Gaussian Quadrature

MATH 375

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Fall 2006

Introduction

Consider the definite integral:

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

The Newton-Cotes formulae discussed so far have used equally spaced nodes in the interval $[a, b]$ of the form $x_j = a + jh$ for $j \in \mathbb{Z}$ where

$$h = \frac{b-a}{n}$$

for some $n \in \mathbb{N} \cup \{0\}$.

The approximation method known as **Gaussian Quadrature** makes an adaptive choice of nodes that minimizes the error in the approximation.

Basic Idea

Choose x_i and c_i for $i = 1, 2, \ldots, n$ such that

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} c_i f(x_i).$$

Note: The constants c_i are arbitrary, but $x_i \in [a, b]$ for $i = 1, 2, \ldots, n$.
There are $2n$ values to be selected.

Objective

- The efficacy of this approach will be judged by the considering the size of the class of polynomials for which this approximation formula gives exact results.
- With $2n$ degrees of freedom, we should expect the upper limit of the **precision** of this method to be $2n - 1$.

Example

- Let $[a, b] = [-1, 1]$ and $n = 2$.
- We want to choose x_1, x_2, c_1, and c_2 so that

$$\int_{-1}^{1} f(x)\,dx \approx c_1 f(x_1) + c_2 f(x_2).$$

- The approximation should be exact for any polynomial of degree 3 or less.

If we let

$$P(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$$

then

$$\int_{-1}^{1} P(x)\,dx = a_0 \int_{-1}^{1} 1\,dx + a_1 \int_{-1}^{1} x\,dx + a_2 \int_{-1}^{1} x^2\,dx + a_3 \int_{-1}^{1} x^3\,dx$$

Each of the remaining definite integrals involves an integrand of degree 3 or less. Gaussian Quadrature should be exact for each of these.

Applying Gaussian Quadrature to each remaining integral yields:

$$\begin{aligned}
\int_{-1}^{1} 1\,dx &= 2 = c_1 + c_2 \\
\int_{-1}^{1} x\,dx &= 0 = c_1 x_1 + c_2 x_2 \\
\int_{-1}^{1} x^2\,dx &= \frac{2}{3} = c_1 x_1^2 + c_2 x_2^2 \\
\int_{-1}^{1} x^3\,dx &= 0 = c_1 x_1^3 + c_2 x_2^3
\end{aligned}$$

Solution to Nonlinear System

Solving this system gives us

$$c_1 = 1, \quad c_2 = 1, \quad x_1 = -\frac{\sqrt{3}}{3}, \quad x_2 = \frac{\sqrt{3}}{3}.$$

Therefore

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

Example

$$\begin{aligned}\int_{-1}^{1} e^x \sin \pi x \, dx &= \frac{\pi(e^2-1)}{e(\pi^2+1)} \quad \text{(exact value)}\\ &\approx 0.679326\\ &\approx 1.18409 \quad \text{(Gaussian Quadrature)}\\ &\approx 0 \quad \text{(Simpson's Rule)}\end{aligned}$$

Legendre Polynomials

- Generalize the previous simple case to the case where $n > 2$.
- Use the **Legendre Polynomials**, $\{P_0(x), P_1(x), \ldots\}$, where
  - $\deg P_n = n$
  - If $P(x)$ is a polynomial of degree less than n, then

$$\int_{-1}^{1} P(x) P_n(x)\, dx = 0.$$

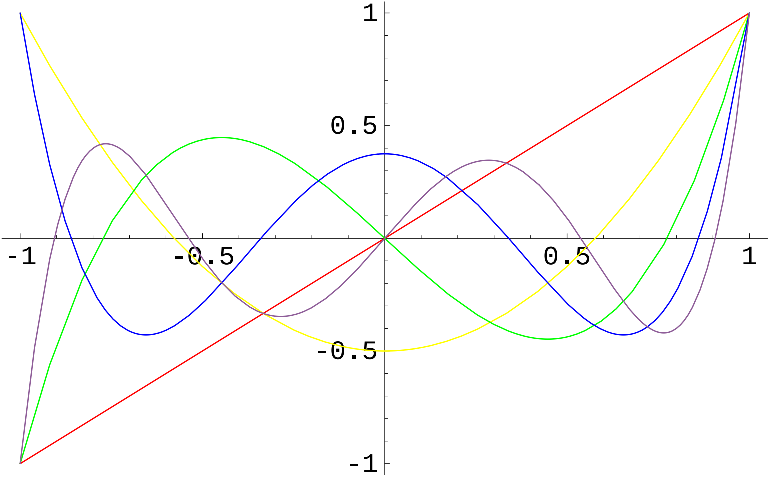
Properties of Legendre Polynomials

- The set of Legendre Polynomials forms an infinite-dimensional inner product space.
- First five Legendre polynomials

$$\begin{aligned} P_0(x) &= 1 \\ P_1(x) &= x \\ P_2(x) &= x^2 - \frac{1}{3} \\ P_3(x) &= x^3 - \frac{3}{5}x \\ P_4(x) &= x^4 - \frac{6}{7}x^2 + \frac{3}{35} \end{aligned}$$

- Higher degree Legendre polynomials can be generated using the **Gram-Schmidt Orthogonalization Process**.

