(x)dx = \frac{h}{3} (f(x_0) + 4f(x_1) + f(x_2)) - \frac{f^{(4)}(\xi)}{90} h^5.$$



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

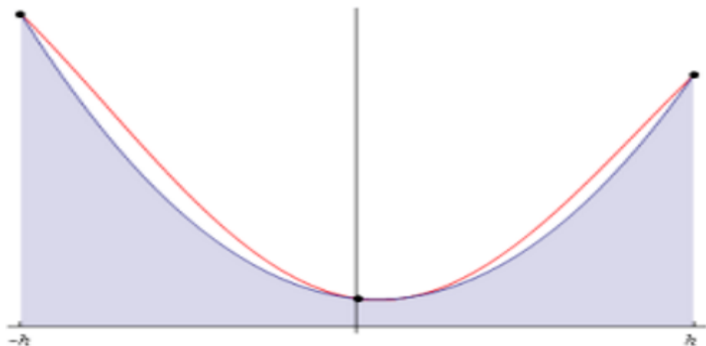
$$\int_a^b f(x) dx = \frac{h}{3} (f(x_0) + 4f(x_1) + f(x_2)) - \frac{f^{(4)}(\xi)}{90} h^5.$$



Wrong: slopes differ at midpoint.

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

$$\int_a^b f(x) dx = \frac{h}{3} (f(x_0) + 4f(x_1) + f(x_2)) - \frac{f^{(4)}(\xi)}{90} h^5.$$



Right: slopes match at midpoint.

Example: approximate $\int_0^2 f(x)dx$: Simpson wins

| | (a) | (b) | (c) | (d) | (e) | (f) |
|-------------|-------|--------|--------------|----------------|----------|-------|
| $f(x)$ | x^2 | x^4 | $(x+1)^{-1}$ | $\sqrt{1+x^2}$ | $\sin x$ | e^x |
| Exact value | 2.667 | 6.400 | 1.099 | 2.958 | 1.416 | 6.389 |
| Trapezoidal | 4.000 | 16.000 | 1.333 | 3.326 | 0.909 | 8.389 |
| Simpson's | 2.667 | 6.667 | 1.111 | 2.964 | 1.425 | 6.421 |

Degree of precision

- ▶ **Degree of precision:** the largest positive integer n such that quadrature formula is exact for x_k , for each $k = 0, 1, \dots, n$.

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DoP = 1 for Trapezoidal Rule, **DoP** = 3 for Simpson.