Applied Math

Quadrature

Federico Pichi

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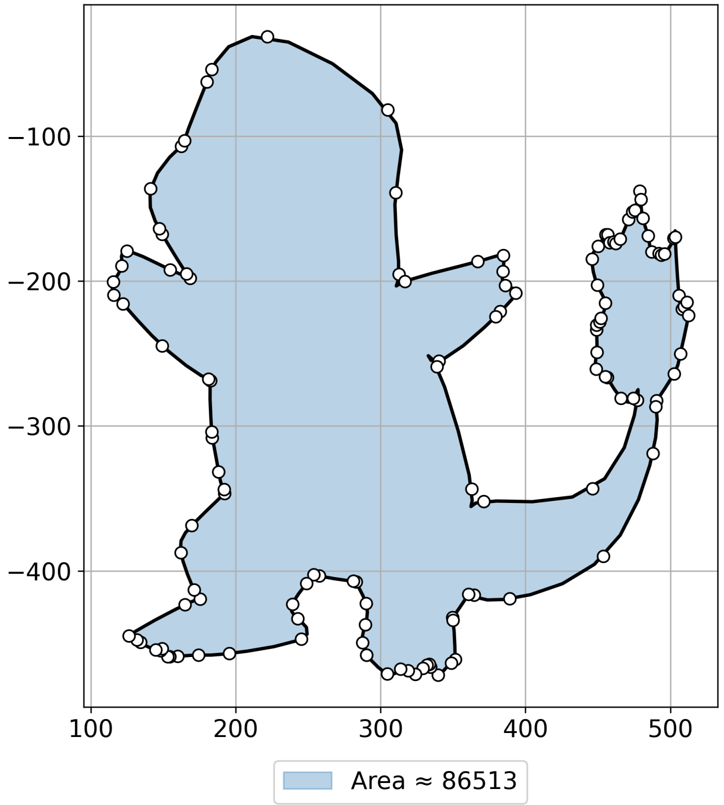
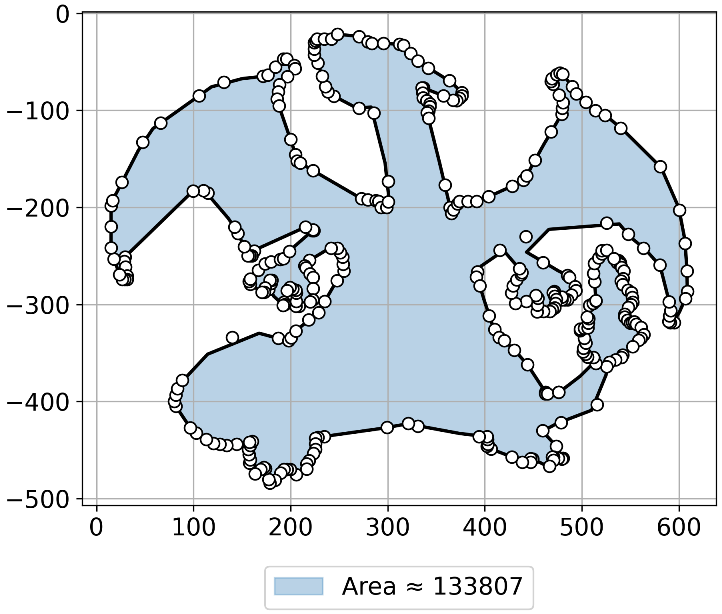
Motivations

- **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





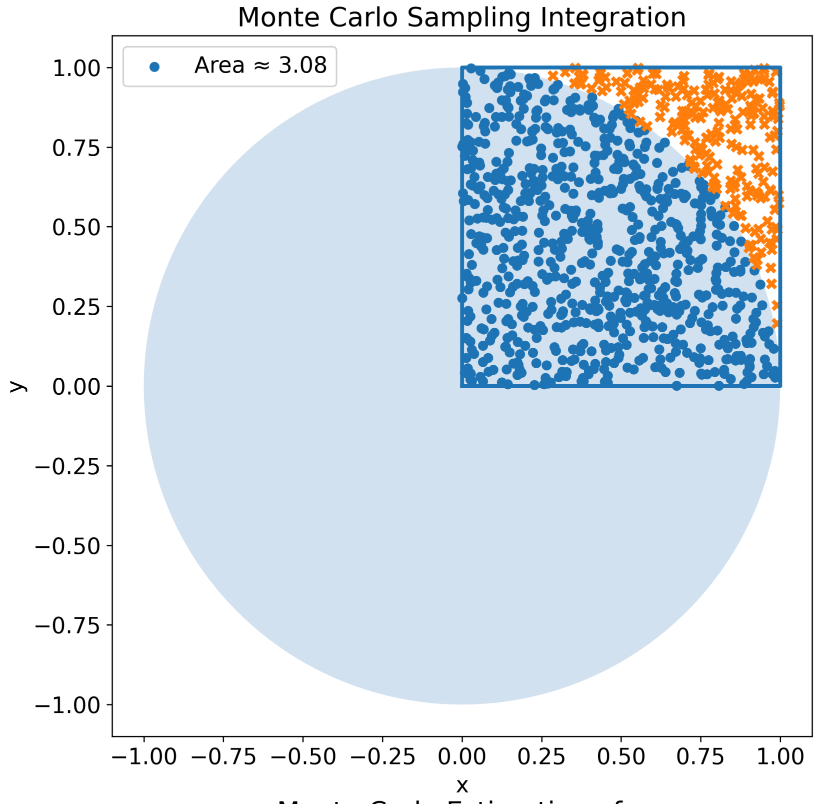
Methodologies and Challenges

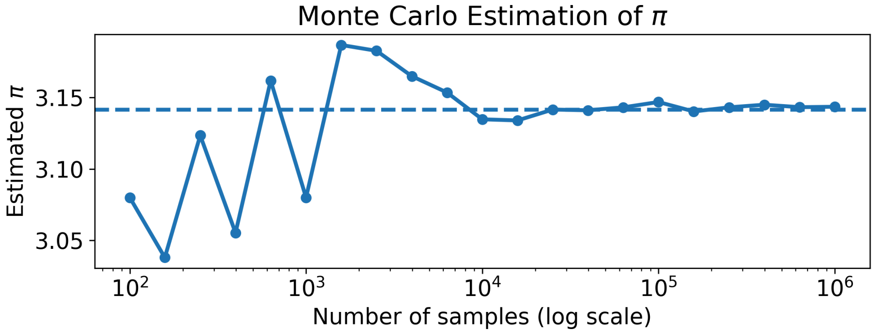
1. Deterministic Quadrature: fixed rules with known nodes and weights (Newton–Cotes, Gaussian, Clenshaw–Curtis)

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

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

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

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

- If $h_n = \max_{i=0}^{n-1} x_{i+1} - x_i$, for any choice of x_i such that $h_n \xrightarrow{n\to\infty} 0$ and ξ_i, we have a finite limit $\lim_{n\to\infty} R_n = R$, 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.
  $\rightsquigarrow$ 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 $f : \mathbb{R} \to \mathbb{R}$ 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

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

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

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

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

$\rightsquigarrow$ 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 $I(f) = F(b) - F(a)$.
$\rightsquigarrow$ 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

