Numerical Methods for Integration

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Four distinct numerical techniques of integration were exercise. Romberg integration, Gauss-Legendre quadrature, Gauss-Laguerre quadrature, and Monte Carlo simulations were employed in solving multidimensional integrals as they related to specific physics problems. Romberg integration extrapolated results of the simple trapezoidal rule producing more precise numerical approximations. Both forms of Gaussian Quadrature produced exact results in one and two dimensional integrals. . Monte Carlo Simulations handled multidimensional integrals (> 2) producing quick accurate results.

## Introduction

*Romberg Integration*

Romberg integration consists of a lower diagonal matrix populated with extrapolated integral values stemming from the first column. The first column is calculated utilizing the trapezoidal rule. The trapezoidal rule integrates functions by successively evaluating the function at discrete points assigning a predictive and repeating weight to each evaluation.

$$\int_{x_0}^{x_n} f(x)\,dx \approx h\left(\frac{f_0}{2}+f_1+f_2+..+f_{n-1}+\frac{f_n}{2}\right) \quad (1)$$

The number of discrete points, n, is calculated by

$$n = 2^m \quad (2)$$

Where m is the row number of the Romberg table with an initial value of zero. Taylor expanding equation (1) about x=a and x=b, error correction terms are found.

$$\int_{x_0}^{x_n} f(x)\,dx \approx \frac{h}{2}[f(a)+f(b)] + \frac{h^2}{4}[f'(a)-f'(b)] + \frac{h^3}{12}[f''(a)+f''(b)]... \quad (3)$$

The even ordered terms are canceled when one taylor expands f'(x) about x=a and x=b. The result, known as the Euler-McLaurin rule, expresses the integral as a trapezoidal rule sum with correction terms.

$$\int_{x_0}^{x_n} f(x)\,dx \approx h\left(\frac{f_0}{2}+f_1+f_2+..+f_{n-1}+\frac{f_n}{2}\right) + \frac{h^2}{12}(f'_0-f'_n)-\frac{h^4}{720}(f'''_0-f'''_n)... \quad (4)$$

Romberg integration aims to increase numerical accuracy by eliminating the leading term in the Euler-McClaurin rule. An increase in “n” leads to a decrease in “h”. An interval with twice as many points will have one quarter the amount of error accounting only for the first order correction term. Using this fact, the generalized formula for an entry in the Romberg table is derived.

$$T_{m+k,k} = \frac{4^k T_{m+k,k-1} - T_{m+k-1,k-1}}{4^k - 1} \quad (5)$$

From equation (5), a lower diagonal matrix is computed with increasing numerical accuracy. Romberg integration breaks down when the derivative terms at the end points are infinite. A ratio test of the first Romberg column provides a provision to gauge the rate of convergence of the trapezoidal rule.

$$R_m = \frac{T_{m-1,0}-T_{m,0}}{T_{m,0}-T_{m+1,0}} \approx 4 \quad (6)$$

Should $R_m$ not approximately equal four, a change of variables in the integrand is necessary.

*Gauss-Legendre Quadrature*

Gaussian quadrature numerically evaluates integrals by expressing them as a sum of the integrand multiplied by a weighting function.

$$\int_a^b f(x) \approx \sum_{m=1}^{N} W_m f(x_m) \tag{7}$$

Both the weights and discrete independent variable values must be calculated. The condition put on equation (7) is that quadrature representation for the integral be exact for polynomials of degree 2N-1 and below.

$$\sum_{k=1}^{N} \left[\frac{1}{k}(b^k - a^k) = W_1 {x_1}^{k-1} + W_2 {x_2}^{k-1}\right] \tag{8}$$

The result is 2N non-linear equations with 2N unknowns. In order to solve for the abscissas', utilizing the form

$$\int_a^b f(x) w(x)\, dx \approx \sum_{m=1}^{N} W_m f(x_m) \tag{9}$$

f(x) is set to be a polynomial of order up to 2N-1. If f(x) is divided by φ , which is an orthogonal function relevant to w(x) and the integration limits, f(x) can be expressed as

$$f(x) = q_{N-1}(x)\phi_N(x) + r_{N-1} \tag{10}$$

q and r are functions of order N-1. This substituted into equation (9) yields

$$\int_a^b q_{N-1}(x)\phi_n(x) w(x) = \sum_{m=1}^{N} W_m q_{N-1}\phi_n(x) \tag{11}$$

All of the φ functions are complete allowing a recasting of q.

