

Numerical integration continued

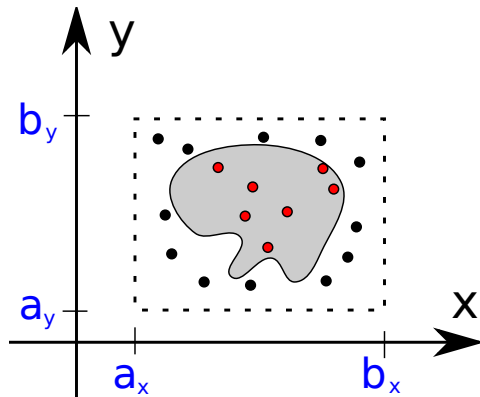
Eugeniy E. Mikhailov

The College of William & Mary



Lecture 10

Toy example - area of the pond



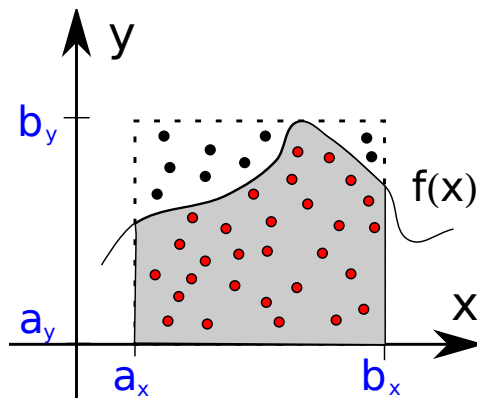
$$A_{pond} = \frac{N_{inside}}{N_{total}} A_{box}$$

where

$$A_{box} = (b_x - a_x)(b_y - a_y)$$

- Points must be **uniformly** and randomly distributed across the area.
- The smaller the enclosing box the better it is.

Naive Monte Carlo integration



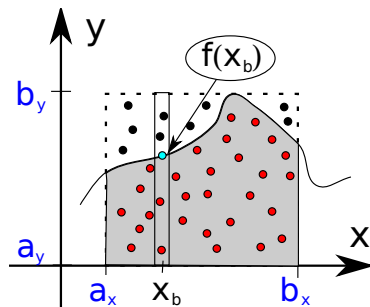
$$\int_{a_x}^{b_x} f(x) dx = \frac{N_{\text{inside}}}{N_{\text{total}}} A_{\text{box}}$$

where

$$A_{\text{box}} = (b_x - a_x)(b_y - a_y)$$

- Points must be **uniformly** and randomly distributed across the area.
- The smaller the enclosing box the better it is. So $\max(f(x)) \rightarrow b_y$

Monte Carlo integration derived



Notice that if we choose a small stripe around the bin value x_b , then subset of points in that stripe gives an estimate for $f(x_b)$.

Thus why bother spreading points around area?

Let's choose a uniform random distribution of points x_i inside $[a_x, b_x]$

$$\int_{a_x}^{b_x} f(x) dx \approx \frac{b_x - a_x}{N} \sum_{i=1}^N f(x_i)$$

Error estimate for Monte-Carlo method

It can be shown that error of the numerical integration (E) is given by the following expressions

Monte Carlo method

$$E = O \left((b_x - a_x) \sqrt{\frac{\langle f^2 \rangle - \langle f \rangle^2}{N}} \right)$$

where

$$\langle f \rangle = \frac{1}{N} \sum_{i=1}^N f(x_i)$$
$$\langle f^2 \rangle = \frac{1}{N} \sum_{i=1}^N f^2(x_i)$$

The term under $\sqrt{\quad}$ is the estimate of the function standard deviation.

Error estimate for other methods

Rectangle method

$$E = \mathcal{O}\left(\frac{(b_x - a_x)h}{2} f'\right) = \mathcal{O}\left(\frac{(b_x - a_x)^2}{2N} f'\right)$$

Trapezoidal method

$$E = \mathcal{O}\left(\frac{(b_x - a_x)h^2}{12} f''\right) = \mathcal{O}\left(\frac{(b_x - a_x)^3}{12N^2} f''\right)$$

Simpson method

$$E = \mathcal{O}\left(\frac{(b_x - a_x)h^4}{180} f^{(4)}\right) = \mathcal{O}\left(\frac{(b_x - a_x)^5}{180N^4} f^{(4)}\right)$$

Multidimensional integration with interval splitting

$$\int_{a_x}^{b_x} \int_{a_y}^{b_y} f(x, y) dx dy = \int_{a_x}^{b_x} dx \int_{a_y}^{b_y} dy f(x, y)$$

Note that last integral is the function of only x

$$\int_{a_y}^{b_y} dy f(x, y) = F(x)$$

$$\int_{a_x}^{b_x} \int_{a_y}^{b_y} f(x, y) dx dy = \int_{a_x}^{b_x} dx F(x)$$

Thus we replaced multidimensional integral as consequent series of single dimension integrals, which we already know how to do.

3D case would look like this

$$\int_{a_x}^{b_x} \int_{a_y}^{b_y} \int_{a_z}^{b_z} f(x, y, z) dx dy dz = \int_{a_x}^{b_x} dx \int_{a_y}^{b_y} dy \int_{a_z}^{b_z} dz f(x, y, z)$$

Multidimensional integration with Monte Carlo

Note that if we would like to split integration region by N points in every of D dimensions, then evaluation time grows $\sim N^D$, which renders Rectangle, Trapezoidal, Simpson, and alike method useless.

Monte Carlo method is a notable exception, it looks very simple even for multidimensional case and maintains the same $\sim N$ evaluation time.

3D case would look like this

$$\int_{a_x}^{b_x} dx \int_{a_y}^{b_y} dy \int_{a_z}^{b_z} dz f(x, y, z) \approx \frac{(b_x - a_x)(b_y - a_y)(b_z - a_z)}{N} \sum_{i=1}^N f(x_i, y_i, z_i)$$

A general case

$$\int_V dV f(\vec{x}) = \int_V dx_1 dx_2 dx_3 \dots dx_D f(\vec{x}) \approx \frac{V}{N} \sum_{i=1}^N f(\vec{x}_i)$$

where V is the multidimensional volume, \vec{x}_i randomly and uniformly distributed points in the volume V

Matlab functions for integration

1D integration

- `integral`
- `trapz`
- `quad`

2D and 3D

- `integral2`
- `integral3`

There are many others as well. See Numerical Integration help section.

Matlab's implementations are more powerful than those which we discussed but deep inside they use similar methods.