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

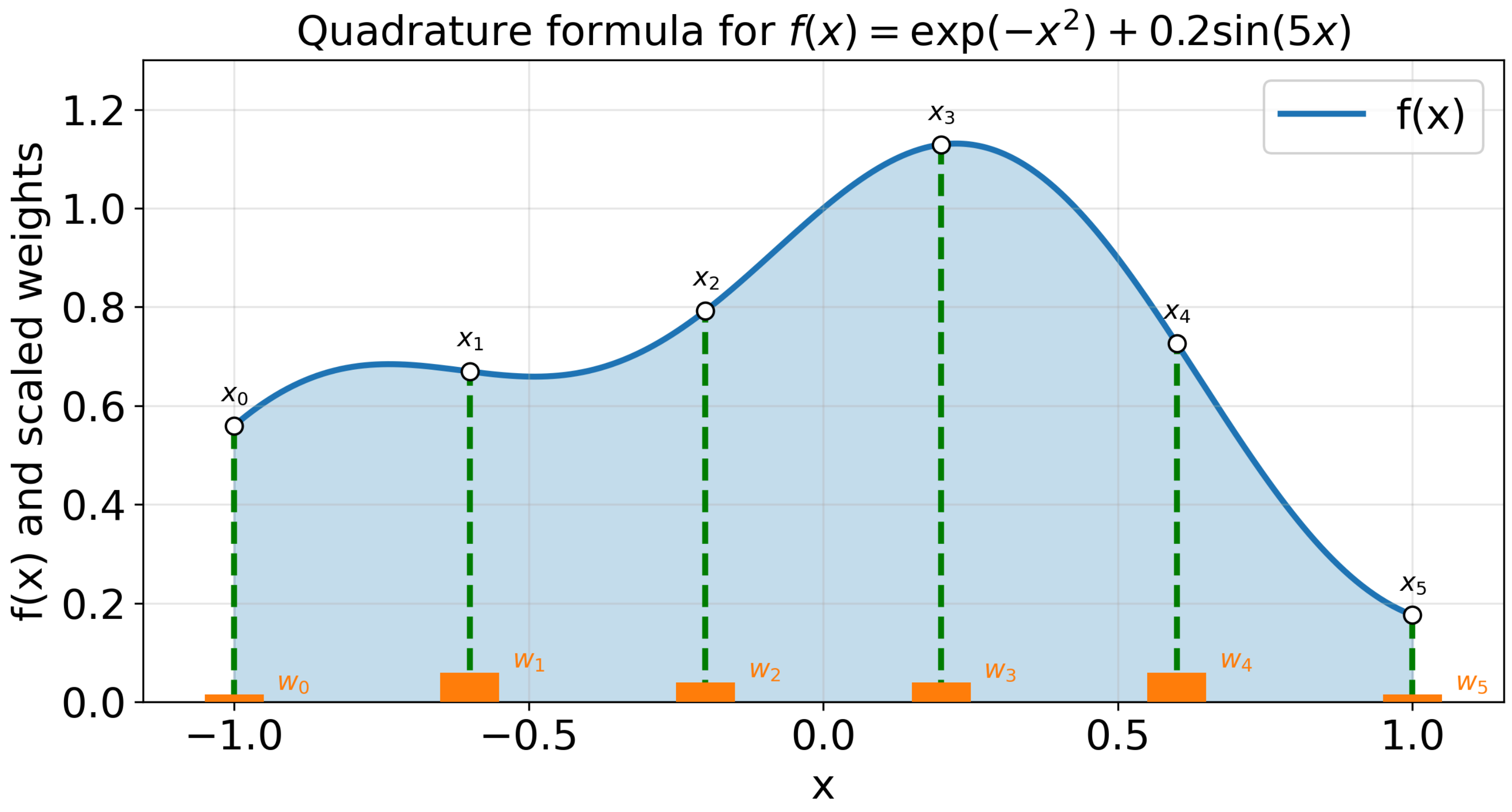
and the error of the quadrature formula is defined as $E_n = I - I_n$.

- 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. $I_n(f) \doteq I(f_n)$.
$\rightsquigarrow$ 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 $w_i = \int_a^b l_i(x)\,dx$.

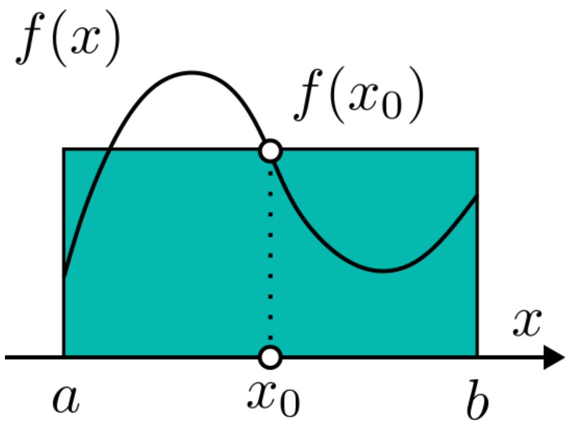
The **degree of exactness** of a quadrature rule is the maximum $r \geq 0$ for which $I_n(f) = I(f), \forall f \in \mathbb{P}_r$.

- 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 $I_n(\Pi_n f) = I(\Pi_n f)$.
- 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 $[a, b]$

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



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

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

$\rightsquigarrow$ midpoint rule is exact for constant and affine functions, since $f''(\xi) = 0, \forall \xi \in (a, b)$, so that $r = 1$.

Composite midpoint formula

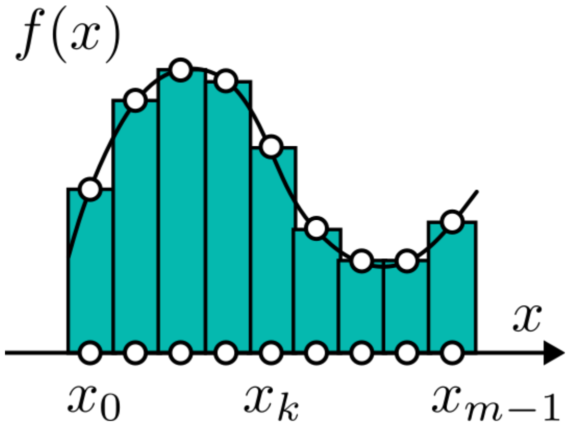
If the width of the integration interval $[a, b]$ is not sufficiently small, the quadrature error can be quite large.

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

$\rightsquigarrow$ consider $m \geq 1$ subintervals of width $H = (b-a)/m$, and quadrature nodes $x_k = a + (2k+1)H/2$ for $k = 0, \ldots, m-1$, 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 $\xi \in (a, b)$.
$\rightsquigarrow$ 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**

