Applied Math

Quadrature

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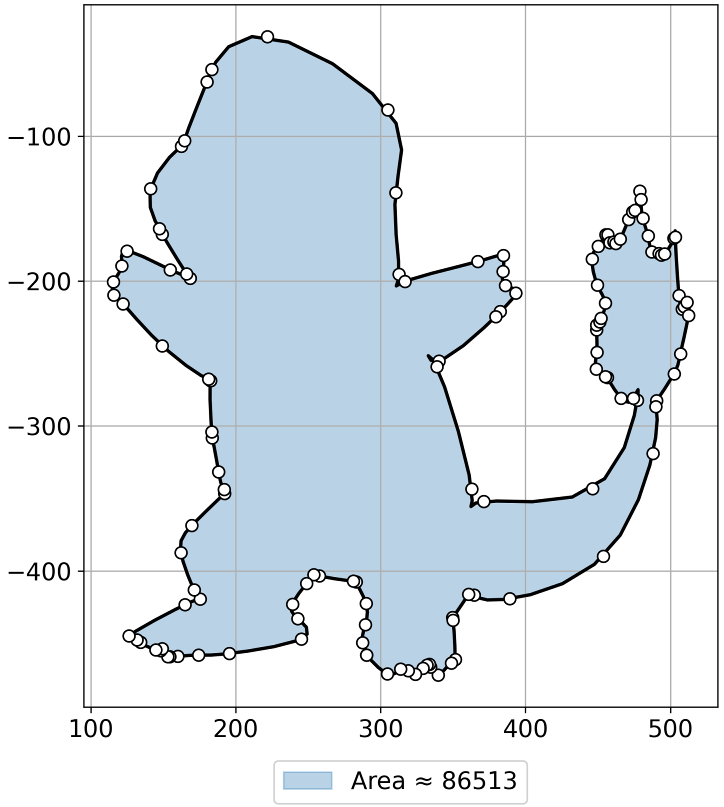
Outline

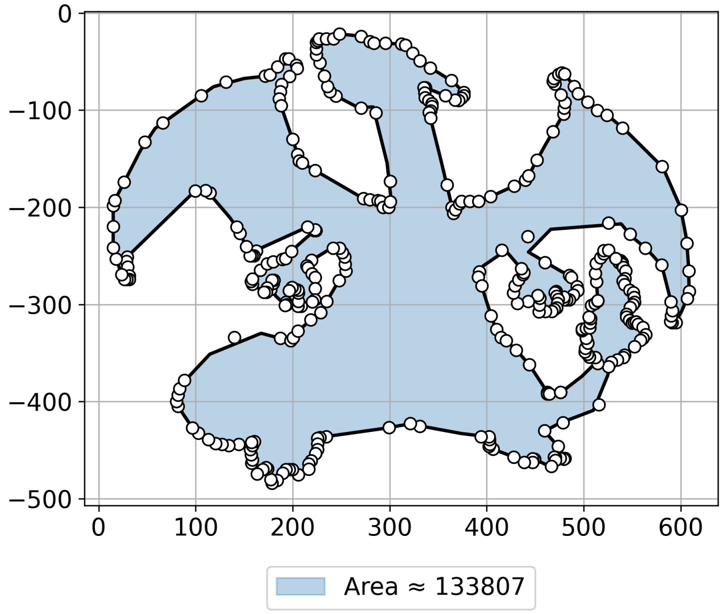
- Introduction
- Integration Problem
- Numerical Quadrature
  - Midpoint Rule
  - Trapezoidal Rule
  - Simpson's Rule
- Composite Formulae
- Method of Undetermined Coefficients
- Newton-Cotes Formulae

