Numerical Integration

- Problem Formulation
- Lagrange Quadrature
- Gauss Quadrature

Contents

Problem Formulation

We are interested in computing integrals of the form

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

for given functions $f : \mathbb{R} \to \mathbb{R}$.

In this lecture, we assume (for simplicity) that f is sufficiently often differentiable.

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Integration of Polynomials

For the special case that the function f is polynomial, the integral

$$\int_a^b f(x)\,\mathrm{d}x = \int_a^b \sum_{i=0}^{n} c_i x^i \,\mathrm{d}x$$

can be computed explicitly. We find

$$\int_a^b f(x)\,\mathrm{d}x = \int_a^b \sum_{i=0}^{n} c_i x^i \,\mathrm{d}x = \sum_{i=0}^{n} \frac{c_i}{i+1}\left(b^{i+1} - a^{i+1}\right) ,$$

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Integration using Lagrange Interpolation

Since we know how to integrate polynomials, one strategy to approximate the general integral

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

is to first approximate f by a polynomial and then use the integral over this polynomial as an approximation for the integral over f.

One way to do this is by Lagrange interpolation. For this aim, we choose points $x_0, \ldots, x_n \in [a, b]$ and compute

$$p(x) = \sum_{i=0}^{n} f(x_i) L_i(x) = \sum_{i=0}^{n} f(x_i) \prod_{j \neq i} \frac{x - x_j}{x_i - x_j} \,.$$

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Newton-Cotes Formulas

An important special case of Lagrange interpolation is obtained for equidistant points:

- Closed Newton-Cotes methods choose:

$$x_i = a + i * H, \quad i = 0, \ldots, n, \quad \text{with} \quad H = \frac{b-a}{n} \; .$$

- Open Newton-Cotes methods choose:

$$x_i = a + (i+1) * H, \quad i = 0, \ldots, n, \quad \text{with} \quad H = \frac{b-a}{n+2} \; .$$

Newton-Cotes Formulas

Using the coordinate transformation $x = a + tH$ with $t \in [0, n]$ we can compute the Lagrange polynomials

$$L_i(t) = \prod_{j=0, j\neq i}^{n} \frac{x - x_j}{x_i - x_j} = \prod_{j=0, j\neq i}^{n} \frac{t - j}{i - j}$$

The so-called Newton-Cotes coefficients

$$\alpha_i = \int_0^n \prod_{j=0, j\neq i}^{n} \frac{t - j}{i - j} \, \mathrm{d}t$$

can be computed "once and forever".The integral approximation is then given by

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

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Example: Simpson's rule

For $n = 2$ the coefficients of the closed Newton-Cotes methods are

- $\alpha_0 = \int_0^2 \frac{t-1}{0-1} \frac{t-2}{0-2} \, \mathrm{d}t = \frac{1}{3}$.
- $\alpha_1 = \int_0^2 \frac{t-0}{1-0} \frac{t-2}{1-2} \, \mathrm{d}t = \frac{4}{3}$.
- $\alpha_2 = \int_0^2 \frac{t-0}{2-0} \frac{t-1}{2-1} \, \mathrm{d}t = \frac{1}{3}$.
- The corresponding approximation formula

$$\int_a^b f(x) \, \mathrm{d}x \approx \frac{H}{3} \left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right)$$

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Integration Error

We use the divided difference notation

$$\begin{aligned} f[x_i] &= f(x_i) \\ f[x_i, x_{i+1}, \ldots, x_{i+k}] &= \frac{f[x_{i+1}, x_{i+2}, \ldots, x_{i+k}] - f[x_i, x_{i+1}, \ldots, x_{i+k-1}]}{x_{i+k} - x_i}\,, \end{aligned}$$

which is defined recursively. If $x_{i+k} = x_i$, replace the divided difference by the corresponding derivative of f, see Hermite interpolation.