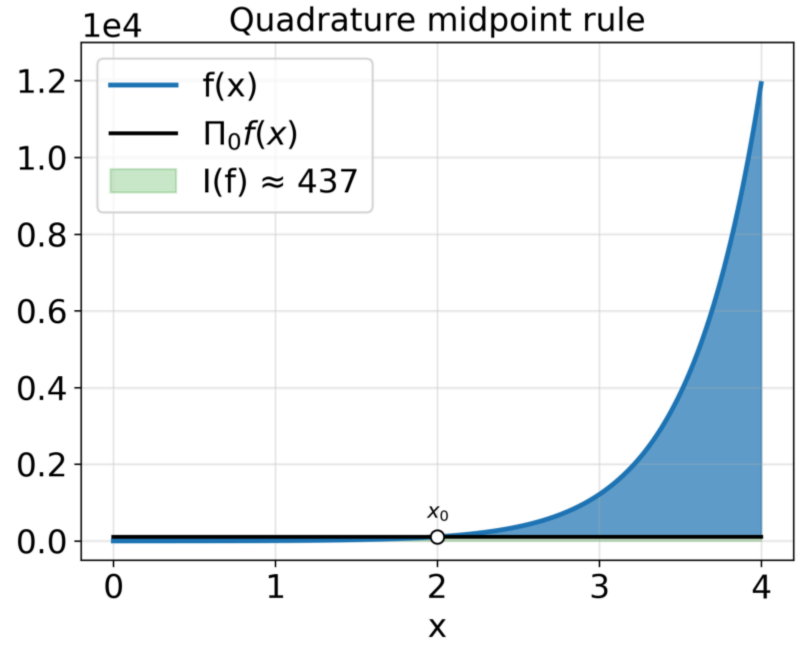
$$\int_0^4 xe^{2x}\,dx = \left[\frac{x}{2}e^{2x} - \frac{1}{4}e^{2x}\right]_0^4 = \frac{1}{4}(7e^8 - 1) = 5217$$

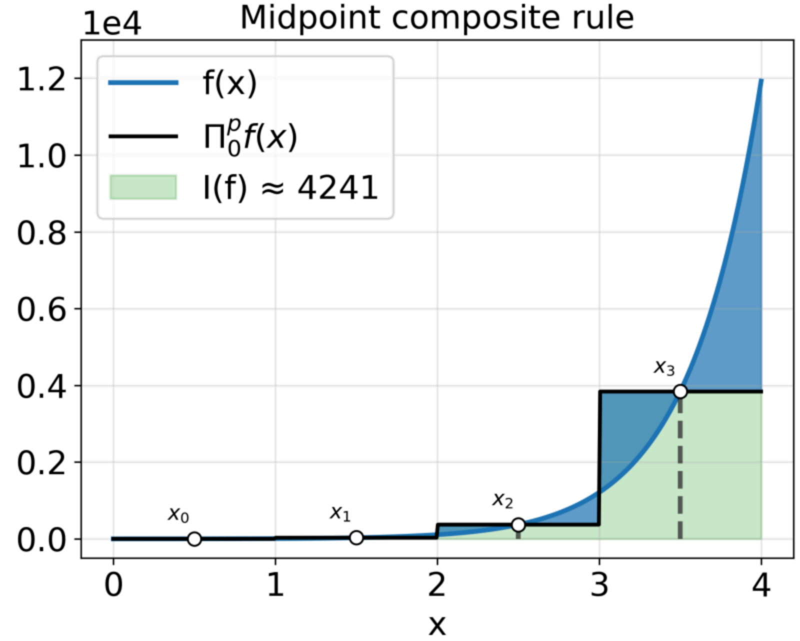
- **Midpoint rule**

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

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

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





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 $\Pi_1 f(t) = (1 - t) f(a) + t f(b)$, thus

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

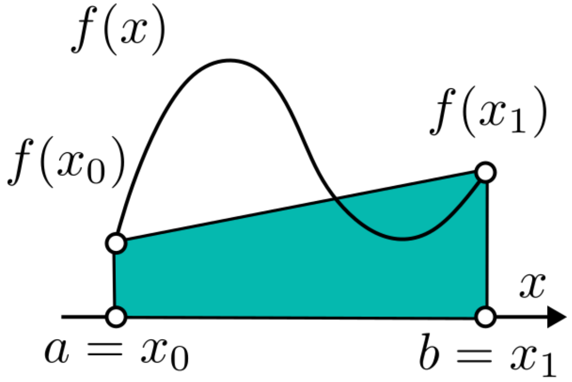
Trapezoidal (composite) formula

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

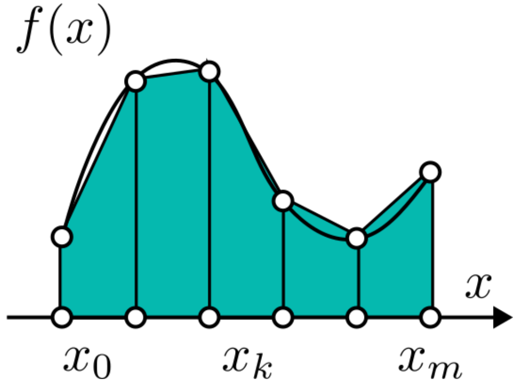
$$I_1(f) = \frac{b-a}{2}[f(a) + f(b)], \quad \text{with} \quad E_1(f) = -\frac{h^3}{12} f''(\xi),$$

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

$\rightsquigarrow$ 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 $k = 0, \ldots, m$, 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**

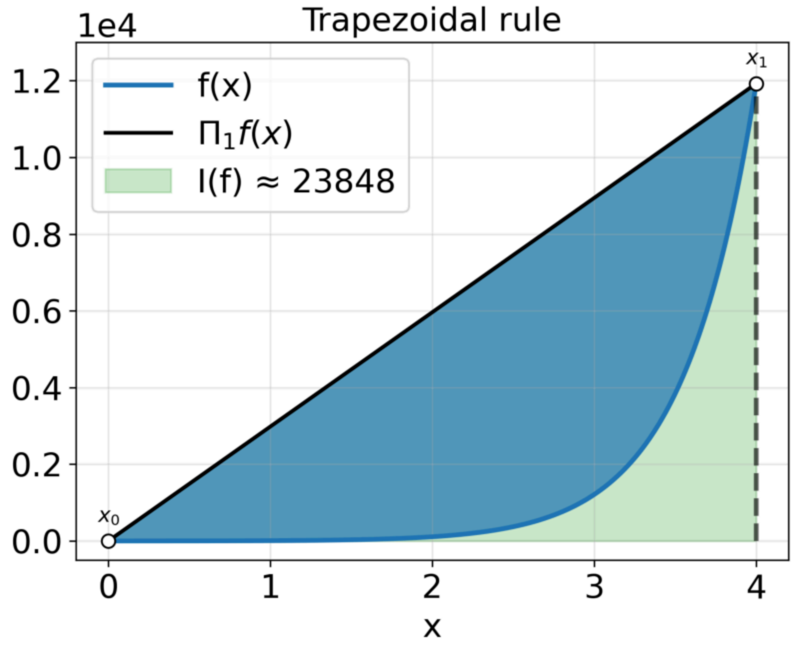
$$\int_0^4 xe^{2x}\,dx = \left[\frac{x}{2}e^{2x} - \frac{1}{4}e^{2x}\right]_0^4 = \frac{1}{4}(7e^8 - 1) = 5217$$