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





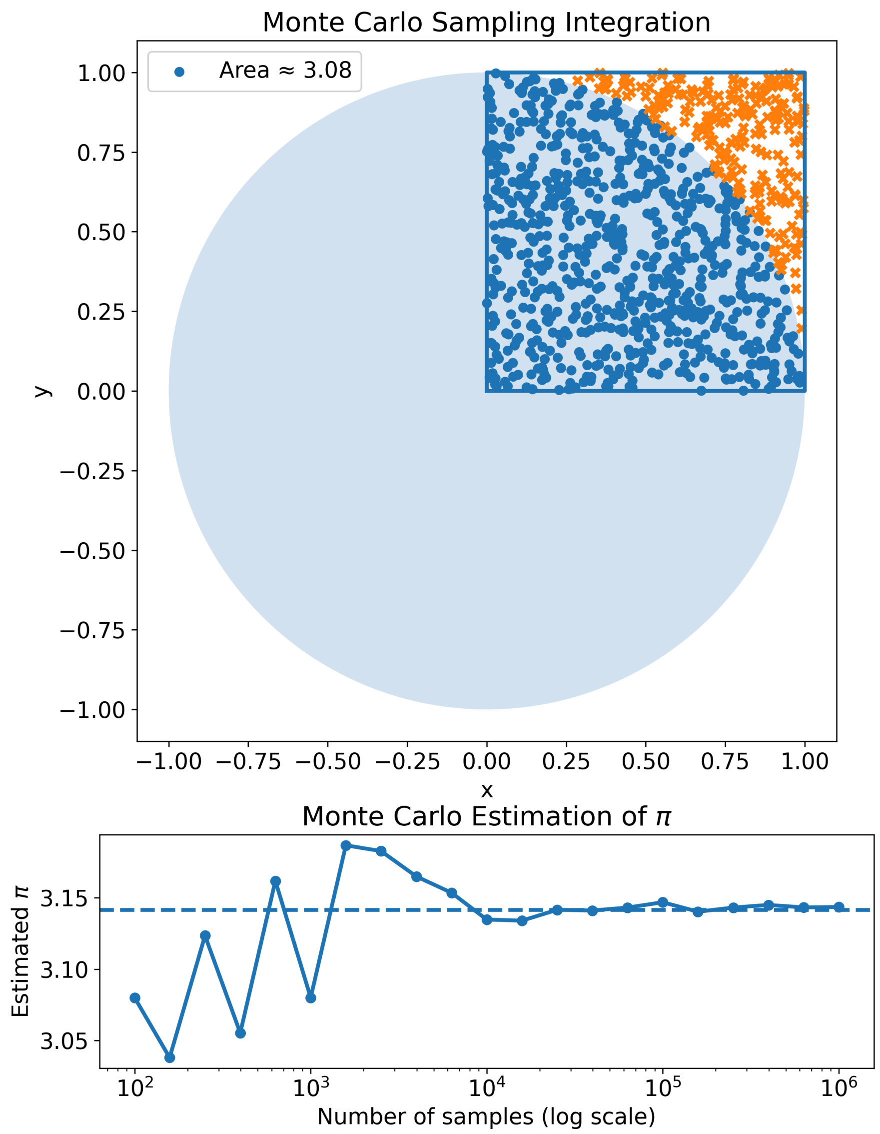
Methodologies and Challenges

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

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

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

$\leadsto$ 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

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

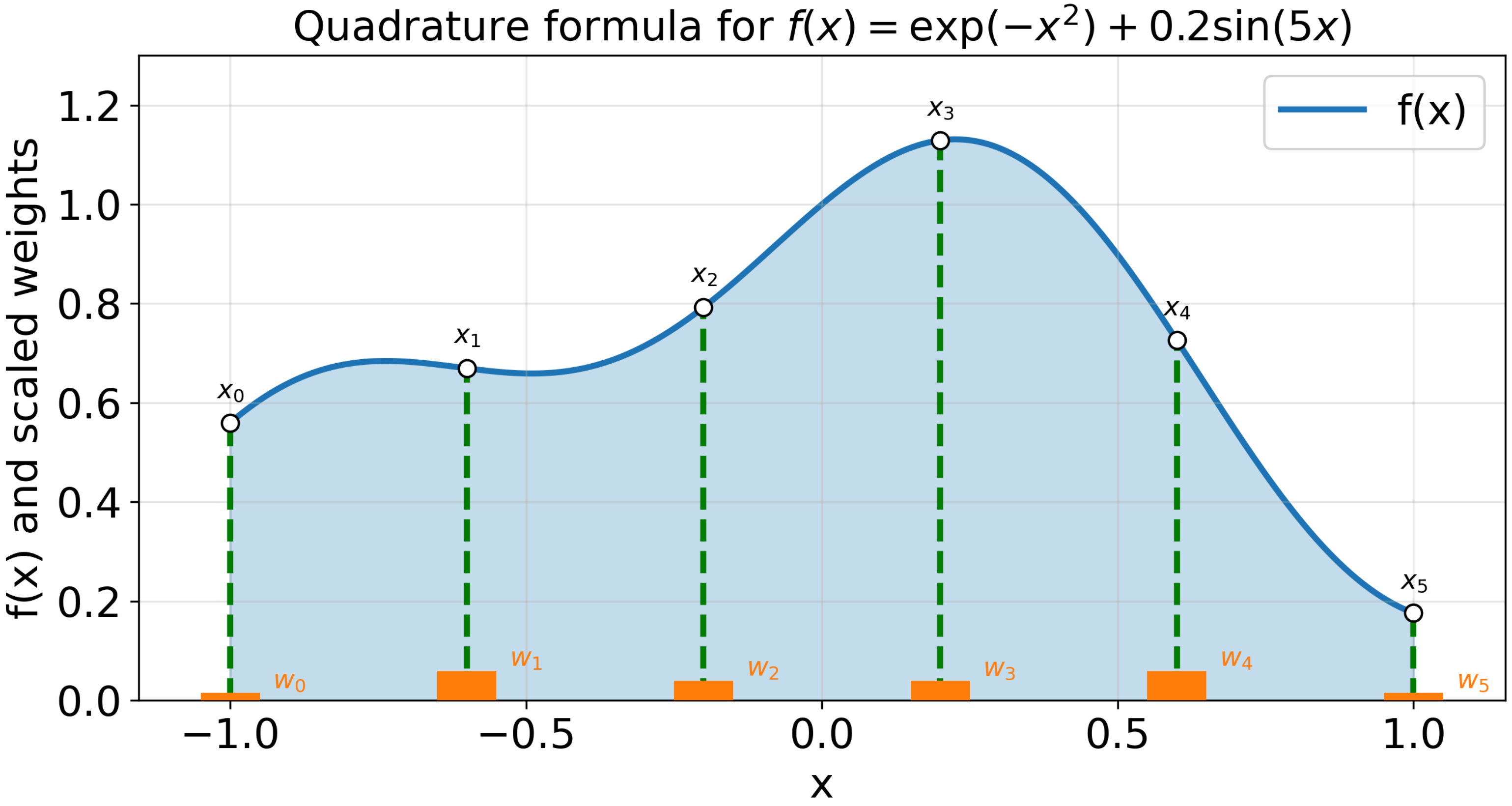
and the error of the quadrature formula is defined as $E_n = I - I_n$.

