Basics in Applied Mathematics – Part I: Numerics

Lecture 9: Numerical integration — quadrature rules, composite rules, Gaussian quadrature

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Recap of Lecture 8 (1/2): the interpolation polynomial

Sections 6.2–6.3

Theorem 6.1 (interpolation polynomial)

For distinct nodes $x_0, \dots, x_n$ and arbitrary values $y_0, \dots, y_n$ there is exactly one $p \in \mathcal{P}_n$ with $p(x_i) = y_i$ for $i = 0, \dots, n$, given by the **Lagrange form**

$$p(x) = \sum_{i=0}^{n} y_i \, L_i(x), \qquad L_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}, \qquad L_i(x_k) = \delta_{ik}.$$

Theorem 6.2 (interpolation error)

Let $f \in C^{n+1}([a,b])$ and let $p \in \mathcal{P}_n$ interpolate f at distinct nodes $x_0, \dots, x_n \in [a,b]$. Then for every $x \in [a,b]$ there is $\xi = \xi(x) \in (a,b)$ with

$$f(x) - p(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \, \omega(x), \qquad \omega(x) = \prod_{j=0}^{n} (x - x_j).$$

Recap of Lecture 8 (2/2): low degree, many pieces

Sections 6.3–6.4

Linear interpolation ($n = 1$, $h = x_1 - x_0$): $$\max_{[x_0,x_1]} |f - p| \le \frac{h^2}{8} \max_{[x_0,x_1]} |f''| \tag{6.1}$$

Runge: at equidistant nodes, high degree can diverge — even for smooth f.

Chebyshev nodes minimise $\max_{[-1,1]} |\omega|$ (Theorem 6.7): choosing the nodes well pays off.

Today: Chapter 7 — numerical integration: integrate the interpolation polynomial,

- with low degree on many pieces (composite rules),
- with well-chosen nodes (Gaussian quadrature).

Compute $I(f) := \int_a^b f(x)\,\mathrm{d}x \quad (a < b)$ when f

- has no elementary antiderivative, e.g. e^{-x^2} or $\sin(x)/x$,
- is known only at some points, or
- is expensive to evaluate.

Idea: integrate the interpolation polynomial p of f instead of f:

$$\int_a^b f(x)\,\mathrm{d}x \;\approx\; \int_a^b p(x)\,\mathrm{d}x = \sum_{i=0}^{n} f(x_i) \int_a^b L_i(x)\,\mathrm{d}x.$$

Definition 7.1 (quadrature rule, degree of exactness)

A **quadrature rule** on $[a, b]$ is a weighted sum of function values,

$$Q(f) := \sum_{i=0}^{n} w_i \, f(x_i), \qquad \text{distinct } \textbf{nodes } x_0, \ldots, x_n \in [a, b], \quad \textbf{weights } w_0, \ldots, w_n \in \mathbb{R}.$$

Q is **exact of degree** m if $Q(p) = I(p)$ for all $p \in \mathcal{P}_m$. If Q is exact of degree 0, the largest such m is the **degree of exactness** of Q.

Q and I are linear: exact of degree $m \iff Q(x^k) = I(x^k)$ for $k = 0, \ldots, m$.

Can a rule with $n+1$ nodes be exact for all polynomials?

No. For $\omega(x) := \prod_{i=0}^{n}(x - x_i)$, ω^2 a polynomial of degree $2n+2$:

$$Q(\omega^2) = \sum_{i=0}^{n} w_i \, \omega(x_i)^2 = 0 \; < \; I(\omega^2). \qquad \text{Degree of exactness } \leq 2n+1.$$

Lemma 7.2 (interpolatory rules)

Let $x_0, \dots, x_n \in [a, b]$ be distinct nodes with Lagrange basis polynomials L_i (Theorem 6.1). The **interpolatory rule**, obtained by integrating the interpolation polynomial $p \in \mathcal{P}_n$ of f,

$$Q(f) := \int_a^b p(x)\,\mathrm{d}x = \sum_{i=0}^{n} w_i f(x_i), \qquad w_i := \int_a^b L_i(x)\,\mathrm{d}x,$$

is exact of degree at least n. Conversely, every quadrature rule with the nodes $x_0, \dots, x_n$ that is exact of degree at least n is the interpolatory rule.