$$q_{N-1}(x) = \sum_{i=0}^{N-1} q_i \phi_i(x) \tag{12}$$

Substituting equation (12) into (11) it can be seen that given the properties of orthogonal functions, the right hand side goes to 0. To ensure the left hand side goes to zero as well, the zero's of the φ (x) function must be found. For finite limits and and w(x) = 1, these are the zero's of the Legendre polynomials. The weights, W, are then defined as

$$W_i = \int_a^b l_{i,N}(x)\, dx$$
$$l_{i,N}(x) = \sum_{m=1}^{N} \frac{(x - x_i)}{(x_j - x_i)}, \; i \neq j \tag{13}$$

*Gauss-Laguerre Quadrature*

Gauss-Laguerre handles integrals with infinite limits of integration. Recasting the integral

$$\int_0^\infty g(x)\, dx = \int_0^\infty e^{-x} f(x)\, dx \tag{14}$$

It can be shown that with the use of orthogonal functions and the same reasoning outlined for Gauss-Legendre, that the abscissas are the zeros of the Laguerre polynomials.

*Monte Carlo*

The method of Monte Carlo integration numerically evaluates an integrand randomly numerous times in an effort to achieve a working average of the function. The average is then multiplied by the integrating range.

$$\int_a^b f(x) = (b-a) < f(x) > \tag{15}$$

Where

$$< f(x) >_N = \frac{1}{N} \sum_{i=1}^{N} f(x_i) \tag{16}$$

Substituting equation (16) into equation (15), the full method of Monte Carlo integration is derived.

$$\int_a^b f(x) = (b-a) \frac{1}{N} \sum_{i=1}^{N} f(x_i) \tag{17}$$

What must be stressed is that the $x_i$ points are chosen at random, uniformly distributed within the interval [a,b]. This method can be expanded out to any dimension that is required for the given integrand.

An increase in accuracy of the Monte Carlo method is achieved through *importance sampling*. Importance sampling judiciously chooses points in the interval [a,b] where the value of the function

contributes the most to the average.

If the analytical form of the integrand f(x) is known, another integrable function, g(x) may chosen so that

$$g(x) \approx f(x) \tag{18}$$

Multiplying the integrand by g(x) / g(x)

$$\int_a^b f(x)\,dx = \int_a^b \frac{f(x)}{g(x)} g(x)\,dx = \int_{y^{-1}(a)}^{y^{-1}(b)} \frac{f(x)}{g(x)}\,dy \tag{19}$$

Where

$$y(x) = \int^x g(t)\,dx \tag{20}$$

If g(x) is a close enough approximation to f(x), the integrand of equation (19) equates to one and the integral is sampled randomly and uniformly over y. This method places more points in regions where the value of f(x) is large, allowing for a better estimate of the average.

Monte Carlo methods are employed thousands of times on the same integral, in which each successive value for the integral is "binned" into a histogram. This binning, when graphed, shows the spread of the obtained integral values, which is proportional to 1/ √N where N is the number of points used in each successive Monte Carlo run. An increase in N leads to a decrease in the width of the histogram.

Results from probability theory explain where the resultant Monte Carlo estimate lies with respect to the exact average. The standard deviation of the Monte Carlo technique is defined as

$$\sigma_N = \sqrt{\frac{\frac{1}{N}\sum f(x_i)^2 - \left(\frac{1}{N}\sum f(x_i)\right)^2}{N-1}} \tag{21}$$

Probability states that the resultant average for the Monte Carlo method has a 68.3% probability of being within one standard deviation of the true mean. This result allows equation (15) to be rewritten as

$$\int_a^b f(x) \approx (b-a)(\langle f(x)\rangle_N \pm \sigma_N) \tag{22}$$

With a 68.3% confidence level. To Increase the confidence level, the number of standard deviations allowed must be increased.

**Applications**

In order to ensure that the Romberg method of integration employed by the written C code, the methodology was employed on the function

$$I = \int_{-1}^{1} \sqrt{1-x^2}\,dx \tag{23}$$

This was done as there was a provided table of Romberg values for equation (23) in which to verify the coded methods. The ratio test method was also verified against a table for equation (23).

Romberg integration was also employed against the function

$$I = \int_{-1}^{1} \sqrt{(1-x^2)(2-x)}\,dx \tag{24}$$

The ratio test was employed against the first column of the produced Romberg table to insure convergence. A change of variables was planned if the ratio test failed.