- 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 $w_i = \int_a^b l_i(x)\, dx$.

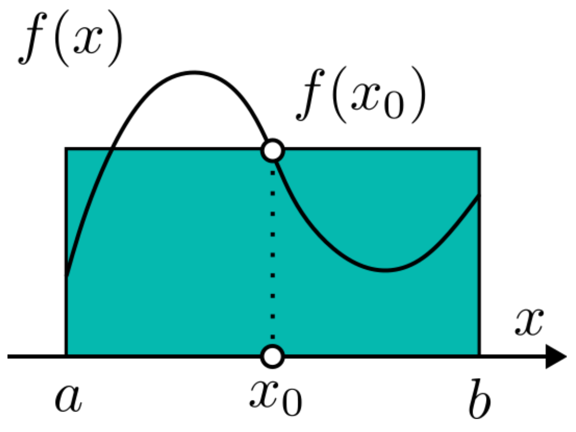
The **degree of exactness** of a quadrature rule is the maximum $r \geq 0$ for which $I_n(f) = I(f), \forall f \in \mathbb{P}_r$.

- 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

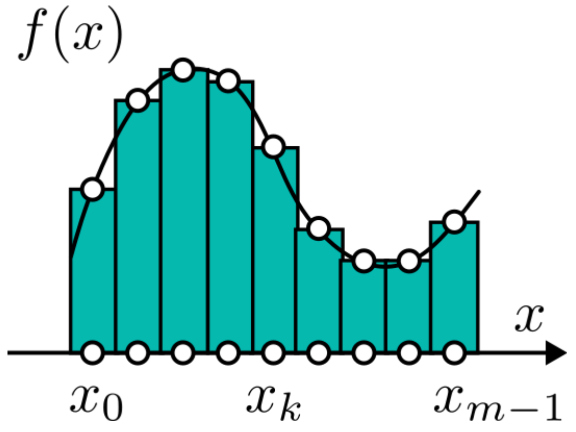
$$E_0(f) = \frac{h^3}{3} f''(\xi), \quad \text{where } h = \frac{b-a}{2}, \text{ and } \xi \in (a, b).$$

$\rightsquigarrow$ 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**

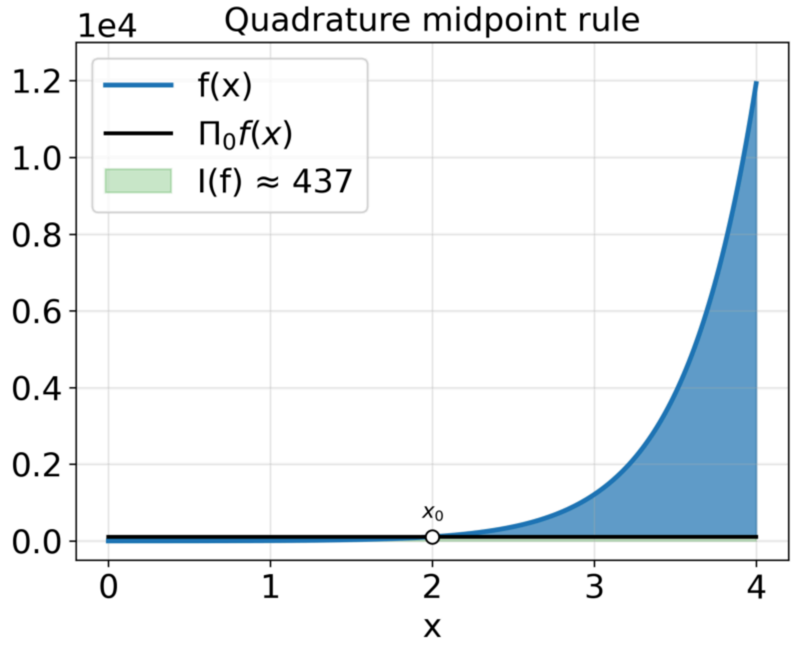
$$\int_0^4 xe^{2x}\,dx = \left[\frac{x}{2}e^{2x} - \frac{1}{4}e^{2x}\right]_0^4 = \frac{1}{4}(7e^8 - 1) = 5217$$

