A brief note on numerical integration

We will explore three techniques of numerical integration –

- Midpoint or Rectangle rule
- Trapezoidal rule
- Simpson's rule
- Monte Carlo

Consider integrating the function $f(x)$ over the interval $[a,\, b]$,

$$I = \int_a^b f(x)\, dx \approx \sum_{i=1}^{N} w(x_i)\, f(x_i) \tag{1}$$

where N should preferably be large. Chances are you actually do not know how to integrate this, hence resorting to numerical methods, where integration is replaced with weighted sum as shown in (1). Later we will see that this statement has a bearing on how to determine the accuracy of the numerical method.

Midpoint / Rectangle method

1. Let us divide the integration range $[a,\, b]$ in N equal parts of width h
$$h = \frac{b-a}{N} \tag{2}$$
2. Determine the midpoint of each intervals
$$x_1 = \frac{(a)+(a+h)}{2},\; x_2 = \frac{(a+h)+(a+2h)}{2},\; x_3 = \frac{(a+2h)+(a+3h)}{2},\; \ldots \tag{3}$$
3. Evaluate $f(x_i)$ and calculate the following sum to arrive at the answer
$$M_N = \sum_{i=1}^{n} h\, f(x_i) \quad \Rightarrow \quad \lim_{N\to\infty} M_N = \int_a^b f(x)\, dx \tag{4}$$
where the weight function $w = 1$ for all x_i.

So, how do you know the answer obtained in (4) is accurate enough *i.e.* how large N need to be. We will discuss this issue later.

Trapezoidal rule

The trapezoidal rule for estimating definite integrals uses trapezoids rather than rectangles (as done in Midpoint method) to approximate the area under a curve.

1. As before in (2), we have N intervals each of width h. This h forms the width of each trapezoids, however this is not the weight function as in Midpoint method.

2. Let the endpoints of each interval be at $x_0,\ x_1,\ x_2,\ \ldots\ x_N$ where

$$x_0 = a,\ x_1 = x_0 + h,\ x_2 = x_0 + 2h,\ \ldots\ x_n = x_0 + Nh = b \tag{5}$$

3. Evaluate the $f(x_i)$ and calculate the area of each trapezoids,

$$T_i = \frac{h}{2}\Big(f(x_{i-1}) + f(x_i)\Big) \tag{6}$$

4. Sum over the T_i's to obtain the answer

$$\begin{aligned} T_N &= \sum_{i=1}^{N} T_i = \frac{h}{2}\Big(f(x_0) + 2f(x_1) + 2f(x_2) + \cdots + 2f(x_{N-1}) + f(x_N)\Big) \qquad (7) \\ &= \sum_{i=1}^{N} w(x_i)\, f(x_i) \quad \Rightarrow \quad \lim_{N\to\infty} T_N = \int_a^b f(x)\, dx \end{aligned}$$

where $w(x_0) = w(x_N) = 1$ and $w(x_1) = w(x_2) = \cdots = w(x_{N-1}) = 2$. Once again, we will come back to the accuracy question later. But contrary to the expectation trapezoidal rule tends to be less accurate than the midpoint rule.

Simpson's rule

In Midpoint method the area under the curve is estimated by rectangles *i.e.* piecewise constant functions. In Trapezoidal rule the area is estimated by trapeziums *i.e.* piecewise linear functions. In the Simpson's rule we will approximate the curves in an interval with a quadratic functions, hence we need three points – two are the interval boundaries and the other is the average of the two.

$$\text{For} \int_{x_0}^{x_2} f(x)\, dx \ \text{ we need } \ (x_0,\ f(x_0)),\ (x_1,\ f(x_1)) \text{ and } (x_2,\ f(x_2)) \tag{8}$$

where $x_1 = (x_0 + x_2)/2$. The calculation of the integral above in (8) proceeds as,

$$\begin{aligned} \int_{x_0}^{x_2} f(x)\, dx &\approx \int_{x_0}^{x_2} \Big(Ax^2 + Bx + C\Big)^2 dx \\ &= \left(\frac{A}{3}x^3 + \frac{B}{2}x^2 + Cx\right)\Bigg|_{x_0}^{x_2} \\ &= \frac{A}{3}\left(x_2^3 - x_0^3\right) + \frac{B}{2}\left(x_2^2 - x_0^2\right) + C\left(x_2 - x_0\right) \\ &= \frac{x_2 - x_0}{6}\Big(2A\left(x_2^2 + x_2x_0 + x_0^2\right) + 3B\left(x_2 + x_0\right) + 6C\Big) \qquad (9) \end{aligned}$$

