1. Basic idea of integration

Integration of functions is an important calculation in computational physics, both as a fundamental task and as a component of larger problems. Many integrals do not have closed forms and require numerical computation.

What is the definition of an integral?

An integral is defined by the limit:

$$\int_a^b \mathrm{d}x f(x) = \lim_{\mathrm{d}x \to 0} \left[\mathrm{d}x \sum_{i=1}^{(b-a)/\mathrm{d}x} f(x_i) \right] \tag{1}$$

where x_i are spaced between a and b with separations $\mathrm{d}x$.

What is a simple numerical estimate of an integral?

Just to perform this sum with some finite $\mathrm{d}x$:

$$\int_a^b \mathrm{d}x f(x) = \left[\mathrm{d}x \sum_{i=1}^{(b-a)/\mathrm{d}x} f(x_i) \right] \tag{2}$$

where x_i are spaced between a and b with separations $\mathrm{d}x$.

This is just a particular case of the more general form that most integration methods take, which is that it can be approximated as some linear combination of evaluations of the function:

$$\int_a^b \mathrm{d}x f(x) = \sum_{i=1}^{N} f(x_i) w_i \tag{3}$$

2. Trapezoid rule

The simple estimate above can be thought of as approximating the function as piecewise constant. Obviously there are better approximations that can be made! Better algorithms for integration generally boil down to better models of the function. In this respect, integration is closely allied to interpolation of functions.

The trapezoid rule is the result of integrating a linear interpolation of the function. Each term in the integral will become:

$$\frac{1}{2}\mathrm{d}x \left(f_i + f_{i+1} \right) \tag{4}$$

The next term is:

$$\frac{1}{2}\mathrm{d}x \left(f_{i+1} + f_{i+2} \right) \tag{5}$$

For equally spaced points, then $w_i = \mathrm{d}x$, except for $w_1 = w_N = \mathrm{d}x/2$.

For what sort of function is the trapezoid rule exactly correct?

For a linear function. Of course, this property is not very useful!!

3. Simpson's rule

Simpson's rule represents the next level of sophistication in interpolation. Here, the function is approximated locally around the points $i-1$, i, $i+1$, as a quadratic:

$$f(x) = \alpha' + \beta' x + \gamma' x^2 \tag{6}$$

This is not a very convenient form. Let us instead use:

$$f(x) = \alpha + \beta\left(\frac{x - x_i}{\mathrm{d}x}\right) + \gamma\left(\frac{x - x_i}{\mathrm{d}x}\right)^2 = \alpha + \beta y + \gamma y^2 \tag{7}$$

with a change of variable to $y = (x - x_i)/\mathrm{d}x$. For a set of three points, $i-1$, i, and $i+1$, you can fit the parabola using the fact:

$$\begin{aligned} f_{i-1} &= \alpha - \beta + \gamma \\ f_i &= \alpha \\ f_{i+1} &= \alpha + \beta + \gamma \end{aligned} \tag{8}$$

This can be easily solved:

$$\begin{aligned} \alpha &= f_i \\ \gamma &= \frac{f_{i+1} + f_{i-1}}{2} - f_i \\ \beta &= \frac{f_{i+1} - f_{i-1}}{2} \end{aligned} \tag{9}$$

What is the integral over the region defined by these three points?

The integral over the region defined by these three points :

$$\begin{aligned} \int_{x_{i-1}}^{x_{i+1}} \mathrm{d}x f(x) &= \mathrm{d}x \int_{-1}^{1} \mathrm{d}y \left(\alpha + \beta y + \gamma y^2\right) \\ &= \mathrm{d}x \left[\alpha y + \frac{\beta}{2} y^2 + \frac{\gamma}{3} y^3\right]_{-1}^{1} \\ &= \mathrm{d}x \left[2\alpha + \frac{2\gamma}{3}\right] \end{aligned} \tag{10}$$

Plugging in α and γ:

$$\int_{x_{i-1}}^{x_{i+1}} \mathrm{d}x f(x) = \mathrm{d}x \left(2 f_i + \frac{f_{i+1} + f_{i-1}}{3} - \frac{2}{3} f_i\right) = \mathrm{d}x \left(\frac{1}{3} f_{i-1} + \frac{4}{3} f_i + \frac{1}{3} f_{i+1}\right) \tag{11}$$

Simpson's rule comes from using this approximation across the length from a to b, by dividing the interval into an even number of segments, and integrating each separately. This yields a full summation:

$$\int_a^b \mathrm{d}x f(x) = \sum_{i=1}^{N} = \mathrm{d}x \left[\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{2}{3}f_3 + \frac{4}{3}f_4 + \ldots + \frac{2}{3}f_{N-2} + \frac{4}{3}f_{N-1} + \frac{1}{3}f_N\right] \tag{12}$$

Because this is applied to two segments at a time, it requires an even number of segments, which means N must be odd.

The weights for the three points used in in Simpson's rule are set to exactly integral a quadratic function — a second degree polynomial. What must N be to exactly integrate an M-degree polynomial?

$N = M + 1$. We can show this as follows. Each of the N points x_k yields a linear equality:

$$f_k = \sum_{j=0}^{M} \alpha_j x^j \tag{13}$$

that can be used to determine the coefficients of the function, and thus its integral. So this yields a system of N linear equations, with $M + 1$ unknowns. So to guarantee a solution, you need $N = M + 1$.

These methods are good methods, but it turns out we can be even cleverer. But before we do so, we have a little bit of work to do.

4. Rescaling of integrals

It may appear trivial, but just as in differentiation, there are rescaling of integrals that can be performed for various reasons of convenience or otherwise.

