Integrals, Integral Equations and Gaussian Quadrature

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Abstract

We first provide motivation by giving Integral equations that we routinely solve as examples. We then describe the method of Gaussian quadrature with some examples. Finally we show how to solve an integral equation that is usually encountered in quantum mechanical bound state problem.

1 Introduction

Physicists deal with integrals, integral equations and integro-differential equations everyday. For example, the most general Schroedinger equation in position space with nonlocal potential is an integro-differential equation. Schroedinger equation in momentum space is a homogeneous integral equation and Lippman-Schwinger equation, which is a Schroedinger equation with scattering boundary condition is an inhomogeneous integral equation. Here, we give a simple but most frequently encountered integral equation as an example. Consider the Schreodinger equation in momentum space. Most students are familiar with the position space representation of the Schroedinger equation, which is a second order partial differential equation. It is of the form

$$[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)]\Psi(\bar{r}) = E\Psi(\bar{r}) \tag{1}$$

This equation is never solved in this 3-dimensional form. Before it can be solved, the angular dependence must be separated. For simplicity of presentation, we will consider the systems where the orbital angular momentum l is a good quantum number. After the separation of variables, we obtain

$$[-\frac{\hbar^2}{2\mu}(\frac{1}{r}\frac{d^2}{dr^2}r) + \frac{\hbar^2 l(l+1)}{2\mu r^2} - V(r)]R(r) = ER(r) \tag{2}$$

The above equation can be solved for bound states or scattering problems by employing appropriate boundary conditions. Now, in momentum representation, the analogous 3-dimensional equation for bound states is

$$\frac{\mathbf{p}^2}{2\mu}\Phi(\mathbf{p}) + \int \langle \mathbf{p}|V|\mathbf{p}'\rangle \Phi(\mathbf{p}')d\mathbf{p}' = E\Phi(\mathbf{p}) \tag{3}$$

Here $\langle \mathbf{p}|V|\mathbf{p}'\rangle$ is the Fourier transform of the r-space potential $V(r)$ and is given by (We will use the units where $\hbar = c = 1$)

$$\langle \mathbf{p}|V|\mathbf{p}'\rangle = \frac{1}{(2\pi)^3}\int exp(-i\mathbf{p}\cdot\mathbf{r})V(r)d\mathbf{r} \tag{4}$$

Just like the position space Schroedinger equation, we do not solve this 3-dimensional integral equation directly. We will follow the way it is done in position space and seperate the anguular variables first. Now, to do the angular separation, we perform the partial wave decomposition for potentials that do not couple orbital angular momentum as follows,

$$\Phi(\mathbf{p}) = \phi_l(p)Y_l^m(\hat{p}) \tag{5}$$

$$\langle \mathbf{p}|V|\mathbf{p}'\rangle = \sum_{l=0}^{\infty}\sum_{m=-l}^{m=l} V_l(p,p')Y_l^m(\hat{p})Y_l^{m^*}(\hat{p}') \tag{6}$$

After this equation(3) becomes

$$\frac{p^2}{2\mu}\phi_l(p) + \int_0^\infty V_l(p,p')\phi_l(p){p'}^2dp' = E\phi_l(p) \tag{7}$$

where $V_l(p,p')$ is the l^{th} partial wave component of $\langle \mathbf{p}|V|\mathbf{p}'\rangle$ and is given by

$$V_l(p.p') = 2\pi\int_{-1}^{1}\langle \mathbf{p}|V|\mathbf{p}'\rangle P_l(x)dx \tag{8}$$

where $x = \cos\theta$ and we have used the following identities.

$$\int Y_l^m(\hat{p})Y_l^{m^*}(\hat{p}d\hat{p} = \delta_{ll'}\delta_{mm'} \tag{9}$$

$$\int_{-1}^{1} P_l(x)P_{l'}(x)dx = \frac{2\delta_{ll'}}{2L+1} \tag{10}$$

$$\sum_{m=-l}^{l} Y_l^m(\hat{p})Y_l^{m^*}(\hat{p} = \frac{2l+1}{4\pi}P_l(x) \tag{11}$$

