Numerical Integration

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Plan for today

- General problem of estimating the integral of a continuous function $f(x)$ on a finite support
- Specific problems in which properties of the integrand can be used to our advantage
  What properties of $f(x)$ can we use make our live easier?

Setup

Commonly, the integral I of a function $f(x)$ over finite support $a \leq x \leq b$ is introduced via the area below the curve $\gamma : (x, f(x))$. This isually called a Riemann-type integral.

For this lecture we will stick to this type of integrals. However, note that there are other measures that can be used to determine an integral (see Lebesque-type integrals).

For this first lecture, we will stick to one-dimensional, definite integrals:

$$I \equiv \int_a^b \mathrm{d}x\, f(x)$$

Moreover, we will focus on integrals of smooth, continuous functions.

Constant approximation

Usually, the first step in introducing students to the concept of integration is the constant approximation of the integral through summation of K rectangles of equal widths:

$$I_K^{\text{rect}} \equiv \frac{(b-a)}{K} \sum_{k=1}^{K} f(x_k) \qquad x_k = a + (b-a)\frac{k}{K}$$

Variations of this use different heights of the rectangles (left-hand, right-hand, central).

In the limit of infinitely many rectangles K or infinitely small steps $(b-a)/K$ the approximation can be expected to converge toward the true integral I:

$$\lim_{K\to\infty} I_K^{\text{rect}} = I$$

More sophisticated approximations

We can now try to be more sophisticated. Let's approcximate the function not by a sequence of rectangles, but by a sequence of trapezoids!

$$I_K^{\text{trap}} \equiv \frac{(b-a)}{K} \sum_{k=0}^{K-1} \frac{f(x_k) + f(x_{k+1})}{2}\,, \qquad x_k = a + (b-a)\frac{k}{K}$$

Compare the two approximations piece by piece:

$$\begin{aligned}
\frac{K\, I_K^{\text{rect}}}{b-a} &= 0 & &+ f(x_1) & &+ f(x_2) & &+ \dots & &+ f(x_{K-1}) & &+ f(x_K) \\
\frac{K\, I_K^{\text{trap}}}{b-a} &= \frac{1}{2} f(x_0) & &+ f(x_1) & &+ f(x_2) & &+ \dots & &+ f(x_{K-1}) & &+ \frac{1}{2} f(x_K)
\end{aligned}$$

This looks familiar!

Wait a minute, I know this!

- For the rectangles, we use a constant approximation of f within a small interval.
- For the trapezoid, we use a linear approimation of f within a small interval.

We have covered this: Let's interpolate the function f on an equidistant grid with grid size $(b-a)/K$, and then integrate the interpolating polynomial!
Polynomial interpolation yields one unique function, regardless of its representation. For this part, the representation via Lagrange basis polynomials $\ell_k(x)$ is benefitial:

$$L(x) \equiv \sum_k f(x_k)\ell_k(x)$$

We can then proceed to integrate:

$$I \approx \int_a^b \mathrm{d}x\, L(x) = \sum_k f(x_k) \int_a^b \mathrm{d}x\, \ell_k(x)$$

Newton-Coates Quadrature

Isaac Newton and Roger Cotes had this idea before us!

Closed Newton-Cotes formulas

$$I_K^{\mathrm{NC}} = \sum_{k=0}^{K} \omega_k^{(K)} f(x_k)\,, \qquad x_k = a + (b-a)\frac{k}{K}$$

where the weights $\omega_k^{(K)}$ depend on the index k and the degree of the interpolating polynomial K.

The open Newton-Cotes formulas are obtained by interpolating equidistantly only within the support, and not on its boundaries.

