

Applied Math

Quadrature

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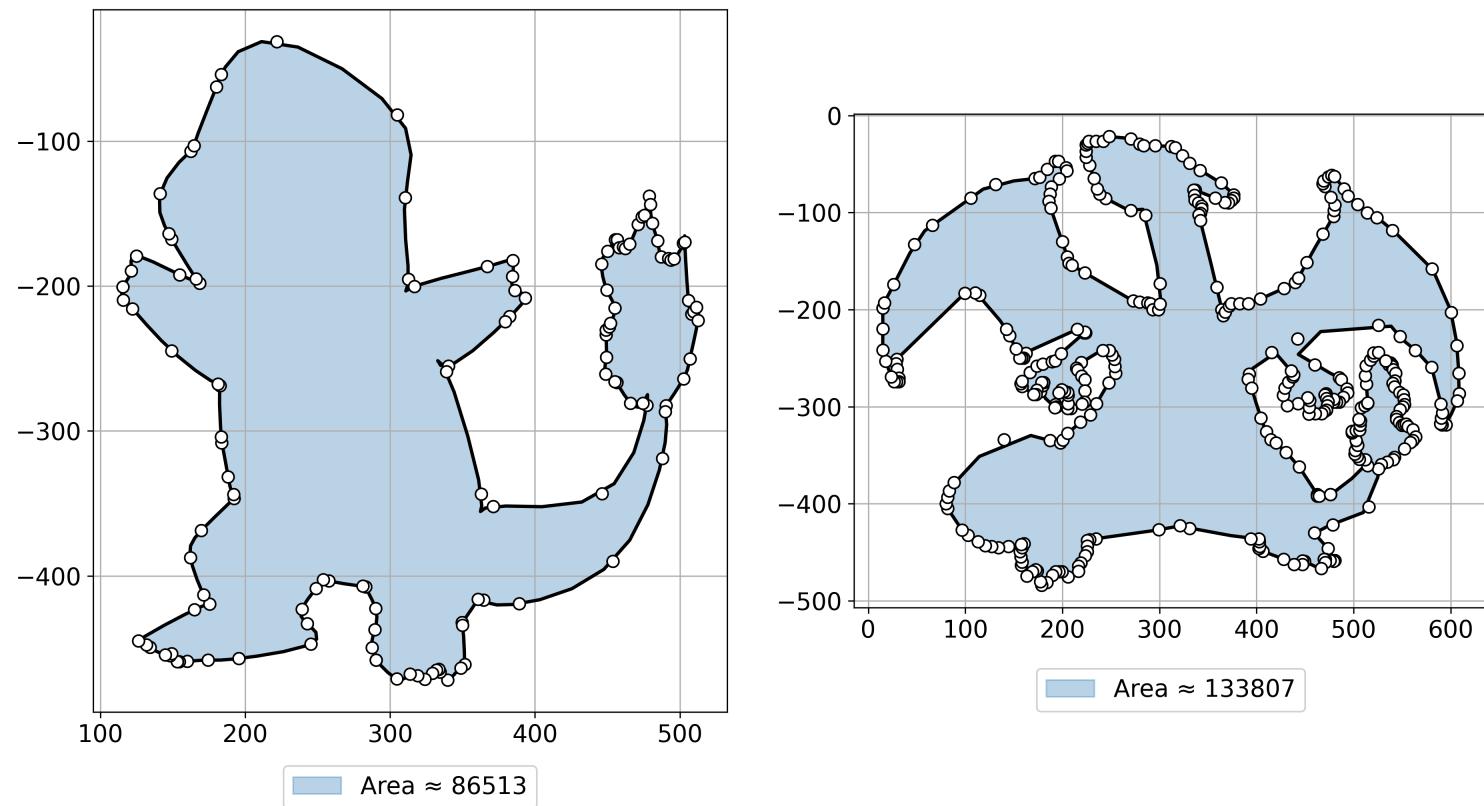
Outline

- Introduction
- Integration Problem
- Numerical Quadrature
 - Midpoint Rule
 - Trapezoidal Rule
 - Simpson's Rule
- Composite Formulae
- Method of Undetermined Coefficients
- Newton-Cotes Formulae
- Hermite quadrature
- Clenshaw-Curtis quadrature
- Gaussian quadrature

Motivations

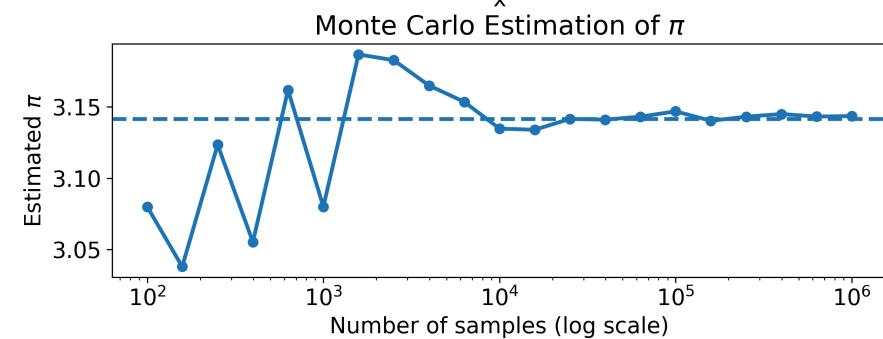
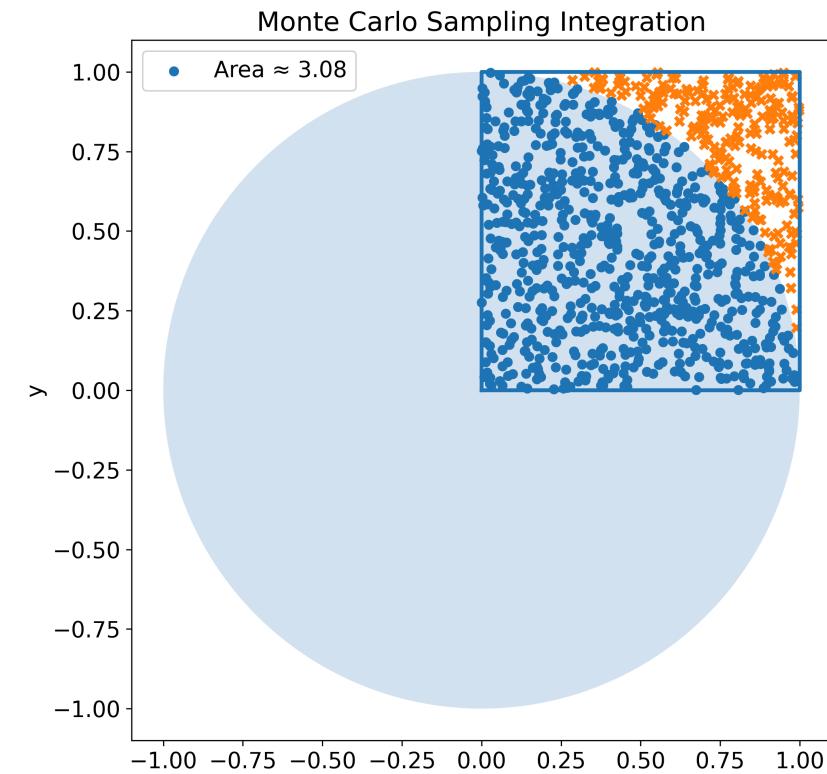
- **No closed-form integrals:**
 - many functions cannot be integrated analytically.
- **Data-defined functions:**
 - integrating noisy, sampled, or simulation-based expressions.
- **Efficient approximations:**
 - needed in loops, solvers, and real-time systems.
- **Arbitrary domains:**
 - handles curves, surfaces, and multidimensional regions.
- **Core to numerical PDEs solvers:**
 - FEM, spectral, and variational methods rely on repeated integrals.
- **Uncertainty quantification:**
 - Computes expectations and probabilistic integrals.

Real motivations



Methodologies and Challenges

1. Deterministic Quadrature: fixed rules with known nodes and weights (Newton–Cotes, Gaussian, Clenshaw–Curtis)
2. Adaptive Quadrature: refines the grid where the integrand is difficult (Adaptive Simpson)
3. Monte Carlo Quadrature: Random sampling-based integration (Monte Carlo, Quasi–Monte Carlo, Importance sampling)
4. Sparse Grids and High-Dimensional Quadrature: extending 1d setting to higher dimensions with fewer points (Smolyak quadrature, Sparse Gauss)



Integration problem

Given a function $f : \mathbb{R} \rightarrow \mathbb{R}$ we want to approximate the definite integral over the interval $[a, b]$

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

From the partition $a = x_0 < x_1 < \dots < x_{n-1} < x_n = b$, $I(f)$ is defined as the limit of **Riemann** sums

$$R_n = \sum_{i=0}^{n-1} (x_{i+1} - x_i) f(\xi_i), \quad \text{and} \quad \xi_i \in [x_i, x_{i+1}], \text{ for } i = 0, \dots, n-1.$$

- If $h_n = \max_{i=0}^{n-1} x_{i+1} - x_i$, for any choice of x_i such that $h_n \xrightarrow{n \rightarrow \infty} 0$ and ξ_i , we have a finite limit $\lim_{n \rightarrow \infty} R_n = R$, and f is said to be Riemann integrable on $[a, b]$.
- One could use a finite Riemann sum with large n to achieve the desired accuracy.
~~> if x_i and ξ_i are not carefully chosen, it requires too many evaluations of the integrand function f .
- We seek efficient methods which are highly accurate and low cost (number of function evaluations).
- More general concepts of integration (Lebesgue) but unsuitable for numerical computation.

Existence, Uniqueness and Stability

- If $f : \mathbb{R} \rightarrow \mathbb{R}$ is bounded and continuous a.e. on $[a, b]$, then the Riemann integral $I(f)$ exists.
 - This sufficient condition is also necessary, so unbounded functions are not Riemann integrable.
- Since all the Riemann sums must have the same limit, the Riemann integral is **unique** by definition.

The **conditioning** of an integration problem is the sensitivity to perturbations in f and $[a, b]$.

- Consider \tilde{f} is a perturbation f , defining the ∞ -norm as $\|f\|_\infty = \max_{x \in [a, b]} |f(x)|$, we have

$$|I(\tilde{f}) - I(f)| = \left| \int_a^b (\tilde{f}(x) - f(x)) dx \right| \leq \int_a^b |\tilde{f}(x) - f(x)| dx \leq (b - a) \|\tilde{f} - f\|_\infty$$

- Consider a perturbation $\tilde{b} > b$, then we have

$$\left| \int_a^{\tilde{b}} f(x) dx - \int_a^b f(x) dx \right| = \left| \int_b^{\tilde{b}} f(x) dx \right| \leq (\tilde{b} - b) \max_{[-b, \tilde{b}]} |f(x)|.$$

⤳ the **absolute condition number** is at most $\tilde{b} - b$, realized when $\tilde{f}(x) = f(x) + c$.

⤳ integration is inherently **well-conditioned** because of averaging or smoothing process.

Numerical Quadrature

Idea. Find the antiderivative F of f , i.e. $F'(x) = f(x)$, and use FTC to evaluate $I(f) = F(b) - F(a)$.
~~ some integrals have no closed form, e.g. $f(x) = \exp(-x^2)$, and others are complicated to evaluate.

- The numerical approximation of definite integrals is known as **numerical quadrature** (different from numerical integration of ODEs), approximating areas of irregular/curved figures with small squares.

Goal. We approximate the integral by a weighted sum by w_i of **integrand values** $f(x_i)$ (known or to evaluate) at a finite number n of sample points x_i (fixed or adaptive) in the interval of integration $[a, b]$.