Two nodes a, b, $h := b - a$: the weights?

$$w_0 = \int_a^b \frac{x-b}{a-b}\,\mathrm{d}x = \frac{h}{2}, \qquad w_1 = \int_a^b \frac{x-a}{b-a}\,\mathrm{d}x = \frac{h}{2} \qquad \Longrightarrow \qquad Q(f) = \frac{h}{2}\big(f(a) + f(b)\big) :$$

the **trapezoidal rule**.

The midpoint rule and the trapezoidal rule

Newton–Cotes rules: interpolatory, equidistant nodes; *closed* (with a and b) or *open* (interior nodes).

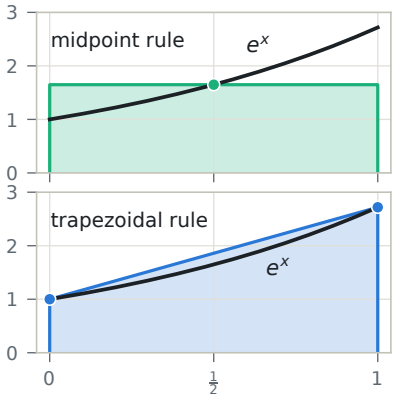
With $h = b - a$ and $m = \frac{a+b}{2}$:

rule	nodes	$Q(f)$
midpoint	m	$h\, f(m)$
trapezoidal	$a,\ b$	$\frac{h}{2}\big(f(a) + f(b)\big)$

$f(x) = e^x$ on $[0, 1]$: **which rule is more accurate?**

$I(f) - Q_{\mathrm{M}}(f) = \quad 0.0696$
$I(f) - Q_{\mathrm{T}}(f) = -0.1409$

The midpoint rule: half the error, opposite sign.



Theorem 7.3 (local errors of the midpoint and trapezoidal rules)

Let $h = b - a$, $m = \frac{a+b}{2}$ and $f \in C^2([a,b])$.

(i) There is $\xi \in (a,b)$ with $I(f) - h\,f(m) = \dfrac{h^3}{24} f''(\xi)$.

(ii) There is $\xi \in (a,b)$ with $I(f) - \dfrac{h}{2}\big(f(a) + f(b)\big) = -\dfrac{h^3}{12} f''(\xi)$.

The midpoint rule has **one** node and is exact of degree 1 — like the trapezoidal rule with two nodes. **Why?**

Proposition 7.4 (symmetric rules)

Let Q be a quadrature rule on $[a, b]$ that is exact of degree $2q$ for some $q \in \mathbb{N}_0$ and **symmetric** with respect to the midpoint m, that is, its nodes and weights satisfy

$$x_{n-i} = a + b - x_i \quad \text{and} \quad w_{n-i} = w_i \qquad \text{for all } i.$$

Then Q is exact of degree $2q + 1$.

Blackboard: proof.

- Midpoint rule: exact of degree 0 and symmetric $\implies$ exact of degree 1.

The composite trapezoidal rule

More accuracy: higher degree or more pieces?

N subintervals of length $h = \frac{b-a}{N}$, nodes $x_k = a + kh$, $k = 0, \dots, N$; the trapezoidal rule on each subinterval:

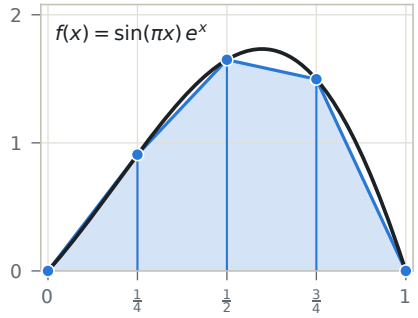
$$T_h(f) := \sum_{k=0}^{N-1} \frac{h}{2}\big(f(x_k) + f(x_{k+1})\big),$$

$$T_h(f) = h\big(\tfrac{1}{2}f(x_0) + f(x_1) + \cdots + f(x_{N-1}) + \tfrac{1}{2}f(x_N)\big).$$

$N+1$ function values.