Now, let us take $h = (x_2 - x_0)/2$ and rearranging the terms using $x_1 = (x_2 + x_0)/2$ in (9) we get

$$\begin{aligned}\int_{x_0}^{x_2} f(x)\,dx &\approx \frac{h}{3}\Big(\big(Ax_2^2 + Bx_2 + C\big) + \big(Ax_0^2 + Bx_0 + C\big) + A\left(x_2^2 + 2x_2x_0x_0^2\right) \\ &\qquad +2B\left(x_2 + x_0\right) + 4C\Big) \\ &= \frac{h}{3}\Big(f(x_2) + f(x_0) + A\left(2x_2\right)^2 + 2B\left(2x_2\right) + 4C\Big) \\ &= \frac{h}{3}\Big(f(x_0) + 4f(x_1) + f(x_2)\Big) \qquad (10)\end{aligned}$$

Similarly for $\int_{x_2}^{x_4} f(x)dx = h(f(x_2) + 4f(x_3) + f(x_4))$ and so on. Therefore, in the final step we get the answer from Simpson's rule as,

$$S_N = \frac{h}{3}\Big(f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + \cdots + 2f(x_{N-2}) + 4f(x_{N-1}) + f(x_N)\Big) \qquad (11)$$

$$= \sum_{i=1}^{N} w(x_i)\,f(x_i) \quad \Rightarrow \quad \lim_{N\to\infty} S_N = \int_a^b f(x)\,dx$$

where, the weight functions are $w(x_0) = w(x_N) = 1$, for odd i the $w(x_i) = 4$ and for the even i the $w(x_i) = 2$. It is interesting to note that

$$S_{2N} = \frac{2}{3}\,M_N + \frac{1}{3}\,T_N \qquad (12)$$

Let us now address the problem of accuracy of the above numerical integrations. If we already know the actual answer of the integration in (1) to be I, then the absolute and relative errors obviously are

$$\text{Abosulte error: } \left|X_N - I\right| \quad \text{and Relative error: } \left|\frac{X_N - I}{I}\right| \times 100\% \qquad (13)$$

where $X_N \in M_N,\, T_N,\, S_N$. But often, the very reason for doing numerical integration is that we do not have or calculate an I, and in that case all we can calculate is the upper bound of the error that each method will yield. If $f(x)$ is a continuous function over $[a,\, b]$, having a second derivative $f''(x)$ for Midpoint and Trapezoidal and fourth derivative $f''''(x)$ for Simpson over this interval, then the estimated upper bounds for the error in using numerical integration schemes to estimate $\int_a^b f(x)\,dx$ are

$$\text{Midpoint : } \quad \text{Error in } M_N \leq \frac{(b-a)^3}{24N^2}\,\left|f''(x)\right|_{\max} \qquad (14)$$

$$\text{Trapezoidal : } \quad \text{Error in } T_N \leq \frac{(b-a)^3}{12N^2}\,\left|f''(x)\right|_{\max} \qquad (15)$$

$$\text{Simpson : } \quad \text{Error in } S_N \leq \frac{(b-a)^5}{180N^4}\,\left|f''''(x)\right|_{\max} \qquad (16)$$

The requirement of upper bound for the error determines N. Two things to keep in mind – (i) N chosen should be the smallest integer value greater than or equal to N (basically `ceil(N)`), (ii) the actual estimate may, in fact, be much better approximation than is indicated by error bound. It may sound strange, but it is often true, that taking N larger than what you obtain from the error bounds can actually detoriate the accuracy, contrary to what the limit $N \to \infty$ suggests.

