Numerical Integration

Often in physics problems one needs to evaluate a definate integral. If it is not possible to find the "anti-derivative" of the integrand then numerical methods may be the only way to solve the problem. In our class we will introduce some simple methods of numerically evaluating one dimensional integrals, which include the trapezoid rule, Simpson's rule, and Gaussian quadrature.

Rectangle and Trapezoid Rules

Consider the definate integral, $\int_a^b f(x)\,dx$. The integral is equal to the area under the curve $f(x)$ from a to b. Our task is then to estimate the area under this curve. The simplest way is to divide the total area under the curve into small rectangles and add up the areas of each small rectangle. Let the base of each rectangle be on the x-axis and the height be the value $f(x)$. We divide the x-axis into small segments of equal length h. Then the sum of the areas of the rectangles is given by

$$\begin{aligned}\int_a^b f(x)\,dx &\approx hf(a) + hf(a+h) + hf(a+2h) + \cdots + hf(b-h) \\ &\approx h(f(a) + f(a+h) + f(a+2h) + \cdots + f(b-h))\end{aligned}$$

The smaller that h is, the better the approximation. We can write this expression in summation notation as follows:

$$\int_a^b \approx \sum_{n=0}^{N-1} h\, f(a+nh) \tag{1}$$

where n is an integer and $h = (b-a)/N$. The larger that N is, the more accurate is the sum.

One can do slightly better by using trapezoids instead of rectangles. The area of a trapezoid with a base h, a left height of $f(a)$ and a right height of $f(a+h)$ is $h(f(a) + f(a+h))/2$. Using trapezoids instead of rectangles yields

$$\begin{aligned}\int_a^b f(x)\,dx &\approx h\frac{f(a)+f(a+h)}{2} + h\frac{f(a+h)+f(a+2h)}{2} + \cdots \\ &\approx h(\frac{f(a)}{2} + f(a+h) + f(a+2h) + \cdots + f(a+(N-1)h) + \frac{f(b)}{2})\end{aligned}$$

$$\int_a^b f(x)\,dx \;\approx\; h(\frac{f(a)}{2} + \sum_{n=1}^{N-1} h\, f(a+nh) + \frac{f(b)}{2})$$

where n is an integer and $h = (b-a)/h$. As before, the approximation gets better as $N \to \infty$. Also note that this expression is exact if $f(x)$ is a line.

Simpson's Rule

The trapeziod rule used two values of $f(x)$ for each interval, and is exact if $f(x)$ is a line. One can do a little bit better using equal spacing and three values of $f(x)$. We will derive in class the following formula for the area under a parabola using values of the function evaluated at $x-h$, x, and $x+h$:

$$AREA = h(\frac{f(x-h)}{3} + \frac{4f(x)}{3} + \frac{f(x+h)}{3}) \tag{2}$$

We can do the same treatment with parabola fits that we did with trapezoids. We divide the interval from a to b into N equal segments. For each consequitive triplet of segments we can use the parabola formula above. The sum over all the segments is:

$$\begin{aligned}\int_a^b f(x)\,dx \;\approx\;& h((\frac{f(a)}{3} + \frac{4f(a+h)}{3} + \frac{f(a+2h)}{3}) + \\ & (\frac{f(a+2h)}{3} + \frac{4f(a+3h)}{3} + \frac{f(a+4h)}{3}) + \\ & (\frac{f(a+4h)}{3} + \frac{4f(a+5h)}{3} + \frac{f(a+6h)}{3}) + \cdots)\end{aligned}$$

Notice that the even increments of h are counted twice resulting in a 2/3 factor on even multiples of h:

$$\begin{aligned}\int_a^b f(x)\,dx \;\approx\;& h(\frac{f(a)}{3} + \frac{4f(a+h)}{3} + \frac{2f(a+2h)}{3} + \\ & \frac{4f(a+3h)}{3} + \frac{2f(a+4h)}{3} + \frac{4f(a+5h)}{3} + \\ & \cdots + \frac{4f(a+(N-1)h)}{3} + \frac{f(b)}{3})\end{aligned}$$

where $h = (b-a)/N$ and N must be an even number. N must be even so that the function is evaluated at an odd number of points. This is to insure that the triplet of evenly spaced segments fits properly into the interval between a and b.

The parabolic formula for numerical integration is called Simpson's Rule. It is exact if $f(x)$ is a parabola.

Gaussian Quadrature

The rectangle, trapeziod and Simpson rules have the same general form. The approximation to the definate integral is equal to the sum over values of $f(x)$ evaluated at different points times a weight:

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

where the w_i are the weights for the points x_i. In the rectangle, trapezoid, and Simpson rules the x_i are equally spaced: $x_i = a + i\,h$. For the rectangle rule, the w_i are: $(1, 1, 1, \cdots, 1, 0)$. For the trapezoid rule, the w_i are: $(1/2, 1, 1, 1, \cdots, 1, 1/2)$. In the case of Simpson's rule, the w_i are: $(1/3, 4/3, 2/3, 4/3, \cdots, 2/3, 4/3, 1/3)$.

Gauss determined a way to choose the x_i and the w_i so the sum on the right is the best approximation to the definite integral. Using his method, the sum on the left is exact for $f(x)$ a polynomial up to order $2N+1$. The points and weights can be found in tables. We list below the values for $a = -1$, $b = 1$, and $N = 5$ (Gauss-Legendre quadrature):

x_i	w_i
+.90618	.23693
+.53847	.47863
0	.56889
-.53847	.47863
-.90618	.23693

Usually one looks up the Gauss points and weights in available tables in the literature. Explainations and proofs of Gaussian quadrature are also found in the literature for the interested student. We will not have time in this course to derive the formulas for Gaussian Quadrature.