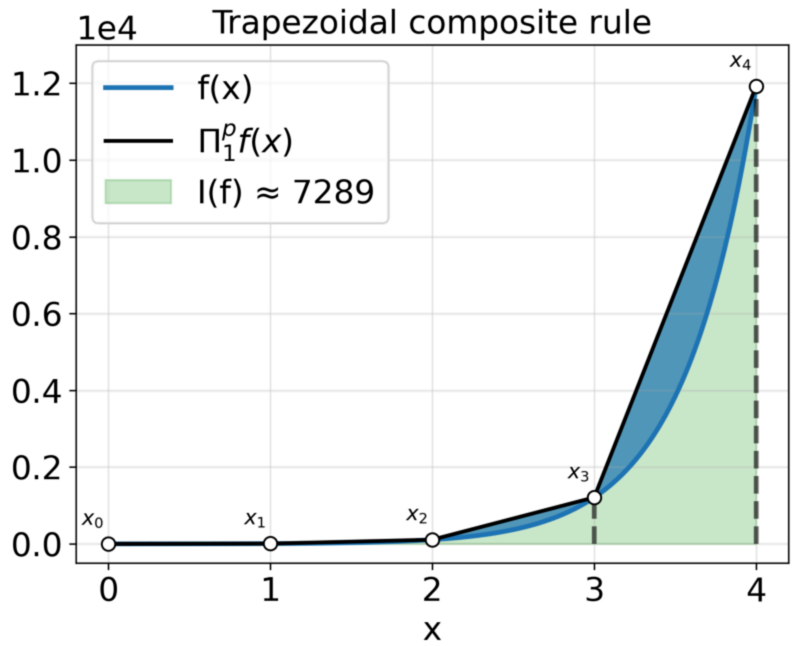
- **Trapezoidal rule**

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

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

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





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

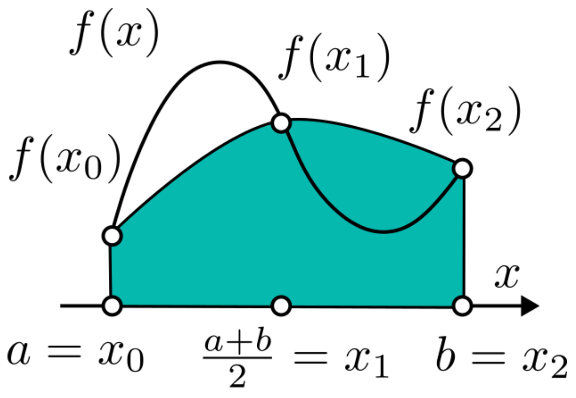
$$\Pi_2 f(t)=\frac{t(1-t)}{2}f(x_0)+(1-t)^2f(x_1)+\frac{t(t+1)}{2}f(x_2),\quad \text{so that}$$

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

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

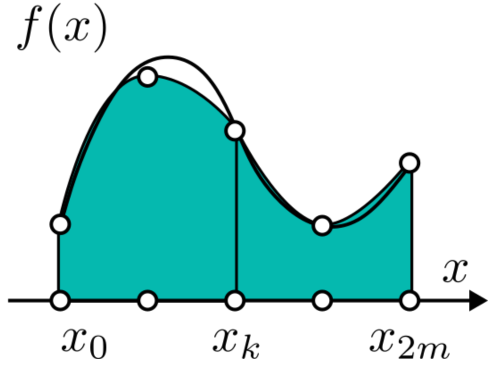
$$I_2(f) = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right], \quad \text{with} \quad E_2(f) = -\frac{h^5}{90} f''''(\xi).$$



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

For the **composite** rule we replace f with its piecewise interpolant Π_2^p.

Given $m \geq 1$ of width $H = (b-a)/m$, and quadrature nodes $x_k = a + kH/2$ for $k = 0, \ldots, 2m$, 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**

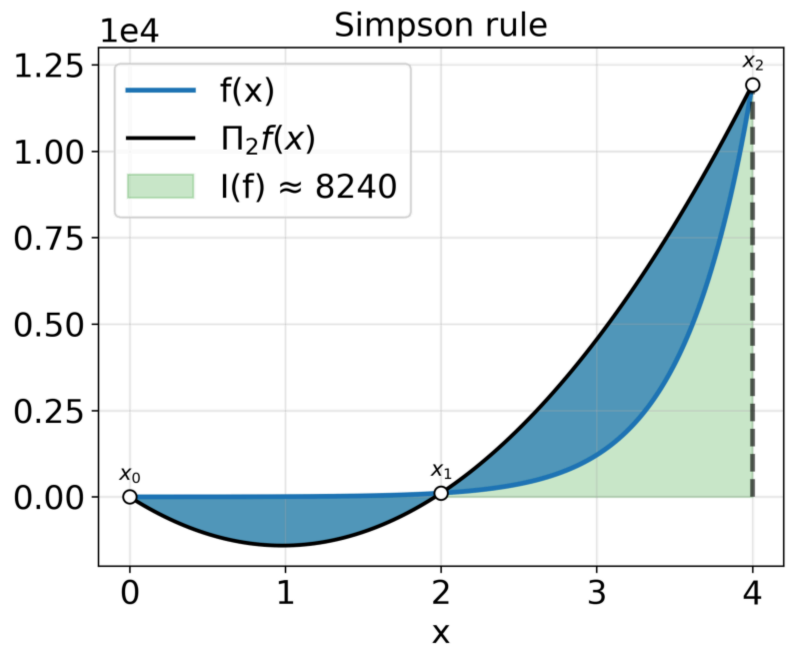
$$\int_0^4 xe^{2x}\, dx = \left[\frac{x}{2}e^{2x} - \frac{1}{4}e^{2x}\right]_0^4 = \frac{1}{4}(7e^8 - 1) = 5217$$

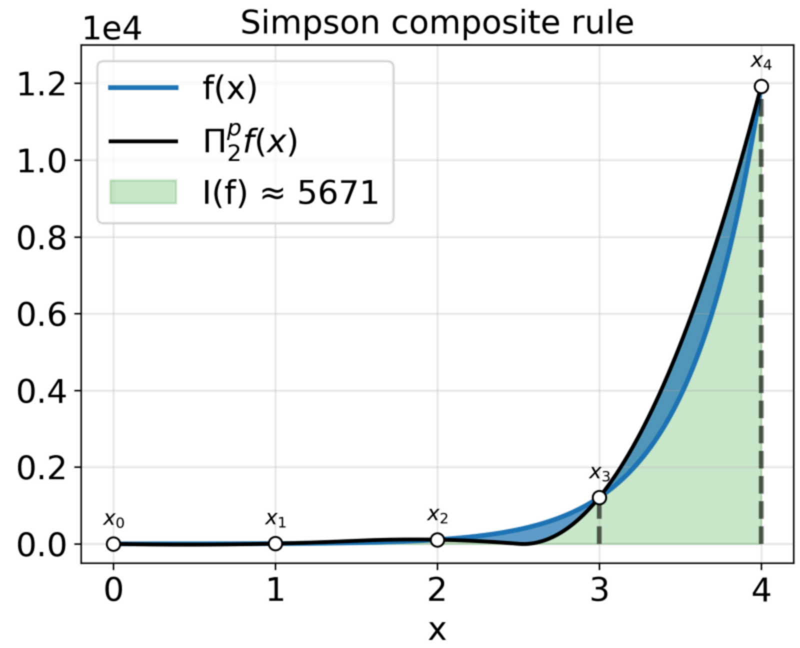
- **Simpson rule**

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

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

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





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.

$\rightsquigarrow$ 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

$$\begin{aligned}
w_0 \cdot 1 + w_1 \cdot 1 + \cdots + w_n \cdot 1 &= \int_a^b 1 \, dx = [x]_a^b = b - a \\
w_0 \cdot x_0 + w_1 \cdot x_1 + \cdots + w_n \cdot x_n &= \int_a^b x \, dx = [x^2/2]_a^b = (b^2 - a^2)/2 \\
&\vdots \\
w_0 \cdot x_0^n + w_1 \cdot x_1^n + \cdots + w_n \cdot x_n^n &= \int_a^b x^n \, dx = [x^{n+1}/(n+1)]_a^b = (b^{n+1} - a^{n+1})/(n+1)
\end{aligned}$$

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 $x_0, \ldots, x_n$, 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 $I_n(f) \overset{n\to\infty}{\longrightarrow} I(f)$ 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

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

$\rightsquigarrow$ 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 $n \geq 0$.