Monte Carlo integration

The Monte Carlo integration starts with choosing random numbers X_i with a *probability distribution function* (PDF) $p(x)$. If the *domain* of X *i.e.* $X \in D$ and it is discrete, as in tossing of coin $X \in \{h, t\}$ or rolling of a dice $X \in \{1, 2, 3, 4, 5, 6\}$ etc., then the $p(x)$ gives the probability or relative frequency with which a particular X occurs, $p(x) = \text{Prob}(X = x)$. For a continuous domain, however, $p(x)\,dx$ is the probability for X to assume any value on an interval dx around x. Two important properties of PDF $p(x)$ are

$$0 \leq p(x) \leq 1 \quad \text{and} \quad \sum_{x_i \in D} p(x_i) = 1 \;\text{ or }\; \int_D p(x)\,dx = 1 \tag{17}$$

As an example, consider $p(x) =$ constant or uniformly distributed over a domain $D = [a, b]$

$$\begin{aligned} \int_a^b p(x)\,dx &= \int_a^b \mathcal{C}\,dx = 1 \\ \Rightarrow p(x) &= \mathcal{C} = \frac{1}{b-a} \end{aligned} \tag{18}$$

Another widely used PDF is Gaussian distribution $\mathcal{N}(\mu, \sigma)$,

$$p(x) = \frac{1}{\sigma\sqrt{2\pi}}\, e^{-\frac{(x-\mu)^2}{2\sigma^2}} \tag{19}$$

Suppose $f(x)$ is a function on the, say discrete, domain of X whose PDF is $p(x)$ and evaluated over M random X, then

$$\langle f \rangle = \frac{1}{M} \sum_{i=1}^{M} f(x_i)\, p(x_i) \tag{20}$$

$$\sigma_f^2 = \frac{1}{M} \sum_{i=1}^{M} \Big(f(x_i) - \langle f \rangle \Big)^2 p(x_i) = \langle f^2 \rangle - \langle f \rangle^2 \tag{21}$$

Suppose we assemble N such independent $\langle f\rangle$ and their corresponding σ_f, then the *global* average and variance will be

$$\langle\langle f\rangle\rangle = \frac{1}{N}\sum_{i=1}^{N}\langle f\rangle_i \quad \text{and} \quad \sigma_N^2 = \frac{\sigma_f^2}{N} \quad \Rightarrow \quad \sigma_N \sim \frac{1}{\sqrt{N}} \tag{22}$$

The error on the measurement of f thus decreases as $1/\sqrt{N}$. So if we want Monte Carlo estimate of $\int_a^b f(x)dx$, then the method is certainly at disadvantage when compared to, say, Trapezoidal or Simpson where errors fall as $1/N^2$ and $1/N^4$ respectively. But it is true for one or fewer dimensions, as we move to higher dimensions (*i.e.* large number of variables) Monte Carlo becomes significantly efficient.

In Monte Carlo integration, we wish to estimate the integral $\int_a^b f(x)dx$ and for this we define an *estimator*, given a random variable X drawn from a PDF $p(x)$, as

$$\mathcal{F}_N = \frac{1}{N}\sum_{i=1}^{N}\frac{f(X_i)}{p(X_i)} \tag{23}$$

Then the average of the estimator $\mathcal{F}_N$ is

$$\langle\mathcal{F}_N\rangle = \int_a^b \mathcal{F}_N\, p(x)\, dx = \int_a^b f(x)\, dx \tag{24}$$

with the variance as in (21). For our particular case of uniform PDF in $[a, b]$,

$$\mathcal{F}_N = \frac{b-a}{N}\sum_{i=1}^{N} f(X_i) \tag{25}$$

The above expression (25) looks very similar to Midpoint expression (4). Therefore, the steps involve in Monte Carlo integration methods are,

1. Choose a N, say 10 or 20 or 50 or whatever.

2. Draw N number of random variables X_i from its domain $[a, b]$. Usually the in-built random numbers in any language return uniform random numbers in the range $[0, 1]$. To convert it to $[a, b]$ one may use

$$X = a + (b-a)\xi \quad \text{where,} \quad \xi \in [0, 1]$$

3. For each X_i calculate $f(X_i)$ and determine $\mathcal{F}_N$ using eqn. (25) and σ_f using

$$\sigma_f^2 = \frac{1}{N}\sum_{i=1}^{N} f(X_i)^2 - \left(\frac{1}{N}\sum_{i=1}^{N} f(X_i)\right)^2 \tag{26}$$

4. Either tabulate or plot $\mathcal{F}_N$ versus N. Also keep track of σ_f for each N.

5. Go to step (1), increase N by 10 or whatever times and repeat the above cycle.

As N becomes larger and larger, you will find $\mathcal{F}_N$ converging to a value but decrease in error or σ_f will be rather slow ($\sim 1/\sqrt{N}$).