Kinetic Monte Carlo Review Notes

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Monte Carlo Methods

- Solve complex problems using random sampling from a probability distribution (i.e. stochastic description).
- Useful to evolve a physical system to a new state from an esemble of potential future states.

Integrating a function MC sampling

• If we want to evaluate the integral of a function over some domain we can numerically approximate this using the midpoint rule:

$$\int_{a}^{b} f(x)dx = \frac{b-a}{N} \sum_{i=1}^{N} f(x_{i})$$
 (1)

• There is an alternative way to do this using probablity theory to determine the expectation value of a function f(x) for random variable x:

$$\int_{a}^{b} p(x)f(x)dx = \frac{b-a}{N} \sum_{i=1}^{N} f(x_{i})$$
 (2)

where p(x) is a uniform probability distribution over the interval [a, b].

- The difference between numerically evaluating Equation 1 and Equation 2, is that Equation 1 is evaluated over a grid of points and Equation 2 is randomly sampled points.
- The error of MC integration is $\propto \frac{1}{\sqrt{N}}$ as a result of central limit theorem

Example integrating a function using MC sampling¹

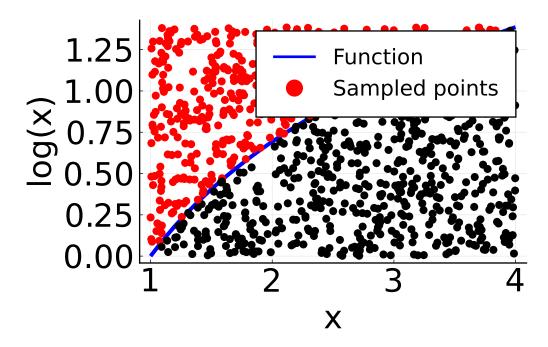


Figure 1: Random sampled points from uniform distribution over the interval [1,4]. The black points are those that are accepted.

Example integrating a function using MC sampling

Backmatter

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¹A more detailed notebook implementing the code can be viewed here

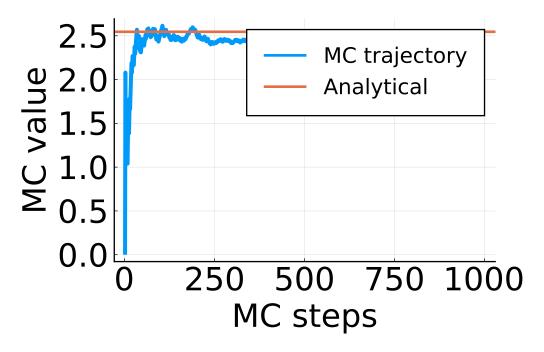


Figure 2: Integration of log(x) using MC.



i Note

This presentation can be viewed online at https://stefanbringuier.github.io/KMCNotes. A report formated PDF of this presentation can be downloaded here.

? Tip

To export revealjs presentations to pdf, press 'e' then 'ctrl-p' 'save as pdf'

References & footnotes