Monte Carlo

Simulated experiments and Integration

Introduction

- Based on introducing artificial dynamics based upon random numbers (which does not mean it is *any* dynamics)
- Popular for static properties but not for dynamical

Types of Monte Carlo

- Direct Monte Carlo
- Monte Carlo Integration
- Metropolis Monte Carlo

Direct Monte Carlo

- Random numbers are used to model the effect of complicated processes. Details are not crucial
- Useful when the computations are too difficult or too vaguely defined to be solved by numeric or algebraic methods
- Example:
  - Traffic

Monte Carlo Integration

- To calculate integrals using random numbers
- Efficient when the integration is over high-dimensional volumes

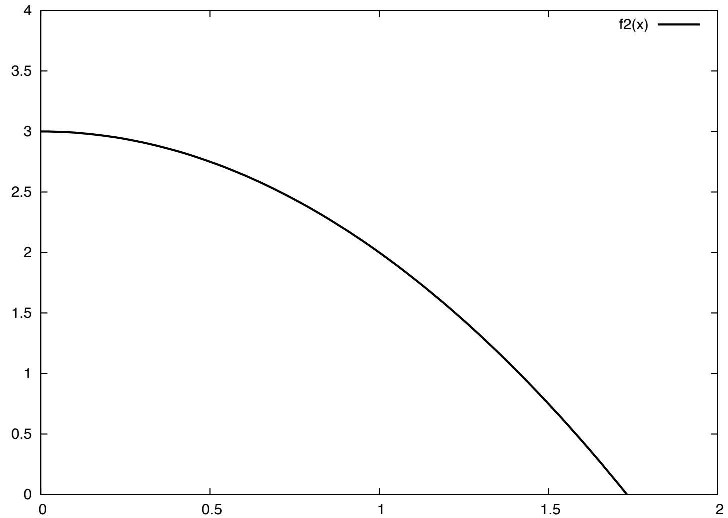
Metropolis Monte Carlo

- A sequence of distributions of a system is generated in a so-called Markov chain
- Allows to study the static properties of physical systems

Random numbers

- Topic covered

Monte Carlo Integration



$$\int f(x)dx = A\frac{\text{Number of points below the curve}}{\text{Number of points}}$$

- The statistical error is proportional to $\frac{1}{\sqrt{N}}$

When is MC integration interesting?

- MC vs. quadrature (step *h*)

$$I = \int_a^b dx f(x) \approx \frac{(b-a)}{N} \sum_{i=1}^{N} \omega_i f_i(x_i)$$

- Quadrature methods using equidistant values for x_i, error goes as $\propto h^k \propto N^{-k}$, $k \geq 1$

- We assume for simplicity that the integration volume is a hypercube with side L. This contains $N = \left(\frac{L}{h}\right)^d$ so the error scales with $N^{-k/d}$

- However for MC error is of the order $1/\sqrt{N}$

- So if $d > 2k$ MC is more efficient

Stratified sampling

- Reduction of the error in MC

$$\sigma^2 = \frac{(b-a)^2}{N} \left(\bar{f^2} - \bar{f}^2 \right)$$

- Subdivision of the integration hypercube in smaller, equally sized volumes

Importance sampling

- Problem with a cube: Samples volume homogeneously

$$I = \int_a^b f(x)dx \quad ; \quad \int_a^b \rho(x)dx = 1$$

$$\frac{f(x)}{\rho(x)} \approx 1$$

$$I = \int_a^b f(x)dx = \int_a^b \rho(x) \left[\frac{f(x)}{\rho(x)}\right] dx$$

Importance sampling

- We choose random numbers according to the distribution

$$\rho(x)$$

- The variance is

$$\sigma^2 = \frac{1}{N}\left[\int_a^b dx \rho(x)\left[\frac{f(x)}{\rho(x)}\right]^2 - \left(\int_a^b dx \rho(x) \frac{f(x)}{\rho(x)}\right)^2\right]$$

Note on random numbers

- MC integration is not susceptible to correlations in the random number generator
- Correlations influence the order in which the points are generated but this does not affect the sum