The next thing we want to do is to solve Eq. 7. In order to do that, we expand the wavefunction $\phi_l(p)$ in terms of known orthonormal set of basis functions. i.e

$$\phi_l(p) = \sum_{n=1}^{N} C_n g_n(p) \tag{12}$$

where the functions $\{g_n(p)\}$ are known functions and form a complete orthonormal set. After the expansion, we multiply with $g_m(p)p^2$ and by integrating over dp we obtain our desired matrix eigenequation

$$\sum_{n=1}^{N} C_n \{ \int_0^\infty \frac{p^2}{2\mu} g_m(p) g_n(p) p^2 dp + \int_0^\infty \int_0^\infty V_l(p,p') g_m(p) g_n(p') p^2 p'^2 dp dp' \} = C_m \tag{13}$$

Since the terms in the braces depends only on the indices n and m, by naming it D_{mn}, we get

$$\sum_{n=1}^{N} D_{mn} C_n = E C_m \tag{14}$$

Obviously, from this matrix eigenvalue equation, we can solve for the eigen energies and also the eigenvectors where the expansion coefficients C_n are the componenets of the eigenvectors. Note that, for an $N \times N$ matrix, we will get N number of eigenvalues (E's) and for each eigenvalue, there is a corresponding eigenvector given by a set of C_n's. Once an eigenvalue (Energy) is known, we can construct the wavefunction for that state from the corresponding C_n's by using Eq. 12.
All this can be done, provided that we have the matrix D_{mn}. Obviously, in order to find the matrix elements of the matrix D, we must be able to evaluate the integrals in Eq. 13. Only in the rarest of circumstances, the integrals involved can be done analytically. In the following, I present a very accurate and most commonly used numerical integration method.

Gaussian Quadrature

In this section, I will describe how to use Gaussian quadrature method without proofs. Gaussian quadrature was designed by Karl Fredric Gauss. It simply states that

$$\int_{-1}^{+1} f(x)dx \;=\; \sum_{i=1}^{N} f(x_i) w_i + \text{Error} \tag{15}$$

Here the Error term is usually very small and I will not mention it again. In the above formula, x_i are the root of the Legendre polynomial $P_N(x)$. Since the N^{th} order Legendre polynomial has N number of roots, we say that we are

using N number of integration points. w_i are called the weights and they are given by

$$w_i = \frac{1}{[1-x_i^2][P'_N(x_i)]^2} \tag{16}$$

Where $P'_N(x_i)$ is the derivitive of $P_N(x)$ evaluated at x_i.

We first illustrate the method for a very simple case. Consider $N = 2$. In this case, $P_2(x) = \frac{1}{2}(3x^2 - 1)$ and $P'_2(x) = 3x$. Therefore, we obtains the roots of P_2 which are $x_1 = -\sqrt{1/3}$ and $x_2 = \sqrt{1/3}$. By using the formula for the weight, we obtain $w_1 = 1$ and $w_2 = 1$. As an example, consider the integral

$$\int_1^1 x^2 dx = \frac{2}{3} \tag{17}$$

Now by direct application of the Gaussian integration formula, we obtain

$$\begin{aligned} \int_1^1 x^2 dx &= \sum_{i=1}^{2} x_i^2 w_i & (18)\\ &= x_1^2 w_1 + x_2^2 w_2 & (19)\\ &= \frac{2}{3} & (20) \end{aligned}$$

Note that this gives us an exact answer. Gaussian quadrature is designed so that if the integrand is an N^{th} order polynomial, exact result can be achieved by using N point integration. So far, the limits are from -1 to 1 and it is not directly applicable for most integrals of interest. In order to remedy that, we consider the next example with different limits.

