Numerical Integration

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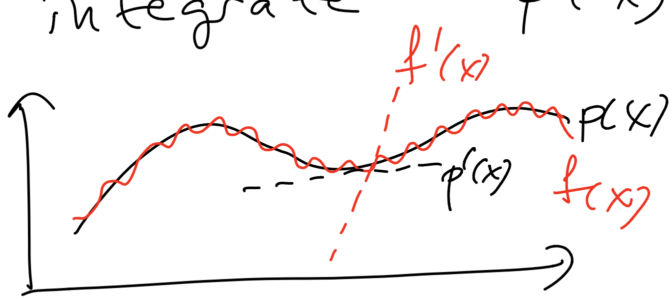
$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt$$

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

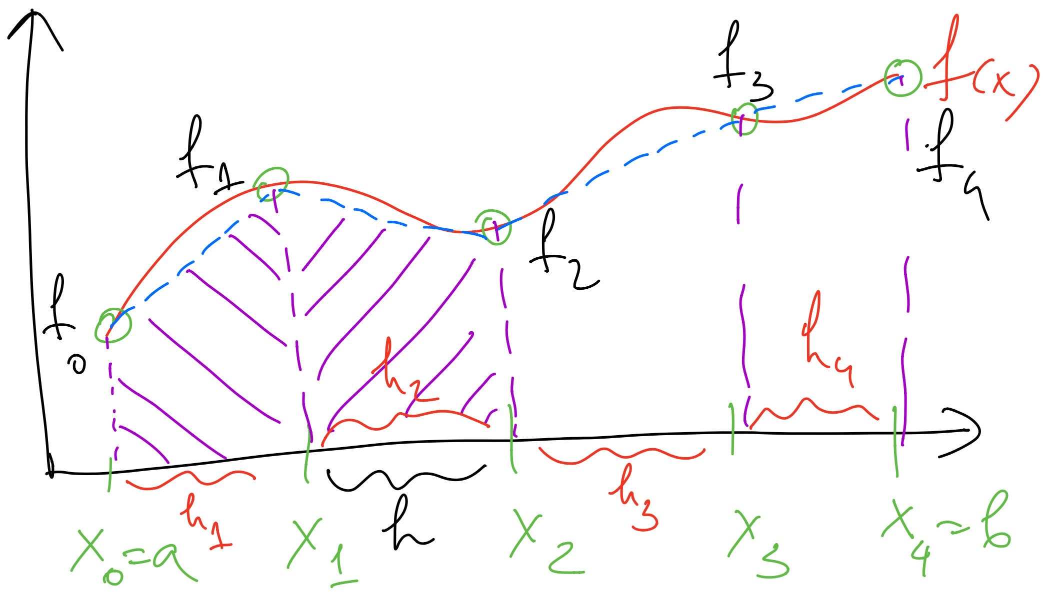
quadrature

Idea:

Approximate $f(x)$ by $p(x)$, and integrate $p(x)$ instead



E.g. Piecewise linear interp.



$$\begin{cases} x_k = a + k \cdot h \,, & k = 0, \dots, n \\ h = \dfrac{b-a}{n} \,, & f_k = f(x_k) \end{cases}$$

Area under $f \simeq$ Sum of areas of four trapezoids

$$I \simeq \cancel{h} \cdot \left(\frac{f_0 + f_1}{2} h_1 + \frac{f_1 + f_2}{2} h_2 + \frac{f_2 + f_3}{2} h_3 + \frac{f_3 + f_4}{2} h_4 \right)$$