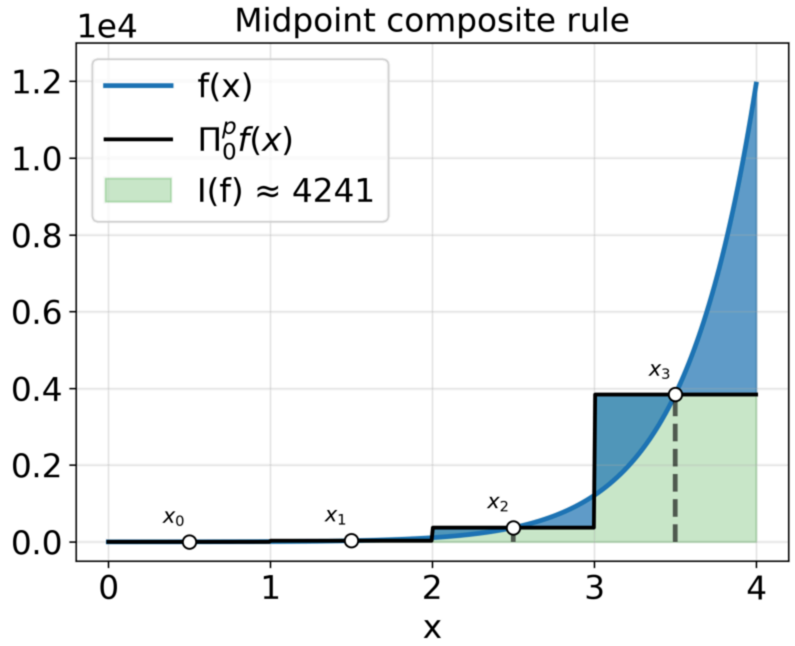
- **Midpoint rule**

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

- **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

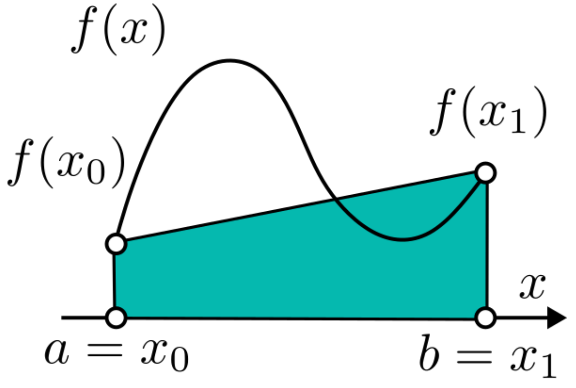
$$\begin{aligned}
\int_a^b f(x)\, dx \approx \int_a^b \Pi_1 f(x)\, dx &= h \int_0^1 \Pi_1 f(t)\, dt \\
&= f(a)h \int_0^1 (1 - t)\, dt + f(b)h \int_0^1 t\, dt \\
&= f(a)h \left[t - \frac{t^2}{2} \right]_0^1 + f(b)h \left[\frac{t^2}{2} \right]_0^1 = \frac{h}{2} [f(a) + f(b)].
\end{aligned}$$

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

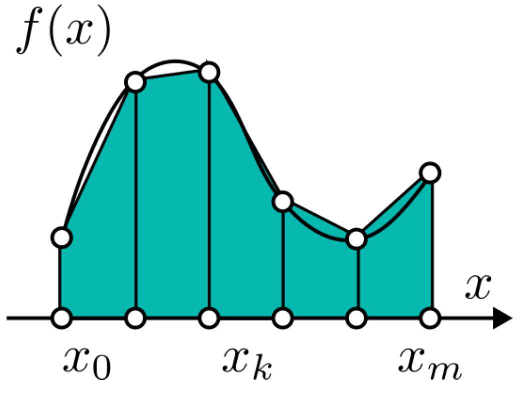
$$I_1(f) = \frac{b-a}{2}[f(a) + f(b)], \quad \text{with} \quad E_1(f) = -\frac{h^3}{12} f''(\xi),$$

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**

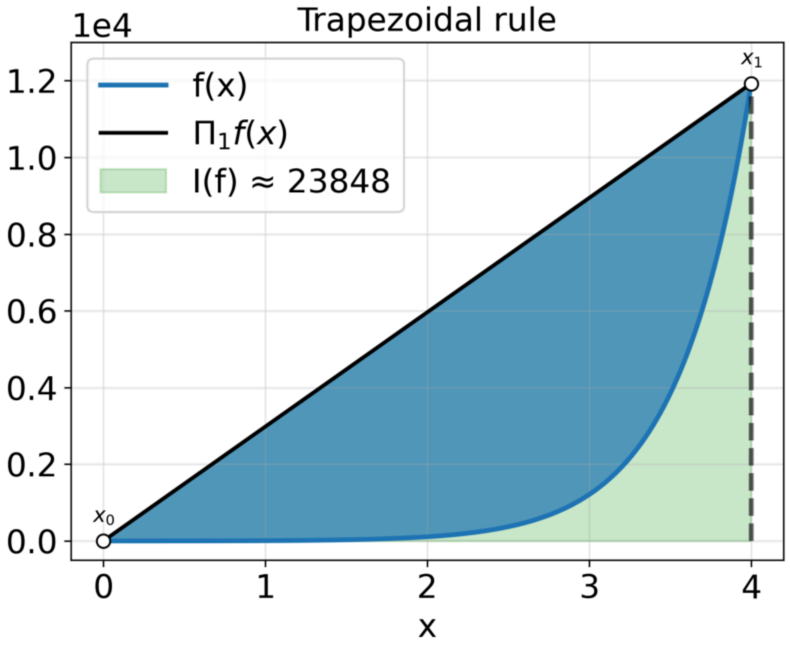
$$\int_0^4 xe^{2x}\,dx = \left[\frac{x}{2}e^{2x} - \frac{1}{4}e^{2x}\right]_0^4 = \frac{1}{4}(7e^8 - 1) = 5217$$