Example: $\int_0^1 \sin(\pi x) e^x \, \mathrm{d}x = \frac{\pi(e+1)}{1+\pi^2} = 1.0747$;
$N = 4$: $T_h(f) = 1.0134$, error $6.1 \cdot 10^{-2}$.

More pieces (Lecture 8: Runge).



Theorem 7.5 (error of the composite trapezoidal rule)

If $f \in C^2([a,b])$, there is $\xi \in (a,b)$ with

$$I(f) - T_h(f) = -\frac{b-a}{12}\, h^2 f''(\xi), \qquad \text{in particular} \qquad |I(f) - T_h(f)| \le \frac{b-a}{12}\, h^2 \max_{[a,b]} |f''|.$$

Blackboard: proof.

Halving h (doubling N) divides the error **bound** by 4.

Example ($\max_{[0,1]} |f''| \approx 22.9$): $h = \frac{1}{4}$: bound 0.12, actual error 0.061.

Experimental order of convergence (EOC)

For the errors $e_h := |I(f) - Q_h(f)| > 0$ and $e_H > 0$ with step sizes $h < H$:

$$\mathrm{EOC} := \frac{\log(e_h/e_H)}{\log(h/H)}.$$

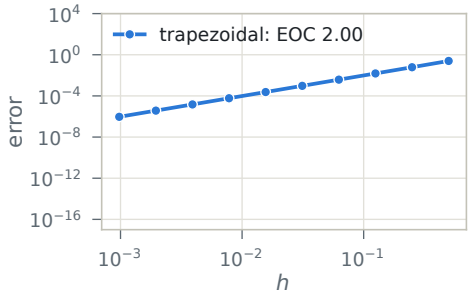
If $I(f) - Q_h(f) = Ch^p + o(h^p)$ with $C \neq 0$, then $\mathrm{EOC} \to p$ $(h, H \to 0,\ h/H$ fixed).

$e_{1/4} = 6.13 \cdot 10^{-2}$, $e_{1/8} = 1.52 \cdot 10^{-2}$: **EOC = ?** $\log_2(6.13/1.52) \approx 2.01$.

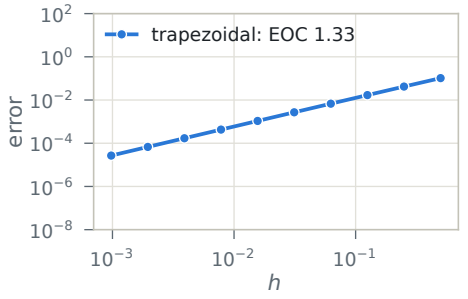
Experiment: smooth and non-smooth integrands

Composite trapezoidal rule, $h = 2^{-1}, \dots, 2^{-10}$ $(N = 2, \dots, 1024)$:

$\int_0^1 \sin(\pi x) e^x \, \mathrm{d}x$ (smooth)



$\int_0^1 x^{1/3} \, \mathrm{d}x = \frac{3}{4}$ (non-smooth)



$f(x) = x^{1/3}$, $f'(x) = \frac{1}{3} x^{-2/3}$ unbounded at 0: **what do you expect?**

EOC $1.33 \approx \frac{4}{3}$ instead of 2: $f \notin C^2([0,1])$, and the order drops.

Newton–Cotes: nodes fixed, $n+1$ weights chosen $\implies$ degree $\geq n$.
Nodes free as well: $2n+2$ parameters $\implies$ degree $2n+1$? (the maximum, Definition 7.1)

One node on $[-1,1]$: where, and with which weight, to be exact of degree 1?

$Q(1) = w_0 \stackrel{!}{=} I(1) = 2, \quad Q(x) = 2x_0 \stackrel{!}{=} I(x) = 0 \quad \implies \quad x_0 = 0,\ w_0 = 2$: the midpoint rule.
Degree 2 is impossible: $Q(x^2) = 0 \neq \frac{2}{3}$.