$$I \simeq h\left(\frac{f_0+f_n}{2}+\sum_{j=1}^{n-1} f_j\right)$$

$$I = \int_a^b f(x)\,dx \approx h \cdot \sum_{j=0}^{n} f(x_j)$$

Don't forget this

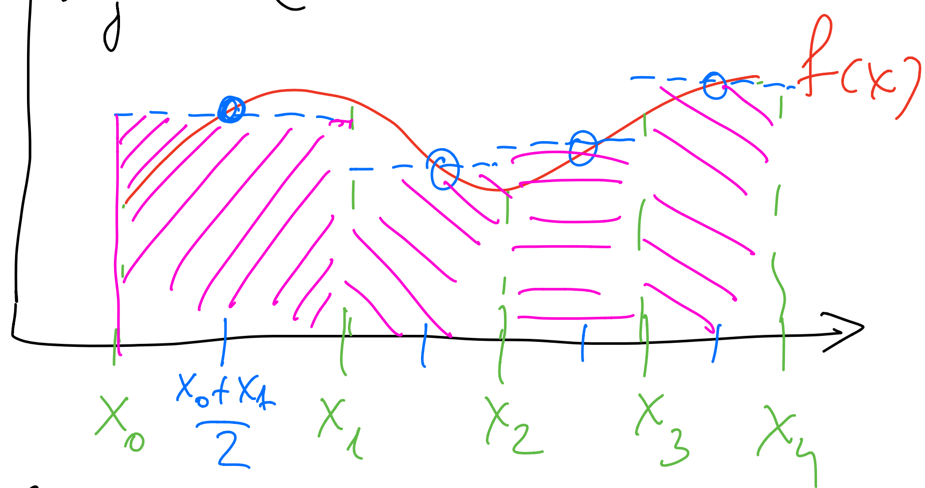
$$\boxed{-\frac{h}{2}\,\frac{f(x_0)+f(x_n)}{2}}$$

Composite trapezoidal rule

Composite midpoint rule

Piecewise constant interpolation

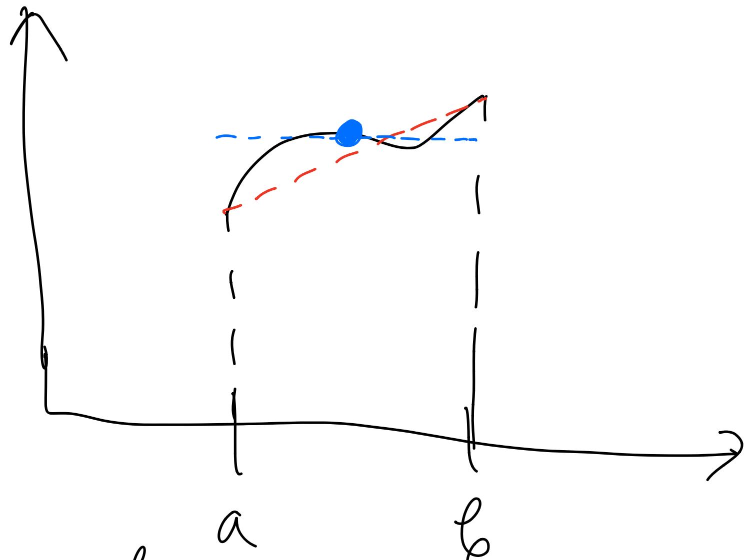
$$x_j = a + (j - 1/2)h$$



$$\int_a^b f(x)\,dx = \int_a^{x_1} f\,dx + \int_{x_1}^{x_2} f\,dx + \int_{x_2}^{x_3} f\,dx + \int_{x_3}^{x_4} f\,dx$$

$$I = h \sum_{j=1}^{n} f(x_j)$$

Composite midpoint rule



error? $\int_a^b f(x)\,dx \simeq \frac{f(a)+f(b)}{2}\cdot(b-a)$

① Taylor series

For midpoint $\quad X_{mid} = \frac{a+b}{2}$

$$f(x) \simeq f(X_{mid}) + f'(X_{mid})(x - X_{mid}) + \frac{1}{2} f''(\xi(x))(x - x_{mid})^2$$

ξ between x and X_{mid}

Do this at home

$$\mathcal{E} = \int_{x-h/2}^{x+h/2} f(t)\,dt - \underbrace{f(x)\cdot h}_{\text{midpoint}}$$