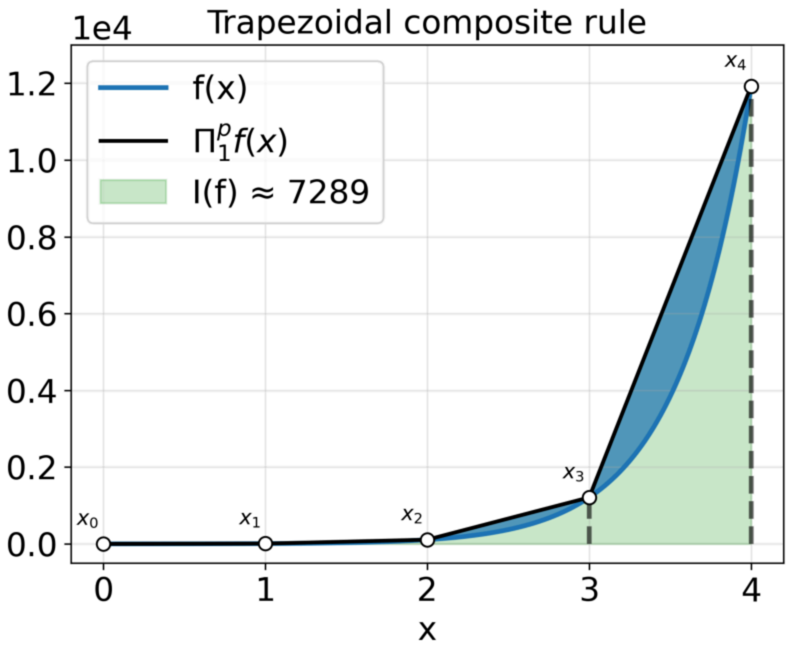
- **Trapezoidal rule**

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

- **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

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

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

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 $r = 3$.

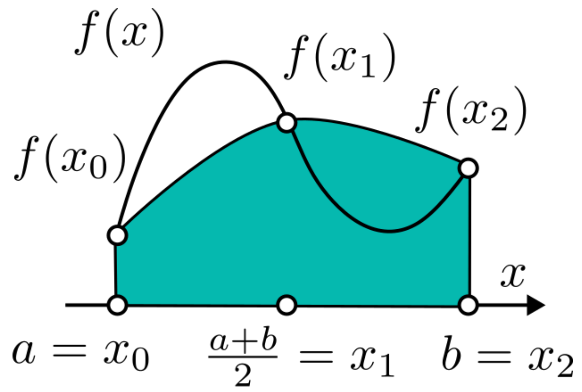
For the **composite** rule we replace f with its piecewise interpolant Π_2^p.

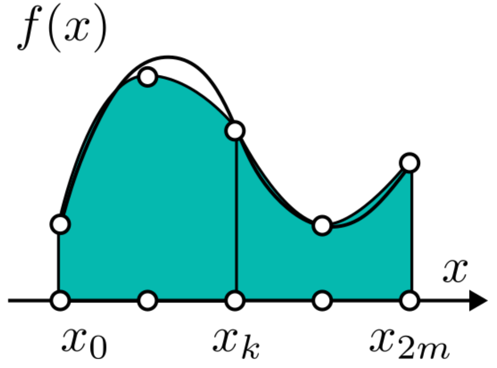
Given $m \geq 1$ of width $H = (b-a)/m$, and quadrature nodes $x_k = a + kH/2$ for $k = 0, \ldots, 2m$, we get

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

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**

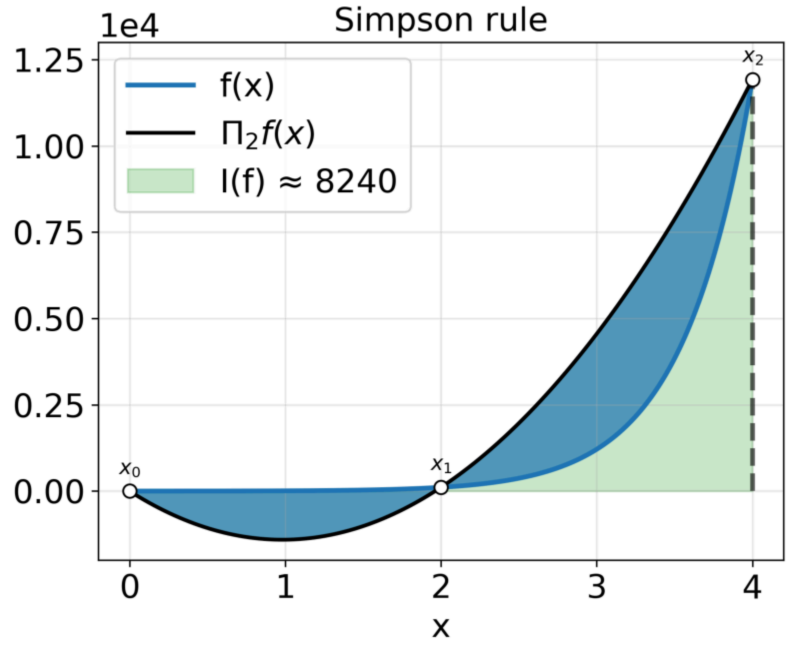
$$\int_0^4 xe^{2x}\,dx = \left[\frac{x}{2}e^{2x} - \frac{1}{4}e^{2x}\right]_0^4 = \frac{1}{4}(7e^8 - 1) = 5217$$