The integral $I(f)$ is approximated by an $n + 1$ -point **quadrature rule**, which has the form

$$I_n(f) = \sum_{i=0}^n w_i f(x_i),$$

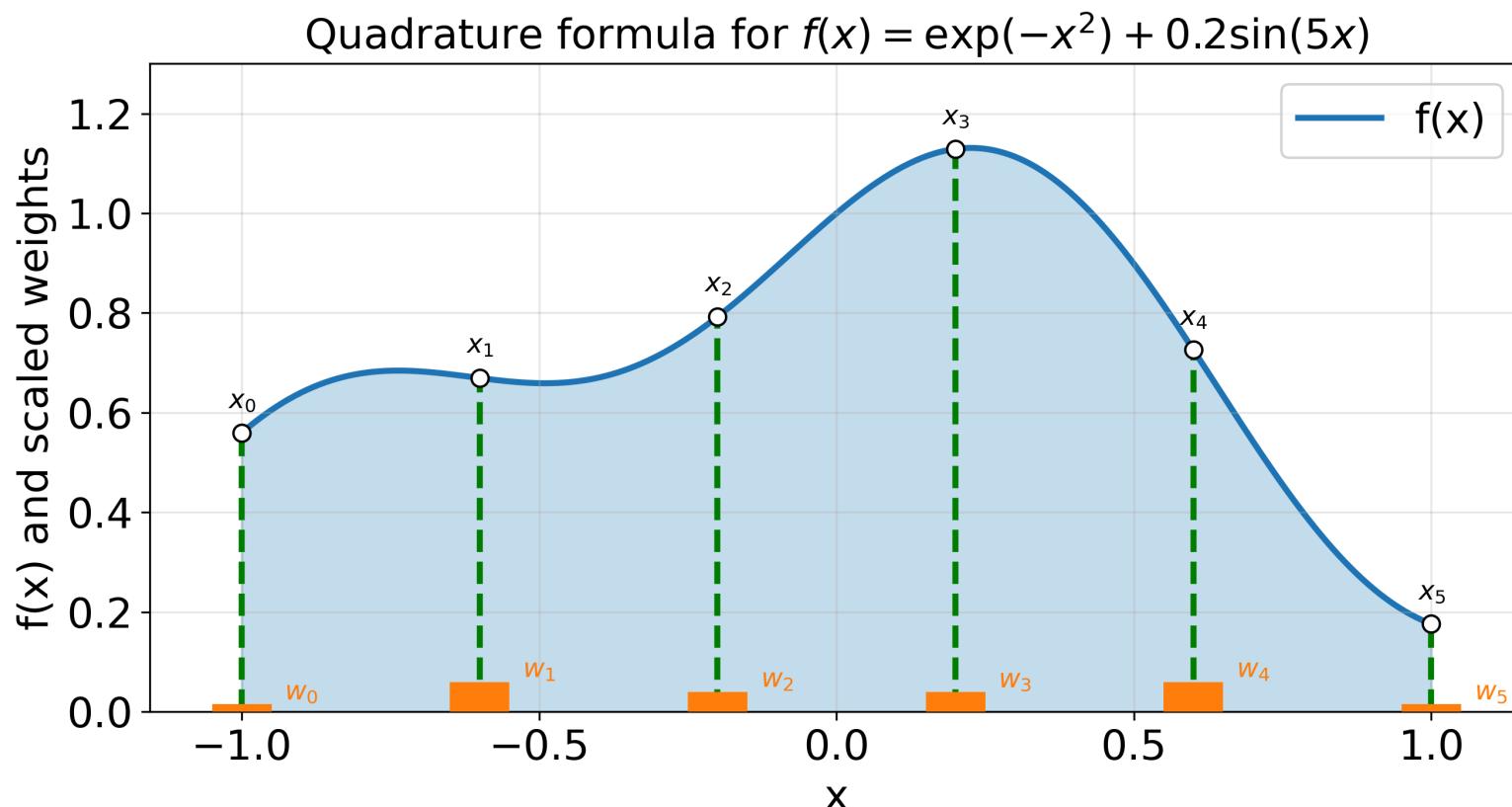
and the error of the quadrature formula is defined as $E_n = I - I_n$.

- How should sample points be chosen?
- How should their contributions be weighted?

Numerical example

Integrate the function $f(x)$ with 6 nodes and chosen weights $\{w_i\}_{i=0}^5$ via the quadrature formula

$$I_5(f) = \sum_{i=0}^5 w_i f(x_i) = w_0 f(x_0) + w_1 f(x_1) + \cdots + w_5 f(x_5)$$



Interpolatory quadrature rules

Idea. Replace the integrand function f , with an easier function f_n to integrate, s.t. $I_n(f) \doteq I(f_n)$.
~~~ the interpolating Lagrange polynomial  $f_n = \Pi_n f$  over a set of  $n + 1$  nodes  $\{x_i\}_{i=0}^n$ , obtaining

$$I_n(f) = \sum_{i=0}^n f(x_i) \int_a^b l_i(x) dx,$$

where we directly define the weights from the characteristic polynomials as  $w_i = \int_a^b l_i(x) dx$ .

The **degree of exactness** of a quadrature rule is the maximum  $r \geq 0$  for which  $I_n(f) = I(f), \forall f \in \mathbb{P}_r$ .

- Any interpolatory quadrature rule that with  $n + 1$  distinct nodes has at least  $n$  degree of exactness.
  - Indeed, if  $f \in \mathbb{P}_n$ , then  $\Pi_n f = f$  implies  $I_n(\Pi_n f) = I(f)$ .
- A quadrature rule with  $n + 1$  distinct nodes and degree of exactness  $\geq n$  is necessarily interpolatory.

## Midpoint or Rectangle formula

Replacing  $f$  over  $[a, b]$  with the constant function  $f_0 = \Pi_0 f = f(x_0)$ ,  
that is  $f$  at the midpoint of  $[a, b]$

$$I_0(f) = (b - a)f\left(\frac{a + b}{2}\right), \quad \text{where } w_0 = b - a, \text{ and } x_0 = \frac{a + b}{2}.$$

If  $f \in C^2([a, b])$ , expanding it with Taylor at the 2-order around  $x_0$

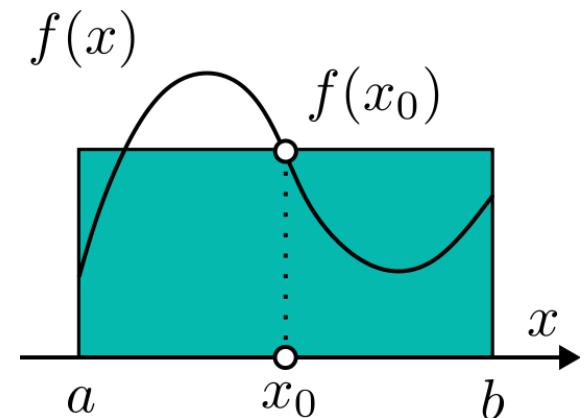
$$f(x) = f(x_0) + f'(x_0)(x - x_0) + f''(\eta(x))(x - x_0)^2/2,$$

thus, integrating on  $[a, b]$  and using the integral mean-value theorem we get

$$E_0(f) = \frac{h^3}{3}f''(\xi), \quad \text{where } h = \frac{b - a}{2}, \text{ and } \xi \in (a, b).$$

~ mid-point rule is exact for constant and affine functions, since

$f''(\xi) = 0, \forall \xi \in (a, b)$ , so that  $r = 1$ .



## Composite midpoint formula

If the width of the integration interval  $[a, b]$  is not sufficiently small, the quadrature error can be quite large.

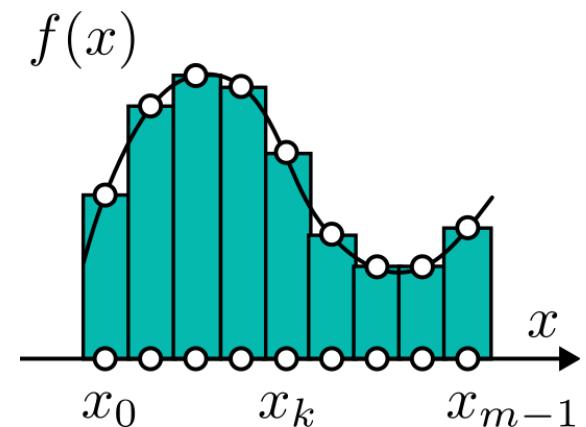
**Idea.** Replace the integrand  $f$  with its piecewise Lagrange polynomial  $\Pi_0^p f$  and obtain a **composite** formula over a partition of the interval.

~~ consider  $m \geq 1$  subintervals of width  $H = (b - a)/m$ , and quadrature nodes  $x_k = a + (2k + 1)H/2$  for  $k = 0, \dots, m - 1$ , we get

$$I_{0,m}(f) = H \sum_{k=0}^{m-1} f(x_k), \quad \text{with} \quad E_{0,m}(f) = \frac{b-a}{24} H^2 f''(\xi)$$

where  $f \in C^2([a, b])$ ,  $H = \frac{b-a}{m}$  and  $\xi \in (a, b)$ .

~~ the degree of exactness is  $r = 1$ .



## Numerical example

Use the midpoint rule with constant  $n = 0$   
interpolant of the function  $f(x) = xe^{2x}$  with 1 node

$$I(f) = \int_0^4 xe^{2x} dx.$$

- Exact value

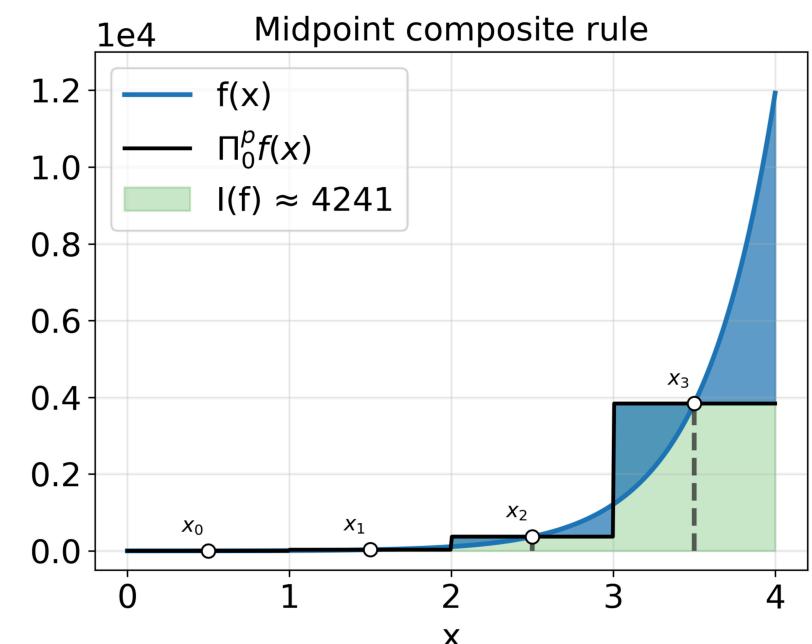
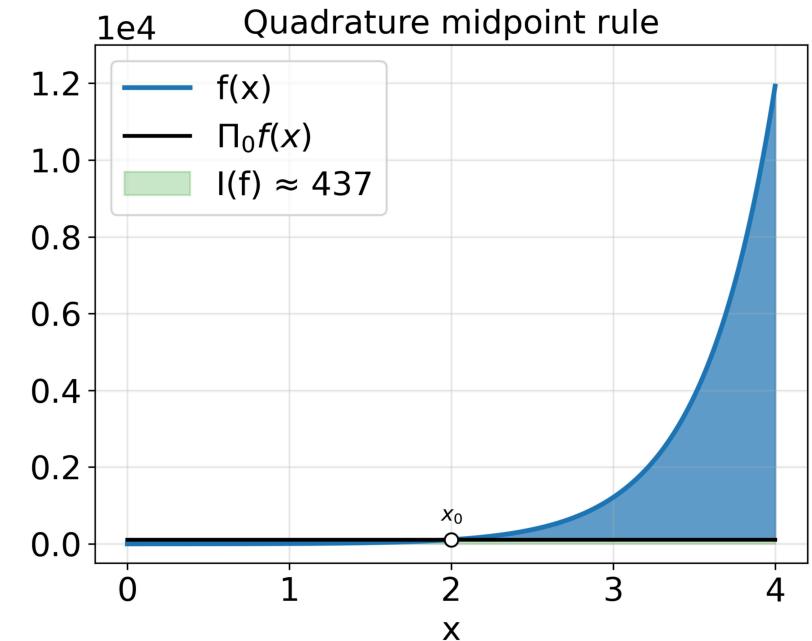
$$\int_0^4 xe^{2x} dx = \left[ \frac{x}{2} e^{2x} - \frac{1}{4} e^{2x} \right]_0^4 = \frac{1}{4} (7e^8 - 1) = 5217$$

- Midpoint rule

$$I(f) \approx (4 - 0)f\left(\frac{4 - 0}{2}\right) = 8e^4 = 437$$

- Midpoint composite rule ( $m = 4$ )

$$\begin{aligned} I(f) &\approx \frac{4 - 0}{4} [f(0.5) + f(1.5) + f(2.5) + f(3.5)] \\ &= 0.5[e + 3e^3 + 5e^5 + 7e^7] = 4241 \end{aligned}$$



## Derivation of more accurate formulae

Let's consider the **Lagrange polynomial** of degree  $n = 1$  with  $a = x_0, b = x_1$ , and  $x \in [a, b]$

$$\Pi_1 f(x) = l_0(x)f(x_0) + l_1(x)f(x_1) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1),$$

We perform the change of variable

$$t = \frac{x - x_0}{x_1 - x_0} \in [0, 1], \quad dx = h dt, \quad \text{where} \quad h = x_1 - x_0$$

which implies that:  $x = x_0$  when  $t = 0$ ,  $x = x_1$  when  $t = 1$ , and  $\Pi_1 f(t) = (1 - t)f(a) + tf(b)$ , thus

$$\begin{aligned} \int_a^b f(x) dx &\approx \int_a^b \Pi_1 f(x) dx = h \int_0^1 \Pi_1 f(t) dt \\ &= f(a)h \int_0^1 (1 - t) dt + f(b)h \int_0^1 t dt \\ &= f(a)h \left[ t - \frac{t^2}{2} \right]_0^1 + f(b)h \left[ \frac{t^2}{2} \right]_0^1 = \frac{h}{2}[f(a) + f(b)]. \end{aligned}$$

## Trapezoidal (composite) formula

Replacing  $f$  over  $[a, b]$  with the Lagrange interpolant  $f_1 = \Pi_1 f$  of degree 1, where  $w_0 = w_1 = (b - a)/2$ , and  $x_0 = a, x_1 = b$  so that

$$I_1(f) = \frac{b - a}{2} [f(a) + f(b)], \quad \text{with} \quad E_1(f) = -\frac{h^3}{12} f''(\xi),$$

where  $h = b - a$  and  $\xi \in (a, b)$ .

