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 $g : [a, b] \to \mathbb{R}$, 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: $x_1, x_2, \cdots, x_{k+1}$ are the quadrature " points" or "nodes" of the rule and $\omega_1, \omega_2, \cdots, \omega_{k+1}$ 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 $x_1, x_2, \cdots, x_{k+1}$, and then the integral of the polynomial is computed exactly.
Then

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

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

The order of precision of an interpolator 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):

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

Thus,

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

(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 smaller as we want. Exactly like we did for Lagrange interpolation, we will construct piecewise integration rules, also called **composite integration rules.**

Given $f : [a, b] \to \mathbb{R}$ (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 $h = (b - a)/N$:
$I_1 = [x_1, x_2], \cdots, I_j = [x_j, x_{j+1}], \cdots, I_N = [x_N, x_{N+1}]$. 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.

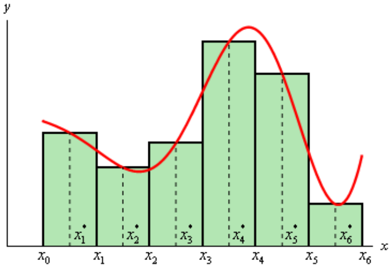
Composite midpoint rule

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

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

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



Composite midpoint rule: pseudocode

Composite midpoint rule

Input: f, a, b, N.

h $= (b-a)/N$

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

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

end

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

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

end

$S = 0$

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

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

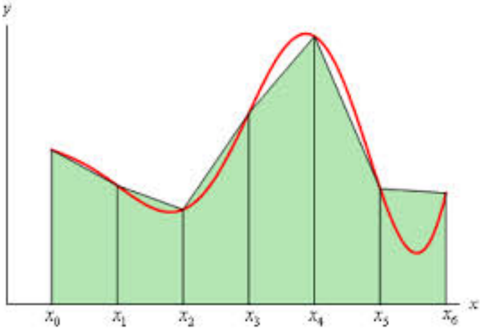
end

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

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

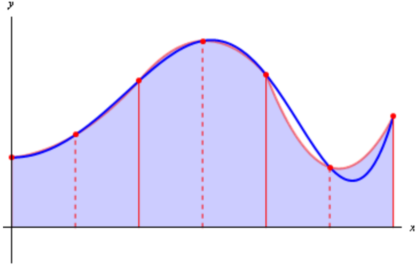


Composite Simpson rule

$f(x)_{|[a,b]} \simeq f_2(x)$ 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: prove the formula using slide 2/15 in each interval...



Composite Midpoint rule: error bound

$$ERR = \Big| \sum_{j=1}^{N} \underbrace{\int_{x_j}^{x_{j+1}} (f(x) - f(x_j^M))\, dx}_{E_j} \Big|$$

Use in each I_j the Taylor expansion centered in x_j^M

$$f(x) = f(x_j^M) + (x - x_j^M) f'(x_j^M) + \frac{(x - x_j^M)^2}{2!} f''(z) \qquad (\text{ for } z \text{ between } x \text{ and } x_j^M)$$

$$\begin{aligned} E_j &= \underbrace{\int_{x_j}^{x_{j+1}} (x - x_j^M) f'(x_j^M)\, dx}_{=0} + \int_{x_j}^{x_{j+1}} \frac{(x - x_j^M)^2}{2!} f''(z)\, dx \\ &\le \frac{1}{2} \max_{[I_j]} |f''(x)| \int_{x_j}^{x_{j+1}} (x - x_j^M)^2\, dx = \frac{\max_{[I_j]} |f''(x)|}{24} h^3 \end{aligned}$$

Composite Midpoint rule: error bound

The global error is the sum of the error in each subinterval.

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

(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 $ERR \to 0$ for $h \to 0$ quadratically with h (halving h reduces the error by 4).

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 $]-1,1[$:

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

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

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

$n=4$ ... 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

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

It is easy to check that the map is linear, 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).