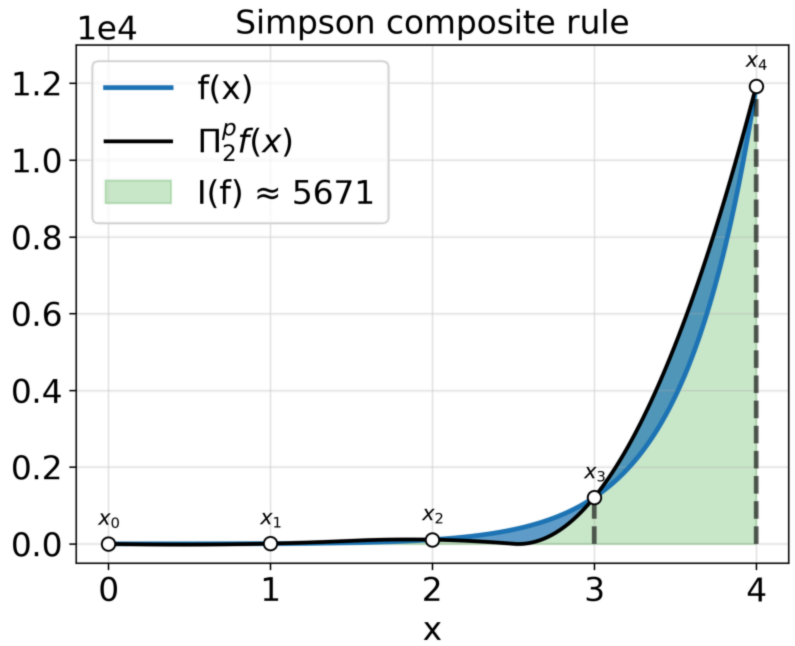
- **Simpson rule**

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

- **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 $n = 1$

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

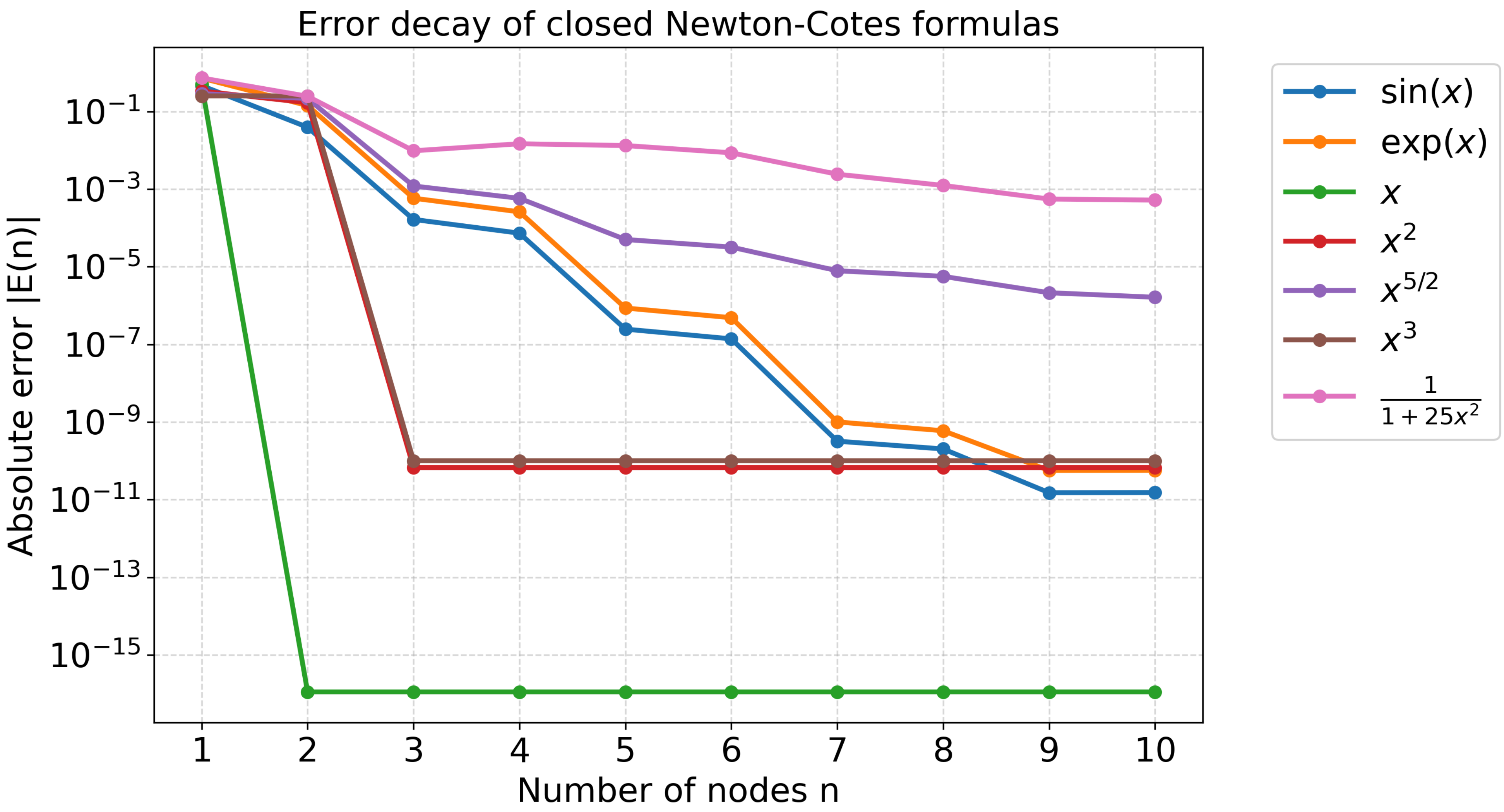
- **Simpson's 1/3 Rule**: quadratic interpolant $n = 2$

