MA 322: Scientific Computing

Department of Mathematics
Indian Institute of Technology Guwahati

February 21, 2023

Chapter 4: Numerical Integrations or Quadratures

Gaussian quadrature formula

It is to be noted that the zeros of different orthogonal polynomials are also used to evaluate $\int_a^b f(x)\mathrm{d}x$ for various choice of a, b, and $w(x)$.

Interval	$w(x)$	Orthogonal polynomials	Known as
$[-1,1]$	1	Legendre polynomials	Gauss-Legendre quadrature
$[-1,1]$	$\frac{1}{\sqrt{1-x^2}}$	Chebyshev polynomials (1st kind)	Gauss-Chebyshev quadrature
$[-1,1]$	$\sqrt{1-x^2}$	Chebyshev polynomials (2nd kind)	Gauss-Chebyshev quadrature
$[0,\infty)$	e^{-x}	Laguerre polynomials (2nd kind)	Gauss-Laguerre quadrature
$(-\infty,\infty)$	e^{-x^2}	Hermite polynomials (2nd kind)	Gauss-Hermite quadrature

Gaussian quadrature formula

Let $\{\phi_n(x)\}_{n\geq 0}$ be the orthogonal polynomials on (a, b) with respect to the weight function $w(x) \geq 0$. Denote the zeros of $\phi_n(x)$ by

$$a < x_1 < \cdots < x_n < b.$$

Define A_n by

$$\phi_n(x) = A_n x^n + \ldots$$

Write $\phi_n(x) = A_n(x - x_{n,1})(x - x_{n,2}) \cdots (x - x_{n,n})$. Let

$$a_n = \frac{A_{n+1}}{A_n}$$

$$\gamma_n = \langle \phi_n, \phi_n \rangle := \int_a^b w(x)[\phi_n(x)]^2 \mathrm{d}x > 0.$$

Gaussian quadrature formula

Theorem

For each $n \geq 1$, there is a unique numerical integration formula

$$I_n(f) = \sum_{j=1}^{n} w_j f(x_j) \approx \int_a^b w(x) f(x) \mathrm{d}x = I$$

of degree of precision $2n-1$. Assuming $f \in C^{2n}[a,b]$, the formula for $I_n(f)$ and its error is given by $\displaystyle\int_a^b w(x) f(x) \mathrm{d}x = \sum_{j=1}^{n} w_j f(x_j) + \frac{\gamma_n}{A_n^2 (2n)!} f^{(2n)}(\eta)$, *for some $a < \eta < b$. The nodes $\{x_j\}$ are zeros of $\phi_n(x)$, and the weights $\{w_j\}$ are given by*

$$w_j = \frac{-a_n \gamma_n}{\phi_n'(x_j) \phi_{n+1}(x_j)}, \quad j = 1, 2, \ldots, n.$$

Legendre polynomials

- Solution of the following SL problem

$$(1-x^2)y'' - 2xy' + n(n+1)y = 0, \qquad -1 < x < 1,$$

is Legendre polynomial of degree n given by

$$P_n(x) = \frac{1}{2^n n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^2-1)^n, \quad n = 0, 1, 2, \cdots .$$

- Legendre polynomials are orthogonal (with respect to weight 1),

$$\langle P_m, P_n \rangle := \int_{-1}^{1} 1 \cdot P_m(x) P_n(x)\,\mathrm{d}x = \begin{cases} 0, & m \neq n \\ \frac{2}{2n+1}, & m = n \end{cases}$$

Chebyshev polynomials (First kind)

- One of the two linearly independent solutions of the following SL problem

$$(1-x^2)y'' - xy' + n^2 y = 0, \qquad -1 < x < 1,$$

is Legendre polynomial (first kind) of degree n given by

$$T_n(x) = \frac{(-2)^n n!}{(2n)!}\sqrt{1-x^2}\,\frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^2-1)^{n-1/2}, \quad n = 0, 1, 2, \cdots .$$

- Legendre polynomials, $T_n(x)$, are orthogonal (with respect to weight $1/\sqrt{1-x^2}$),

$$\langle T_m, T_n \rangle := \int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} T_m(x) T_n(x)\, \mathrm{d}x = \begin{cases} 0, & m \neq n \\ \pi/2, & m = n \neq 0 \\ \pi, & m = n = 0 \end{cases}$$

Chebyshev polynomials (Second kind)

