

Recall: Lagrange interpolation

For distinct nodes $\xi_0, \dots, \xi_k \in [a, b]$, the unique polynomial of degree at most k interpolating f is

$$\Pi_k(x) = \sum_{i=0}^k f(\xi_i) \ell_i(x), \quad \ell_i(x) = \prod_{j \neq i} \frac{x - \xi_j}{\xi_i - \xi_j}.$$

Indeed, $\ell_i(\xi_j) = \delta_{ij}$; uniqueness follows because a nonzero polynomial of degree at most k cannot have $k + 1$ distinct roots. If $f \in C^{k+1}([a, b])$, for each x not among the nodes there exists ζ in the interval spanned by the nodes and x such that

$$f(x) - \Pi_k(x) = \frac{f^{(k+1)}(\zeta)}{(k+1)!} \prod_{i=0}^k (x - \xi_i).$$

Integrating Π_k produces an interpolatory quadrature formula.

See Lecture 20 (Interpolation) for the proofs and piecewise error bounds.

Numerical integration

(a.k.a quadrature formulas or quadrature rules)

Quadrature rules are used to approximate integrals of functions that we are not able to compute exactly.

Given $g : [a, b] \rightarrow \mathbb{R}$, the most common quadrature rules look like

$$\int_a^b g(x) dx \simeq \sum_{i=1}^{k+1} \omega_i g(x_i)$$

where: $x_1, x_2, \dots, x_{k+1}$ are the quadrature “points” or “nodes” of the rule and $\omega_1, \omega_2, \dots, \omega_{k+1}$ are called quadrature “weights”

Definition: The order of precision of a quadrature rule is the maximum degree of the polynomials which are integrated exactly by the rule.

Among the numerous quadrature rules, we shall see the so-called interpolatory rules.

Interpolatory quadrature rules

The function g is approximated by its Lagrange interpolant $\Pi_k(x)$ (of degree $\leq k$) with respect to the given nodes $x_1, x_2, \dots, x_{k+1}$, and then the integral of the polynomial is computed exactly.

Then

$$\begin{aligned}\int_a^b g(x) dx &\simeq \int_a^b \Pi_k(x) dx = \int_a^b \sum_{i=1}^{k+1} g(x_i) L_i(x) dx \\ &= \sum_{i=1}^{k+1} g(x_i) \underbrace{\int_a^b L_i(x) dx}_{\omega_i}\end{aligned}$$

The order of precision of an interpolatory formula will be **at least** k : indeed if $g \in \mathbb{P}_k$ (where $\mathbb{P}_k$ is the space of polynomials of degree $\leq k$) then g is integrated exactly

Error analysis for interpolatory quadrature rules

Bounds for the quadrature error are derived by the bounds for the interpolation error (see the slides on Lagrange interpolation):

$$\max_{x \in [a,b]} |g(x) - \Pi_k(x)| \leq \frac{(b-a)^{k+1}}{(k+1)!} \max_{x \in [a,b]} |g^{(k+1)}(x)| \quad (*)$$

Thus,

$$\begin{aligned} \left| \int_a^b g(x) dx - \int_a^b \Pi_k(x) dx \right| &= \left| \int_a^b (g(x) - \Pi_k(x)) dx \right| \leq \int_a^b |g(x) - \Pi_k(x)| dx \\ &\leq \int_a^b \max_{[a,b]} |g(x) - \Pi_k(x)| dx = (b-a) \max_{[a,b]} |g(x) - \Pi_k(x)| \\ &\leq \frac{(b-a)^{k+2}}{(k+1)!} \max_{x \in [a,b]} |g^{(k+1)}(x)| \end{aligned} \quad (1)$$

(Observe that if $g \in \mathbb{P}_k$, then $g^{(k+1)}(x) \equiv 0$. Hence, the quadrature error is $= 0$)

This estimate is obtained using the generic bound for the interpolation error. Sharper estimates can be obtained by analysing each rule directly, as we shall see.

