

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?

What is a simple numerical estimate of an integral?

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:

$$\int_a^b dx f(x) = \sum_{i=1}^N f(x_i) w_i \quad (1)$$

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:

$$\frac{1}{2} dx (f_i + f_{i+1}) \quad (2)$$

The next term is:

$$\frac{1}{2} dx (f_{i+1} + f_{i+2}) \quad (3)$$

For equally spaced points, then $w_i = dx$, except for $w_1 = w_N = dx/2$.

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

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:

$$f(x) = \alpha' + \beta' x + \gamma' x^2 \quad (4)$$

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

$$f(x) = \alpha + \beta \left(\frac{x - x_i}{dx} \right) + \gamma \left(\frac{x - x_i}{dx} \right)^2 = \alpha + \beta y + \gamma y^2 \quad (5)$$

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

$$\begin{aligned} f_{i-1} &= \alpha - \beta + \gamma \\ f_i &= \alpha \\ f_{i+1} &= \alpha + \beta + \gamma \end{aligned} \tag{6}$$

This can be easily solved:

$$\begin{aligned} \alpha &= f_i \\ \gamma &= \frac{f_{i+1} + f_{i-1}}{2} - f_i \\ \beta &= \frac{f_{i+1} - f_{i-1}}{2} \end{aligned} \tag{7}$$

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

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:

$$\int_a^b dx f(x) = \sum_{i=1}^N = dx \left[\frac{1}{3}f_1 + \frac{4}{3}f_2 + \frac{2}{3}f_3 + \frac{4}{3}f_4 + \dots + \frac{2}{3}f_{N-2} + \frac{4}{3}f_{N-1} + \frac{1}{3}f_N \right] \tag{8}$$

4. Gaussian quadrature

5. Romberg Integration

6. Dealing with singularities and infinities

7. NumPy implementation