- The second member of the linearly independent solutions of the following SL problem
$$(1-x^2)y'' - xy' + n^2 y = 0, \qquad -1 < x < 1,$$
is Legendre polynomial (second kind) of degree n given by
$$U_n(x) = \frac{(-1)^n (n+1)\sqrt{\pi}}{2^{n+1}(n+1/2)!} \frac{1}{\sqrt{1-x^2}} \frac{\mathrm{d}^n}{\mathrm{d}x^n}(x^2-1)^{n+1/2}, \quad n = 0, 1, 2, \cdots .$$
- Legendre polynomials, $U_n(x)$, are orthogonal (with respect to weight $\sqrt{1-x^2}$),
$$\langle U_m, U_n \rangle := \int_{-1}^{1} \sqrt{1-x^2}\, U_m(x) U_n(x)\, \mathrm{d}x = \begin{cases} 0, & m \neq n \\ \pi/2, & m = n \end{cases}$$

Laguerre polynomial

- Solution of the following SL problem

$$xy'' + (1-x)y' + ny = 0, \qquad 0 \le x < \infty,$$

is Laguerre polynomial of degree n given by

$$L_n(x) = \frac{e^x}{n!}\frac{\mathrm{d}^n}{\mathrm{d}x^n}(e^{-x}x^n), \quad n = 0, 1, 2, \cdots .$$

- Legendre polynomials, $U_n(x)$, are orthogonal (with respect to weight e^{-x}),

$$\langle L_m, L_n \rangle := \int_0^\infty e^{-x} L_m(x) L_n(x)\, \mathrm{d}x = \begin{cases} 0, & m \neq n \\ 1, & m = n \end{cases}$$

Hermite polynomial

- Solution of the following SL problem

$$y'' + 2xy' + 2ny = 0, \qquad -\infty < x < \infty,$$

is Hermite polynomial of degree n given by

$$H_n(x) = \frac{1}{2}(-1)^n\sqrt{\pi}e^{x^2}\frac{\mathrm{d}^{n+1}}{\mathrm{d}x^{n+1}}\mathrm{erf}(x), \quad n = 0, 1, 2, \cdots .$$

- Legendre polynomials, $U_n(x)$, are orthogonal (with respect to weight e^{-x^2}),

$$\langle H_m, H_n\rangle := \int_{-\infty}^{\infty} e^{-x^2} H_m(x)H_n(x)\,\mathrm{d}x = \begin{cases} 0, & m \neq n \\ 2^n\ n!\ \sqrt{\pi}, & m = n \end{cases}$$

The Exponentially Convergent Trapezoidal Rule

Authors: Lloyd N. Trefethen and J. A. C. Weideman | AUTHORS INFO & AFFILIATIONS

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Abstract

It is well known that the trapezoidal rule converges geometrically when applied to analytic functions on periodic intervals or the real line. The mathematics and history of this phenomenon are reviewed, and it is shown that far from being a curiosity, it is linked with computational methods all across scientific computing, including algorithms related to inverse Laplace transforms, special functions, complex analysis, rational approximation, integral equations, and the computation of functions and eigenvalues of matrices and operators.

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[Submitted on 23 Jan 2021]

Exactness of quadrature formulas

Lloyd N. Trefethen

The standard design principle for quadrature formulas is that they should be exact for integrands of a given class, such as polynomials of a fixed degree. We show how this principle fails to predict the actual behavior in four cases: Newton-Cotes, Clenshaw-Curtis, Gauss-Legendre, and Gauss-Hermite quadrature. Three further examples are mentioned more briefly.

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[Submitted on 20 Oct 2014]

Fast computation of Gauss quadrature nodes and weights on the whole real line

Alex Townsend, Thomas Trogdon, Sheehan Olver

A fast and accurate algorithm for the computation of Gauss-Hermite and generalized Gauss-Hermite quadrature nodes and weights is presented. The algorithm is based on Newton's method with carefully selected initial guesses for the nodes and a fast evaluation scheme for the associated orthogonal polynomial. In the Gauss-Hermite case the initial guesses and evaluation scheme rely on explicit asymptotic formulas. For generalized Gauss-Hermite, the initial guesses are furnished by sampling a certain equilibrium measure and the associated polynomial evaluated via a Riemann-Hilbert reformulation. In both cases the n-point quadrature rule is computed in $\mathcal{O}(n)$ operations to an accuracy that is close to machine precision. For sufficiently large n, some of the quadrature weights have a value less than the smallest positive normalized floating-point number in double precision and we exploit this fact to achieve a complexity as low as $\mathcal{O}(\sqrt{n})$.

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