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Gaussian Quadrature

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Abstract

This paper discusses the theory and implementation of Gaussian quadrature.

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1 Introduction

In a calculus course, students study Riemannian sums as a prelude to learning how to integrate. Typically, the curriculum involves:

1. left-hand, midpoint, and right-hand Riemann sums
2. the trapezoidal rule
3. Simpson's rule

A student is then usually asked to write a program to implement these integration schemes and compare the results. These schemes have a few things in common:

1. They have a beautiful and accessible geometrical interpretation.
2. The "formulas" follow the pattern:

$$\int_a^b f(x)\,dx \;\approx\; \sum_{i=0}^{N} w_i\, f(x_i) \tag{1}$$

3. They use equally spaced intervals (the x_i are equally spaced).
4. No researcher would touch them with a ten meter pole.

They're taught for pedagogical reasons: accessibility of the underlying concepts. But nobody in their right mind would actually *use* them because there are better algorithms that give more accurate results for less work.

The two widespread numerical integration techniques that researchers *do* use are Gaussian quadrature and Romberg integration.

2 Introducing Gaussian Quadrature

Like elementary techniques, Gaussian quadrature approximates integrals with eqn(1), but gridpoints $\{x_i\}$ are no longer equally spaced and weights $\{w_i\}$ are chosen craftily. Actually, Gaussian quadrature is a *class* of integration techniques, and each one is best suited for a different type of integral. For example, integrals of the form:

$$\int_a^b e^{-x} f(x)\, dx$$

are best integrated using *Gauss-Laguerre quadrature*. The most common and widely applicable technique is called *Gauss-Legendre quadrature*. All Gaussian quadrature is based on the following theorem:

Definition 1 Let $q(x)$ be a polynomial of degree N, such that:

$$\int_a^b q(x)\, \rho(x)\, x^k\, dx \;=\; 0 \tag{2}$$

where k is any integer on $[0, N-1]$, and ρ is some weighting function. Let $\{x_i\}$ be the N roots of $q(x)$. Construct the integration formula:

$$\int_a^b f(x)\rho(x)\, dx \;\approx\; \sum_{i=0}^{N} w_i\, f(x_i) \tag{3}$$

We are *guaranteed* that for *some* set of $\{w_i\}$ the approximation is exact if $f(x)$ is a polynomial of degree $< 2N$.

We know we can always fit an $N-1$ degree polynomial to a set N points[1]. This theorem says, by carefully choosing the gridpoints and weights, we can exactly fit an $N-1$ degree polynomial to a $< 2N$ degree polynomial. Amazing!

The point of this is that if the function we want to integrate is approximated well by a high-degree polynomial, this theorem guarantees that eqn(1) will be near equality.

[1] 2 points define a line, 3 points define a parabola, etc.

3 Three-point Gauss-Legendre Quadrature

This is the most widespread Gaussian quadrature scheme and is characterized by:

- Astonishingly, it uses only 3 gridpoints: not very computationally intensive!
- It takes $\rho(x) = 1$.
- Integration is on $[-1, 1]$. We can transform any integral onto this range using:

$$\int_a^b f(x)\,dx \;=\; \frac{b-a}{2}\int_{-1}^{1} f(u)\,du \qquad\qquad x = \frac{1}{2}(b+a) + \frac{1}{2}(b-a)u$$

This means, we're looking for a formula that looks like:

$$\int_{-1}^{1} f(x)\,dx \;=\; \sum_{i=1}^{3} w_i\, f(x_i)$$

3.1 Step 1: Find $q(x)$

Because we're deriving a three-point rule, $q(x)$ is a cubic:

$$q(x) \;=\; c_0 + c_1 x + c_2 x^2 + c_3 x^3 \tag{4}$$

From theorem 1, we know that for $N = 3$:

$$\int_{-1}^{1} q(x)\,dx \;=\; \int_{-1}^{1} q(x)\,x\,dx \;=\; \int_{-1}^{1} q(x)\,x^2\,dx \;=\; 0 \tag{5}$$

Plugging eqn(4) into eqn(5) and performing the integrals, we get:

$$2c_0 + \frac{2}{3}c_2 \;=\; \frac{2}{3}c_1 + \frac{2}{5}c_3 \;=\; \frac{2}{3}c_0 + \;=\; \frac{2}{5}c_2 \;=\; 0$$

The solution[2] to this set of linear equations is:

$$q(x) \;=\; \frac{5}{2}x^3 - \frac{3}{2}x$$

which is the Legendre polynomial $P_3(x)$. In general, $q(x)$ for the N-point Gaussian quadrature is $P_N(x)$.