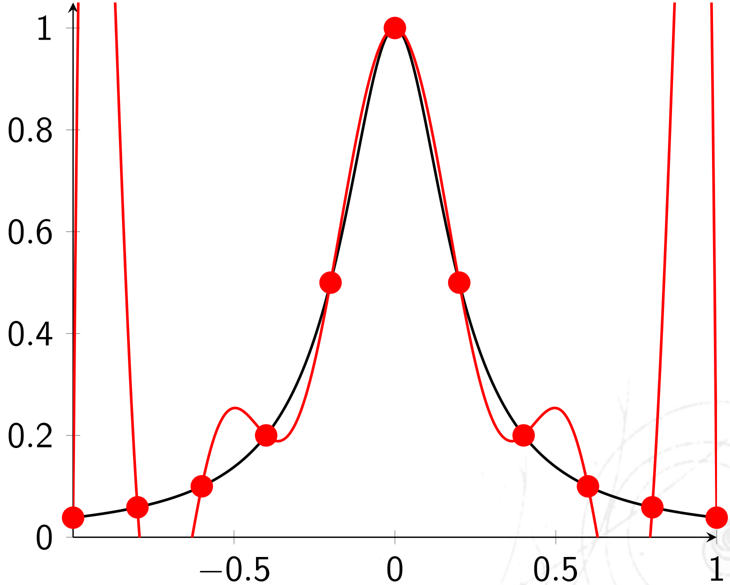
Consistency check

Any given (closed) Newton-Coates formula must fulfill

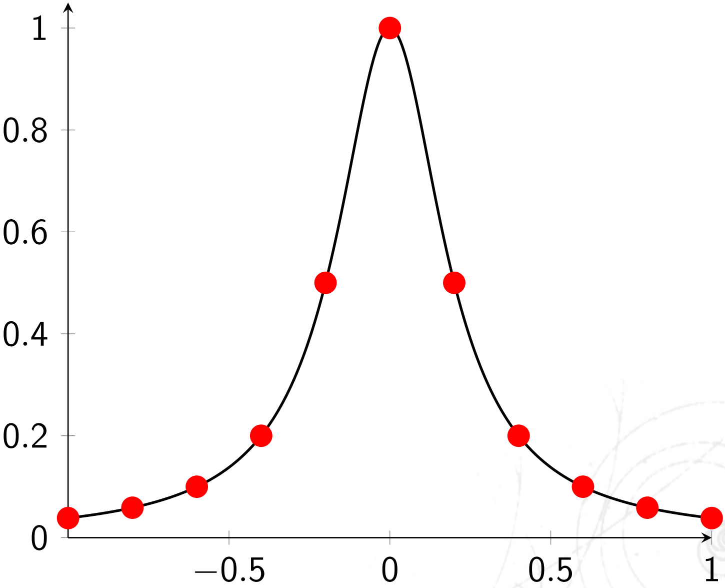
$$\sum_{k=0}^{K} \omega_k^{(K)} = 1$$

To be proven in the exercises.

Pathological example 1



Conclusion 1: We know how to fix it!



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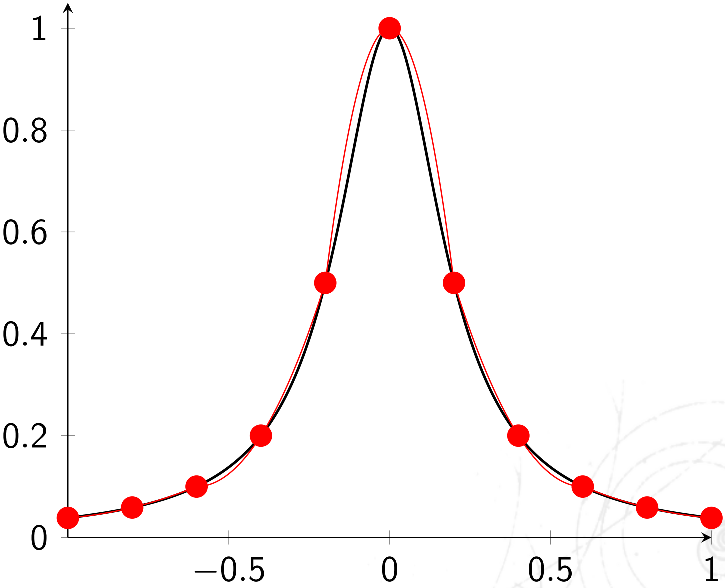


Conclusion 1: We know how to fix it!

When interpolating a function, we saw that using splines fixes the problem of oscillating interpolating polynomials.

We can now use this to stabilise our interpolation formula as well.

- Let M be the number of intervals in which we want to integrate.
- Let N be the degree of the interpolating polynomial in each interval.
- Enforce that the interpolating function is continous, but not differentiable at the interval boundaries.

The integral can then be approximated as

$$I = \sum_{m=1}^{M-1} \int_{x_{m\cdot N}}^{x_{(m+1)\cdot N}} \mathrm{d}x\, f(x) = \frac{b-a}{M} \sum_{m=1}^{M-1} \sum_{n=0}^{N} \omega_k f(x_{m\cdot N+n}) = \frac{b-a}{N\cdot M} \sum_{k=0}^{K=N\cdot M} \Omega_k f(x_k)$$

with $x_i = a + (b-a)\frac{i}{N\cdot M}$.