Use of quadrature rules

It should be clear by now that if we want a good approximation of an integral we have to use properly the rules in order to make the error as small as we want. Exactly like we did for Lagrange interpolation, we will construct piecewise integration rules, also called **composite integration rules**.

Given $f : [a, b] \rightarrow \mathbb{R}$ (smooth enough), subdivide $[a, b]$ in N subintervals, for simplicity of notation all equal. We have then a uniform subdivision of $[a, b]$ into intervals of length $h = (b - a)/N$:

$I_1 = [x_1, x_2], \dots, I_j = [x_j, x_{j+1}], \dots, I_N = [x_N, x_{N+1}]$. In each subinterval we approximate f with a Lagrange interpolant polynomial of degree k .

Thus,

$$\int_a^b f(x) dx = \sum_{j=1}^N \int_{x_j}^{x_{j+1}} f(x) dx \simeq \sum_{j=1}^N \int_{x_j}^{x_{j+1}} \Pi_k(x) dx$$

Let us see some examples.

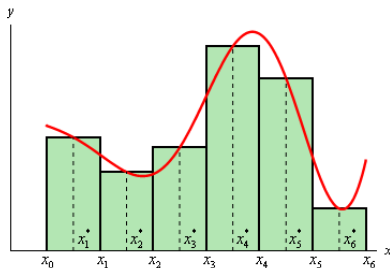
Composite midpoint rule

x_j^M = midpoint of the interval I_j : $x_j^M = (x_j + x_{j+1})/2$

$f(x)|_{[a,b]} \simeq f_0(x)$ piecewise constant function given by

$$f_0(x)|_{I_j} = f(x_j^M) \quad j = 1, 2, \dots, N$$

$$\int_a^b f(x) dx \simeq \int_a^b f_0(x) dx = \sum_{j=1}^N \int_{x_j}^{x_{j+1}} f(x_j^M) dx = h \sum_{j=1}^N f(x_j^M)$$



Composite midpoint rule: pseudocode

Composite midpoint rule

Input: f , a , b , N .

$h = (b - a)/N$

for $i = 1, 2, \dots, N + 1$

$x_i = a + (i - 1)h$

end

for $i = 1, 2, \dots, N$

$x_i^M = (x_i + x_{i+1})/2$

end

$S = 0$

for $i = 1, 2, \dots, N$

$S = S + f(x_i^M)h$

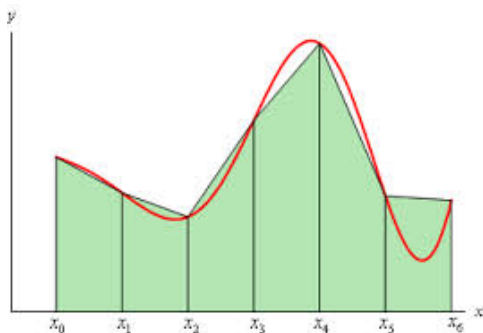
end

Output: S .

Composite trapezoidal rule

$f(x)|_{[a,b]} \simeq f_1(x)$ piecewise linear function which, on each interval I_j , is the Lagrange interpolant of degree ≤ 1 with respect to the endpoints of I_j

$$\int_a^b f(x) dx \simeq \int_a^b f_1(x) dx = \sum_{j=1}^N \int_{x_j}^{x_{j+1}} \Pi_1(x) dx = \frac{h}{2} \sum_{j=1}^N [f(x_j) + f(x_{j+1})]$$

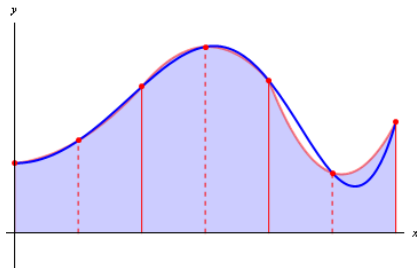


Composite Simpson rule

$f(x)|_{[a,b]} \simeq f_2(x)$ piecewise quadratic function which, on each interval I_j , is the Lagrange interpolant of degree ≤ 2 with respect to the endpoints and the midpoint of I_j

$$\int_a^b f(x) dx \simeq \int_a^b f_2(x) dx = \frac{h}{6} \sum_{j=1}^N [f(x_j) + 4f(x_j^M) + f(x_{j+1})]$$

Exercise: derive the weights from the Lagrange basis (Lecture 20).