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

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

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

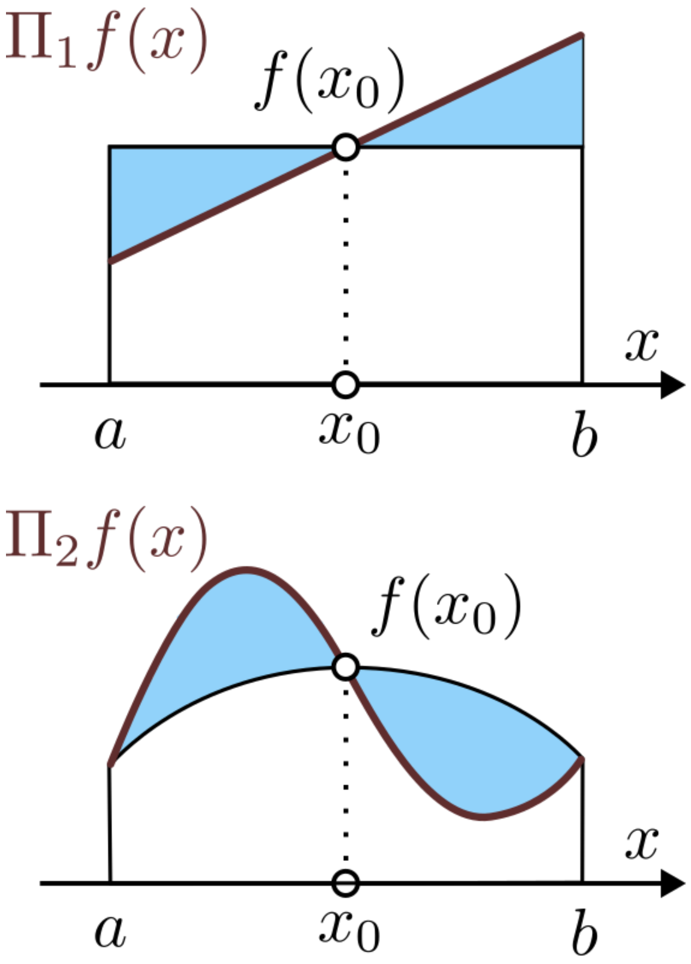
Newton-Cotes errors



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

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

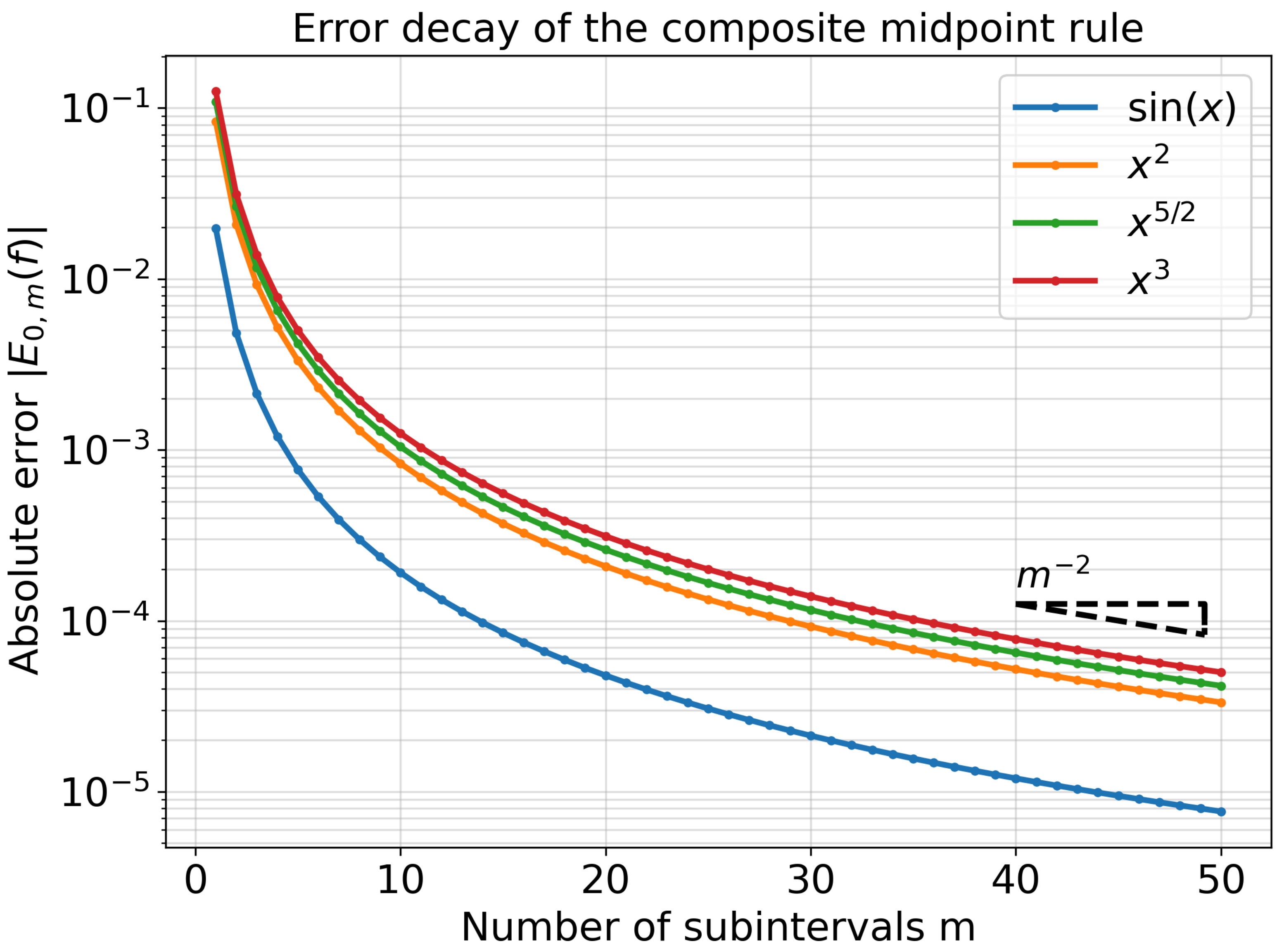