$\rightsquigarrow$ 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: $x_k = x_0 + kh$,
$\Psi(0) = a$, $\Psi(n) = b$

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

Open: $x_k = x_0 + (k+1)h$,
$\Psi(-1) = a$, $\Psi(n+1) = b$

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

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

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 $i = 0, \ldots, n-1$

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 $i = 0, \ldots, n$

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

$$M_n = \begin{cases} \int\limits_0^n \pi_{n+1}(t)dt < 0 & \text{for } \textbf{closed} \text{ formulae,} \\ \int\limits_{-1}^{n+1} \pi_{n+1}(t)dt > 0 & \text{for } \textbf{open} \text{ formulae.} \end{cases}$$

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

$$K_n = \begin{cases} \int\limits_0^n t\, \pi_{n+1}(t) dt < 0 & \text{for } \textbf{closed} \text{ formulae,} \\ \int\limits_{-1}^{n+1} t\, \pi_{n+1}(t) dt > 0 & \text{for } \textbf{open} \text{ formulae.} \end{cases}$$

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

Newton-Cotes errors

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

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

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

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

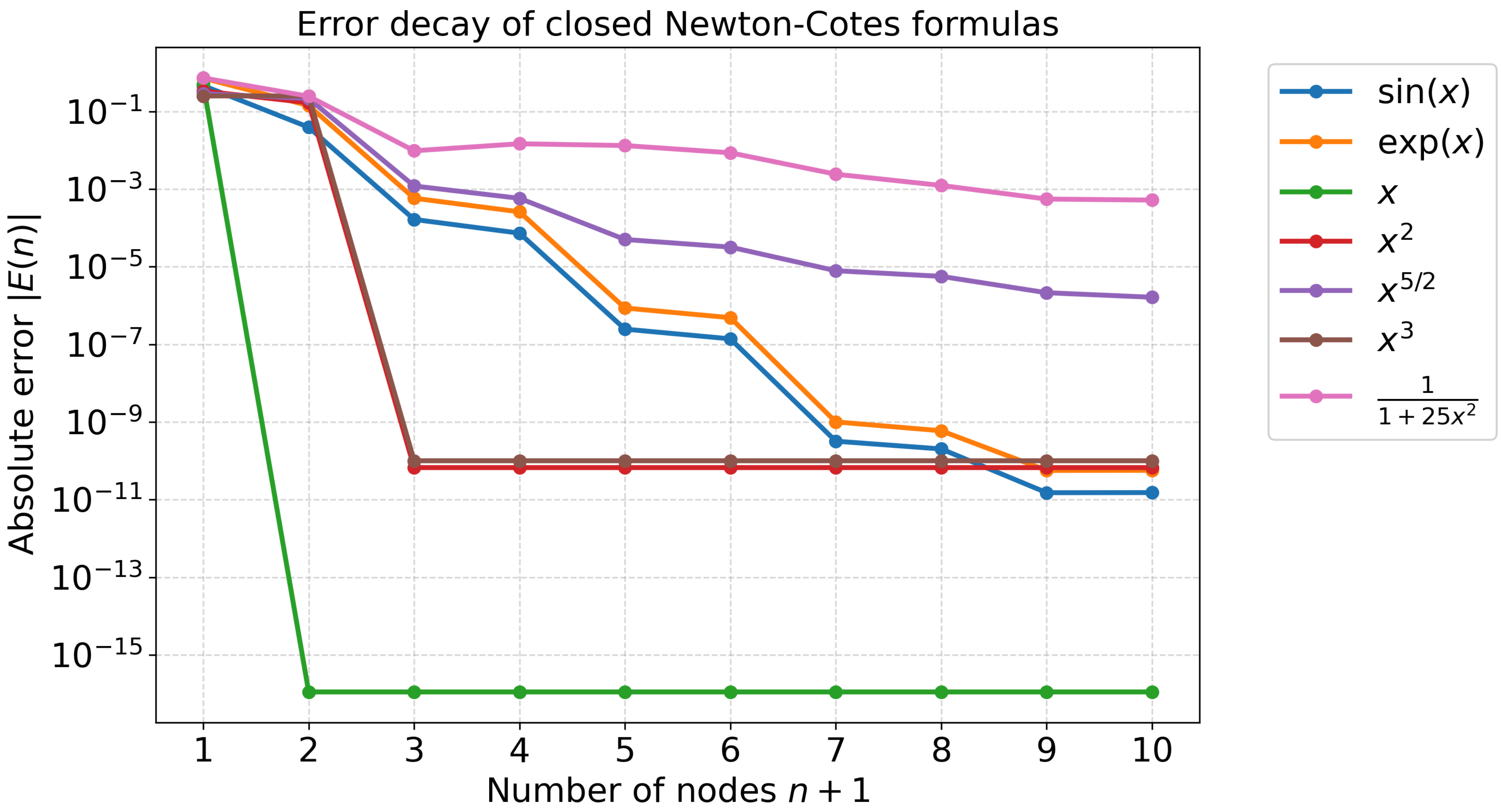
- **Simpson's 1/3 Rule**: quadratic interpolant $n = 2$

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

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

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

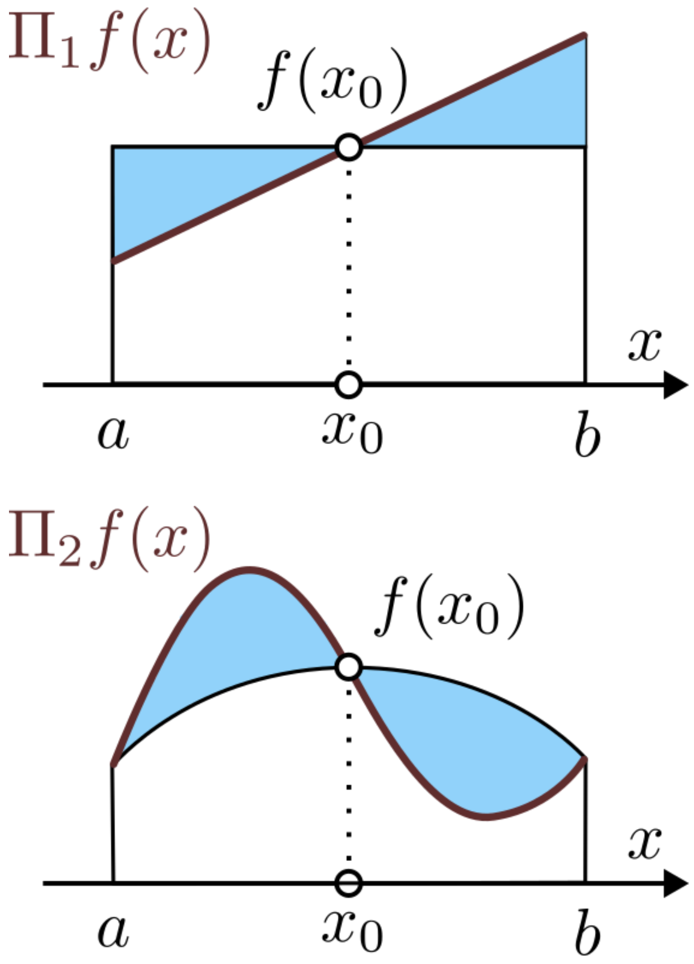
Newton-Cotes errors



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 $\sum_{i=0}^{n} |w_i| \xrightarrow{n\to\infty} \infty$, 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, $E_{n,m}(f) \overset{m\to\infty}{\longrightarrow} 0$, i.e., as $H \to 0$, 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