~~~ The trapezoidal quadrature has degree of exactness  $r = 1$ .

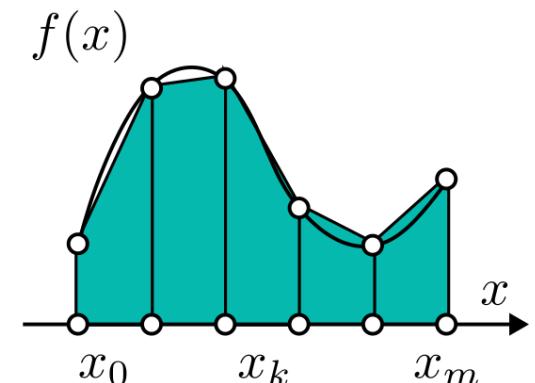
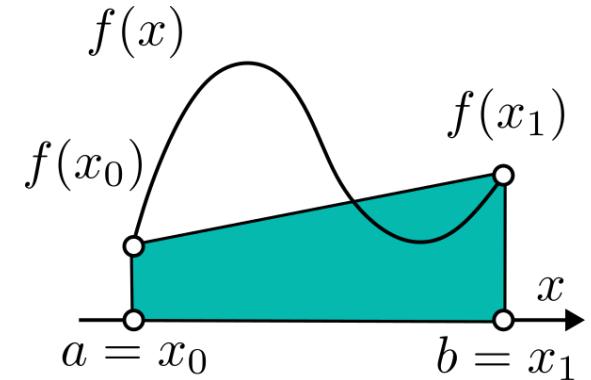
For the **composite** rule we replace f with its piecewise interpolant Π_1^p .

Given $m \geq 1$ of width $H = (b - a)/m$, and quadrature nodes

$x_k = a + kH$ for $k = 0, \dots, m$, we get

$$I_{1,m}(f) = \frac{H}{2} \sum_{k=0}^{m-1} [f(x_k) + f(x_{k+1})], \quad \text{with} \quad E_{1,m}(f) = -\frac{b - a}{12} H^2 f''(\xi),$$

where $f \in C^2([a, b]), \xi \in (a, b)$ and the degree of exactness is $r = 1$.



Numerical example

Use the trapezoidal rule with linear $n = 1$ interpolant of the function $f(x) = xe^{2x}$ with 2 nodes

$$I(f) = \int_0^4 xe^{2x} dx.$$

- **Exact value**

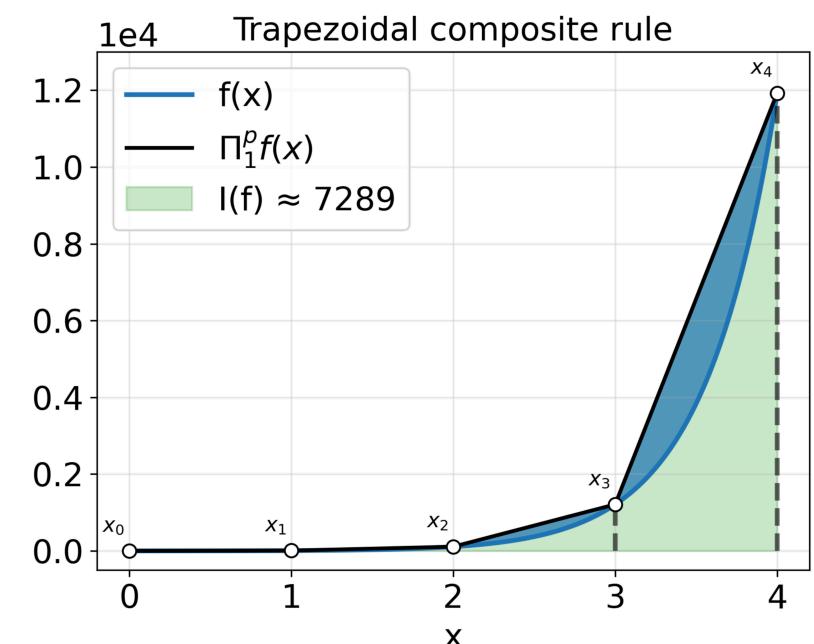
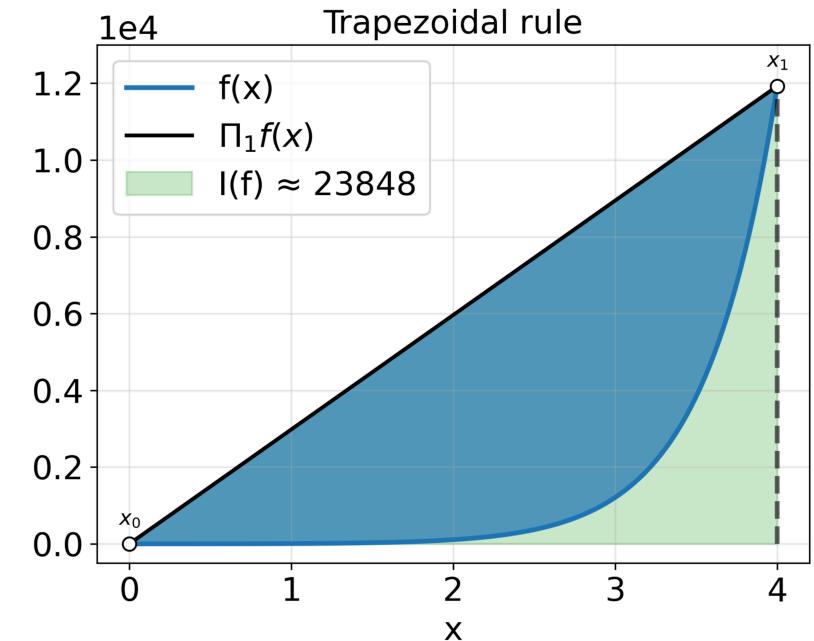
$$\int_0^4 xe^{2x} dx = \left[\frac{x}{2}e^{2x} - \frac{1}{4}e^{2x} \right]_0^4 = \frac{1}{4}(7e^8 - 1) = 5217$$

- **Trapezoidal rule**

$$I(f) \approx \frac{4-0}{2}[f(4) + f(0)] = 2(4e^8 + 0) = 23848$$

- **Trapezoidal composite rule ($m = 4$)**

$$\begin{aligned} I(f) &\approx \frac{4-0}{4} \left[\frac{1}{2}f(0) + f(1) + f(2) + f(3) + \frac{1}{2}f(4) \right] \\ &= e^2 + 2e^4 + 3e^6 + 2e^8 = 7289 \end{aligned}$$



Derivation of more accurate formulae

Let's consider the **Lagrange polynomial** of degree $n = 2$ with $a = x_0$, $(a + b)/2 = x_1$, and $b = x_2$,

$$\begin{aligned}\Pi_2 f(x) &= l_0(x)f(x_0) + l_1(x)f(x_1) + l_2(x)f(x_2) \\ &= \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)}f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}f(x_2),\end{aligned}$$

We perform the change of variable $t = (x - x_1)/h \in [-1, 1]$, $dx = h dt$, where $h = (x_2 - x_0)/2$ which implies that: $x = x_0$ when $t = -1$, $x = x_1$ when $t = 0$, $x = x_2$ when $t = 1$ and

$$\Pi_2 f(t) = \frac{t(1-t)}{2}f(x_0) + (1-t)^2f(x_1) + \frac{t(t+1)}{2}f(x_2), \quad \text{so that}$$

$$\begin{aligned}\int_a^b f(x) dx &\approx h \int_{-1}^1 \Pi_2 f(t) dt = f(x_0) \frac{h}{2} \int_{-1}^1 t(t-1) dt + f(x_1) h \int_{-1}^1 (1-t^2) dt + f(x_2) \frac{h}{2} \int_{-1}^1 t(t+1) dt \\ &= f(x_0) \frac{h}{2} \left(\frac{t^3}{3} - \frac{t^2}{2} \right) \Big|_{-1}^1 + f(x_1) h \left(t - \frac{t^3}{3} \right) \Big|_{-1}^1 + f(x_2) \frac{h}{2} \left(\frac{t^3}{3} + \frac{t^2}{2} \right) \Big|_{-1}^1 \\ &= \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)].\end{aligned}$$