The simplest rescaling is linear, which just rescales the limits of the integral:

$$I = \int_a^b \mathrm{d}x f(x) = \frac{b-a}{b'-a'} \int_{a'}^{b'} \mathrm{d}x' f(x(x')) \tag{14}$$

which simply follows from the tranformation:

$$\begin{aligned} x' &= (x-a)\left(\frac{b'-a'}{b-a}\right) + a' \\ \mathrm{d}x' &= \mathrm{d}x \left(\frac{b'-a'}{b-a}\right) \end{aligned} \tag{15}$$

or:

$$
\begin{aligned}
x &= (x' - a')\left(\frac{b-a}{b'-a'}\right) + a' \\
\mathrm{d}x &= \mathrm{d}x'\left(\frac{b-a}{b'-a'}\right)
\end{aligned} \tag{16}
$$

This is a pretty trival rescaling, but it can be useful if you can rescale an integral to a previously calculated integral. We will use this below in the specific case: $a' = -1$, $b' = 1$:

$$
I = \int_a^b \mathrm{d}x f(x) = \frac{b-a}{2}\int_{-1}^{1} \mathrm{d}x' f(x(x')) \tag{17}
$$

This will allow us to develop some useful algorithms for the specific range -1 to 1, which can then be generalized to any finite range.

If we want to alter $[-1, 1]$ to an infinite range that is possible too. For example:

$$
\begin{aligned}
x &= a\frac{1+x'}{1-x'} \\
dx &= a\left(\frac{1}{1-x'} + \frac{1+x'}{(1-x')^2}\right) \\
&= a\mathrm{d}x'\frac{1-x'+1+x'}{(1-x')^2} \\
&= \mathrm{d}x'\frac{2a}{(1-x')^2}
\end{aligned} \tag{18}
$$

which lets us rewrite an infinite range:

$$
I = \int_0^\infty \mathrm{d}x f(x) = \int_{-1}^{1} \mathrm{d}x' \frac{2ax'}{(1-x')^2} f(x(x')) \tag{19}
$$

In this case, a is a choice to be made, and $x = a$ when $x' = 0$. So there are better choices for a than others – you want it to be somewhere near where the integral is expected to reach about half its total.

The other forms of weighting are given in the book, and may be derived similarly.

5. Gaussian quadrature

Now we have all the tools to derive one of the workhorse algorithms for integrating function, which is Gaussian quadrature. Gaussian quadrature has the advantage that it yields a systematic way to write an algorithm for integration which utilizes N points, that is *exact* for any polynomial of order $2N - 1$ or less. Note that this is much better than we found before, the path we were on for Simpson's rule, which utilized $N+1$ points to exactly integrate a polynomial of N points. It turns out that the improvement is gained by choosing the points carefully.

We will show how to do this for the integral:

$$\int_{-1}^{1} \mathrm{d}x f(x) \tag{20}$$

where $f(x)$ is a $2N-1$ degree polynomial (or less). Clearly we can rescale the limits as necessary above for the problem at hand.

We are seeking an exact formula for the integral of this function which is:

$$\int_{-1}^{1} \mathrm{d}x f(x) = \sum_{i=1}^{N} w_i f(x_i) \tag{21}$$

The derivation of this is neat. Note that the derivation in the book is extremely confusing and contains at least one error.

We will use the Legendre polynomials to aid us. In fact, it will be the roots of the Legendre polynomials (where they are zero) that turn out to be the locations of the integration points.

NEED TO INTRODUCE LEGENDRE POLYNOMIALS HERE

We start by noting that $f(x)$ can be in general factored in the following way:

$$f(x) = q(x)P_N(x) + r(x) \tag{22}$$

where we choose $q(x)$ to be an $N-1$-degree polynomial. The first term is therefore a polynomial of order $2N-1$, or less. Since we can choose the coefficients of the $q(x)$ polynomial to be whatever we want, we can always match the coefficients of all the polynomial terms of order N or greater in $f(x)$. This leaves a remainder $r(x)$ which is an $N-1$-degree polynomial (or less).

The integral:

$$\int_{-1}^{1} \mathrm{d}x q(x) P_N(x) = 0 \tag{23}$$

because the Legendre polynomials are always orthogonal to lower-order polynomials.

So:

$$\int_{-1}^{1} \mathrm{d}x f(x) = \int_{-1}^{1} \mathrm{d}x r(x) \tag{24}$$

Since $r(x)$ is an $N-1$-degree polynomial or less, there is a way to integrate the function with N points or less, as we found above.

The locations of these points can be found as follows. The integral is now known to be writable as:

$$\int_{-1}^{1} \mathrm{d}x f(x) = \sum_{i=1}^{N} w_i f(x_i) = \sum_{i+1}^{N} w_i q(x_i) P_N(x_i) + \sum_{i+1}^{N} w_i r(x_i) \tag{25}$$

If we choose the points x_i to be the N roots of the Legendre polynomial of order N, then:

$$\int_{-1}^{1} \mathrm{d}x f(x) = \sum_{i=1}^{N} w_i r(x_i) \tag{26}$$

where:

$$r(x) = \sum_{j=0}^{N-1} \alpha_j x_j \tag{27}$$

This is great, and we also know how to set the w_i. These are derived in the same way as for Simpson's rule. Using the appropriate linear set of equations analogous to Equation 13, you can express the solution for the coefficients α_j in terms of values of the function $f(x_i)$, which by design is equal to $r(x_i)$ at the chosen points, and then given the closed form of the integral of the polynomial, this translates into a form for w_i.

6. NumPy implementation