Kinetic Monte Carlo Notes

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Monte Carlo Methods

- Solve complex problems using random sampling from a probablity 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:

$$\int_a^b f(x)dx = \frac{b-a}{N} \sum_{i=1}^{N} f(x_i) \tag{0.1}$$

- 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:

$$\int_a^b p(x)f(x)dx = \frac{b-a}{N} \sum_{i=1}^{N} f(x_i) \tag{0.2}$$

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

- The difference between numerically evaluating Equation 0.1 and Equation 0.2, is that Equation 0.1 is evaluated over a grid of points and Equation 0.2 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 sampling[1]

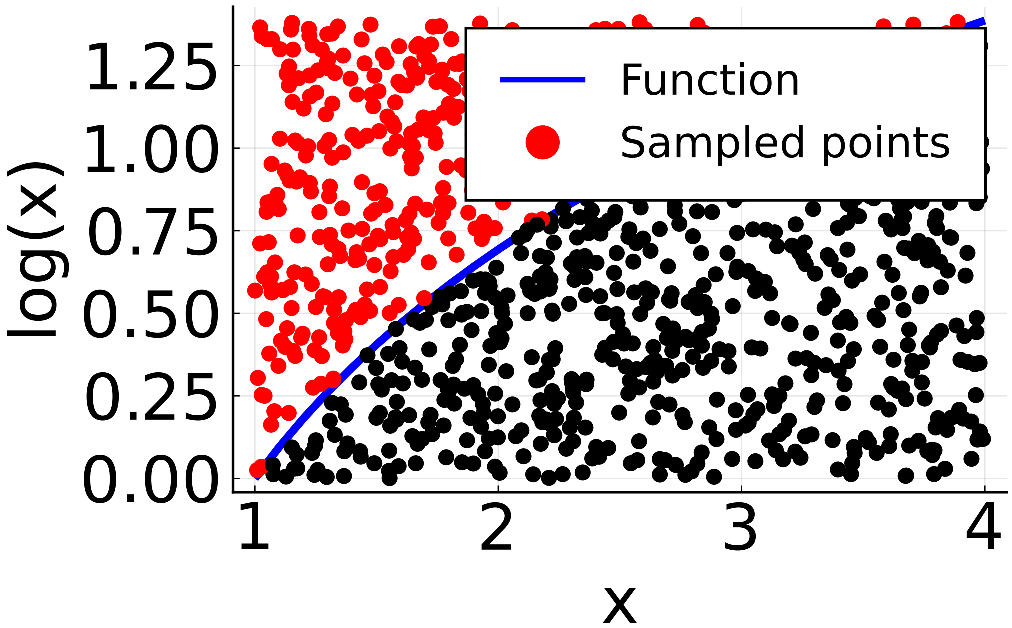

Figure 0.1: Random sampled points from uniform distribution over the interval $[1, 4]$. The black points are those that are accepted.

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

Example integrating a function using MC sampling

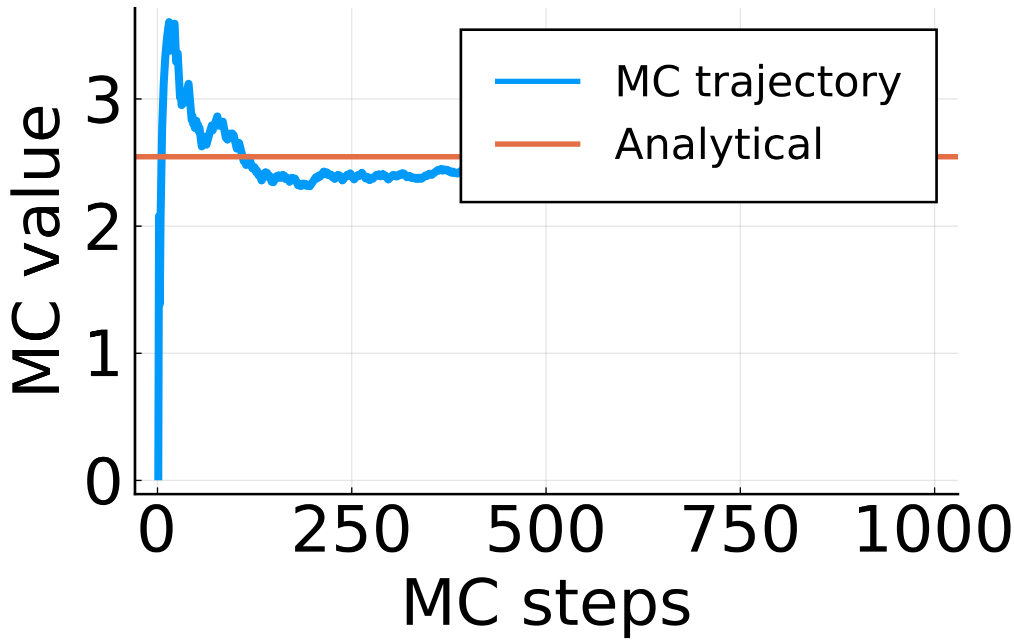

Figure 0.2: Integration of $log(x)$ using MC.

Statistical Thermodynamics & Ensemble Properties

- Microscopic $\rightarrow$ Macroscopic description
  - How positions and momenta of 10^{23} particles relates to bulk temperature, pressure, or volume.
- Ensembles use probablity of specific microstate. Probability theory provides average of a function or variable, $\langle X \rangle$:

$$\langle X \rangle = \frac{1}{N} \sum_{i=1}^{N} n_i X_i = \sum_{i=1}^{N} \underbrace{p_i}_{\text{PDF}} X_i \tag{0.3}$$

- If $\langle X \rangle$ is continous, Equation 0.3 is an integral.
- p_i is the probablity the system is in state i. The probablity density function (PDF) has the property that its normalized, i.e. $\sum_{i=1}^{N} p_i = 1$

Statistical Thermodynamics & Ensemble Properties

- The consqequence of Equation 0.3 is that microscopic collections (i.e. ensemble of systems) can be used to calculate macroscopic properties.
- Choice of $p_i = \frac{z_i}{Z}$ depends on macroscopic conditions which manifest through the partition function:

$$Z = \sum_i e^{-\beta X_i} \tag{0.4}$$

- For a macroscopic system that has constant particles, volume and temperature, i.e., canonical.
  - $\beta = \frac{1}{k_b T}$ and $X_i = E_i$ where Boltzmann factor is $z_i = e^{-\frac{E_i}{k_b T}}$

$$\langle E \rangle = \frac{1}{Z} \sum_i e^{-\frac{E_i}{k_b T}} E_i \tag{0.5}$$

Backmatter

Connect with me!

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> **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