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

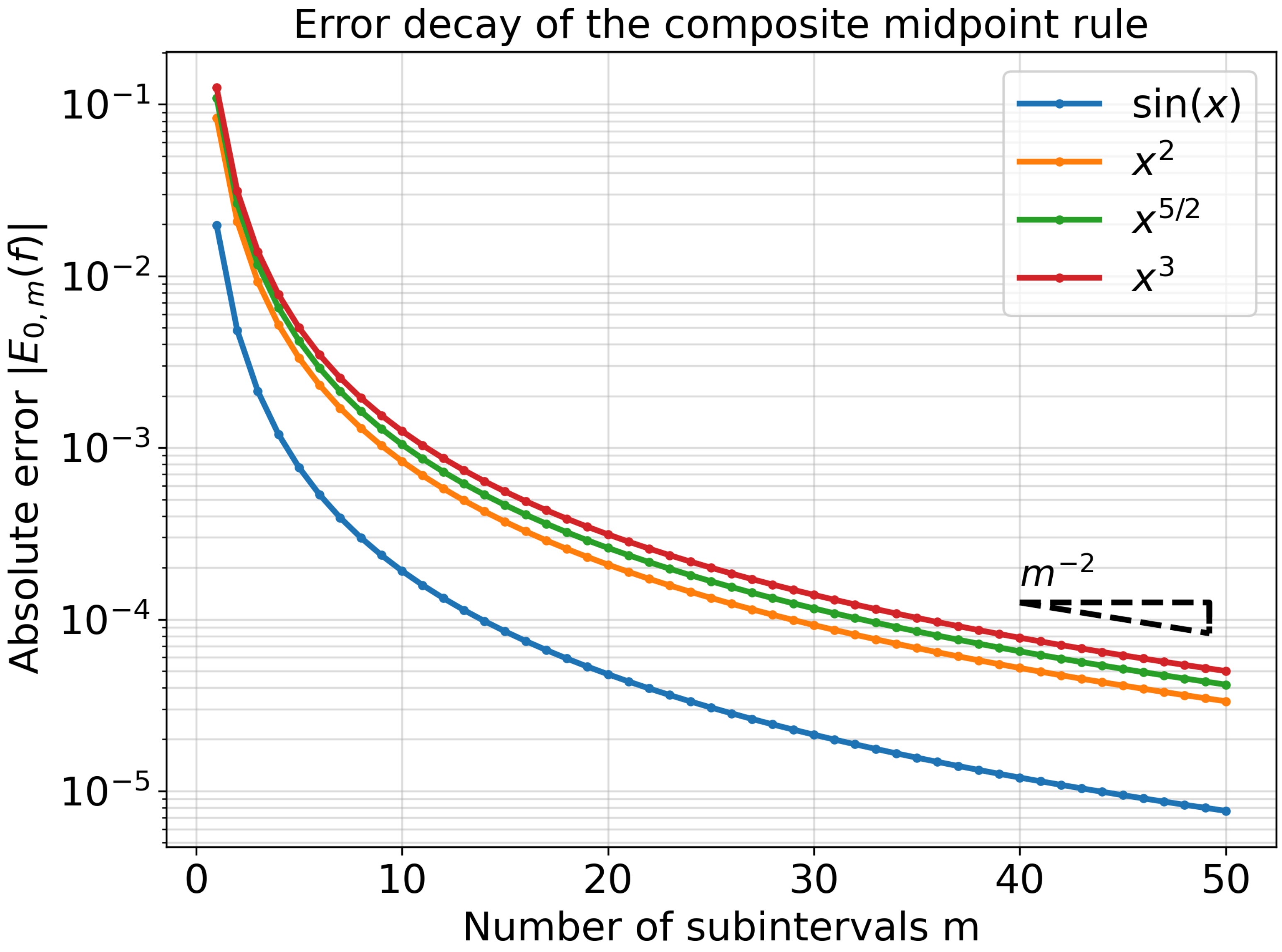
Moreover

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

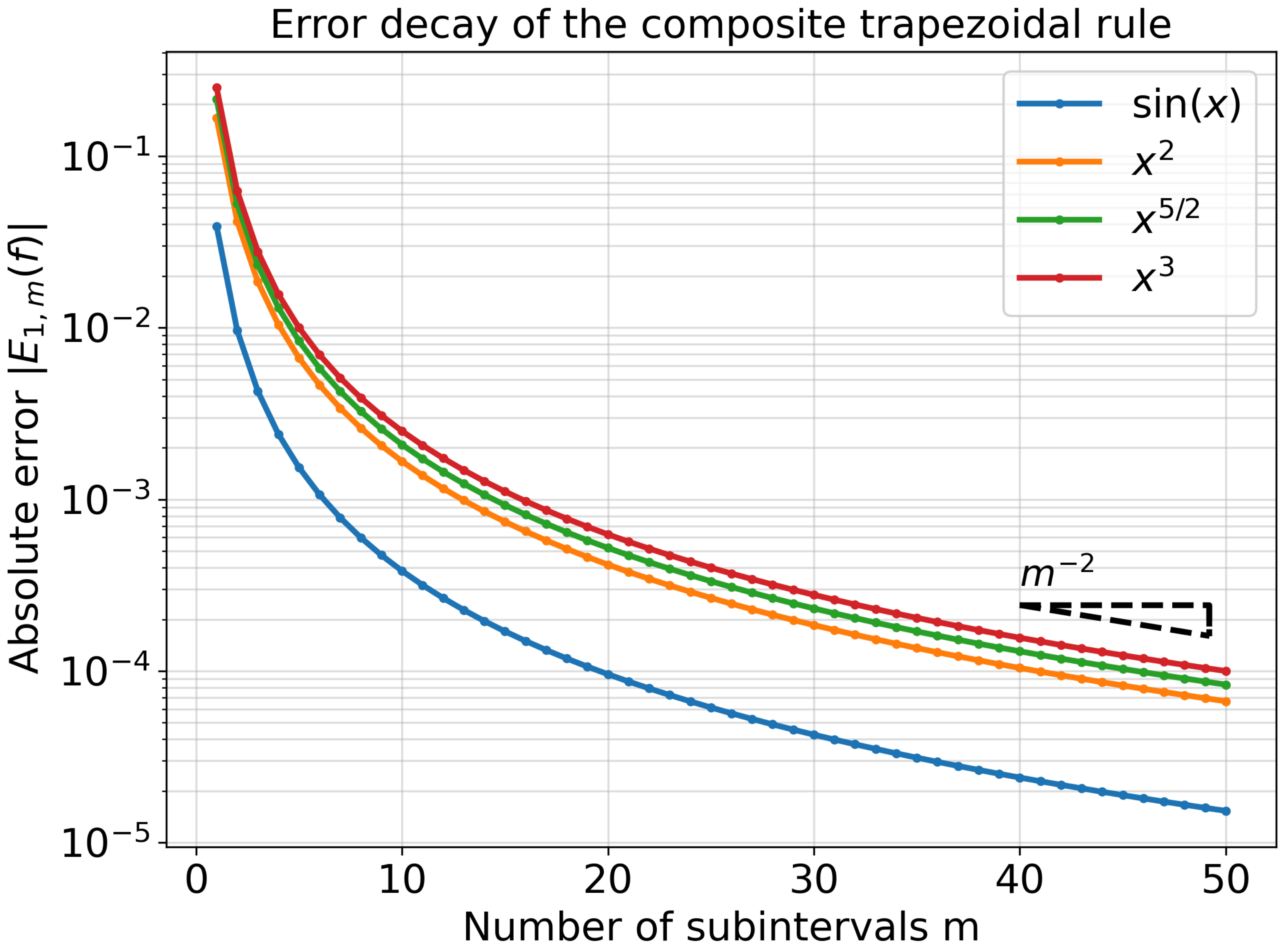
where the module of continuity of the function f is defined as