$$= \frac{h^3}{24} f''(\xi)$$

$$\xi \in \left[x-\frac{h}{2}, x+\frac{h}{2}\right)$$

#2 Use formula for error of polynomial interpolant for trapezoidal rule

$$\mathcal{E}_1(x) = f(x) - P_1(x) = \frac{1}{2} f''(\xi(x))(x-a)(x-b)$$

linear interpolant $\quad \xi(x) \in [a, b]$

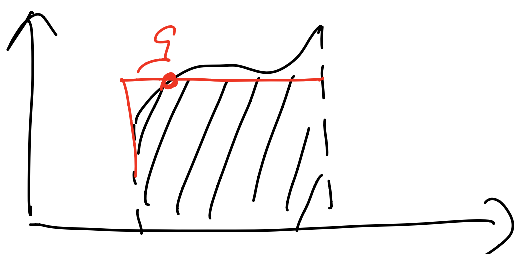
$$\mathcal{E} = \int f(x)\,dx - \underbrace{\int p_1(x)\,dx}_{\text{trapezeidal rule}} =$$

$$\mathcal{E} = \int_a^b \mathcal{E}_1(x)\,dx = \frac{1}{2}\int_a^b f''(\xi(x))(x-a)(x-b)\,dx$$

ξ

Mean-value theorem for integrals

continuous $\rightarrow$ $\int_a^b f(x)\,dx = f(\xi)(b-a)$



$$\mathcal{E} = \frac{f''(\xi)}{2}\int_{x=a}^{b}(x-a)(x-b)\,dx, \quad \xi \in [a,b]$$

$$\begin{cases} \mathcal{E}_{trap} = -\dfrac{h^3}{12} f''(\xi) \\ \qquad\qquad\qquad\qquad\qquad \xi \in [a,b] \\ \mathcal{E}_{mid} = \dfrac{h^3}{24} f''(\xi) \end{cases}$$

$$\mathcal{E}_{mid/trap} \sim O(h^3) \cdot f''(\xi)$$

<u>Composite rule error</u>

$$\left| I - I_{trap} \right| \leq \left| \sum_{k=1}^{n} \frac{h^3}{12} f''(\xi_k) \right|$$

$$\xi_k \in [x_{k-1}, x_k]$$

$$\left| f''(x) \right| < M, \quad x \in [a,b]$$

$$|I - I_{trap}| < \frac{M}{12} h^3 \cdot n$$

$$= \frac{M}{12} h^{\cancel{3}\,2} \cdot \frac{b-a}{\cancel{h}}$$

$$\mathcal{E}_{\text{comp. trap}} \leq \frac{h^2}{12} \cdot M = O(h^2)$$

Same for composite midpoint.

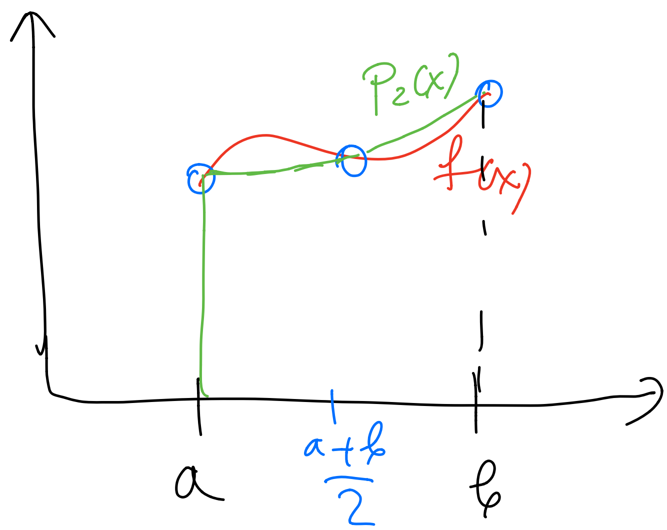
Composite midpoint / trapezoidal rule are second-order accurate

$$\varepsilon \sim \frac{1}{n^2}$$

$$\begin{cases} n \to 2n \\ \mathcal{E} \to \frac{\mathcal{E}}{4} \end{cases}$$

Warning: This is an <u>overestimate</u>
See Euler-MacLaurin theorem (trap. rule)