Composite midpoint rule: local error

Assume $f \in C^2([a, b])$, $I_j = [x_j, x_{j+1}]$, $h = x_{j+1} - x_j$, and $m_j = (x_j + x_{j+1})/2$. Taylor's formula gives

$$f(x) = f(m_j) + (x - m_j)f'(m_j) + \frac{1}{2}(x - m_j)^2 f''(\zeta_x).$$

The integral of the linear term over I_j vanishes. Hence

$$\begin{aligned} |E_j| &= \left| \int_{I_j} (f(x) - f(m_j)) dx \right| \\ &\leq \frac{\|f''\|_{\infty, I_j}}{2} \int_{I_j} (x - m_j)^2 dx = \frac{h^3}{24} \|f''\|_{\infty, I_j}. \end{aligned}$$

The composite error satisfies $ERR = |\sum_j E_j| \leq \sum_j |E_j|$.

Composite Midpoint rule: error bound

The absolute global error is bounded by the sum of the absolute local errors.

$$ERR \leq \sum_{j=1}^N |E_j| \leq \frac{\max_{[a,b]} |f''(x)|}{24} h^3 N = \frac{\max_{[a,b]} |f''(x)|}{24} (b-a) h^2$$

(we used $Nh = b - a$ and $\max_{[I_j]} |f''(x)| \leq \max_{[a,b]} |f''(x)|$).

We see that the error is zero if $f'' \equiv 0$ in each I_j , i.e., if f is a piecewise polynomial of degree 1. Hence, the order of precision of the midpoint rule is actually 1 (even though we are projecting onto piecewise constants!)

To summarize:

$$ERR \leq C h^2 \quad \text{with } C = \frac{\max_{[a,b]} |f''(x)|}{24} (b-a)$$

The $ERR \rightarrow 0$ for $h \rightarrow 0$ quadratically with h (halving h reduces this error bound by a factor of 4).

Trapezoidal error bound * NOT FOR THE EXAM *

Assume $f \in C^2([a, b])$ and panels of length $h = (b - a)/N$. On $I_j = [x_j, x_{j+1}]$, integrate the linear interpolant:

$$Q_j = \frac{h}{2}(f(x_j) + f(x_{j+1})).$$

The interpolation remainder yields

$$\begin{aligned}|E_j| &\leq \frac{\|f''\|_{\infty, I_j}}{2} \int_{x_j}^{x_{j+1}} (x - x_j)(x_{j+1} - x) dx \\ &= \frac{h^3}{12} \|f''\|_{\infty, I_j}.\end{aligned}$$

Thus $ERR \leq (b - a)h^2 \|f''\|_{\infty}/12$. The rule has degree of precision 1 and composite error of order 2.

Simpson error bound * NOT FOR THE EXAM *

Assume $f \in C^4([a, b])$. Here h is the full panel length and m_j is its midpoint:

$$Q_j = \frac{h}{6} (f(x_j) + 4f(m_j) + f(x_{j+1})).$$

Simpson's remainder formula gives, for some $\zeta_j \in I_j$,

$$E_j = \int_{I_j} f(x) dx - Q_j = -\frac{h^5}{2880} f^{(4)}(\zeta_j).$$

Consequently,

$$ERR \leq \sum_{j=1}^N |E_j| \leq \frac{(b-a)h^4}{2880} \|f^{(4)}\|_{\infty}.$$

The degree of precision is 3, although the interpolant is quadratic. If the node spacing is $\delta = h/2$, the same bound is $(b-a)\delta^4 \|f^{(4)}\|_{\infty}/180$.

Hints on Gaussian rules * NOT FOR THE EXAM *

Conclusions The order of precision of an interpolatory quadrature rule using n nodes is at least $n - 1$ (that is, the rule integrates exactly polynomials of degree up to $n - 1$).

