

Appendix D

Overview of interpolatory, polynomial quadrature rules

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 $g : [c, d] \rightarrow \mathbb{R}$, the most common quadrature rules look like

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

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

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

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

The order of precision of an interpolator formula will be **at least** k (if $g \in \mathbb{P}_k$, it is integrated exactly)

Example: second-order formula using a three-point interpolant on a uniform grid.

Polynomial interpolant on nodes $[x(j), (x(j+1)+x(j))/2, x(j+1)]$:

$$\frac{1}{h} \left[f(x_j) \left(\frac{h-x}{2} \right)^2 + 4 f\left(\frac{x_j+x_{j+1}}{2}\right) \left(\frac{h-x}{2} \right) + f(x_{j+1}) \right]$$

Resulting quadrature rule (SIMPSON'S RULE):

$$\frac{1}{6} \left[f(x_j) \left(\frac{h-x}{2} \right)^3 + 3 f\left(\frac{x_j+x_{j+1}}{2}\right) \left(\frac{h-x}{2} \right)^2 + f(x_{j+1}) \left(\frac{h-x}{2} \right) \right]$$

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):

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

Thus,

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

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

Given $f : [a, b] \rightarrow \mathbb{R}$ (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 $h = (b - a)/N$:
 $h_1 = [x_1, x_2], \dots, h_j = [x_j, x_{j+1}], \dots, h_N = [x_N, x_{N+1}]$. In each subinterval we approximate f with a Lagrange interpolant polynomial of degree k .
Thus,

THIS IS A "COMPOSITE" QUADRATURE RULE

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

Let us see some examples.

Composite midpoint rule

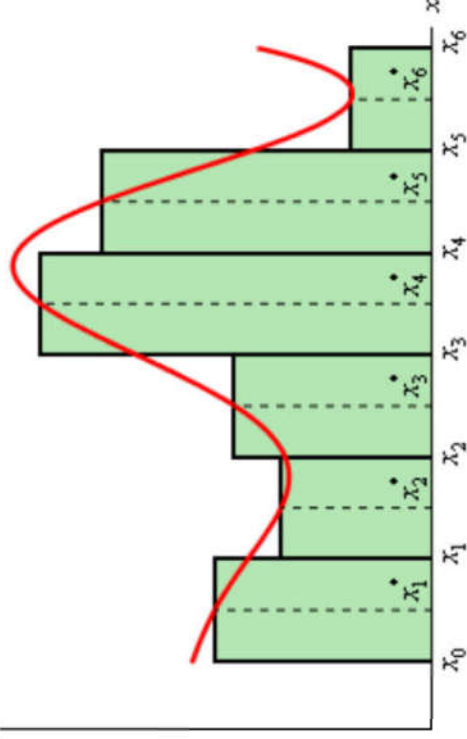
x_j^M = midpoint of the interval I_j : $x_j^M = (x_j + x_{j+1})/2$

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

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

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

REMARK: IT CAN BE PROVED THAT THE MID-POINT QUADRATURE RULE IS TWICE AS ACCURATE AS THE TRAPEZOIDAL RULE.



Composite midpoint rule: pseudocode on the blackboard

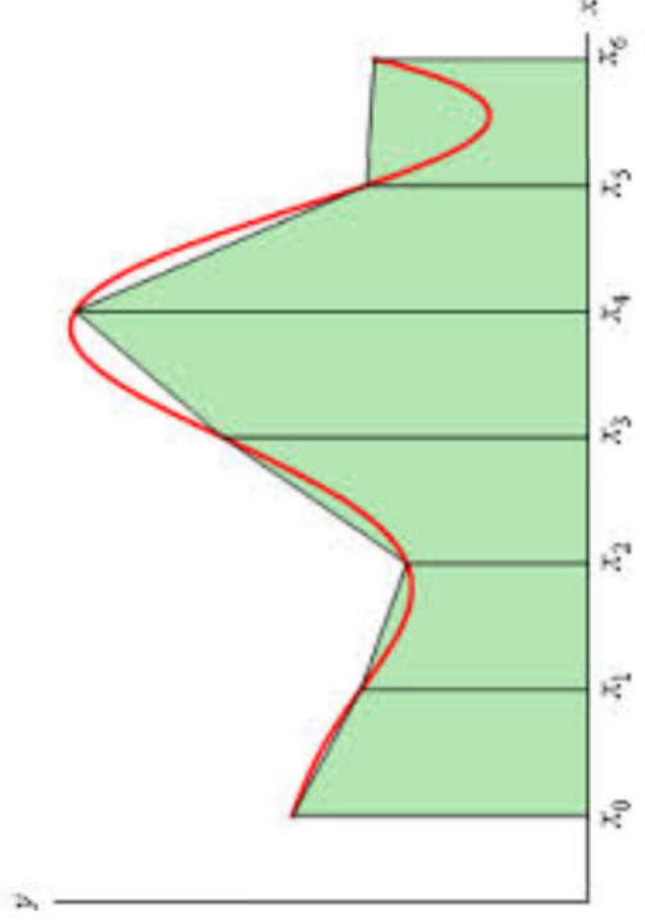
TRY THIS! CLASS EXERCISE! COMPARE WITH SIMPSON'S RULE.

integral = midpoint (f, a, b, N)
% Computes $\int_a^b f(x) dx$ by the composite m.p. rule over N elements
h = (b-a) / N
for i = 1:N+1
 x(i) = a + (i-1)*h
end
for i = 1:N
 x^M(i) = (x(i) + x(i+1)) / 2 % Quadrature points
end
integral = 0
for i = 1:N
 integral = integral + h * f(x^M(i))
end