The (composite) Cavalieri-Simpson formula

Replacing f over $[a, b]$ with the Lagrange interpolant $f_2 = \Pi_2 f$ of degree 2, where $w_0 = w_2 = (b - a)/6$, $w_1 = 4(b - a)/6$, $x_0 = a$, $x_1 = (a + b)/2$ and $x_2 = b$ so that if $h = (b - a)/2$ and $\xi \in (a, b)$, we obtain

$$I_2(f) = \frac{b - a}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right], \quad \text{with} \quad E_2(f) = -\frac{h^5}{90} f''''(\xi).$$

~~~ The Cavalieri-Simpson quadrature has degree of exactness  $r = 3$ .

For the **composite** rule we replace  $f$  with its piecewise interpolant  $\Pi_2^p$ .

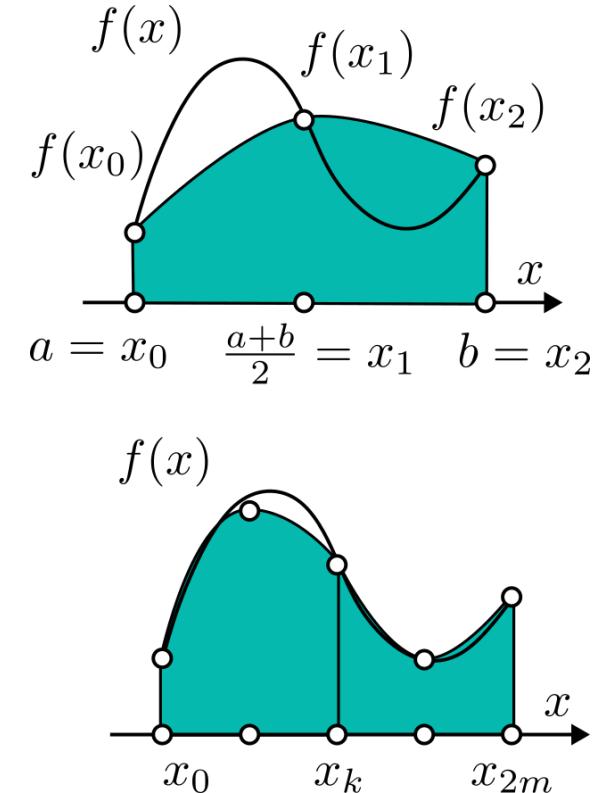
Given  $m \geq 1$  of width  $H = (b - a)/m$ , and quadrature nodes

$x_k = a + kH/2$  for  $k = 0, \dots, 2m$ , we get

$$I_{2,m}(f) = \frac{H}{6} \left[ f(x_0) + 2 \sum_{i=1}^{m-1} f(x_{2i}) + 4 \sum_{j=0}^{m-1} f(x_{2j+1}) + f(x_{2m}) \right],$$

where  $f \in C^4([a, b])$ , and  $\xi \in (a, b)$ , the degree of exactness is  $r = 3$  and

$$E_{2,m}(f) = -\frac{b - a}{180} \frac{H^4}{2} f''''(\xi).$$



# Numerical example

Use the **Simpson** rule with quadratic  $n = 2$   
 interpolant of the function  $f(x) = xe^{2x}$  with 3 nodes

$$I(f) = \int_0^4 xe^{2x} dx.$$

- **Exact value**

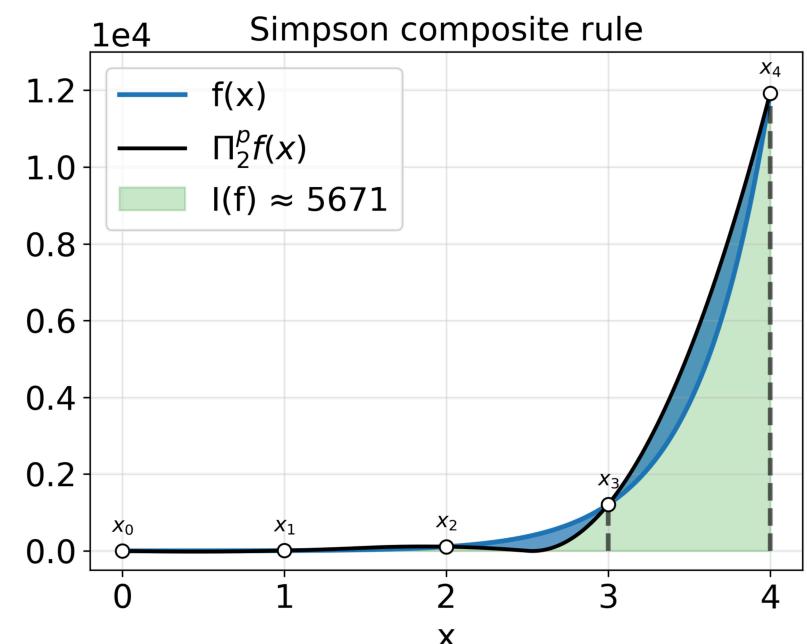
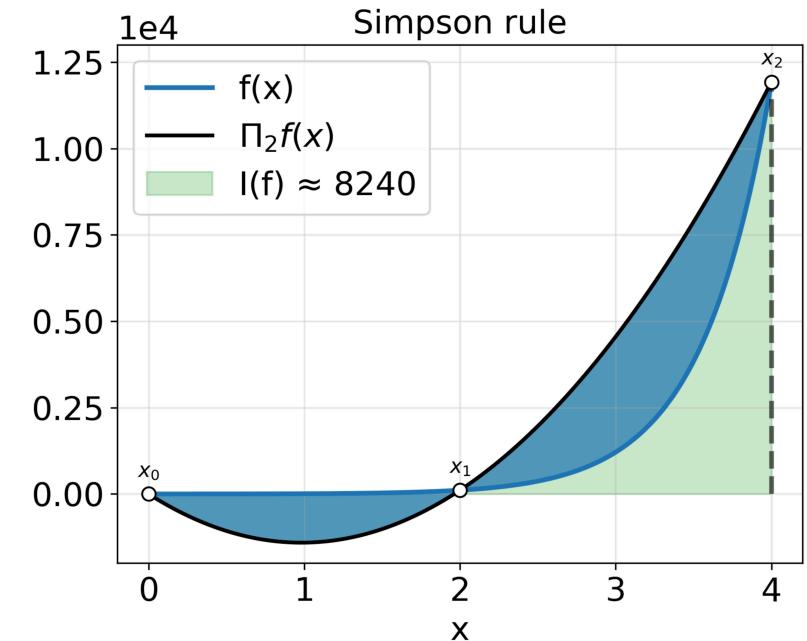
$$\int_0^4 xe^{2x} dx = \left[ \frac{x}{2} e^{2x} - \frac{1}{4} e^{2x} \right]_0^4 = \frac{1}{4} (7e^8 - 1) = 5217$$

- **Simpson rule**

$$I_2(f) = \frac{4-0}{6} [f(0) + 4f(2) + f(4)] = 2(8e^4 + 4e^8)/3 = 8240$$

- **Simpson composite rule ( $m = 2$ )**

$$\begin{aligned} I_{2,m}(f) &= \frac{4-0}{12} [f(0) + 4f(1) + 2f(2) + 4f(3) + f(4)] \\ &= [4e^2 + 4e^4 + 12e^6 + 4e^8]/3 = 5671 \end{aligned}$$



# Method of undetermined coefficients

- Quadrature rules can be derived using polynomial interpolation.
- The integral of the original function is approximated by the integral of the **interpolant of degree  $n$** .
- The polynomial is used to determine the **nodes** and **weights** for a given quadrature rule.

~~~ An alternative derivation of the quadrature rules is called the **method of undetermined coefficients**

- find the weights s.t. the rule integrates the first $n + 1$ polynomial basis functions exactly ($\deg \leq n$)
- solve a system of $n + 1$ equations and unknowns, e.g. for monomial basis the **moment equations** are

$$w_0 \cdot 1 + w_1 \cdot 1 + \cdots + w_n \cdot 1 = \int_a^b 1 \, dx = [x]_a^b = b - a$$

$$w_0 \cdot x_0 + w_1 \cdot x_1 + \cdots + w_n \cdot x_n = \int_a^b x \, dx = [x^2/2]_a^b = (b^2 - a^2)/2$$

⋮

$$w_0 \cdot x_0^n + w_1 \cdot x_1^n + \cdots + w_n \cdot x_n^n = \int_a^b x^n \, dx = [x^{n+1}/(n+1)]_a^b = (b^{n+1} - a^{n+1})/(n+1)$$

Method of undetermined coefficients

The system of moment equations is thus given by the transpose of the **Vandermonde** matrix

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ x_1 & x_2 & \cdots & x_n \\ \vdots & \vdots & \ddots & \vdots \\ x_1^n & x_2^n & \cdots & x_n^n \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_n \end{bmatrix} = \begin{bmatrix} b - a \\ (b^2 - a^2)/2 \\ \vdots \\ (b^{n+1} - a^{n+1})/(n + 1) \end{bmatrix}$$

$\exists!$ solution for distinct nodes which correspond to the weights $\{w_i\}_{i=0}^n$ given by the Lagrange basis.

Example. Deriving the three-point quadrature rule $I_2(f) = w_0 f(x_0) + w_1 f(x_1) + w_2 f(x_2)$

$$\begin{bmatrix} 1 & 1 & 1 \\ a & (a + b)/2 & b \\ a^2 & ((a + b)/2)^2 & b^2 \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} b - a \\ (b^2 - a^2)/2 \\ (b^3 - a^3)/3 \end{bmatrix}$$

from which we obtain the Simpson's 1/3 rule with $w_0 = \frac{b-a}{6}$, $w_1 = \frac{2(b-a)}{3}$ and $w_2 = \frac{b-a}{6}$.

Naïve error bound and stability

- The significance of the **degree of exactness** is that it characterizes the accuracy of a given rule.

If I_n is an interpolatory quadrature rule, and Π_n is the polynomial interpolant of degree $\leq n$ at the nodes x_0, \dots, x_n , then the following **naïve error bound** for the approximate integral holds

$$|I(f) - I_n(f)| = |I(f - \Pi_n f)| \leq (b - a) \|f - \Pi_n f\|_\infty \leq \frac{b - a}{4(n + 1)} h^{n+1} \|f^{(n+1)}\|_\infty \leq \frac{h^{n+2}}{4} \|f^{(n+1)}\|_\infty$$

\rightsquigarrow higher accuracy when n larger, or h smaller, or both, thus $I_n(f) \xrightarrow{n \rightarrow \infty} I(f)$ provided $f^{(n)}$ is bounded.

As concerns the **stability** of the numerical quadrature, let's consider a perturbation \tilde{f} of f , then we have

$$|I_n(\tilde{f}) - I_n(f)| = |I_n(\tilde{f} - f)| = \left| \sum_{i=0}^n w_i (\tilde{f}(x_i) - f(x_i)) \right| \leq \sum_{i=0}^n (|w_i| \cdot |\tilde{f}(x_i) - f(x_i)|) \leq \left(\sum_{i=0}^n |w_i| \right) \|\tilde{f} - f\|_\infty$$

\rightsquigarrow the absolute condition number of the quadrature rule is at most $\sum_{i=0}^n |w_i|$.

Given $\sum_{i=0}^n w_i = b - a$, if the weights are all nonnegative, then it is equal to $b - a$, while if some weights are negative, then it can be much larger and the quadrature rule can be unstable.

Newton-Cotes formulae

Lagrange-based quadratures with $n + 1$ equispaced nodes in $[a, b]$.

Midpoint ($n = 0$), trapezoidal ($n = 1$) and Simpson ($n = 2$) are instances of **Newton-Cotes** formulae.

- **closed formulae**, if $x_0 = a, x_n = b$, and $h = \frac{b-a}{n}$ where $n \geq 1$,
- **open formulae**, if $x_0 = a + h, x_n = b - h$, and $h = \frac{b-a}{n+2}$ where $n \geq 0$.

~~ Quadrature weights $\{w_i\}_{i=0}^n$ of Newton-Cotes formulae depend explicitly on n and h , but not on $[a, b]$.

With the change of variable $x = \Psi(t) = x_0 + th$, we obtain $l_i(x) = \prod_{k=0, k \neq i} \left(\frac{t-k}{i-k} \right) = \phi_i(t)$, s.t

Closed: $x_k = x_0 + kh,$

$\Psi(0) = a, \Psi(n) = b$

Open: $x_k = x_0 + (k+1)h,$

$\Psi(-1) = a, \Psi(n+1) = b$

$$w_i = \int_a^b l_i(x) dx = h \int_0^n \phi_i(t) dt \doteq h\alpha_i$$

$$w_i = \int_a^b l_i(x) dx = h \int_{-1}^{n+1} \phi_i(t) dt \doteq h\alpha_i$$

$$\rightsquigarrow I_n(f) = h \sum_{i=0}^n \alpha_i f(x_i)$$

Newton-Cotes formulae

The coefficients α_i do not depend on a, b, h and f , but only depend on n . By symmetry we obtain

Closed: $\alpha_i = \alpha_{n-i}$ for $i = 0, \dots, n - 1$

| n | 1 | 2 | 3 | 4 | 5 | 6 |
|------------|---------------|---------------|---------------|-----------------|-------------------|-------------------|
| α_0 | $\frac{1}{2}$ | $\frac{1}{3}$ | $\frac{3}{8}$ | $\frac{14}{45}$ | $\frac{95}{288}$ | $\frac{41}{140}$ |
| α_1 | 0 | $\frac{4}{3}$ | $\frac{9}{8}$ | $\frac{64}{45}$ | $\frac{375}{288}$ | $\frac{216}{140}$ |
| α_2 | 0 | 0 | 0 | $\frac{24}{45}$ | $\frac{250}{288}$ | $\frac{27}{140}$ |
| α_3 | 0 | 0 | 0 | 0 | 0 | $\frac{272}{140}$ |

Open: $\alpha_i = \alpha_{n-i}$ for $i = 0, \dots, n$

| n | 1 | 2 | 3 | 4 | 5 | 6 |
|------------|---|---------------|----------------|-----------------|------------------|----------------------|
| α_0 | 2 | $\frac{3}{2}$ | $\frac{3}{8}$ | $\frac{55}{24}$ | $\frac{66}{20}$ | $\frac{4277}{1440}$ |
| α_1 | 0 | 0 | $-\frac{4}{3}$ | $\frac{5}{24}$ | $-\frac{84}{20}$ | $-\frac{3171}{1440}$ |
| α_2 | 0 | 0 | 0 | 0 | $\frac{156}{20}$ | $\frac{3934}{1440}$ |

Remarks.