(Closed) Newton-Cotes Weights and error estimates

N	$\omega_k^{(N)}$	approx. error
1	$\frac{1}{2}\ \frac{1}{2}$	$\sim (b-a) f''(\xi)$
2	$\frac{1}{6}\ \frac{4}{6}\ \frac{1}{6}$	$\sim (b-a) f^{(4)}(\xi)$
3	$\frac{1}{8}\ \frac{3}{8}\ \frac{3}{8}\ \frac{1}{8}$	$\sim (b-a) f^{(4)}(\xi)$
$\vdots$	$\vdots$	$\vdots$

Comments and observations:

- $\xi \in [a, b]$
- While numerical factors change, the approximation error scales only with an even derivative of the integrand!
- The iterated weights Ω_k can be obtained from shuffling and interweaving the single-interval weights ω_k, e.g.:

$$\Omega_k^{(1)} = \{\frac{1}{2}, 1, 1, \ldots, 1, \frac{1}{2}\}$$
$$\Omega_k^{(2)} = \{\frac{1}{6}, \frac{4}{6}, \frac{2}{6}, \frac{4}{6}, \frac{2}{6}, \ldots, \frac{2}{6}, \frac{1}{6}\}$$

Should we always use equidistant grids?

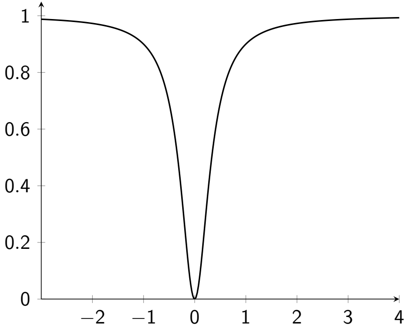
Both open and closed Newton-Cotes formula use fixed-size equidistant grids to interpolate the target function piece by piece.

Should we always do that?

Can it be benefitial to use prior knowledge of the target function in our approximation of the interval? How to incorporate that into the methods that we know?

Pathological example 2

$$I \equiv \int_{-3}^{+4} \mathrm{d}x \left[1 - \frac{\varepsilon}{x^2 + \varepsilon}\right] \qquad \text{with } \varepsilon = \frac{1}{9}$$



Exact result

$$I = 5.57396$$

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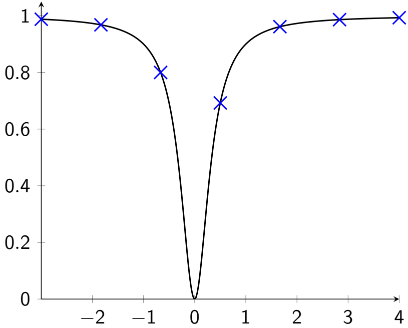

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Entire range, 7 data points

$$I_7 = 6.25746 \qquad \delta_7 = 12.26\%$$

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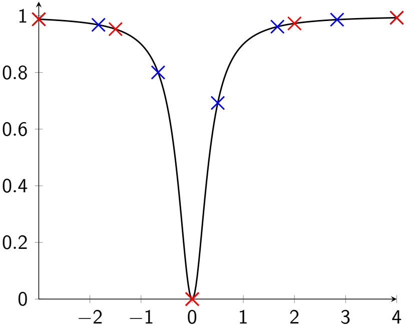

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Two integration, 5 data points

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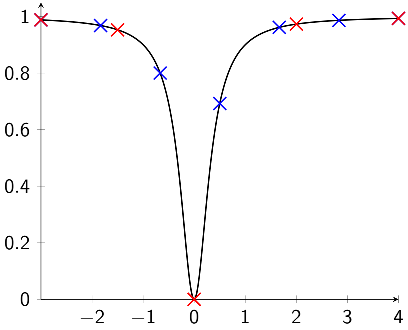

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It is benefitial to arrange the integration intervals around known special points (e.g.: roots, minima, poles!) of the integrand!

Rationale for Gauss quadrature

Given that we ended up (again) using polynomial interpolation to numerically solve a problem, we can ask ourselves the following question:

Is there a method to numerically obtain the exact integral of a polynomial of degree $2N - 1$?

Carl Friedrich Gauß answered in the affirmative!