Composite trapezoidal rule

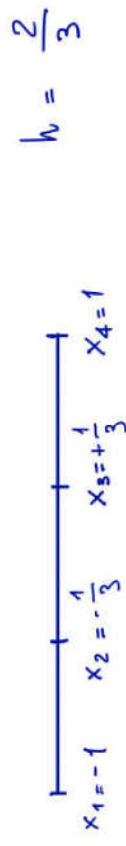
$f(x)|_{[a,b]} \simeq f_1(x)$ piecewise linear function which, on each interval I_j , is the Lagrange interpolant of degree ≤ 1 with respect to the endpoints of I_j

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



Exercise on composite midpoint and trapezoidal rules

Exercise: given the function $f(x) = 9 \cdot x^4$ and the following mesh on $[-1, 1]$:

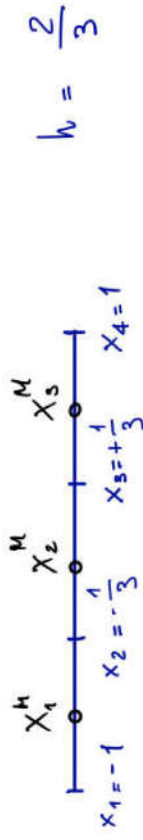


compute the approximation of $\int_{-1}^1 f(x)$ by a

- composite midpoint rule
- composite trapezoidal rule

Exercise on composite midpoint and trapezoidal rules

Exercise: given the function $f(x) = 9x^4$ and the following mesh on $[-1, 1]$:



compute the approximation of $\int_{-1}^1 f(x)$ by a

- composite midpoint rule
- composite trapezoidal rule ← do it yourself

↳ the 3 midpoints (quadrature points) are $x_1^M = -2/3$, $x_2^M = 0$, $x_3^M = 2/3$ and the rule is:

$$\begin{aligned} \int_{-1}^1 f(x) dx &= h (f(x_1^M) + f(x_2^M) + f(x_3^M)) \\ &= \frac{2}{3} \left(\frac{16}{9} + \frac{16}{9} \right) = \frac{64}{27} \end{aligned}$$

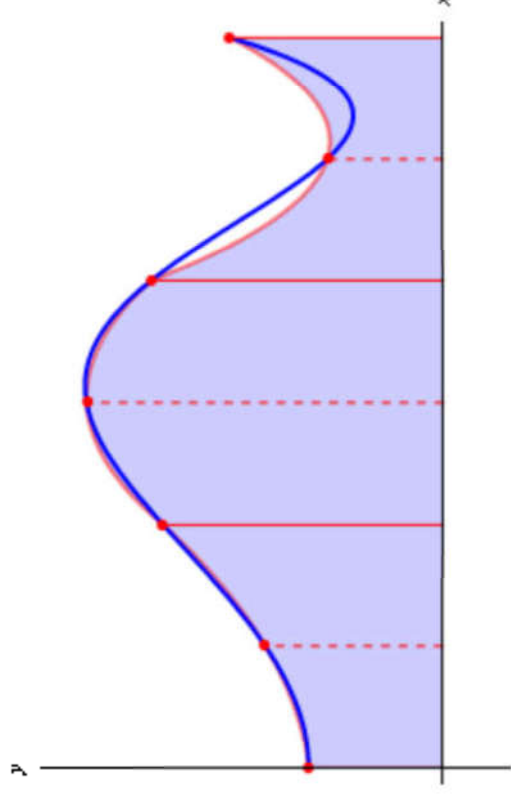
since $f(x_1^M) = f(x_3^M) = 9 \cdot \frac{16}{9 \cdot 9} = \frac{16}{9}$ and $f(x_2^M) = 0$

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

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

$$E_j \leq \frac{(d-c)^{k+2}}{(k+1)!} \max_{x \in [c,d]} |g^{(k+1)}(x)|$$

The first possibility is to use (1), which gives in our case:

$$E_j = \left| \int_{x_j}^{x_{j+1}} f(x) - P_{f_0}(x) dx \right| \leq h^2 \max_{x \in [x_j, x_{j+1}]} |f'(x)| = O(h^2)$$

Then the global error ERR is the sum of the error in each subinterval:

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

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

Composite Midpoint rule: error bound (sharp)

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

Second possibility: use in each I_j the Taylor expansion centered in x_j^M

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

$$E_j = \underbrace{\int_{x_j}^{x_{j+1}} (x - x_j^M) f'(x_j^M) dx}_{=0} + \int_{x_j}^{x_{j+1}} \frac{(x - x_j^M)^2}{2!} f''(z) dx$$

$$\leq \frac{1}{2} \max_{[I_j]} |f''(x)| \int_{x_j}^{x_{j+1}} (x - x_j^M)^2 dx = \frac{\max_{[I_j]} |f''(x)|}{24} h^3$$

Composite Midpoint rule: error bound (sharp)

Again, 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 $\max_{[j]} |f''(x)| \leq \max_{[a,b]} |f''(x)|$).

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:

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

We see that $ERR \rightarrow 0$ for $h \rightarrow 0$ 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 $n - 1$).

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

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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 $] - 1, 1[$:

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

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

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

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

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

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

$$\int_a^b f(x) dx = \int_{-1}^1 f(x(\xi)) d\xi \quad \frac{b-a}{2} \quad \text{can } \xi \equiv 2 \frac{x - X^M}{b-a}$$
$$\text{e } X^M \equiv \frac{b+a}{2}$$

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It is easy to check that the map is linear, given by $x = \frac{b-a}{2}\hat{x} + \frac{a+b}{2}$

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

It is easy to check that the map is 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).