More accurate: Piecewise quadratic interpolation

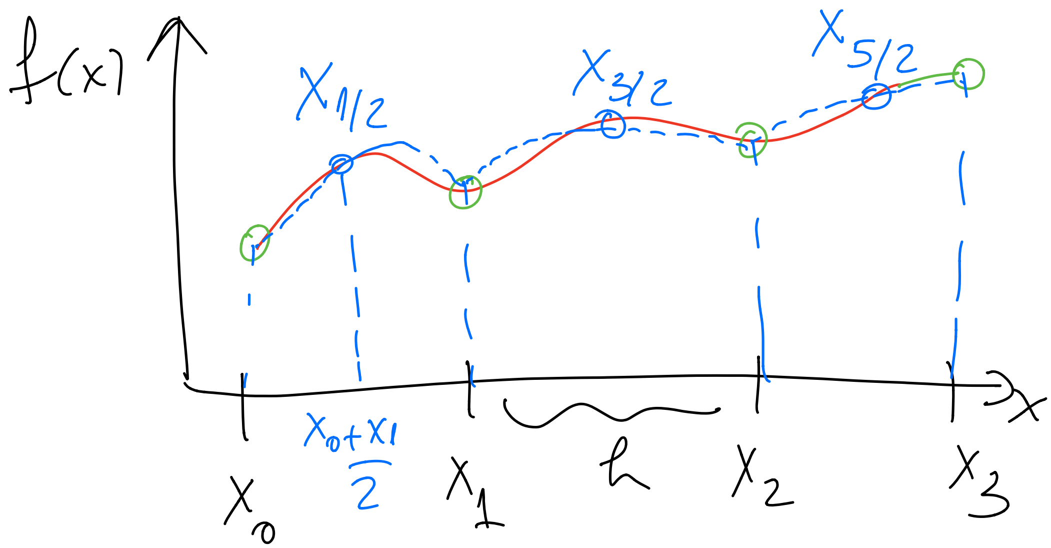


$$\int_a^b f(x)\,dx \approx \int_a^b P_2(x)\,dx$$

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6}\left[f(a)+f(b)+4f\left(\frac{a+b}{2}\right)\right]$$

Simpson's rule

Composite Simpson's rule



$$I = \frac{h}{6}\left[f_0 + f_1 + 4 f_{1/2}\right] + \frac{h}{6}\left[f_1 + f_2 + 4 f_{3/2}\right] + \frac{h}{6}\left[f_2 + f_3 + 4 f_{5/2}\right]$$

$$= \frac{h}{6}\left[f_0 + 4 f_{1/2} + 2 f_1 + 4 f_{3/2}\right.$$

$$+2f_2+4f_{5/2}+f_3]$$

$$\int_a^b f(x)\,dx \approx \frac{h}{6}\left[f(a)+f(b)\right]$$

$$+\frac{h}{3}\sum_{k=1}^{n-1} f(x_k)$$

$$+\frac{2h}{3}\sum_{k=0}^{n-1} f(x_{k+1/2})$$

Composite Simpson's rule

$$\mathcal{E}_{\substack{comp\\Simp}} = \frac{b-a}{2880}\, h^4 \cdot M$$

$$M = \max_{a\le x\le b} |f^{(4)}(x)|$$

$$\mathcal{E}_{comp.\ simp.} = O(h^4)$$

A method is p^{th} order accurate iff it is <u>exact</u> for polynomials of degree (at least) up to $p-1$

Use this to:

1) validate / test formulas

2) derive formulas faster

$$\int_a^b P_2(x)\,dx = w_1 f(a) + w_2 \cdot f\left(\frac{a+b}{2}\right) + w_3 \cdot f(b)$$

unknown weights

$\forall\ P(x) \in \mathcal{P}_2$

Formula is exact for $\{1, x, x^2\}$

(understand why)

$$\int_a^b 1\,dx = w_1 + w_2 + w_3 = b - a$$

$$\int_a^b x\,dx = w_1 a + w_2 \frac{a+b}{2} + w_3 b$$

$$= \frac{b^2 - a^2}{2}$$

$$\int_a^b x^2\,dx = \frac{b^3 - a^3}{3} = w_1 a^2 + w_2 \left(\frac{a+b}{2}\right)^2$$

$$+ w_3 b^2$$

3 linear eqs for 3 unknowns

w_1, w_2, w_3

Solution is $w_1 = w_3 = \dfrac{b-a}{6}$

$$w_2 = \frac{4}{6}(b-a)$$