- There are negative weights in open formulae for $n \geq 2$, potentially causing numerical instability.
- The order of infinitesimal w.r.t. the integration stepsize h is defined as the maximum integer p s.t.

$$|I(f) - I_n(f)| = \mathcal{O}(h^p).$$

Newton-Cotes errors

Theorem 1. For any Newton-Cotes rule with an **even** value of n , the following error characterization holds

$$E_n(f) = \frac{M_n}{(n+2)!} h^{n+3} f^{(n+2)}(\xi),$$

provided $f \in C^{n+2}([a, b])$, $\xi \in (a, b)$, and defining $\pi_{n+1}(t) = \prod_{i=0}^n (t - i)$ and

$$M_n = \begin{cases} \int_0^n \pi_{n+1}(t) dt < 0 & \text{for } \mathbf{closed} \text{ formulae,} \\ \int_{-1}^{n+1} \pi_{n+1}(t) dt > 0 & \text{for } \mathbf{open} \text{ formulae.} \end{cases}$$

The **degree of exactness** is equal to $n + 1$ and the order of **infinitesimal** is $n + 3$.

Newton-Cotes errors

Theorem 2. For any Newton-Cotes rule with an **odd** value of n , the following error characterization holds

$$E_n(f) = \frac{K_n}{(n+1)!} h^{n+2} f^{(n+1)}(\eta),$$

provided $f \in C^{n+1}([a, b])$, $\eta \in (a, b)$, and defining $\pi_{n+1}(t) = \prod_{i=0}^n (t - i)$ and

$$K_n = \begin{cases} \int_0^n t \pi_{n+1}(t) dt < 0 & \text{for } \mathbf{closed} \text{ formulae,} \\ \int_{-1}^{n+1} t \pi_{n+1}(t) dt > 0 & \text{for } \mathbf{open} \text{ formulae.} \end{cases}$$

The **degree of exactness** is thus equal to n and the order of **infinitesimal** is $n + 2$.

Newton-Cotes errors

- **Midpoint Rule:** constant interpolant $n = 0$

$$E_0 = -\frac{h^3}{3} f^{(2)}(\xi), \quad \text{where } h = \frac{b-a}{2}$$

- **Trapezoidal Rule:** linear interpolant $n = 1$

$$E_1 = -\frac{h^3}{12} f^{(2)}(\xi), \quad \text{where } h = b-a$$

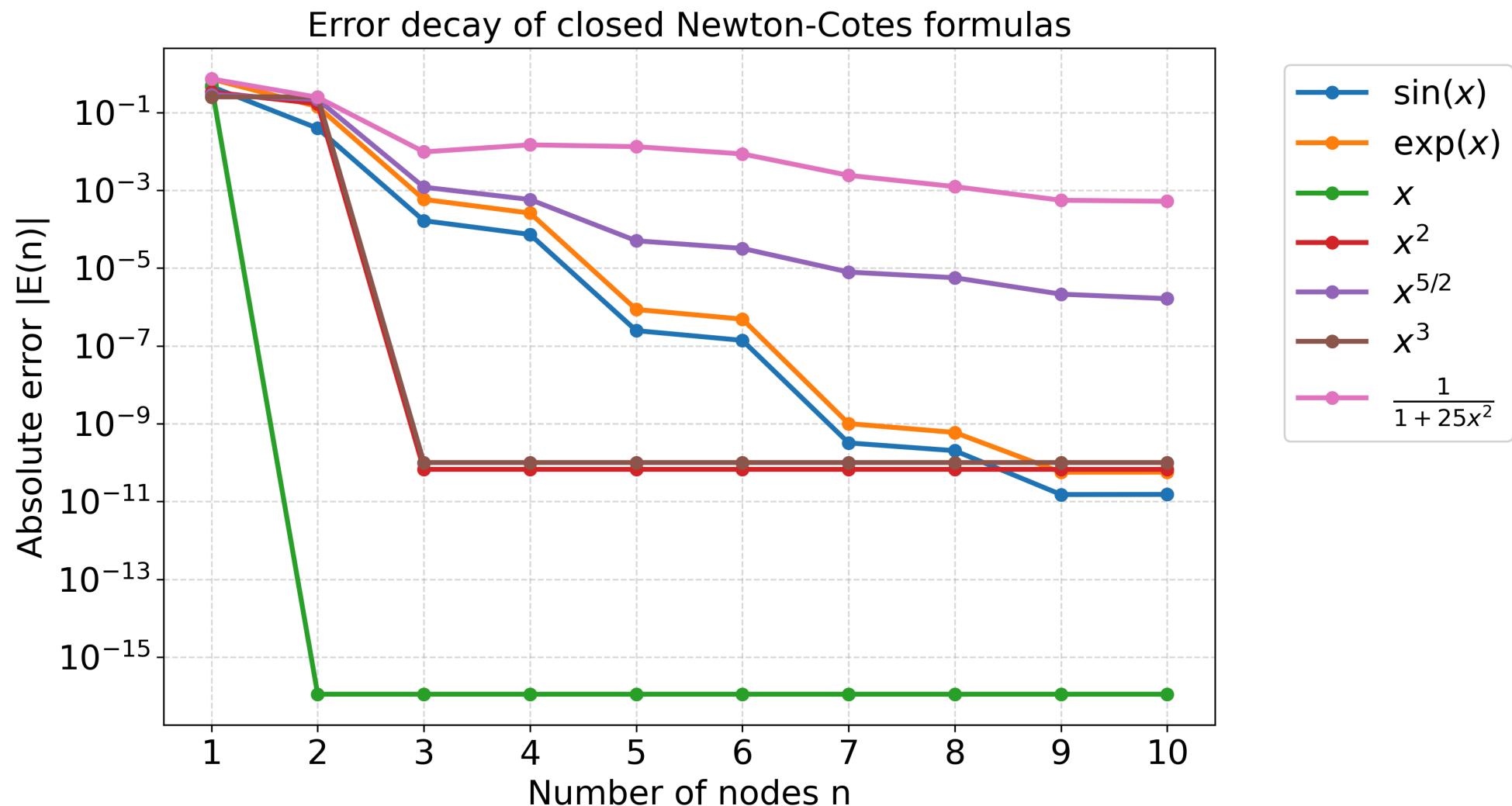
- **Simpson's 1/3 Rule:** quadratic interpolant $n = 2$

$$E_2 = -\frac{h^5}{90} f^{(4)}(\xi), \quad \text{where } h = \frac{b-a}{2}$$

- **Simpson's 3/8 Rule:** cubic interpolant $n = 3$

$$E_3 = -\frac{3h^5}{80} f^{(4)}(\xi), \quad \text{where } h = \frac{b-a}{3}$$

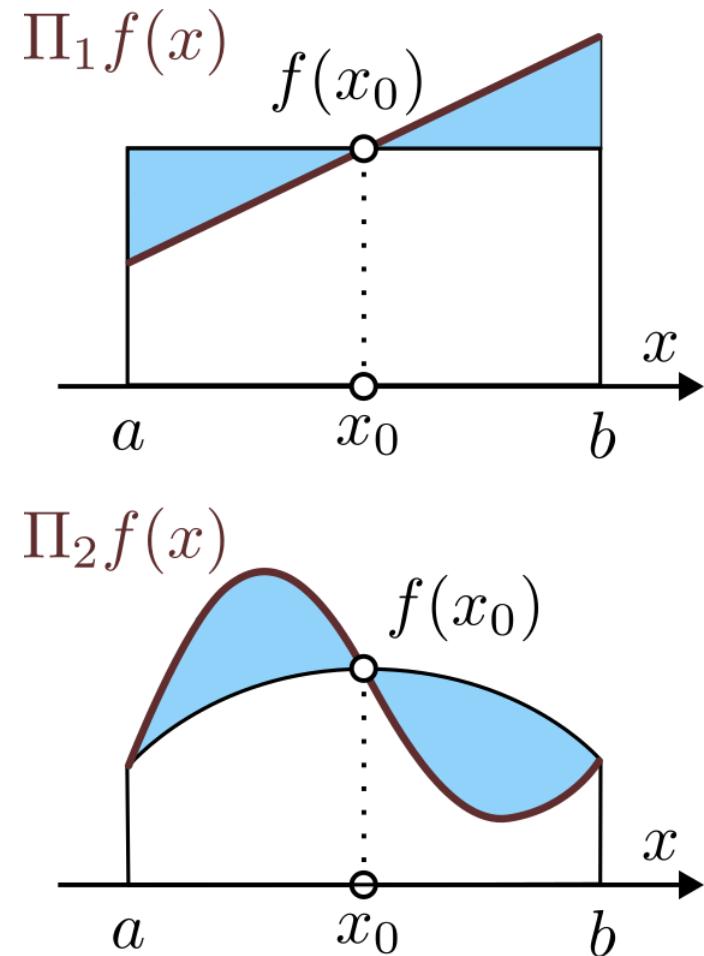
Newton-Cotes errors



Newton-Cotes formulae

Highlights.

- Phenomenon due to **cancellation** of positive and negative errors.
- Every degree n rule with $n \geq 10$ has at least one **negative weight**.
- Since $\sum_{i=0}^n |w_i| \xrightarrow{n \rightarrow \infty} \infty$, NC rules become **ill-conditioned** and unstable for large n .
- Large positive and negative weights can cause cancellation error in **finite-precision** arithmetic.
- **NC** rules do not have the highest possible degree (accuracy) for the number of points used (number of function evaluations required).



Composite Newton-Cotes formulae and errors

Partitioning $[a, b]$ into m subintervals $T_j = [y_j, y_{j+1}]$ with $\{y_j = a + jH\}_{j=0}^m$ where $H = (b - a)/m$. For each subinterval, an interpolatory formula with $n + 1$ nodes $\{x_k^{(j)}\}_{k=0}^n$ and weights $\{w_k^{(j)}\}_{k=0}^n$ is used

$$I(f) = \int_a^b f(x) dx = \sum_{j=0}^{m-1} \int_{T_j} f(x) dx \approx \sum_{j=0}^{m-1} \sum_{k=0}^n w_k^{(j)} f(x_k^{(j)}) \doteq I_{n,m}(f).$$

By using a NC formula with $n + 1$ equispaced nodes the weights $w_k^{(j)} = h\alpha_k$ are still independent of T_j .

Theorem 3. If $I_{n,m}(f)$ is a composite NC rule with n **even**, and $f \in C^{n+2}([a, b])$, the quadrature error is

$$E_{n,m}(f) = I(f) - I_{n,m}(f) = \frac{b-a}{(n+2)!} \frac{M_n}{\gamma_n^{n+3}} H^{n+2} f^{(n+2)}(\xi).$$

If $I_{n,m}(f)$ is a composite NC rule with n **odd**, and $f \in C^{n+1}([a, b])$, the quadrature error is

$$E_{n,m}(f) = I(f) - I_{n,m}(f) = \frac{b-a}{(n+1)!} \frac{K_n}{\gamma_n^{n+2}} H^{n+1} f^{(n+1)}(\eta),$$

Composite Newton-Cotes formulae and errors

Highlights.