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

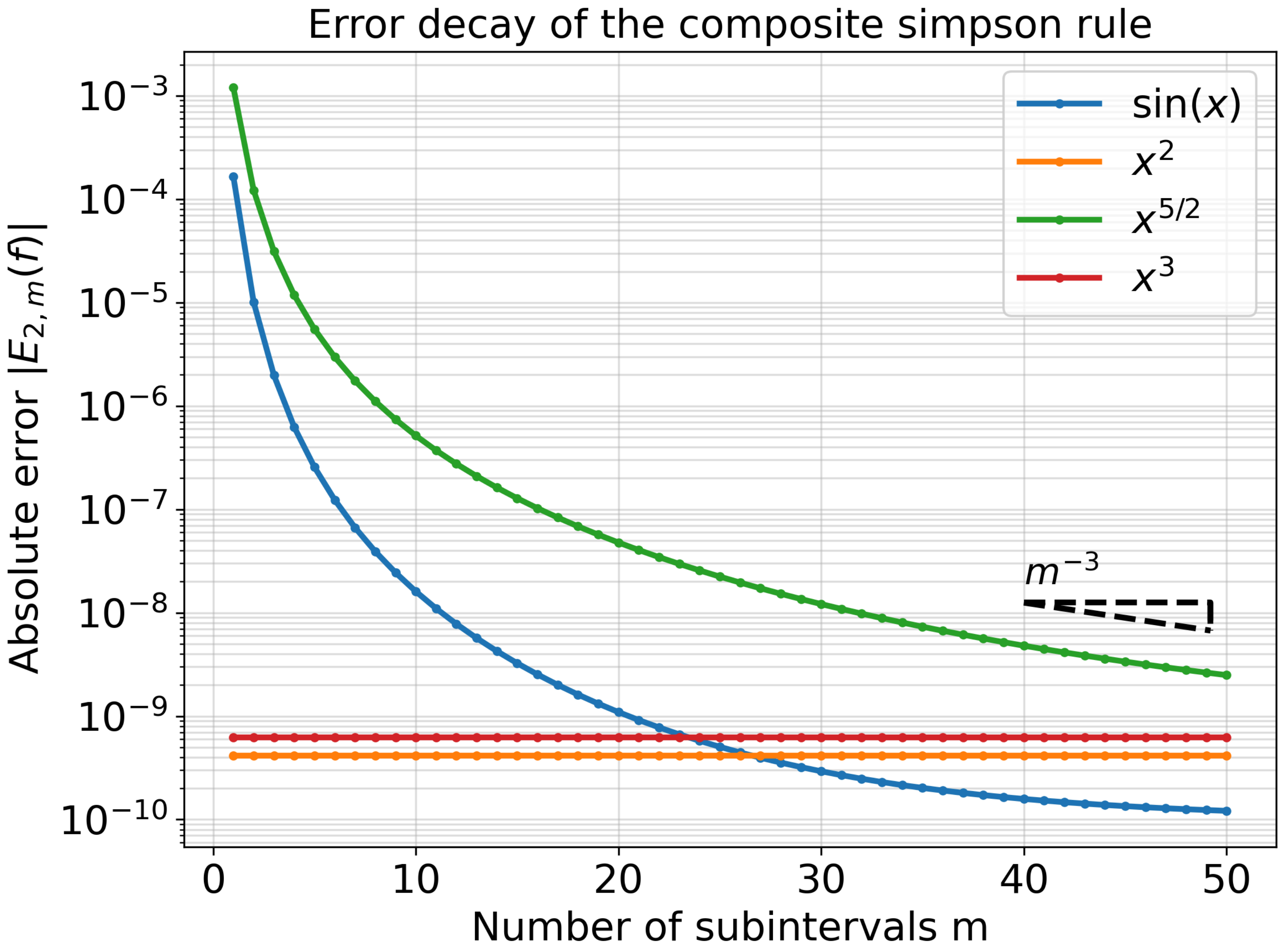
Composite Newton-Cotes formulae and errors



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**

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

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

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

$\rightsquigarrow$ 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

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

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

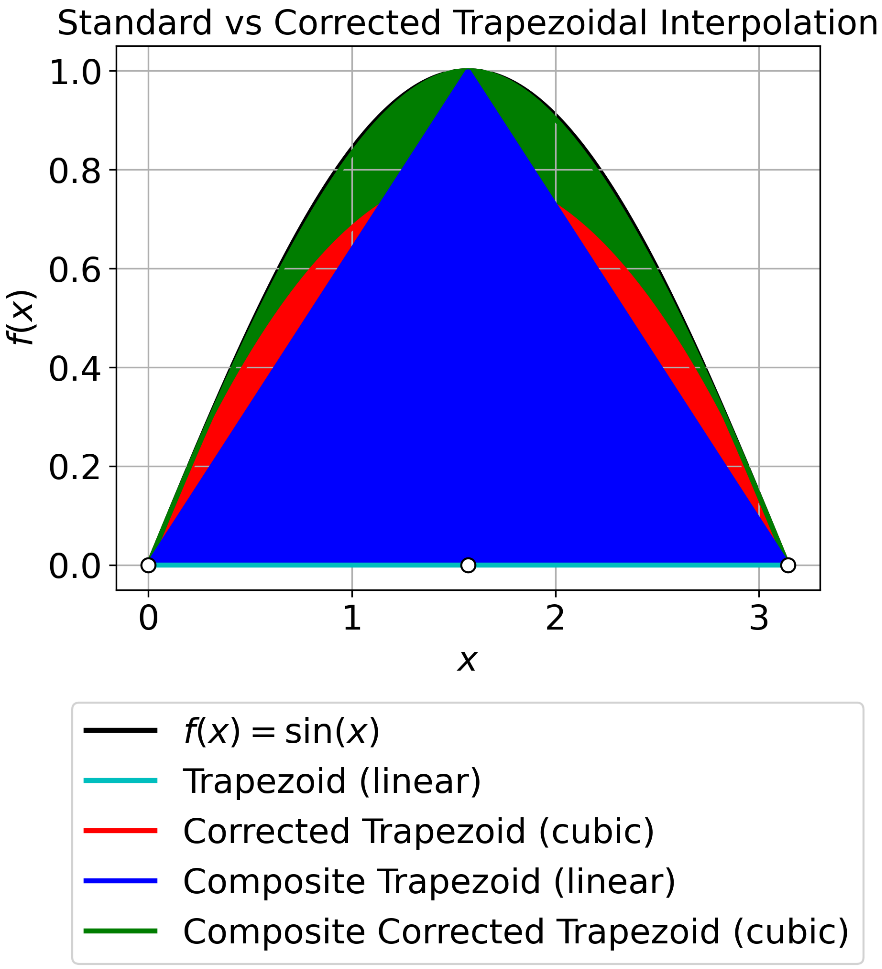
$$I(f) = \int_0^\pi \sin(x)\, dx = [\cos(x)]_\pi^0 = 2.$$

- **Corrected trapezoid rule**

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

- **Corrected composite trapezoid rule**

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



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 $L^2_w(-1, 1)$ as

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

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^2_w 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^2_w, i.e.