Legendre Polynomial Graphs



More Properties

- Roots of the polynomials lie in the interval $(-1, 1)$.
- Roots are symmetric about the origin.
- Roots are distinct.
- For $P_n(x)$ the roots $\{x_1, x_2, \dots, x_n\}$ are the nodes needed by Gaussian Quadrature.

Roots of the Legendre Polynomials

n	$r_{n,i}$	$\tilde{r}_{n,i}$
2	$\pm\frac{\sqrt{3}}{3}$	± 0.5773502692
3	0	0
	$\pm\frac{\sqrt{15}}{5}$	± 0.7745966692
4	$\pm\frac{1}{35}\sqrt{525-70\sqrt{30}}$	± 0.3399810436
	$\pm\frac{1}{35}\sqrt{525+70\sqrt{30}}$	± 0.8611363116
5	0	0
	$\pm\frac{1}{21}\sqrt{245-14\sqrt{70}}$	± 0.5384693101
	$\pm\frac{1}{21}\sqrt{245+14\sqrt{70}}$	± 0.9061798459

Weights

For a fixed n the weights used in Gaussian Quadrature of order n are the values of

$$c_{n,i} = \int_{-1}^{1} \prod_{j=1, j \neq i}^{n} \frac{x - x_j}{x_i - x_j} \, dx = \int_{-1}^{1} L_{n,i}(x) \, dx,$$

where $L_{n,i}(x)$ is the i^{th} Lagrange Basis Polynomial of degree $n - 1$.

n	$c_{n,i}$	$\tilde{c}_{n,i}$
2	1	1
3	$\frac{8}{9}$	0.8888888889
	$\frac{5}{9}$	0.5555555556
4	$\frac{1}{36}(18+\sqrt{30})$	0.6521451549
	$\frac{1}{36}(18-\sqrt{30})$	0.3478548451
5	$\frac{128}{225}$	0.5688888889
	$\frac{1}{900}(322+13\sqrt{70})$	0.4786286705
	$\frac{1}{900}(322-13\sqrt{70})$	0.2369268850

Summary

n	$\tilde{r}_{n,i}$	$\tilde{c}_{n,i}$
2	± 0.5773502692	1
3	0	0.8888888889
	± 0.7745966692	0.5555555556
4	± 0.3399810436	0.6521451549
	± 0.8611363116	0.3478548451
5	0	0.5688888889
	± 0.5384693101	0.4786286705
	± 0.9061798459	0.2369268850

Main Result

Theorem

Suppose that $x_1, x_2, \ldots, x_n$ are the roots of the nth Legendre polynomial $P_n(x)$ and that for each $i = 1, 2, \ldots, n$, the numbers c_i are defined by

$$\int_{-1}^{1} \prod_{j=1, j\neq i}^{n} \frac{x - x_j}{x_i - x_j}\, dx.$$

If $P(x)$ is any polynomial of degree less than 2n, then

$$\int_{-1}^{1} P(x)\, dx = \sum_{i=1}^{n} c_i P(x_i).$$

When $[a, b] \neq [-1, 1] \ldots$

The previous theorem is valid only for integrals of the form

$$\int_{-1}^{1} f(x)\,dx.$$

For the case of

$$\int_{a}^{b} f(x)\,dx$$

we integrate by substitution using

$$\begin{aligned} x &= \frac{(b-a)}{2}t + \frac{(a+b)}{2} \\ dx &= \frac{(b-a)}{2}\,dt. \end{aligned}$$

Under this change of variables

$$\int_{a}^{b} f(x)\,dx = \int_{-1}^{1} f\left(\frac{(b-a)}{2}t + \frac{(a+b)}{2}\right)\frac{(b-a)}{2}\,dt.$$

Using Gaussian Quadrature with $n = 2$,

Example

$$\begin{aligned}\int_1^{1.5} x^2 \ln x \, dx &= \int_{-1}^{1} \left(\frac{t}{4} + \frac{5}{4}\right)^2 \ln\left(\frac{t}{4} + \frac{5}{4}\right) \frac{1}{4} \, dt \\ &\approx 0.192269 \\ \text{Absolute error} &\approx 9.35 \times 10^{-6}\end{aligned}$$

Using Gaussian Quadrature with $n = 3$,

Example

$$\begin{aligned} \int_1^{1.6} \frac{2x}{x^2-4}\,dx &= \int_{-1}^{1} \frac{2(0.3t+1.3)}{(0.3t+1.3)^2-4}\cdot 0.3\,dt \\ &\approx -0.733799 \\ \text{Absolute error} &\approx 1.70\times 10^{-4} \end{aligned}$$