The integration error is now given by

$$\int_a^b f(x)\mathrm{d}x - \left(\frac{b-a}{n}\sum_{i=0}^{n} f(x_i)\alpha_i\right) = \int_a^b f[x_0, \ldots, x_n, x]\prod_{j=0}^{n}(x - x_j)\,\mathrm{d}x$$

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Example

The error of Simpson's formula is bounded by

$$\int_a^b f\left[a, \frac{a+b}{2}, b, x\right](x-a)\left(x-\frac{a+b}{2}\right)(x-b)\,\mathrm{d}x$$

$$= \int_a^b \frac{f\left[a, \frac{a+b}{2}, b, x\right] - f\left[a, \frac{a+b}{2}, b, \frac{a+b}{2}\right]}{x-\frac{a+b}{2}} \underbrace{(x-a)\left(x-\frac{a+b}{2}\right)^2(x-b)}_{\leq 0}\,\mathrm{d}x$$

$$+f\left[a, \frac{a+b}{2}, b, \frac{a+b}{2}\right] \underbrace{\int_a^b (x-a)\left(x-\frac{a+b}{2}\right)(x-b)\,\mathrm{d}x}_{=0}$$

$$\leq \frac{\max_{x\in[a,b]} |f^{(4)}(x)|}{4!} \underbrace{\left|\int_a^b (x-a)\left(x-\frac{a+b}{2}\right)^2(x-b)\,\mathrm{d}x\right|}_{=\frac{(b-a)^5}{120}}$$

Example

Summary: the numerical error of Simpson's formula is bounded by

$$\frac{\max_{x\in[a,b]}|f^{(4)}(x)|}{4!}\frac{(b-a)^5}{120} = \frac{(b-a)^5}{2880}\max_{x\in[a,b]}|f^{(4)}(x)|$$

The error bounds for other Newton-Cotes methods can be worked out analogously.

Contents

Order of Integration Formulas

Let f be a smooth function and $I(f) = \int_a^b f(x)\,\mathrm{d}x$. We say that an integration formula of the form

$$I_n(f) = \sum_{i=0}^{n} \alpha_i f(x_i)$$

has order $q \in \mathbb{N}$ if there exists a constant $C < \infty$ such that

$$|I(f) - I_n(f)| \leq C \max_{\xi \in [a,b]} |f^{(q)}(\xi)|\,|b-a|^q$$

for any q-times differentiable function f.

Maximum Order of Integration Formulas

What is the maximum "order" of integration formulas of the form

$$I(f) = \int_a^b f(x)\,\mathrm{d}x \approx I_n(f) = \sum_{i=0}^{n} \alpha_i f(x_i) \text{ ?}$$

Can we choose the points $x_0, \ldots, x_n \in [a, b]$ in a smart way?

An answer to this question was given by Gauss: the best order we can achieve is

$$|I(f) - I_n(f)| \le \mathbf{O}\left((b-a)^{2n+2}\right) \,.$$

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Maximum Order of Integration Formulas

Let us first show that $m = 2n+2$ is an upper bound on the order. For this aim, we consider the polynomial

$$p(x) = \frac{1}{b-a} \prod_{i=0}^{n} (x - x_i)^2 \; .$$

If we had a interpolation formula with order larger than $2n+2$ it would be exact for $p(x)$, i.e.,

$$0 = I_n(p) = I(p) = \underbrace{\int_a^b p(x)\,\mathrm{d}x}_{\mathbf{O}((b-a)^{2n+2})} > 0 \; .$$

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Gauss Quadrature Rule: Main Idea

How can we construct an interpolation formula with order $2n + 2$?

In the following, we use the devided difference notation

$$f[x_0, \ldots, x_n] = \sum_{i=0}^{n} f(x_i) \prod_{j=0, j\neq i}^{n} \frac{1}{x_i - x_j} .$$

The interpolation based integration formula for $2n + 2$ points,

$x_0, \ldots, x_n, x_{n+1}, \ldots, x_{2n+1}$ can now be written as

$$\begin{aligned} I_{2n+1}(f) &= \sum_{i=0}^{2n+1} f[x_0, \ldots, x_i] \int_a^b \prod_{j=0}^{i-1} (x - x_j)\, \mathrm{d}x \\ &= I_n(f) + \sum_{i=n+1}^{2n+1} f[x_0, \ldots, x_i] \int_a^b \prod_{j=0}^{i-1} (x - x_j)\, \mathrm{d}x \end{aligned}$$