General interval: $x = \frac{a+b}{2} + \frac{b-a}{2}t$ maps polynomials to polynomials of the same degree: nodes $\frac{a+b}{2} + \frac{b-a}{2}x_i$, weights $\frac{b-a}{2}w_i$ on $[a,b]$, the same degree of exactness.

For $n+1$ nodes: the nodes are the roots of **orthogonal polynomials**.

Definition 7.6 (Legendre polynomials)

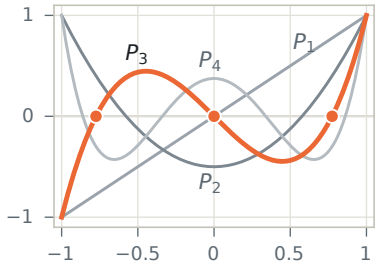
The polynomials $P_0, P_1, P_2, \dots$ with $\deg P_k = k$, $P_k(1) = 1$ and $\int_{-1}^{1} P_k(x) P_l(x)\,\mathrm{d}x = 0$ for $k \neq l$.

They exist and are unique: Gram–Schmidt (Algorithm 3.15) for $1, x, x^2, \dots$ with $(f, g) = \int_{-1}^{1} fg\,\mathrm{d}x$. $P_k \perp \mathcal{P}_{k-1}$.

$P_0 = 1$, $P_1 = x$, $P_2 = \frac{1}{2}(3x^2 - 1)$, $P_3 = \frac{1}{2}(5x^3 - 3x)$.

Check: $P_2 \perp \mathcal{P}_1$?

$\int_{-1}^{1} \frac{1}{2}(3x^2 - 1)\,\mathrm{d}x = \frac{1}{2}(2 - 2) = 0$; $x\,P_2(x)$ is odd.



dots: the roots of P_3

Lemma 7.7 (roots of the Legendre polynomials)

For $n \geq 0$ the polynomial P_{n+1} has $n + 1$ distinct real roots, all in $(-1, 1)$.

Theorem 7.8 (Gauss–Legendre quadrature)

Let $x_0, \dots, x_n$ be the roots of P_{n+1} and let $w_i = \int_{-1}^{1} L_i(x)\,\mathrm{d}x$ be the weights of the interpolatory rule with these nodes. Then:

(i) the rule $Q(f) = \sum_{i=0}^{n} w_i f(x_i)$ is exact of degree $2n+1$;

(ii) all weights are positive, and $\sum_i w_i = 2$;

(iii) no quadrature rule with $n+1$ nodes in $[-1,1]$ is exact of degree $2n+2$.

Blackboard: proof of (i) and (ii); (iii): ω^2 as in Definition 7.1.

$n+1$ function values, exact of degree $2n+1$: the largest possible degree.

Gauss–Legendre rules for $n = 0, 1, 2$

n	P_{n+1}	nodes x_i	weights w_i	exact of degree
0	x	0	2	1 (midpoint rule)
1	$\frac{1}{2}(3x^2-1)$	$\pm 1/\sqrt{3} \approx \pm 0.5774$	$1,\ 1$	3
2	$\frac{1}{2}(5x^3-3x)$	$-\sqrt{3/5},\ 0,\ \sqrt{3/5} \approx \pm 0.7746$	$\frac{5}{9},\ \frac{8}{9},\ \frac{5}{9}$	5

Three nodes, $I(x^k) - Q(x^k)$ in floating-point arithmetic (output in the notes):

k	0	1	2	3	4	5	6	7
$I-Q$	$-4.4 \cdot 10^{-16}$	0	$-3.3 \cdot 10^{-16}$	0	$-1.1 \cdot 10^{-16}$	0	$\mathbf{4.57 \cdot 10^{-2}}$	0

First non-exact degree: $6 = 2n + 2$ (exact value $\frac{2}{7} - \frac{6}{25} = \frac{8}{175}$).