[2] $c_0 = 0$, $c_1 = -a$, $c_2 = 0$, $c_3 = 5a/3$.

3.2 Step 2: Find the roots of $q(x)$

Next we need to find the roots of $P_3(x)$ which are our gridpoints. This step is non-trial, but for the 3-point Legendre-Gauss forumla, it's easily found that $\{x_3\} = \pm\frac{3}{5}, 0$.

Our integration formula so far is:

$$\int_{-1}^{1} f(x)\,dx \;=\; w_1\,f(-\frac{3}{5}) + w_2\,f(0) + w_3\,f(\frac{3}{5})$$

In general, the roots of $q(x)$ for the N-point Gauss Legendre integration will be the roots of $P_N(x)$.

3.3 Step 3: Find the weights

From theorem 1 we know that eqn(3.2) must be exact if $f(x)$ is either 1, x, $\cdots$, x^5. Since we only have 3 unknowns, we can consider $f(x) = \{1, x, x^2\}$ which are the easiest. After some computation, we're left with 3 equations with 3 unknowns:

$$\begin{aligned}
2 &= w_1 + w_2 + w_3 \\
0 &= -\sqrt{\frac{2}{5}}\,w_1 + \sqrt{\frac{2}{5}}\,w_2 \\
\frac{2}{3} &= \frac{3}{5}\,w_1 + \frac{3}{5}\,w_3
\end{aligned}$$

Solving this system of equations we have $w_1 = \frac{5}{9}$, $w_2 = \frac{8}{9}$. $w_3 = \frac{5}{9}$.

Thus, for 3-point Gauss-Legendre quadrature, we have:

$$\int_{-1}^{1} f(x)\,dx \;=\; \frac{5}{9}\,f(-\frac{3}{5}) + \frac{8}{9}\,f(0) + \frac{5}{9}\,f(\frac{3}{5})$$

4 Gauss-Legendre Quadrature

For the error function,

$$\mathrm{erf}(x) \;=\; \frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2}\, dy$$

evaluated at $x = 1$, our humble 3-point Legendre Gauss formula gives 5 digits of accuracy! With only 3 function evaluations! Whoa!

For N-point Gauss-Legendre qudrature, $q(x)$ is the Legendre polynomial of order N, the $\{x_i\}$ are the roots of the Legendre polynomials, and the $\{w_i\}$ are given by:

$$w_i \;=\; \frac{2}{(1 - x_i^2)\,(P_N'(x_i))^2}$$

However, you generally look up $q(x)$, its roots, and the $\{w_i\}$ in a table like Abramowitz and Stegun (in the 9th printing, the tables start with table 25.4 on page 916).

5 General Gaussian Quadrature

$\int_{-1}^{1} f(x)\, dx$	Gaussian or Gauss-Legendre
$\int_{-1}^{1} \frac{F(x)}{\sqrt{1-x^2}}\, dx$	Gauss-Chebyshev (rational)
$\int_{-\infty}^{\infty} e^{-x^2}\, F(x)\, dx$	Gauss-Hermite
$\int_{-\infty}^{\infty} e^{-x}\, F(x)\, dx$	Gauss-Laguerre
$\int_{-1}^{1} \frac{e^{-x}}{\sqrt{x}} F(x)\, dx$	Associated Gauss-Laguerre

6 Conclusion

The main benefit of Gaussian quadrature is very high-order accuracy with *very* few points (typically less than 10). This is great when $f(x)$ is expensive to compute. In general, you want

$$\int_a^b f(x)\, dx \;=\; \int_a^b \rho(x)\, F(x)\, dx$$

$f(x)$ or $F(x)$ to be smooth. For regions where $N \leq 20$ gives poor results, the function is very badly behaved and not well approximated by a high order polynomial. In this case, you'll want to use another scheme for the region of bad behavior.

On the bad side, it's not easy to get an error estimate of your work, and unlike Romberg integration, you can't really iterate this technique.