If the n nodes are **Gauss points** (special points that are defined as roots of Legendre polynomials) the order of precision is higher: precisely, $2n - 1$.

Operatively: Gauss points are computed in the open interval $] - 1, 1[$:

$$n = 1 \qquad \int_{-1}^1 g(x) dx \approx 2g(0)$$

$$n = 2 \qquad \int_{-1}^1 g(x) dx \approx g\left(-\frac{1}{\sqrt{3}}\right) + g\left(+\frac{1}{\sqrt{3}}\right)$$

$$n = 3 \qquad \int_{-1}^1 g(x) dx \approx \frac{5}{9}g\left(-\frac{\sqrt{3}}{\sqrt{5}}\right) + \frac{8}{9}g(0) + \frac{5}{9}g\left(\frac{\sqrt{3}}{\sqrt{5}}\right)$$

$$n = 4 \qquad \dots \text{ see the reference books}$$

Hints on Gaussian rules * NOT FOR THE EXAM *

To compute Gauss points on a generic interval $[a, b]$ and use them for evaluating $\int_a^b g(x) dx$ is simple. Consider the map

$$F : [-1, 1] \rightarrow [a, b], \text{ that is, } \hat{x} \in [-1, 1] \rightarrow x = F(\hat{x}) \in [a, b]$$

It is easy to check that the map is affine, given by $x = \frac{b-a}{2}\hat{x} + \frac{a+b}{2}$. Hence, if $\hat{x}_1$ is a Gauss point in $] -1, 1[$, the point

$$x_1 = \frac{b-a}{2}\hat{x}_1 + \frac{a+b}{2} \text{ is a Gauss point in } [a, b]$$

Instead, the quadrature weights get scaled by a factor $F' = \frac{b-a}{2}$ (use change of variable to prove it).

Quadrature on triangles * NOT FOR THE EXAM *

Let T have vertices $V_i = (x_i, y_i)$, $i = 1, 2, 3$, and positive area. Its barycenter and area are

$$B = \frac{V_1 + V_2 + V_3}{3}, \quad |T| = \frac{1}{2} \left| \det \begin{pmatrix} x_2 - x_1 & x_3 - x_1 \\ y_2 - y_1 & y_3 - y_1 \end{pmatrix} \right|.$$

The barycenter rule and the vertex rule are

$$\int_T g \, dx \, dy \approx |T|g(B), \quad \int_T g \, dx \, dy \approx \frac{|T|}{3} \sum_{i=1}^3 g(V_i).$$

Both are exact for $g \in \mathbb{P}_1 = \text{span}\{1, x, y\}$: their degree of precision is 1.

Triangle midpoint rule * NOT FOR THE EXAM *

Let M_1, M_2, M_3 be the midpoints of the three edges of T . Then

$$\int_T g(x, y) \, dx \, dy \approx \frac{|T|}{3} \sum_{i=1}^3 g(M_i).$$

This rule has degree of precision 2: it integrates exactly every polynomial in

$$\mathbb{P}_2 = \text{span}\{1, x, y, x^2, xy, y^2\}.$$

The formula on an arbitrary triangle follows from the reference triangle by an affine change of variables. Its constant Jacobian rescales all quadrature weights by the area ratio.

Composite quadrature on a triangle mesh

For a polygonal domain $\Omega \subset \mathbb{R}^2$ exactly partitioned into nonoverlapping triangles $\mathcal{T}$,

$$\int_{\Omega} g \, dx \, dy = \sum_{T \in \mathcal{T}} \int_T g \, dx \, dy \approx \sum_{T \in \mathcal{T}} Q_T(g).$$

For example, the composite barycenter formula is

$$\int_{\Omega} g \, dx \, dy \approx \sum_{T \in \mathcal{T}} |T| g(B_T).$$

If the mesh covers only an approximation Ω_h to Ω , the sum instead approximates the integral over Ω_h . The total error also includes the geometric domain approximation.