- The constants in the error are $\gamma_n = (n + 2)$ if the formula is **open**, and $\gamma_n = n$ if it is **closed**.
- The quadrature error with n **even**
 - is *infinitesimal* in H of order $n + 2$
 - has *degree of exactness* equal to $n + 1$.
- The quadrature error with n **odd**
 - is *infinitesimal* in H of order $n + 1$
 - has *degree of exactness* equal to n .
- For n fixed, $E_{n,m}(f) \xrightarrow{m \rightarrow \infty} 0$, i.e., as $H \rightarrow 0$, ensuring the convergence of the quadrature to $I(f)$.
- The **degree of exactness** of composite formulae **coincides** with that of simple formulae
- The **order of infinitesimal** w.r.t. H , is **reduced by 1** w.r.t. the one in h of simple formulae.
- It is convenient to resort to a local interpolation of low degree, e.g. $n \leq 2$, leading to composite quadrature rules with positive weights, with a minimization of the rounding errors.

Composite Newton-Cotes formulae and errors

Convergence of $I_{n,m}(f)$ to $I(f)$ can be obtain wiht less regularity assumptions on f than Theorem 3.

Theorem 4.

Let $f \in C^0([a, b])$ and assume that the weights $w_k^{(j)}$ are nonnegative, then

$$\lim_{m \rightarrow \infty} I_{n,m}(f) = I(f) = \int_a^b f(x) dx, \quad \forall n \geq 0.$$

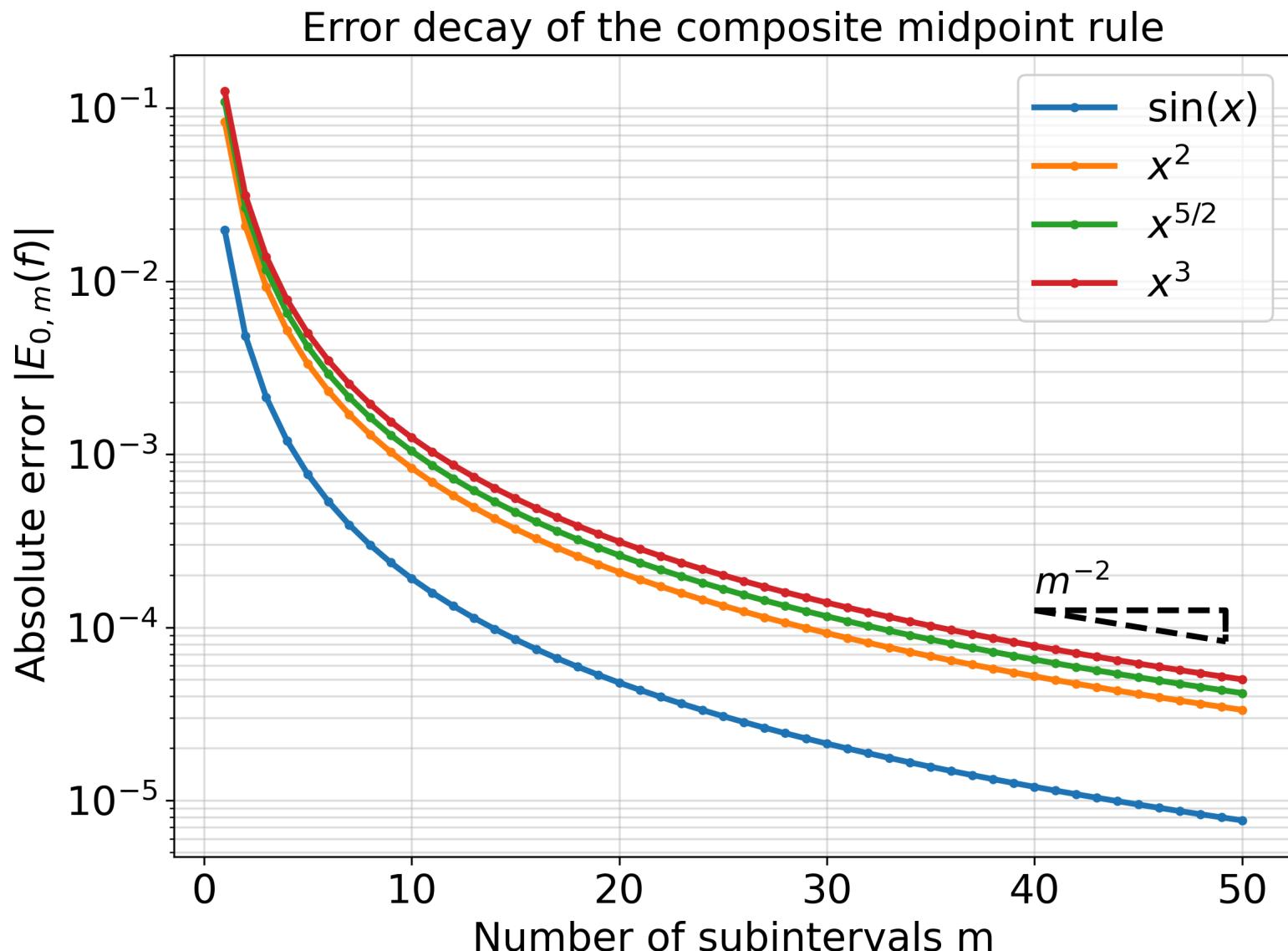
Moreover

$$\left| \int_a^b f(x) dx - I_{n,m}(f) \right| \leq 2(b-a)\Omega(f; H),$$

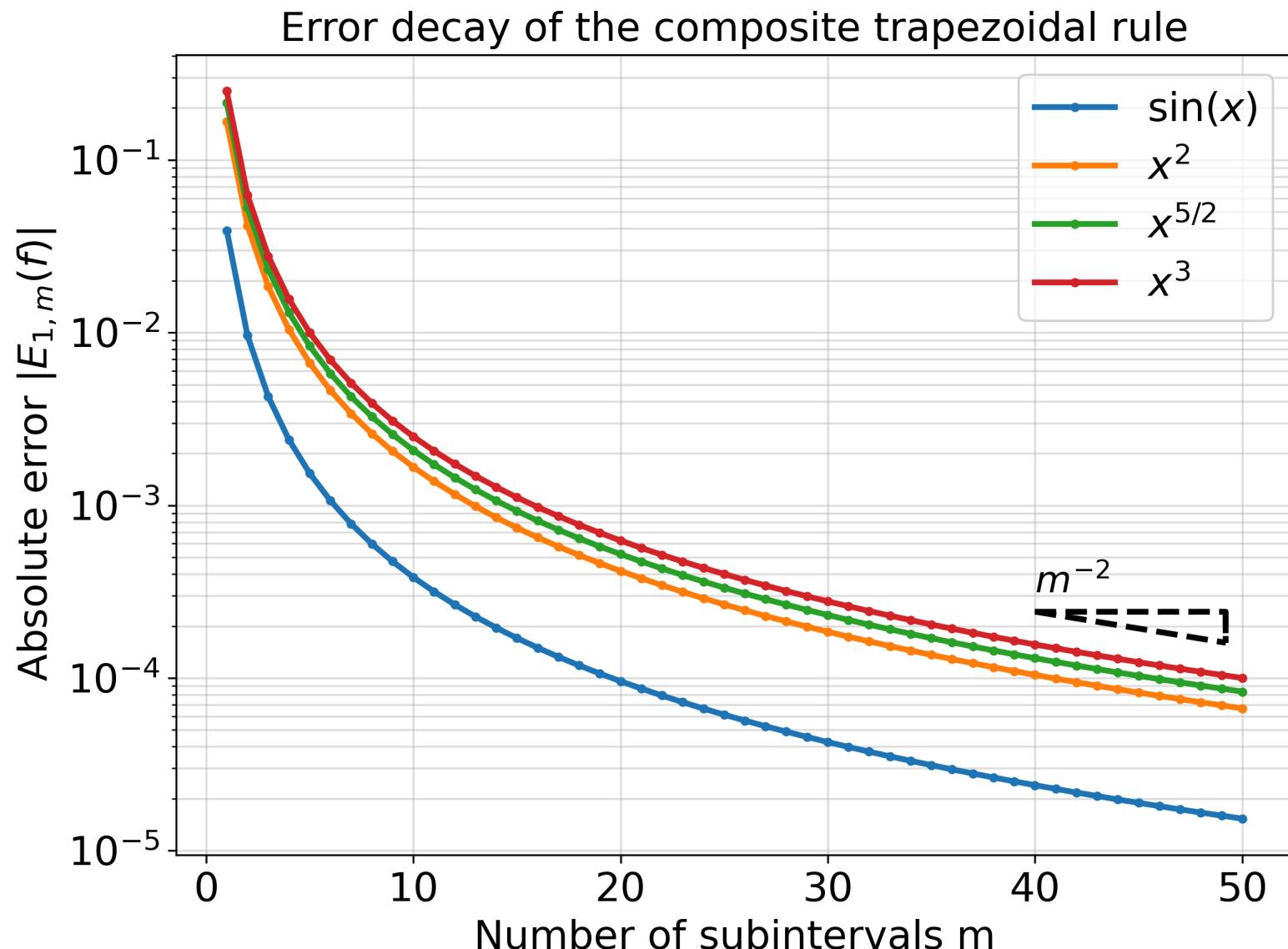
where the module of continuity of the function f is defined as

$$\Omega(f; H) = \sup\{\|f(x) - f(y)\|, x, y \in [a, b], x \neq y, |x - y| < H\}.$$

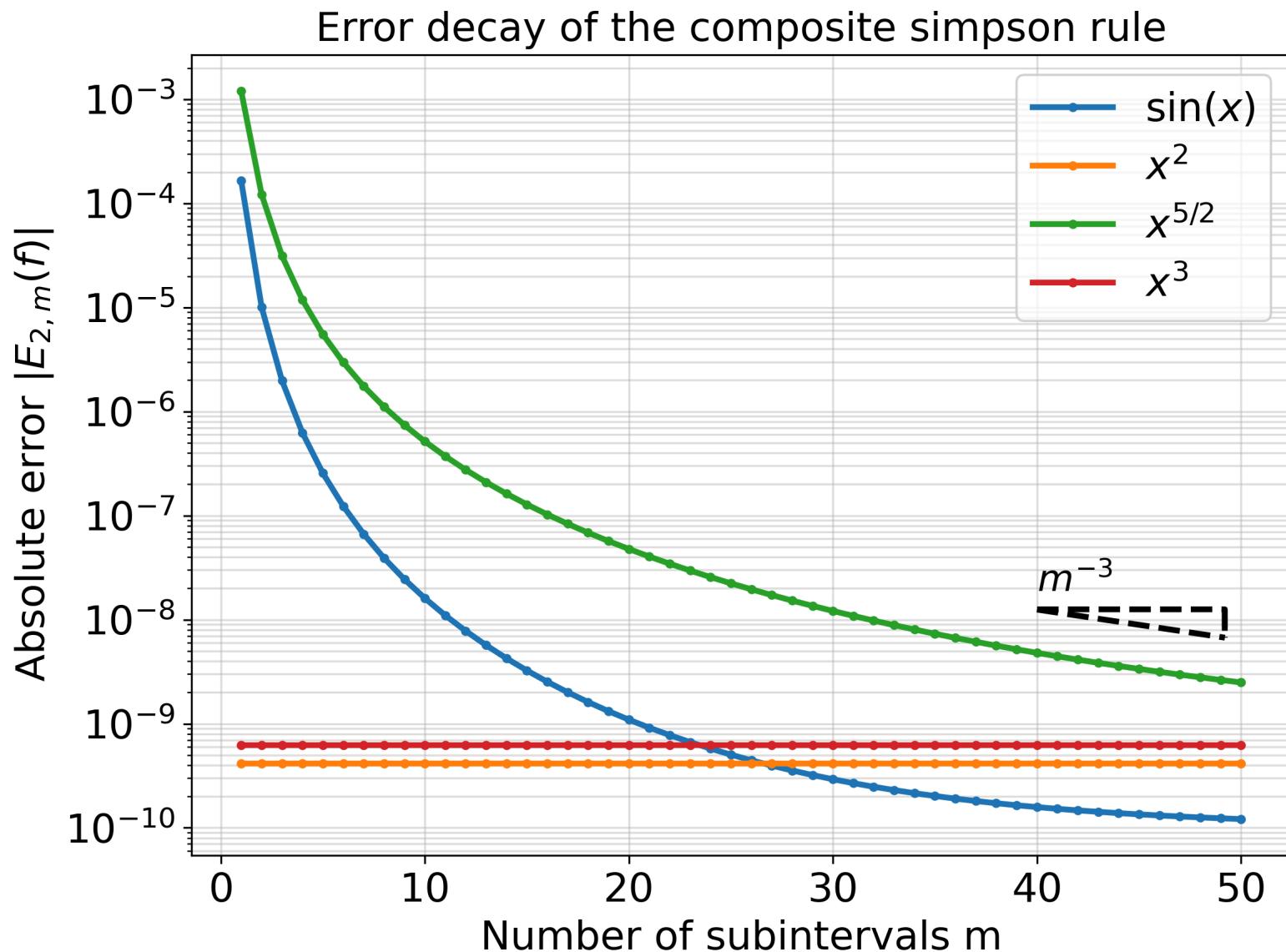
Composite Newton-Cotes formulae and errors



Composite Newton-Cotes formulae and errors



Composite Newton-Cotes formulae and errors



Hermite quadrature

Idea. Exploit (first-order) derivative information to enhance the accuracy via **Hermite** interpolation.