Moreover

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

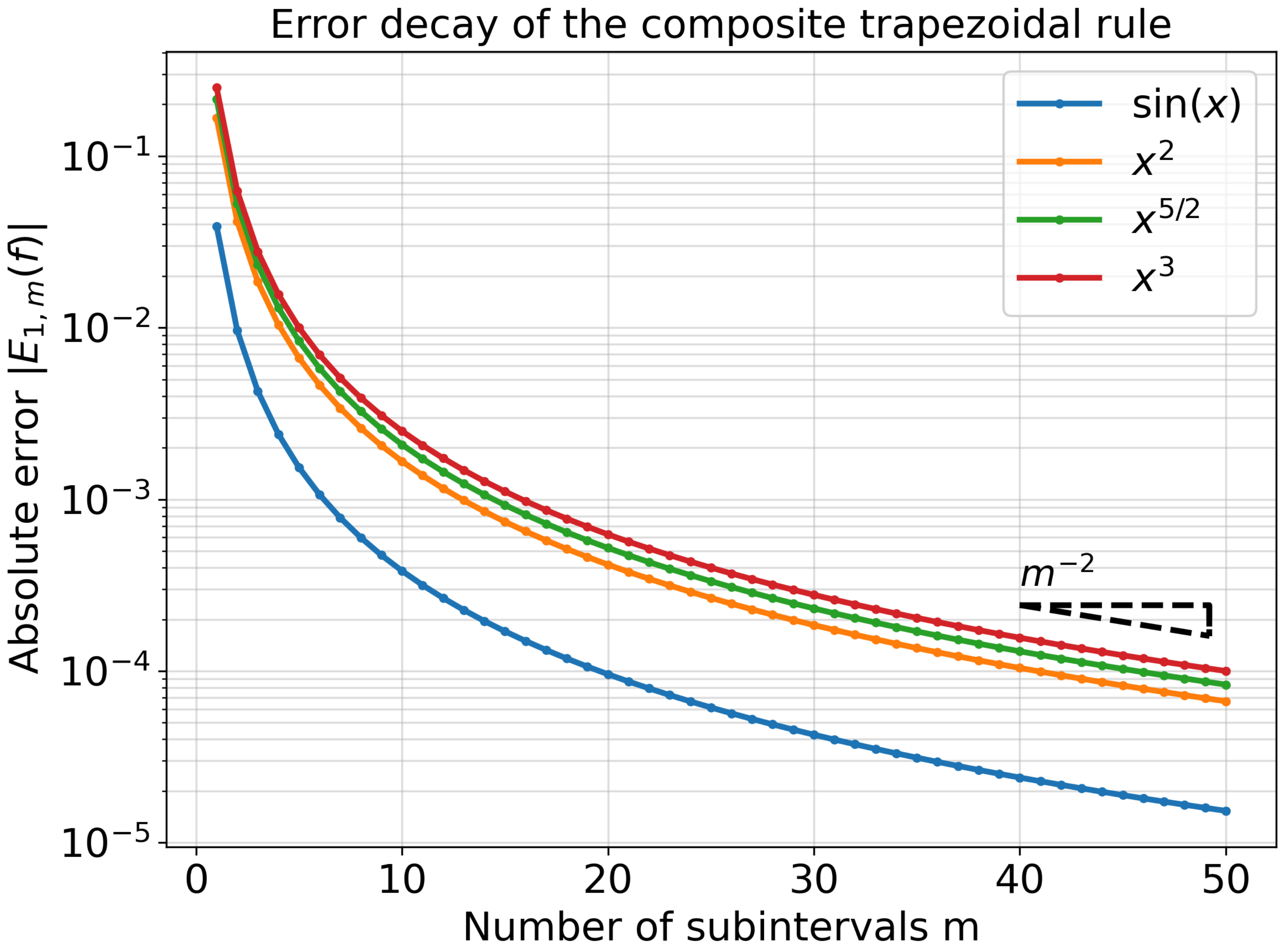
where the module of continuity of the function f is defined as

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

Composite Newton-Cotes formulae and errors



Composite Newton-Cotes formulae and errors



Composite Newton-Cotes formulae and errors