Physics 263: Numerical Integration Background I

This is a very brief introduction to some algorithms for numerical integration. We will imagine we want to calculate an approximation to the one-dimensional integral of $f(x)$ from a to b:

$$I = \int_a^b f(x)\,dx \ .$$

The algorithms for the numerical approximation of I considered here involve breaking up the interval $a < x < b$ into N subintervals, each with width

$$\Delta x = \frac{b-a}{N} \ .$$

The $N+1$ boundaries of these subintervals are defined to be x_i, where

$$x_1 = a\,, \quad x_2 = a + \Delta x\,, \quad x_3 = a + 2\Delta x\,, \quad \cdots \quad x_N = b - \Delta x\,, \quad x_{N+1} = b\,.$$

As a shorthand, we'll define $f_i \equiv f(x_i)$. Our approximations to the integral will take the form of a sum over all the x points:

$$I \doteq \sum_{i=1}^{N+1} f(x_i)\,w_i = \sum_{i=1}^{N+1} f_i\,w_i\,,$$

where the w_i are "weights" that are different for each of the different approximations.

1. **Naive Rule.** The very simplest approximation to the integral in each subinterval is to use rectangles of height $f(x_i)$ and width Δx to approximate the area. We can choose to evaluate the height using the left end or the right end of the interval. If we use the left end, then the approximation for each subinterval is

   $$\int_{x_i}^{x_{i+1}} f(x)\,dx \doteq f(x_i)\Delta x = f_i\,\Delta x$$

   and for the entire integral

   $$\int_a^b f(x)\,dx \approx f_1\,\Delta x + f_2\,\Delta x + \cdots + f_N\,\Delta x \ .$$

   Note that we don't use f_{N+1}, so the weights are

   $$w_i = \Delta x \text{ for } 1 \le i \le N \quad \text{and} \quad w_{N+1} = 0 \ .$$

2. **Trapezoid Rule.** We can do better by approximating the integral in each subinterval as the area of the trapezoid formed by joining the endpoints of the interval. Thus the function is approximated by a straight line. Then for each subinterval,

$$\int_{x_i}^{x_{i+1}} f(x)\,dx \doteq \frac{1}{2}(f_i + f_{i+1})\,\Delta x$$

and when we combine these for the entire integral, the 1/2's add to 1 everywhere except the endpoints:

$$\int_a^b f(x)\,dx \approx \frac{1}{2}f_1\,\Delta x + f_2\,\Delta x + f_3\,\Delta x + \cdots + f_N\,\Delta x + \frac{1}{2}f_{N+1}\,\Delta x\ .$$

Thus the weights are

$$w_i = \Delta x \text{ for } 2 \le i \le N \quad \text{and} \quad w_1 = w_{N+1} = \frac{1}{2}\Delta x\,.$$

3. **Simpson's Rule.**

We can do still better by approximating the function in each small interval by a parabola. Without proof, we will simply state that for each *two* subintervals, the approximation is

$$\int_{x_i}^{x_{i+2}} f(x)\,dx \doteq \frac{1}{3}(f_i + 4f_{i+1} + f_{i+2})\,\Delta x\ .$$

Since we use two at a time, N *must be an even number* (so $N+1$ is odd). When we combine the subinterval approximations, we get the following rule:

$$\int_a^b f(x)\,dx \approx \frac{1}{3}f_1\,\Delta x + \frac{4}{3}f_2\,\Delta x + \frac{2}{3}f_3\,\Delta x + \cdots + \frac{2}{3}f_{N-1}\,\Delta x + + \frac{4}{3}f_N\,\Delta x + \frac{1}{3}f_{N+1}\,\Delta x\ .$$

Thus the weights are

$$w_i = \frac{4}{3}\Delta x \text{ for } i = 2, 4, \cdots, N \quad \text{and} \quad w_i = \frac{2}{3}\Delta x \text{ for } i = 3, 5, \cdots, N-1$$

and the endpoints are

$$w_1 = w_{N+1} = \frac{1}{3}\ .$$

4. **Gaussian Quadrature**

All of the approaches considered above divide the interval $a < x < b$ into equally spaced subintervals. We can derive integration rules that are spectacularly effective for many integrals if we relax these rules and define the "nodes" (this means the x_i's) as zeros of special sets of polynomials (called "orthogonal polynomials"). This approach is called "gaussian quadrature". We won't explain it further here, but look at

`http://library.lanl.gov/numerical/bookcpdf/c4-5.pdf`

for details on how it works.