General idea

We restrict ourselves to the interval $[a, b]$, and to integrals of the type

$$I = \int_a^b \mathrm{d}x\, \omega(x) p(x)$$

Nomenclature:

- $p(x)$ is a polynomial of degree N.
- $\omega(x)$ is the weight function: $\omega(x) > 0$, integrable and has finitely many roots in $[a, b]$.
- $p_i(x)$ are elements of the vector space of orthogonal polynomials under ω:

$$\langle p_i(x), p_j(x) \rangle \equiv \int_a^b \mathrm{d}x\, \omega(x) p_i(x) p_j(x) = \delta_{ij}$$

We can then approximate

$$I \approx \sum_{n=1}^{N} \omega_n f(\xi_n)$$

where the evaluation points ξ_n with $n = 1, \ldots, N$ are not yet defined

General idea cont'd

What happened? Why is this different from Newton-Cotes?

- The evaluation points ξ_n are not equidistant anymore!
- Choose ω_n and ξ_n such that

$$\tilde{p}(x) = p(\xi_n)\left[\prod_{m=1, n\neq m}^{N} \frac{x-\xi_n}{\xi_m-\xi_n}\right]$$

$$0 = \sum_{n=1}^{N} \omega_n p_i(\xi_n) \qquad \forall i < N$$

We can achieve this through

$$\omega_n \equiv \int_a^b \mathrm{d}x\, \omega(x)\left[\prod_{m=1, n\neq m}^{N} \frac{x-\xi_n}{\xi_m-\xi_n}\right]$$

and choosing ξ_n as the roots of $p_N(x)$.

- $\tilde{p}(x)$ corresponds to an interpolating polynomial of degree $N-1$ that interpolates $p(x)$ in the N roots of a (orthogonal) polynomial $p_N(x)$.

Why is this so benefitial

Interpolating polynomial

$$\tilde{p}(x) = \sum_n p(\xi_n) \left[\prod_{m=1, n\neq m}^{N} \frac{x - \xi_n}{\xi_m - \xi_n} \right]$$

We can measure the distance between the interpolating polynomial and any other polynomial of degree $N' = 0, \ldots, N-1 < N$:

$$\langle p_{N'}, p \rangle = 0 = \int_a^b \omega(x) p_{N'}(x) p(x)$$

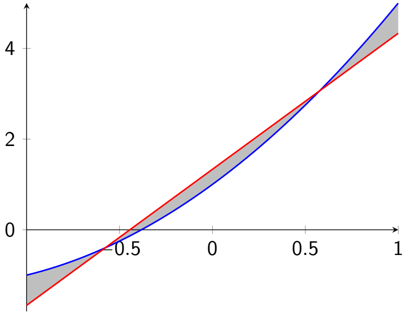
by construction.

Here $p_{N'}(x)p(x)$ is a polynomial of up to degreen $N' + N \leq 2N - 1$. Therefore no quadrature formula of degree $< 2N$ exists which yields a better approximation to I than the Gaussian quadrature.

Example

- Let $p(x) = 1 + 3x + x^2$, with degree $N = 2$.
- Let $\omega(x) = 1$, which impllies usage of the Legendre polynomials.
- Let $\xi_n = \{-1/\sqrt{3}, +1/\sqrt{3}\}$: the roots of P_2.
- Interpolate $p(x)$ in the roots:

$$\tilde{p}(x) = \frac{4}{3} - 3x$$



- The integrals over both $\omega(x)p(x)$ and $\omega(x)\tilde{p}$ coincide: $I = 8/3$.
- The discrete weights are $\omega_1 = \omega_2 = 1$
  $\Rightarrow I \approx p(\xi_1) + p(\xi_2) = \left[\frac{4}{3} - \sqrt{3}\right] + \left[\frac{4}{3} + \sqrt{3}\right] = \frac{8}{3}$.

List of weight functions and associated polynomials

interval $[\boldsymbol{a}, \boldsymbol{b}]$	**weight** $\omega(\boldsymbol{x})$	**name of polynomials**	
$[-1, 1]$	1	$P_n(x)$	Legendre polynomials
$[-1, 1]$	$(1-x^2)^{-1/2}$	$T_n(x)$	Tschebyscheff polynomials
$[-1, 1]$	$(1-x)^{\alpha}(1+x)^{\beta}$	$P_n^{\alpha,\beta}(x)$	Jacobi polynomials
$[0, \infty]$	$\exp(-x)$	$L_n(x)$	Laguerre polynomials
$[-\infty, \infty]$	$\exp(-x^2)$	$H_n(x)$	Hermite polynomials

You can look up this list, as well as the roots ξ_n and the weights ω_n in:

Handbook of mathematical functions, Abramowith and Stegun (1964).

Backup