PHYS-4007/5007: Computational Physics
Course Lecture Notes
Appendix G

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Version 7.0

Abstract

These class notes are designed for use of the instructor and students of the course PHYS-4007/5007: Computational Physics I taught by Dr. Donald Luttermoser at East Tennessee State University.

Appendix G: Numerical Integration Using Gaussian Quadrature

A. Gaussian Quadrature.

1. Often, one cannot choose an evenly spaced interval of grid points to do a numerical integration. From Eq. (VI-21) we have

$$\int_a^b f(x)\,dx \approx w_1 f(x_1) + \cdots + w_N f(x_N) \; . \qquad \text{(G-1)}$$

One then can ask the question, *is there an optimal choice for the grid points (or nodes)* x_i *and the weights* w_i *to solve this integral?*

2. This question leads us to formulate a new class of integration formulas, known collectively as **Gaussian quadrature**.

a) In this class, we will use only the most common formula, namely **Gauss-Legendre quadrature**.

i) There are many other kinds of Gaussian quadrature that treat specific types of integrands, such as the *Gauss-Laguerre* formularization which is optimal for integrals of the form $\int_0^\infty e^{-x} f(x)\,dx$.

ii) The derivation of the other Gaussian formulas (see Table 5.2 in your textbook) is similar to our analysis of Gauss-Legendre quadrature.

b) The theory of Gaussian integration is based on the following theorem.

i) Let $q(x)$ be a polynomial of degree N such that

$$\int_a^b q(x)\rho(x)x^k\,dx = 0 \; , \qquad \text{(G-2)}$$

where $k = 1, 2, ..., N-1$ and $\rho(x)$ is a specified weight function.

ii) Call $x_1, x_2, ..., x_N$ the roots of the polynomial $q(x)$. Using these roots as grid points plus a set of weights $w_1, w_2, \ldots, w_N$ we construct an integration formula of the form

$$\int_a^b f(x)\rho(x)\,dx \approx w_1 f(x_1) + \cdots + w_N f(x_N)\ . \quad \text{(G-3)}$$

iii) There is a set of w's for which the integral formula will be *exact* if $f(x)$ is a polynomial of degree $< 2N$.

c) The weights can be determined from the **Three-Point Gaussian-Legendre Rule**. For example, consider the interval $[-1, 1]$ with $\rho(x) = 1$. This gives us a Gaussian-Legendre formula. For integrals in the interval $[a, b]$, it is easy to transform them as

$$\int_a^b f(x)\,dx = \frac{b-a}{2}\int_{-1}^{1} f(z)\,dz \quad \text{(G-4)}$$

using the change of variable $x = \frac{1}{2}[b + a + (b - a)z]$.

i) The first step is to find polynomial $q(x)$. We want a three-point rule so that $q(x)$ is a cubic:

$$q(x) = c_0 + c_1 x + c_2 x^2 + c_3 x^3\ . \quad \text{(G-5)}$$

ii) From the theorem of Eq. (C-2), we know that

$$\int_{-1}^{1} q(x)\,dx = \int_{-1}^{1} x q(x)\,dx = \int_{-1}^{1} x^2 q(x)\,dx = 0\ . \quad \text{(G-6)}$$

iii) Plugging in and doing each integral we get the equations

$$2c_0 + \frac{2}{3}c_2 = \frac{2}{3}c_1 + \frac{2}{3}c_3 = \frac{2}{3}c_0 + \frac{2}{5}c_2 = 0 \ . \qquad \text{(G-7)}$$

iv) The general solution is $c_0 = 0, c_1 = -a, c_2 = 0, c_3 = 5a/3$, where a is some constant. This arbitrary constant cancels out in the second step.

v) Using this in Eq. (IX-64) gives a polynomial solution of

$$q(x) = \frac{5}{2}x^3 - \frac{3}{2}x \ . \qquad \text{(G-8)}$$

Notice that this is just the Legendre polynomial $P_3(x)$.

vi) Next we need to find the roots of $q(x) = P_3(x)$. This cubic is easy to factor. The roots are $x_1 = -\sqrt{3/5}, x_2 = 0$, and $x_3 = \sqrt{3/5}$. Using the grid points in Eq. (C-5) gives

$$\int_{-1}^{1} f(x)\, dx \approx w_1 f(\sqrt{3/5}) + w_2 f(0) + w_3 f(-\sqrt{3/5}) \ . \qquad \text{(G-9)}$$

vii) Finally, to find the weights. The above formula must be exact for $f(x) = 1, x, ..., x^5$. We can use this to work out values of w_1, w_2, and w_3. It turns out to be sufficient to consider just $f(x) = 1, x$, and x^2 which produces 3 equations:

$$\begin{aligned} 2 &= w_1 + w_2 + w_3 \\ 0 &= -\sqrt{3/5}w_1 + \sqrt{3/5}w_3 \\ \frac{2}{3} &= \frac{3}{5}w_1 + \frac{3}{5}w_3 \ . \end{aligned} \qquad \text{(G-10)}$$

viii) This linear system of equations is easy to solve giving $w_1 = 5/9, w_2 = 8/9, w_3 = 5/9$.

ix) An alternative way of finding the weights is to use the identity

$$w_i = \frac{2}{(1 - x_i^2)\{(d/dx)P_N(x_i)\}^2} \,, \qquad \text{(G-11)}$$

where $N = 3$ in our example. This formula may be derived from the recurrence relation for Legendre polynomials.

d) There are various advantages and disadvantages in using Gaussian integration.

i) Advantage: A very high-order accuracy is obtained for just a few points — often this method yields excellent results using fewer than 10 points.

ii) Disadvantages: (1) The node points and weights must be computed or obtained from tables. This step is nontrivial if you want to use many node points. Using more than $N = 20$ points is rarely worth it since badly behaved functions will spoil the results in any case. (2) Unlike Newton-Cotes integration, the method does not lead itself to iteration nor is it easy to estimate the error.

3. You will typically never have to write your own Gaussian quadrature subroutines since they are included in math libraries and built into some programming languages (*e.g.*, the IDL functions INT_2D( ) and INT_3D( ); the QGAUS subroutine in Numerical Recipes).