A physics application of this method was the integration of Fresnel integrals.

$$C(\nu) = \int_0^{\nu} \cos\left(\frac{\pi \omega^2}{2}\right) d\omega \tag{25}$$

$$S(\nu) = \int_0^{\nu} \sin\left(\frac{\pi \omega^2}{2}\right) d\omega \tag{26}$$

Fresnel integrals arise out of the study of geometric optics and, when coupled describe the intensity of light after diffraction from a straight edge.

$$I = .5\,I_0[(C(\nu)+.5)^2 + (S(\nu)+.5)^2] \tag{27}$$

Numerically integrating equations (24) and (25) allowed for a evaluation of the intensity as a function of distance, υ.

Another physics application of this method was in numerically studying the periodicity of a simple pendulum.

$$T = 4\sqrt{\frac{l}{g}}\,K\left(\sin\left(\frac{\theta_0}{2}\right)\right) \tag{28}$$

Where l is the length of the pendulum, g is the acceleration due to gravity and theta is initial angle above a straight downward hang. K(k) is a complete elliptic integral of the first kind, taking the form

$$K(k) = \int_0^{\frac{\pi}{2}} \frac{1}{\sqrt{1 - k^2 \sin^2(\zeta)}}\,d\zeta \tag{29}$$

Different values of theta were input and the periodicity calculated.

Gauss-Legendre quadrature was implemented on two integrals.

$$\int_0^1 x^7\,dx \tag{30}$$

$$\int_0^1 \mathrm{e}^{-x^2}\,dx \tag{31}$$

Equations (30) and (31) were evaluated with quadratures of N = 2, 3, 4, and 5.

This method was extended out to evaluate the electric potential at a point outside a uniformly charged square.

$$\Phi(x_p, y_p) = \frac{\rho}{4\pi\epsilon_0}\int_{-1}^{1}\int_{-1}^{1} \frac{dxdy}{\sqrt{(x - x_p)^2 + (y - y_p)^2}} \tag{32}$$

Where Xp and Yp are the cartesian coordinates of the point in space being investigated.

Gauss-Laguerre quadrature was implemented against a single integral.

$$\int_0^\infty \frac{x^3}{\mathrm{e}^x - 1}\,dx \tag{33}$$

This was performed with quadratures of N = 2, 4, 6, and 8 points.

Monte Carlo integration was applied to evaluate the function

$$I = \int_0^1 \mathrm{e}^x\,dx \tag{34}$$

Equation (34) was recast using importance sampling to obtain

$$I = \int_0^{\frac{3}{2}} \frac{\mathrm{e}^{\sqrt{1+2y}-1}}{\sqrt{1+2y}}\,dy \tag{35}$$

Where

$$y = \int^x (1+t)\,dt = x + \frac{x^2}{2} \tag{36}$$

The method was applied 10,000 times for a schema of N= 100 points and for N = 400 points.

The final application of Monte Carlo integration was in solving the exchange energy of the first excited state of the helium atom.

The Hamiltonian of the helium atom is defined as

$$H = \frac{P_1^2}{2m_e} + \frac{P_2^2}{2m_e} - Ze^2\left(\frac{1}{|r_1|} + \frac{1}{|r_2|}\right) + \frac{e^2}{|r_1 - r_2|} \tag{37}$$

Where $P_1$ , $P_2$ and $r_1$ , $r_2$ are the momenta and radii of the first and second electron, respectively. “e” is the fundamental charge of an electron and $m_e$ is the mass of an electron.

It is the final term is equation (37) that makes is impossible to solve for the energy levels of the helium atom *exactly.* This term describes the electron-electron coulomb repulsion within the atom and is a positive attribution to the overall energy.

In the first excited state, one electron is promoted to the $|2lm\rangle$ state. Strictly speaking in terms of hydrogenic wave functions, the n=2 excited state is a four-fold degenerate eigenstate of the corresponding hamiltonian.

Utilizing overall anti-symmetric wave functions for helium as a result of the Pauli-exclusion principle in conjunction with first-order perturbation theory, the shift in energy as a result of the coulomb

repulsion can be approximated.

$$\Delta E_J = e^2 \int \int |\phi_{100}(r_1)|^2 |\phi_{2lm}(r_2)|^2 d^3 r_1 d^3 r_2 \quad (38)$$

$$\Delta E_K = e^2 \int \int \phi^*_{100}(r_1)\phi^*_{2lm}(r2)\frac{1}{|r_1 - r_2|} \times \phi_{2lm}(r_1)\phi_{100}(r_2) \quad (39)$$

Where the total shift is

$$\Delta E_T = \Delta E_J + \Delta E_K = J \pm K \quad (40)$$

J and K can take on two values depending on whether the excited electron is in a spin triplet state (Spin = 1, p-orbital) or a spin singlet state (Spin=0, s-orbital). It is these values, $J_{1s1s}$ , $J_{1s2p}$ , $K_{1s1s}$ and $K_{1s2p}$ that Monte Carlo integration was employed to solve. The radii of the electrons were broken down into their respective three dimensional cartesian coordinates and a six dimensional Monte Carlo integration was one 10^3 times for 10^6 points per evaluation. The random number generator utilized in performing the Monte Carlo integration was developed by Steve Park and David Geyer, described in the paper, "Random Number Generators: Good Ones Are Hard to Find," Communications of the ACM, October 1988.