Why is x^7 integrated exactly? The rule is symmetric: $I(x^7) = Q(x^7) = 0$ (as in Proposition 7.4). x^6 is not: the degree of exactness is 5.

(i) Error. For $f \in C^{2n+2}([a,b])$, the rule with $n+1$ nodes on $[a,b]$:

$$I(f) - Q(f) = \frac{(b-a)^{2n+3}\big((n+1)!\big)^4}{(2n+3)\big((2n+2)!\big)^3}\, f^{(2n+2)}(\xi), \qquad \xi \in (a,b);$$

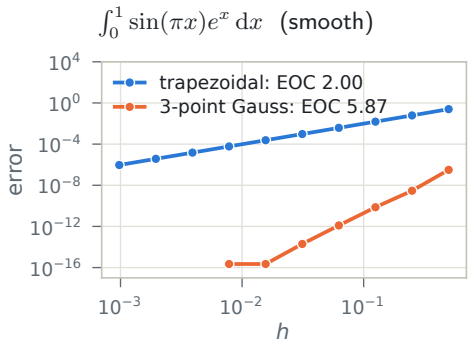
$n=0$: $\frac{h^3}{24} f''(\xi)$ (midpoint rule); $n=2$: $\frac{(b-a)^7}{2016000} f^{(6)}(\xi)$. Analytic f: exponential decay in n.

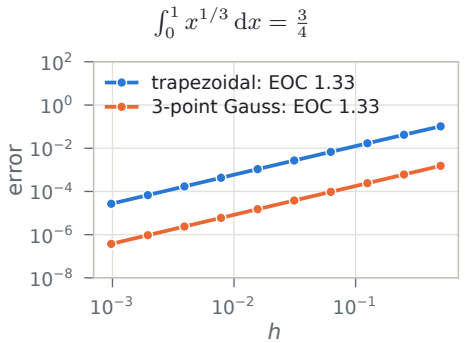
(ii) Stability. Data errors $\le \varepsilon$ change $Q(f)$ by at most $\varepsilon \sum_i |w_i| = \varepsilon(b-a)$, for every n.
Convergence: $Q_n(f) \to I(f)$ for all $f \in C([a,b])$: p with $\max|f-p| \le \varepsilon$ (Weierstrass); for $2n+1 \ge \deg p$,

$$|I(f) - Q_n(f)| \le |I(f-p)| + |I(p) - Q_n(p)| + |Q_n(p-f)| \le (b-a)\varepsilon + 0 + (b-a)\varepsilon.$$

Back to the experiment: the composite 3-point Gauss rule

Sections 7.2, 7.3





Smooth: order 6 (Remark 7.9(i), $n = 2$, on each subinterval) until rounding errors take over.

$x^{1/3}$: again $\frac{4}{3}$; $c \approx -0.00386$ instead of 0.277 — a smaller constant, the same order.

Remedies: $x = t^3$ ($\int_0^1 3t^3 \, \mathrm{d}t$, integrated exactly), a mesh refined near 0, adaptive quadrature.

Summary

- **Quadrature rule** $Q(f) = \sum_i w_i f(x_i)$; interpolatory rule: $w_i = \int L_i$, exact of degree $\geq n$; degree of exactness $\leq 2n+1$; symmetric rules gain one degree.
- **Local errors:** midpoint $\frac{h^3}{24} f''(\xi)$, trapezoidal $-\frac{h^3}{12} f''(\xi)$. **Composite trapezoidal rule:** $-\frac{b-a}{12} h^2 f''(\xi)$.
- **EOC** checks the order; for non-smooth f (e.g. $x^{1/3}$) the order drops on a uniform mesh, also for Gauss rules.
- **Gauss–Legendre:** nodes = roots of P_{n+1}, exact of degree $2n+1$ (optimal), positive weights, convergence for every continuous f.
- **Thursday:** Chapter 8 (ODEs), the last lecture of Part I; Sheet 5. **Friday 20 November:** tutorials (Sheet 4), HS II.
  Test 2: Friday 27 November, 13:45–14:15.