

Numerical Integration

- Problem Formulation
- Lagrange Quadrature
- Gauss Quadrature

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Problem Formulation

We are interested in computing integrals of the form

$$\int_a^b f(x) \, dx$$

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

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

Integration of Polynomials

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

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

can be computed explicitly. We find

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

which can be evaluated with Horner's algorithm.

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Integration using Lagrange Interpolation

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

$$\int_a^b f(x) \, dx$$

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 $x_0, \dots, x_n \in [a, b]$ and compute

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

Newton-Cotes Formulas

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

- Closed Newton-Cotes methods choose:

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

- Open Newton-Cotes methods choose:

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

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

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

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

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

Example: Simpson's rule

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

- $\alpha_0 = \int_0^2 \frac{t-1}{0-1} \frac{t-2}{0-2} dt = \frac{1}{3}.$

- $\alpha_1 = \int_0^2 \frac{t-0}{1-0} \frac{t-2}{1-2} dt = \frac{4}{3}.$

- $\alpha_2 = \int_0^2 \frac{t-0}{2-0} \frac{t-1}{2-1} dt = \frac{1}{3}.$

- The corresponding approximation formula

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

with $H = \frac{b-a}{2}$ is called Simpson's rule.

Integration Error

We use the divided difference notation

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

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

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

Example

The error of Simpson's formula is bounded by

$$\begin{aligned}
 & \int_a^b f \left[a, \frac{a+b}{2}, b, x \right] (x-a) \left(x - \frac{a+b}{2} \right) (x-b) dx \\
 = & \int_a^b \frac{f \left[a, \frac{a+b}{2}, b, x \right] - f \left[a, \frac{a+b}{2}, b, \frac{a+b}{2} \right]}{x - \frac{a+b}{2}} \underbrace{\left(x-a \right) \left(x - \frac{a+b}{2} \right)^2 (x-b)}_{\leq 0} dx \\
 & + f \left[a, \frac{a+b}{2}, b, \frac{a+b}{2} \right] \underbrace{\int_a^b (x-a) \left(x - \frac{a+b}{2} \right) (x-b) dx}_{=0} \\
 \leq & \frac{\max_{x \in [a,b]} |f^{(4)}(x)|}{4!} \underbrace{\left| \int_a^b (x-a) \left(x - \frac{a+b}{2} \right)^2 (x-b) dx \right|}_{=\frac{(b-a)^5}{120}}
 \end{aligned}$$

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.

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Maximum Order of Integration Formulas

What is the maximum order of integration formulas of the form

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

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

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

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

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

$$p(x) = \prod_{i=0}^n (x - x_i)^2 .$$

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

$$0 = I_n(p) = I(p) = \int_a^b p(x) \, dx > 0 .$$

This is a contradiction! Thus, $m = 2n + 2$ is an upper bound on the order.

Gauss Quadrature Rule: Main Idea

The integral term in the equation

$$I_{2n+1}(f) = I_n(f) + \sum_{i=n+1}^{2n+1} f[x_0, \dots, x_i] \int_a^b \prod_{j=0}^{i-1} (x - x_j) dx$$

can be written in the form

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

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

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

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, \dots, 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

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

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 $q \perp L_{n+1}$.

Gauss Quadrature

If x_0, \dots, 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 $\alpha_i = \int_a^b \prod_{j=0, j \neq i}^n \frac{x - x_j}{x_i - x_j} dt$ has order $2n + 2$, i.e.,

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

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

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

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