PHYS 304 5.5-5.10 Notes

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February 2024

1 Higher-order integration methods

The general form of trapezoidal and Simpson rule is,

$$\int_b^a f(x)dx \approx \sum_{k=1}^{N} \omega_k f(x_k) \tag{1}$$

, this is called Newton-Cotes formulas.

Suppose we have N sample points; there can be $(N-1)th$-degree polynomials, assuming that the N points are equally spaced. If we can move the points, i.e., having them equally spaced, it is unnecessary; there can be $2N-1$ degrees for the polynomial. Thus, we would have higher accuracy.

2 Gaussian Quadrature

2.1 Nonuniform sample points

To make a good fit of the function, we need the interpolating polynomials,

$$\phi_k(x) = \prod_{m=1...N, m\neq k} \frac{x - x_m}{x_k - x_m} \tag{2}$$

, which can be represented by the Kronecker Delta function,

$$\phi_k(x_m) = \begin{cases} 1 & m = k \\ 0 & m \neq k \end{cases} \tag{3}$$

We proceed to write our fitting polynomial as,

$$\Phi(x_m) = \sum_{k=1}^{N} f(x_k)\phi_k(x) = f(x_m) \tag{4}$$

, where $\phi_k(x)$ can be integrated to get ω_k in equation 1. The polynomial is unique since it has N coefficients and N constraints. This section tells us that we can calculate the weights by knowing the positions of sample points.

2.2 Sample points for Gaussian quadrature

As we mentioned earlier, reaching the highest order $2N-1$ is possible if we have N freedom for moving x positions. An important point for choosing x is to ensure they coincide with the zeros of the Nth Legendre polynomial $P_N(x)$. To get the weights, we can apply,

$$\omega_k = [\frac{2}{(1-x^2)}(\frac{dP_N}{dx})^{-2}]_{x=x_k} \tag{5}$$

2.3 Gaussian quadrature errors

The method for estimating the error in Gaussian quadrature is called "Gauss-Kronrod quadrature," explained in Appendix C.

3 When to use the appropriate function

Integral Method	Benefit	Appropriate situations
The trapezoidal rule	quick	lab experiments/poorly behaved functions
Simpson's rule	higher accuracy than trapezoidal rule	less suitable for poorly behaved functions
Romberg integration	exceptionally accurate/fewer sample points	equally spaced sample points/smooth functions
Gaussian quadrature	most accurate	unequally spaced sample points

4 Infinite integral

Transform the infinite limit to specific values.

$\int_0^\infty f(x)dx$	$z = \frac{x}{1+x}$ $x = \frac{z}{1-z}$	$\int_0^\infty f(x)dx = \int_0^1 \frac{1}{(1-z)^2} f(\frac{z}{1-z})dz$
$\int_a^\infty f(x)dx$	$z = \frac{x-a}{1+x-a}$ $x = \frac{z}{1-z} + a$	$\int_a^\infty f(x)dx = \int_0^1 \frac{1}{(1-z)^2} f(\frac{z}{1-z} + a)dz$
$\int_{-\infty}^\infty f(x)dx$	$x = \frac{z}{1-z^2}$ $dx = \frac{1+z^2}{(1-z^2)^2}dz$	$\int_{-\infty}^\infty f(x)dx = \int_{-1}^1 \frac{1+z^2}{(1-z^2)^2} f(\frac{z}{1-z})dz$
$\int_{-\infty}^\infty f(x)dx$	$x = \tan(z)$ $dx = \frac{dz}{cos^2 z}$	$\int_{-\infty}^\infty f(x)dx = \int_{-\pi/2}^{\pi/2} \frac{f(\tan z)}{(\cos^2 z} dz$

5 Multiple integration

Sometimes, we encounter multi-variable calculus. For example, if we have a charge distribution in 2-dimension, given the electric field, we need to integrate over both x and y coordinates in Cartesian. Or we can integrate over r and θ in circular coordinates. Either way, we will proceed with more than one variable. Thus, we proceed to come up with a computer program enabling multi-variable calculus.

Suppose we have $I = \int_0^1 \int_0^1 f(x,y)dxdy$. We firstly rewrite a function $F(y)$ as $F(y) = \int_0^1 f(x,y)dx$. Then, we have $I = \int_0^1 F(y)dy$. This way, we separate the multi-variable integral into two single-variable integrals. We can use the Gaussian quadrature shown in the previous section to calculate the weights. We can also combine the weights so that,

$$I \approx \sum_{i=1}^{N} \sum_{j=1}^{N} \omega_i \omega_j f(x_i, y_j) \tag{6}$$

When choosing the 2-dimensional set of sample points, we have various ways to decide. There's no way to tell which one is better. One standard method is called the "Sobol sequence." We can also use the famous "Monte Carlo" method, which will be illustrated in later chapters.

6 Derivatives

1. forward difference

$$\frac{df}{dx} \approx \frac{f(x+h) - f(x)}{h} \tag{7}$$

2. backward difference

$$\frac{df}{dx} \approx \frac{f(x) - f(x+h)}{h} \tag{8}$$

6.1 Errors

When considering the errors on the derivative, we need to consider both the approximate and the rounding errors. However, round error is proportional to $\frac{1}{h}$, while the approximate error is proportional to h, where h is the step we want to minimize. Thus, we take a derivative of the sum of both errors to h and make it equal to zero to get the appropriate h. Then, the error is around,

$$\epsilon = \sqrt{4C|f(x)f''(x)|} \tag{9}$$

To make the estimate more accurate, we can use the central difference for the derivative, which will have error around,

$$\epsilon = (\frac{9}{8}C^2[f(x)]^2|f'''(x)|)^{1/3} \tag{10}$$

6.2 Second derivative

Following the firs derivative, we can calculate the second derivative by,

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{1}{12}h^2 f''''(x) + ... \tag{11}$$

,with an error equal to,

$$\epsilon = (\frac{4}{3}C|f(x)f''''(x)|)^{1/2} \tag{12}$$