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Gauss Quadrature Rule: Main Idea

The integral term in the equation

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can be written in the form

$$\int_a^b \prod_{j=0}^{i-1} (x - x_j)\,\mathrm{d}x = \int_a^b \underbrace{\prod_{j=0}^{n} (x - x_j)}_{\in P_{n+1}} \underbrace{\prod_{j=n+1}^{i-1} (x - x_j)}_{\in P_n}\,\mathrm{d}x \;.$$

Thus, if we succeed in choosing $x_0, \ldots, x_n$ such that

$$\int_a^b \prod_{j=0}^{n} (x - x_j) q(x)\,\mathrm{d}x = 0 \quad \text{for all} \;\; q \in P_n \;,$$

we would have $I_{2n+1}(f) = I_n(f)$.

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we would have $I_{2n+1}(f) = I_n(f)$.

Gauss Quadrature Rule: Main Idea

Let us assume $a = -1$ and $b = 1$. The main idea is to choose the points $x_0, x_1, \ldots, x_n$ such that we have

$$L_{n+1}(x_i) = 0$$

with L_{n+1} being the $(n+1)$-th Legendre polynomial we must have

$$\int_{-1}^{1} \underbrace{\prod_{j=0}^{n} (x - x_j)}_{\sim L_{n+1}(x)} q(x)\,\mathrm{d}x = 0 \quad \text{for all} \;\; q \in P_n \ ,$$

since L_{n+1} is by construction orthogonal on P_n.

Roots of the Legendre Polynomials

Theorem:

The Legendre polynomial L_{n+1} has $n+1$ distinct real roots on the interval $[-1,1]$.

Proof: We define the set

$$S = \{\lambda \in (-1,1) \mid \lambda \text{ is a real root of } L_{n+1} \text{ with odd multiplicity}\}$$

and the polynomial $q(x) = \prod_{\lambda \in S}(x-\lambda)$. Now, the polynomial $q(x) \cdot L_{n+1}(x)$ must be either positive or negative; that is,

$$\langle q, L_{n+1} \rangle \neq 0 \ .$$

For $|S| < n+1$ this is a contradiction to $q \perp L_{n+1}$.

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Gauss Quadrature

If $x_0, \ldots, x_n$ are the $n+1$ roots of the Legendre polynomial L_{n+1} on the interval $[a,b]$, then the corresponding quadrature formula

$$I_n(f) = \sum_{i=0}^{n} \alpha_i f_i(x_i)$$

with $\alpha_i = \int_a^b \prod_{j=0, j\neq i}^{n} \frac{x-x_j}{x_i-x_j}\,\mathrm{d}t$ has order $2n+2$, i.e.,

$$|I(f) - I_n(f)| \leq \mathbf{O}\left((a-b)^{2n+2}\right) \ .$$

Example

For the case $n = 1$, the Legendre polynomial $L_2(x) = \frac{1}{2}(3x^2 - 1)$ has the roots

$$x_{1,2} = \pm\sqrt{\frac{1}{3}}$$

Thus, the first Gauss quadrature formula is given by

$$\int_{-1}^{1} f(x)\,\mathrm{d}x \;\approx\; f\left(-\sqrt{\frac{1}{3}}\right) + f\left(\sqrt{\frac{1}{3}}\right) \;,$$

which is exact for polynomials of order less or equal than $2n + 1 = 3$.

Summary

- The main idea of numerical integration is to first approximate the function f with a polynomial p and then integrate the polynomial.
- For equidistant interpolation points, we obtain the so-called Newton Codes formulas. The coefficients $\alpha_i = \int_0^n \prod_{j=0,j\neq i}^n \frac{t-j}{i-j}\,\mathrm{d}t$ can be worked out "once and forever".
- The maximum order of polynomial interpolation based integration schemes is $2n+2$ (for $n+1$ evaluation points). This order can be achieved by using Gauss quadrature rules.