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

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 $f \in L^2_w(-1, 1)$. The **Chebyshev polynomials** are defined as

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

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

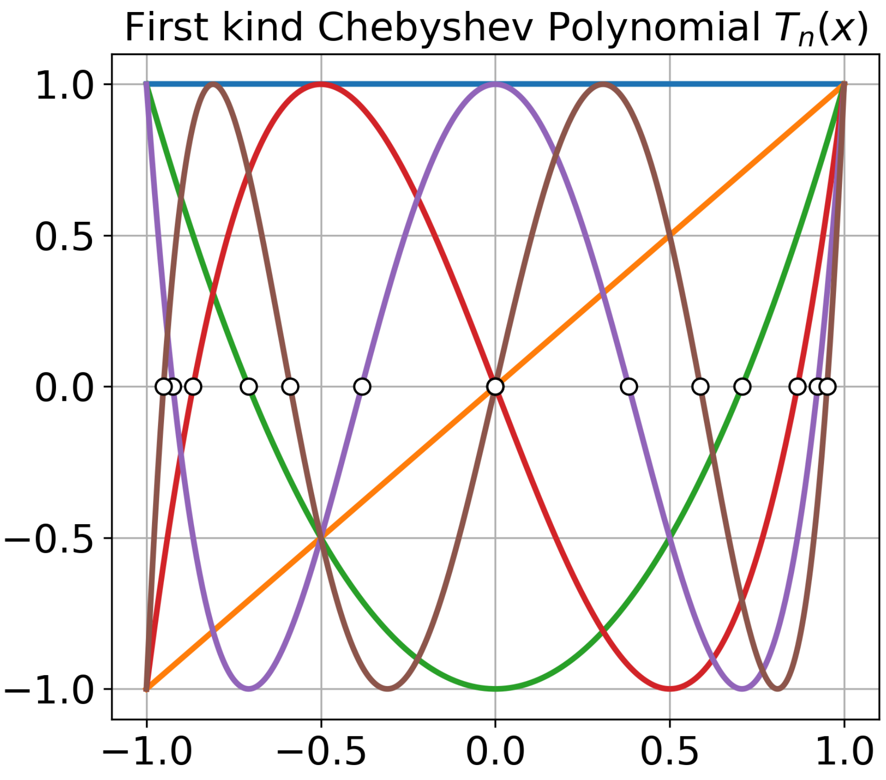
$$\cos(n\theta) = 0 \quad \rightsquigarrow \quad n\theta = \frac{\pi}{2} + m\pi, \; m = 0, \dots, n-1, \quad \rightsquigarrow \quad \theta_k = \frac{(2k-1)\pi}{2n}, \; k = 1, \dots, n,$$

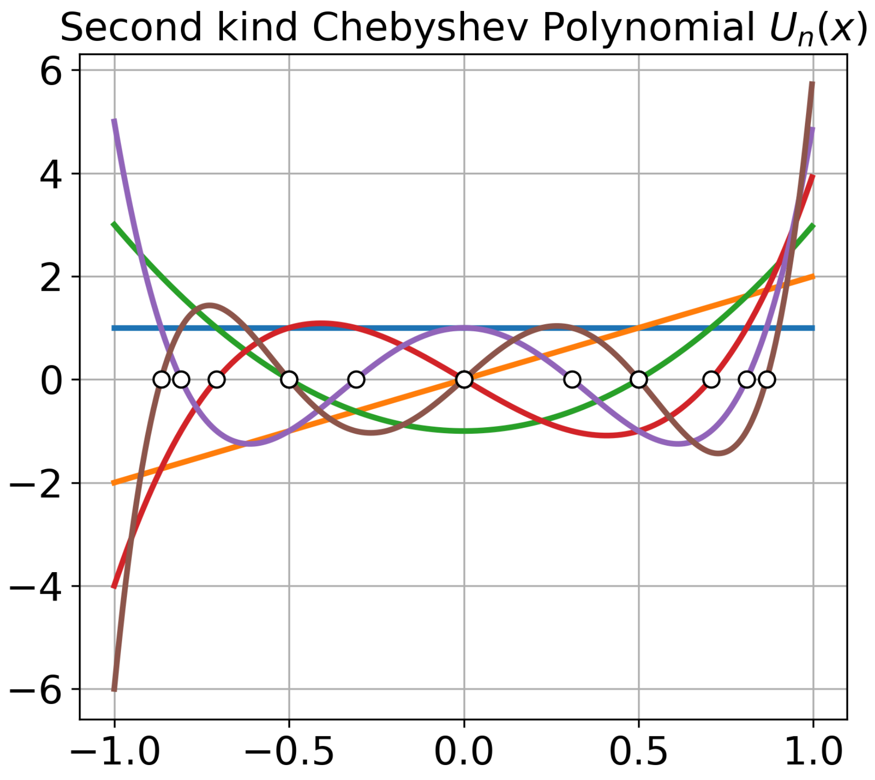
and thus we get the corresponding distinct zeros in x-space as

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

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 $n \to \infty$.
- Clenshaw-Curtis rule are always stable and significantly more accurate than NC.
- Clenshaw-Curtis rule with n nodes have degre 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 weigths 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 $j = 0, \ldots, n$.
- 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 $2n - 1$.

Method of undetermined coefficients

Consider the 2-node quadrrature 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:

$$\begin{aligned} f = 1 \quad &\Rightarrow \quad \int_{-1}^{1} 1\,dx = 2 = \alpha_0 + \alpha_1 \\ f = x \quad &\Rightarrow \quad \int_{-1}^{1} x\,dx = 0 = \alpha_0 x_0 + \alpha_1 x_1 \\ f = x^2 \quad &\Rightarrow \quad \int_{-1}^{1} x^2\,dx = \frac{2}{3} = \alpha_0 x_0^2 + \alpha_1 x_1^2 \\ f = x^3 \quad &\Rightarrow \quad \int_{-1}^{1} x^3\,dx = 0 = \alpha_0 x_0^3 + \alpha_1 x_1^3 \end{aligned} \qquad \Rightarrow \qquad \begin{cases} \alpha_0 & = 1 \\ \alpha_1 & = 1 \\ x_0 & = -\frac{1}{\sqrt{3}} \\ x_1 & = \frac{1}{\sqrt{3}} \end{cases}$$

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

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

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

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

Thus, $\Pi_n^{\mathrm{GL}} f$ converges pointwise to f as $n \to \infty$, for any $f \in C^1([-1, 1])$.
A similar result hold for $\Pi_n^{\mathrm{G}} f$ 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

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

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

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

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

Gaussian quadrature