Given $n + 1$ nodes $\{x_i\}_{i=0}^n$, and $N = 2(n + 1)$ values $f(x_i)$ and $f'(x_i)$, the interpolant is

$$H_{2n+1}f(x) = \sum_{i=0}^n f(x_i)A_i(x) + f'(x_i)B_i(x),$$

where $A_i(x) = (1 - 2(x - x_i)l_i'(x_i))l_i(x)^2$ and $B_i(x) = (x - x_i)l_i(x)^2$, for $i = 0, \dots, n$.

The **Hermite quadrature** formula is then given by

$$I_n(f) = \sum_{i=0}^n w_A^i f(x_i) + w_B^i f'(x_i),$$

where the weight are given by $w_A^i = I(A_i(x))$ and $w_B^i = I(B_i(x))$.

Hermite quadrature

If $n = 1$ one obtain the **corrected trapezoidal formula**

$$I_1^{\text{corr}}(f) = \frac{b-a}{2}[f(a) + f(b)] + \frac{(b-a)^2}{12}[f'(a) - f'(b)],$$

where the weights are given by $w_A^0 = w_A^1 = (b-a)/2$, $w_B^0 = (b-a)^2/12$ and $w_B^1 = -w_B^0$.

Assuming $f \in C^4([a, b])$ the quadrature error is given by

$$E_1^{\text{corr}}(f) = \frac{h^5}{720} f''''(\xi), \quad \text{with } h = b-a \text{ and } \xi \in (a, b).$$

\rightsquigarrow the accuracy increases from $\mathcal{O}(h^3)$ to $\mathcal{O}(h^5)$ (of the same order as the Cavalieri-Simpson rule).

The **composite** formula can be generated in a similar manner

$$I_{1,m}^{\text{corr}}(f) = \frac{b-a}{m} \left[\frac{f(x_0)}{2} + f(x_1) + \cdots + f(x_{m-1}) + \frac{f(x_m)}{2} \right] + \frac{(b-a)^2}{12m^2} [f'(a) - f'(b)]$$

given $f \in C^1([a, b])$ and thanks to the cancellation of the first derivatives at the nodes $\{x_k\}_{k=1}^{m-1}$.

Hermite quadrature

Example. Use the corrected trapezoid rule with cubic $n = 1$ interpolant (!) of $f(x) = \sin(x)$ with 2 nodes and 4 values

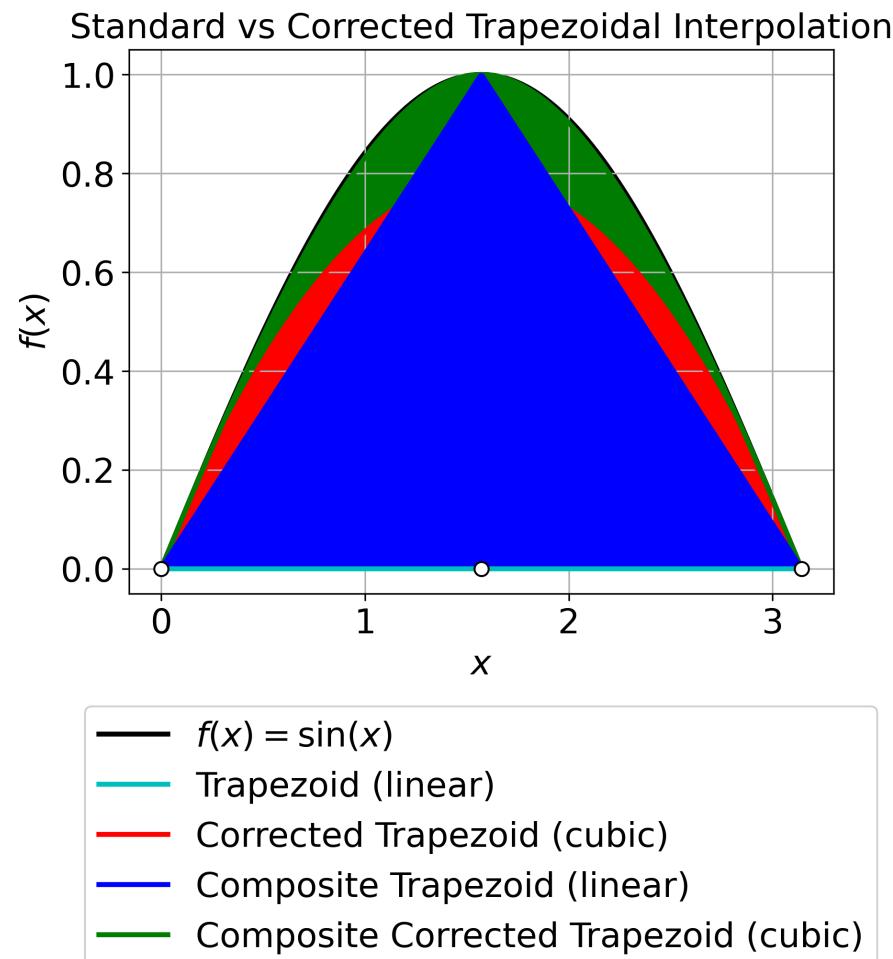
$$I(f) = \int_0^\pi \sin(x) dx = [\cos(x)]_0^\pi = 2.$$

- **Corrected trapezoid rule**

$$\begin{aligned} I_1^{\text{corr}}(f) &= \frac{\pi - 0}{2} [\sin(0) + \sin(\pi)] + \frac{(\pi - 0)^2}{12} [\cos(0) - \cos(\pi)] \\ &= \frac{\pi^2}{6} \approx 1.64 \end{aligned}$$

- **Corrected composite trapezoid rule**

$$\begin{aligned} I_{1,2} *^{\text{corr}} (f) &= \frac{\pi - 0}{2} \left[\frac{\sin(0)}{2} + \sin\left(\frac{\pi}{2}\right) + \frac{\sin(\pi)}{2} \right] + \frac{(\pi - 0)^2}{48} [\cos(0) - \cos(\pi)] \\ &= \frac{\pi}{2} + \frac{\pi^2}{24} \approx 1.98 \end{aligned}$$



Orthogonal polynomials

Orthogonal polynomials, as trigonometric and Chebyshev ones, are fundamental in approximation theory.

Definition 1. Let $w = w(x)$ be a nonnegative integrable weight function on the interval $(-1, 1)$.

Given $\{p_k\}_k$, a sequence of polynomials with $p_k \in \mathbb{P}_k$, they are mutually w -orthogonal if

$$(p_k, p_m)_w = \int_{-1}^1 p_k(x)p_m(x)w(x) dx = 0, \quad \text{for } k \neq m.$$

Definition 2. We define the truncation of order n of the **generalized Fourier sum** of f in $L_w^2(-1, 1)$ as

$$f_n(x) = \sum_{k=0}^n \widehat{f}_k p_k(x) \quad \text{so that} \quad \lim_{n \rightarrow \infty} \|f - f_n\|_w = 0,$$

where $\widehat{f}_k = \frac{(f, p_k)_w}{\|p_k\|_w^2}$ is the k -th Fourier coefficient, and f_n converges in the L_w^2 sense to f .

Theorem 5 The polynomial $f_n \in \mathbb{P}_n$ is the orthogonal projection of f over \mathbb{P}_n in the sense of L_w^2 , i.e.

$$\|f - f_n\|_w = \min_{q \in \mathbb{P}_n} \|f - q\|_w.$$

Chebyshev polynomials

Consider the Chebyshev weight function $w(x) = (1 - x^2)^{-1/2}$ on the interval $(-1, 1)$, and the space of square-integrable functions $f \in L_w^2(-1, 1)$. The **Chebyshev polynomials** are defined as

$$T_k(x) = \cos(k\theta), \quad \text{for } k = 0, 1, \dots, \quad \text{with } \theta = \arccos(x) \in (0, \pi),$$

and can be recursively generated by the three-term formula

$$\begin{cases} T_{k+1}(x) = 2xT_k(x) - T_{k-1}(x), & \text{for } k = 1, 2, \dots, \\ T_0(x) = 1, \quad T_1(x) = x. & \end{cases} \quad \text{so that} \quad (T_k, T_m)_w = \begin{cases} 0, & \text{if } k \neq m, \\ \pi, & \text{if } k = m = 0, \\ \pi/2, & \text{if } k = m \neq 0. \end{cases}$$

Fixed n , if we look for the zeros of the n -th Chebyshev polynomial $T_n(x) = \cos(n\theta)$ we can write