**Results**

Table 1 shows the resulting Romberg table from the integration and extrapolation of equation (23). Clearly from Table 2, it can be seen that the ratio test fails for this particular integral. The substitution x = cos(θ) was made and the integral was reevaluated. Tables 3 and 4 show the resulting Romberg Table and ratio results, respectively. It can be seen through inspection and the values of table 4 that with the change of variables, the integral approximation converges and converges to the correct answer in 3 iterations.

Tables 4 and 5 show the resulting Romberg Table and ratio test values for equation (24). It can be seen from inspection and the ratio test that the integral approximation does not converge quickly and a change of variables is needed. Applying the same substitution as was done for equation (23), convergence of the approximation is achieved.

These two examples show that both the strength and weakness of Romberg integration. For integrals where the derivative at the limits of integration are infinite, Romberg integration breaks down and does not converge. If the functional form of the integrand is known, a change of variables can be applied when Romberg fails and the integral can be approximated again.

Figure 1 displays the value of I / Io from equation (27) as a function of υ. It is seen that as the proportional distance is increased, the relative intensity converges to approximately 56% of the incident intensity.

Straight edge diffraction causes a portion of the incident radiation to be skewed away from the bulk radiation. At large distances, the skewed radiation has diffused away from the incident portion, allowing for less constructive and/or destructive interference as seen be the large deviations in intensity at closer distances.

Figure 2 displays the results of the integration of equation (28). For simplicity, $4\sqrt{l/g}$ was taken to be unity so as to compare when the value of the integral began to deviate from the small angle approximation of (π / 2). It is evident from figure 2 that there is a singularity at θ = π. Physically, this corresponds to the pendulum initially at rest in a vertical position. Albeit an unstable equilibrium position, if unperturbed, the pendulum will remain in the vertical state with a period of ∞.

Figures 3 and 4 show the percent deviation from the small angle approximation value for the integral of π / 2. Equation (41) displays how the relative difference was calculated. Figure 4 is an expansion of figure 3 to illuminate exactly where the integral deviates from the small angle approximation by more than 1%. This value is calculated to be approximately .397 radians.

$$\frac{\left| \int_{calc} T - \int_{exact}^{small\ angle} T \right|}{\int_{exact}^{small\ angle} T} * 100 \quad (41)$$

Tables 9 and 10 display the results of Gauss-Legendre quadrature integration of equations (30) and (31). For the integration of equation (30), an exact solution is achieved for N>=4. Gauss-Legendre integration is intended for strictly polynomials with definite limits of integration. In the case of equation (31), the integral is neither. Again, however it is seen that with increasing N, decreasing error is achieved, as displayed in Table 11.

Figure 5 displays the resulting integral values for the two dimensional integral represented by equation (32). The potential is plotted along the z-axis and is a function of both the x and y distance. The greater the distance away from the origin, the weaker the electric field becomes, as expected.

Figures 6 and 7 display the histogram results for 1000 Monte Carlo integrations of equation (34) with N= 100 and N= 400, respectively. The width of either graph is proportional to the inverse square root of the number of points used in the integration.

$$Width \approx \frac{1}{\sqrt{N}} \qquad (42)$$

The standard deviation was computed to be approximately 3E-4 for N= 400. and 2E-3 for N=100.

The tabulated values for $J_{1s1s}$ , $J_{1s2p}$ , $K_{1s1s}$ and $K_{1s2p}$ were 11.4 eV, 13.2 eV, 1.2 eV and .9 eV, respectively. After 1000 iterations of the Monte Carlo method on equations (38) and (39) for the spin triplet and spin singlet excited states, the following average values for the simulations were calculated; 10.6 eV, 1.1 eV, 15.6 eV and .87 eV. These value yield an average error of 9.21%. This error is on the order of the number of iterations run to produce the average.

Due to the complex nature of the integrands and time constraints, the standard deviation value was not calculated for for any of the four values.

It is recommended that importance sampling be utilized for any further calculations into the helium atom. At its current state, the algorithm for computing the aforementioned values is computationally slow having to perform 10^6 calculations per dimension for 10^3 iterations.