$$I = \int_a^b f(y)dy \tag{21}$$

In order to use our Gaussian quadrature formlula (with limits -1 to 1), we use a linear transformation

$$\begin{aligned} y &= mx + c & (22)\\ dy &= mdx & (23) \end{aligned}$$

What we want is to find the slope m and the y-intercept c so that when $y = a$, the lower limit for x is -1 and for $y = b$, the upper limit for x is $+1$. This gives us two equations with two unknowns and results in $m = (b-a)/2$ and $c = (b+a)/2$. Therefore our integral becomes,

$$\begin{aligned} \int_a^b f(y)dy &= \int_{-1}^{+1} f[y(x)]\ mdx & (24)\\ &= \frac{(b-a)}{2} \sum_{i=1}^{N} f[y_i(x_i)]w_i & (25) \end{aligned}$$

Another most commonly encountered limits of integration are from zero or a to ∞. This can also be done by using the following transformation.

$$y = a + tan[\frac{\pi}{4}(x+1)] \quad (26)$$

$$dy = \frac{\pi}{4}Sec^2[\frac{\pi}{4}(x+1)]dx \quad (27)$$

Obviously, these are not the only transformations possible. One should explore the most suitable transformations for each problem, but the above transformations work well for a large variety of integrals and physical problems.

A note on Legendre polynomials and finding the points and weights.

Legendre polynomials of the first kind $P_l(x)$ are solutions of the Legendre differential equation. The other linearly independent solution is called the Legendre polynomial of the second kind and denoted by $Q_l(x)$. The differential equation is

$$(1-x^2)\frac{d^2w}{dx^2} - 2x\frac{dw}{dx} + l(l+1)w = 0 \quad (28)$$

Analytically, $P_n(x)$ can be generated from the Rodrigues' formula

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n \quad (29)$$

For numerical calculations, it is best suited to use the recurrence relation with starting expressions $P_0(x) = 1$ and $P_1(x) = x$. These can be used in a bootstrap calculation together with the following recurrsion relation

$$P_{n+1}(x) = \frac{1}{n+1}[(2n+1)xP_n(x) - nP_{n-1}(x)] \quad (30)$$

This recurrence relation can be used to generate any $P_l(x)$ for a given x. For a given N, one could find the roots of $P_N(x)$ by any root finding algorithm. Even a simple interval bisection method works well up to $N = 160$. One can avoid finding roots and weights altogether if one is willing to subdivide the range of integration into pieces and using 2 points or 4 points integration for each subdivision. For that purpose, I provide the following table. **NOTE:** The zeros of P_N are symmetric about $x = 0$ therefore we give only the positive one. For example, for $N = 2$, only x_1 and w_1 are given. $x_2 = -x_1$ and weights are always positive and $w_2 = w_1$.

N=2

$x_1 = 0.7735\ 02691\ 89626$ $\qquad$ $w_1 = 1.00000\ 00000\ 00000$

N=4

$x_1 = 0.33998\ 10435\ 84856$ $\qquad$ $w_1 = 0.65214\ 51548\ 62546$

$x_2 = 0.86113\ 63115\ 94053$ $\qquad$ $w_2 = 0.34785\ 48451\ 37454$

N=8

$x_1 = 0.18343\ 46424\ 95650$	$w_1 = 0.36264\ 37833\ 78362$
$x_2 = 0.52553\ 24099\ 16329$	$w_2 = 0.31370\ 66458\ 77887$
$x_3 = 0.79666\ 64774\ 13627$	$w_3 = 0.22238\ 10344\ 53374$
$x_4 = 0.96028\ 98564\ 97536$	$w_4 = 0.10122\ 85362\ 90376$

Test of Convergence

As in any integration method, one must test the convergence of integration. The first thing to test the correctness of your integration program or routine is to test against an integral whose analytical answer is known. For example $\int_{\infty}^{\infty} exp(-x^2)dx = \sqrt{\pi}$ is a good test. Once the correctness of the program is tested, you can test on integrals whose answer is not known. One should start with a small number of integration points first. As you increase the number of integration points (provided that you have a routine to generate Gauss points and weights for any N), the answer should converge to a certain number. You could give a number to your convergence by defining a percentage difference between the last two results as $(A_{n+1} - A_n)/A_{n+1}100\%$.