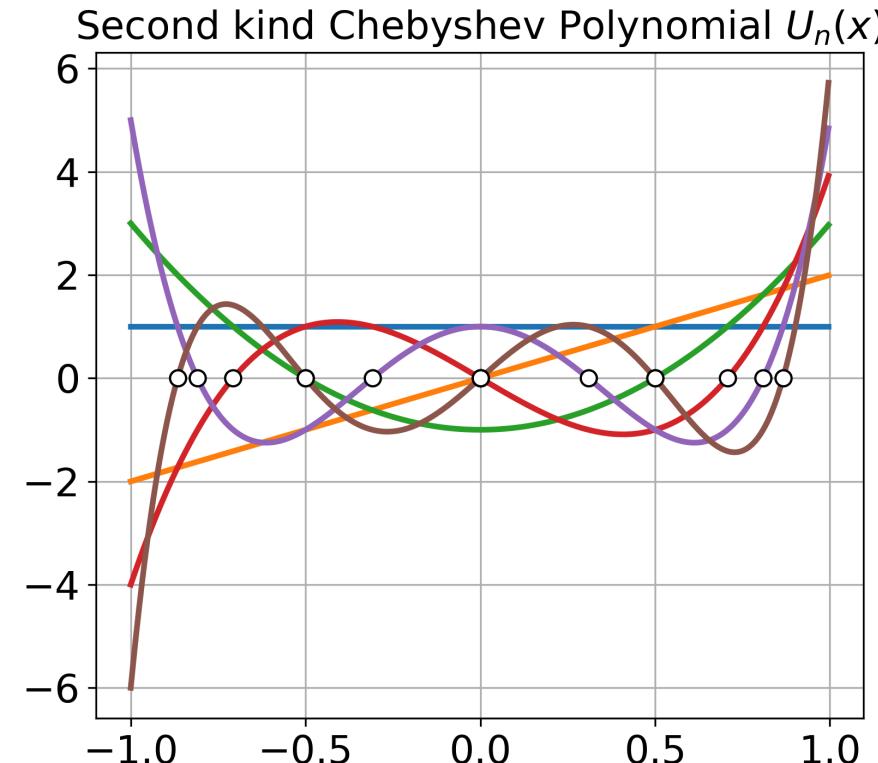
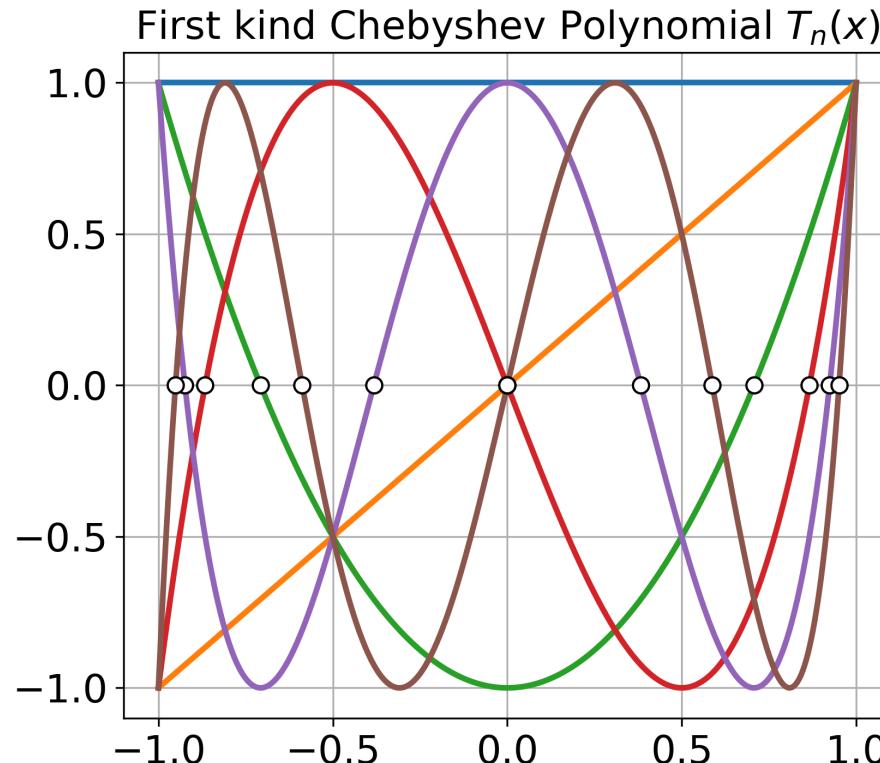
$$\cos(n\theta) = 0 \quad \rightsquigarrow \quad n\theta = \frac{\pi}{2} + m\pi, \quad m = 0, \dots, n-1, \quad \rightsquigarrow \quad \theta_k = \frac{(2k-1)\pi}{2n}, \quad k = 1, \dots, n,$$

and thus we get the corresponding distinct zeros in x -space as

$$x_k = \cos \theta_k = \cos\left(\frac{2k-1}{2n}\pi\right), \quad k = 1, \dots, n,$$

Chebyshev points

- **First kind** Chebyshev polynomial $T_k(x) = \cos(k\theta)$, with $x_k = \cos \theta_k = \cos\left(\frac{2k-1}{2n}\pi\right)$
- **Second kind** Chebyshev polynomial $U_k(x) = \frac{\sin((k+1)\theta)}{\sin(\theta)}$ with $x_k = \cos \theta_k = \cos\left(\frac{k\pi}{n+1}\right)$



Quadrature with Chebyshev points

Remarks.

- Quadrature rules based on the Chebyshev points are referred to as **Clenshaw-Curtis** quadrature.
- Chebyshev points could be a better choice of nodes for interpolatory quadrature rules.
- The weights are positive for any n , and the approximation converges to the exact integral as $n \rightarrow \infty$.
- Clenshaw-Curtis rule are always stable and significantly more accurate than NC.
- Clenshaw-Curtis rule with n nodes have degree of exactness $n - 1$.
- Zeros and extrema of the Chebyshev polynomials have similar stability and accuracy properties.
- Clenshaw-Curtis quadrature does not have maximum possible degree for number of nodes used.
- Chebyshev extrema yield **progressive** quadrature rules.

Gaussian quadrature

Orthogonal polynomials are crucial in devising quadrature formulae with maximal degrees of exactness.
Let $x_0, \dots, x_n \in [-1, 1]$ be $n + 1$ nodes, we approximate the weighted integral with weights α_i

$$I^w(f) = \int_{-1}^1 f(x)w(x) dx \approx \sum_{i=0}^n \alpha_i f(x_i) \doteq I_n^w(f).$$

Denoting by $E_n^w(f) = I^w(f) - I_n^w(f)$ the quadrature error, if $E_n^w(p) = 0$ for any $p \in \mathbb{P}_r$ the formula has degree of exactness r w.r.t. the weight w . Generalization of ordinary integration with weight $w = 1$.

- With Lagrange interpolant we have exactness equal to (at least) n with $\alpha_i = \int_{-1}^1 l_i(x)w(x) dx$.

Question. Choice of nodes such that the degree of exactness is equal to $r = n + m$ for some $m > 0$.

Gaussian quadrature

Theorem 6. For a given $m > 0$, the quadrature formula $I_n^w(f)$ has degree of exactness $n + m$ if and only if it is of interpolatory type and the nodal polynomial ω_{n+1} associated with the nodes x_i is such that

$$\int_{-1}^1 \omega_{n+1}(x)p(x)w(x) dx = 0, \quad \forall p \in \mathbb{P}_{m-1}.$$

Corollary. The maximum degree of exactness of the quadrature formula $I_n^w(f)$ is $2n + 1$.

Setting $m = n + 1$ the nodal polynomial ω_{n+1} satisfies the relation above $\forall p \in \mathbb{P}_n$.

- $\omega_{n+1} \in \mathbb{P}_{n+1}$ is orthogonal to all the polynomials of lower degree, thus $\omega_{n+1} = cp_{n+1}$ and monic.
- its roots x_j coincide with those of p_{n+1} , that is $p_{n+1}(x_j) = 0$, for $j = 0, \dots, n$.
- the abscissae x_j are the **Gauss nodes** associated with the weight function $w(x)$.

$\rightsquigarrow I_n^w(f)$ with coefficients and nodes given by $\alpha_i = \int_{-1}^1 l_i(x)w(x) dx$ and $p_{n+1}(x_j) = 0$, respectively, has degree of exactness $2n + 1$ (maximum with $n + 1$ nodes), and is known as **Gauss quadrature rule**.

- Including the interval's extrema one has the **$(n + 1)$ -Gauss-Lobatto rule** with exactness $2n - 1$. 44

Method of undetermined coefficients

Consider the 2-node quadrature rule with $n = 1$ expressed as $\int_{-1}^1 f(x) dx = \alpha_0 f(x_0) + \alpha_1 f(x_1)$

Imposing exactness for $f = 1, x, x^2, x^3$ we get the nonlinear system of 4 equations and 4 unknowns:

$$f = 1 \Rightarrow \int_{-1}^1 1 dx = 2 = \alpha_0 + \alpha_1$$

$$f = x \Rightarrow \int_{-1}^1 x dx = 0 = \alpha_0 x_0 + \alpha_1 x_1$$

$$f = x^2 \Rightarrow \int_{-1}^1 x^2 dx = \frac{2}{3} = \alpha_0 x_0^2 + \alpha_1 x_1^2$$

$$f = x^3 \Rightarrow \int_{-1}^1 x^3 dx = 0 = \alpha_0 x_0^3 + \alpha_1 x_1^3$$

$$\Rightarrow \begin{cases} \alpha_0 = 1 \\ \alpha_1 = 1 \\ x_0 = -\frac{1}{\sqrt{3}} \\ x_1 = \frac{1}{\sqrt{3}} \end{cases}$$

which has a degree of exactness equal to $2n + 1 = 3$.

Gaussian quadrature by orthogonal polynomials

$$I^w(f) = \int_a^b w(x)f(x) dx \quad \text{where} \quad w(x) > 0 \text{ is the weight function on } [a, b].$$

| Interval | w(x) | Orthogonal polynomials |
|---------------------|---------------------------------|--------------------------------|
| $[-1, 1]$ | 1 | <i>Legendre</i> |
| $[-1, 1]$ | $(1 - x)^s(1 + x)^t, s, t > -1$ | <i>Jacobi</i> |
| $[-1, 1]$ | $1/\sqrt{1 - x^2}$ | <i>Chebyshev</i> (first kind) |
| $[-1, 1]$ | $\sqrt{1 - x^2}$ | <i>Chebyshev</i> (second kind) |
| $[0, \infty]$ | e^{-x} | <i>Laguerre</i> |
| $[-\infty, \infty]$ | e^{-x^2} | <i>Hermite</i> |

Chebyshev quadrature

For the Gaussian rules with Chebyshev weight $w(x) = (1 - x^2)^{-1/2}$, nodes and weights are given by:

- **Gauss-Chebyshev:** $x_j = -\cos \frac{(2j+1)\pi}{2(n+1)}$, and $\alpha_j = \frac{\pi}{n+1}$, for $j = 0, \dots, n$
- **Gauss-Chebyshev-Lobatto:** $x_j = -\cos \frac{\pi j}{n}$, and $\alpha_j = \frac{\pi}{d_j n}$, for $j = 0, \dots, n$, $d_j = 2\chi_{0,n} + \chi_j$.

~~~ The Gauss node, for a fixed  $n \geq 0$ , are the zeros of the Chebyshev polynomial  $T_{n+1} \in \mathbb{P}_{n+1}$ .

~~~ For  $n \geq 1$ , the Gauss-Lobatto nodes  $\{x_j\}_1^{n-1}$  are the zeros of  $T'_n$ , i.e. the extrema of  $T_n$ .

Denoting by $\Pi_n^{\text{GL}} f$ the polynomial of degree n that interpolates f at the Gauss-Lobatto nodes, one has

$$\|f - \Pi_n^{\text{GL}} f\|_\infty \leq C n^{1/2-s} \|f\|_{w,s} = C n^{1/2-s} \left(\sum_{k=0}^s \|f^{(k)}\|_w^2 \right)^{\frac{1}{2}}$$

Thus, $\Pi_n^{\text{GL}} f$ converges pointwise to f as $n \rightarrow \infty$, for any $f \in C^1([-1, 1])$.

A similar result hold for $\Pi_n^G f$ of degree n that interpolates f at the $n + 1$ Gauss nodes x_j .

Legendre quadrature

The **Legendre** polynomial (with quadrature weight $w(x) \equiv 1$) are defined through the three-term relation

$$\begin{cases} L_{k+1}(x) = \frac{2k+1}{k+1}xL_k(x) - \frac{k}{k+1}L_{k-1}(x), & \text{for } k = 1, 2, \dots, \\ L_0(x) = 1, \quad L_1(x) = x. & \end{cases} \quad \text{so that} \quad (T_k, T_m)_w = \begin{cases} 0, & \text{if } k \neq m, \\ \pi, & \text{if } k = m = 0, \\ \pi/2, & \text{if } k = m \neq 0. \end{cases}$$

For every $k = 0, 1, \dots$, we have $L_k \in \mathbb{P}_k$ and $(L_k, L_m) = \delta_{k,m}(k + 1/2) - 1$ for $k, m = 0, 1, 2, \dots$

- For $n \geq 0$, the **Gauss-Legendre** nodes and the coefficients are given by

$$x_j \text{ s.t. } L_{n+1}(x_j) = 0, \quad \text{and} \quad \alpha_j = \frac{2}{(1 - x_j^2)[L'n + 1(x_j)]^2} \quad \text{for } j = 0, \dots, n$$

- For $n \geq 1$, the **Gauss-Legendre-Lobatto** nodes and coefficients are given by

$$\begin{aligned} x_0 &= -1, x_n = 1, \quad x_j \quad \text{s.t.} \quad L'_n(x_j) = 0, \quad \text{for } j = 1, \dots, n-1 \\ \text{and} \quad \alpha_j &= \frac{2}{n(n+1)[L_n(x_j)]^2} \quad \text{for } j = 0, \dots, n \end{aligned}$$

As for Chebyshev, for $\Pi_n^{\text{GLL}} f$ with $n + 1$ GLL nodes one has a similar error decay.

Gaussian quadrature

