Problem set 3: Computational Molecular Physics

Petra Imhof
Department of Physics, Freie Universität Berlin

May 6, 2015

(Please send the solution by e-mail to **tahereh.ghane@gmail.com** by **Mon. 11.05 (4pm)** at the latest.)

1 Probability Estimation

(15 points) Choose your favorite programming language and implement a Monte Carlo algorithm to calculate the probability to obtain either 4, 7 or 9 heads if one flips a coin ten times (choose a reasonably large N).

2 Monte Carlo Integration

(20 points) Choose your favorite programming language and implement a Monte Carlo algorithm to approximate the following integral:
$\int_0^1 \frac{6}{\sqrt{4-x^2}} dx$

(a) Explore what happens with N=100, 1000, 10000 generated points and plot the results of each case.

(b) Obtain the value of π using the results of part (a) (Note: $\int_0^1 \frac{6}{\sqrt{4-x^2}} dx = 6 \cdot ArcSin(x/2)$).

3 Central limit Theorem

(15 points) Consider $\{X_n\}$ be a sequence of independent Bernoulli random variables with parameter p=1/2. i.e a generic term X_n of the sequence has support $R_{X_n} = \{0, 1\}$ and the probability mass function is defined as follow:

$$f(z) = \begin{cases} 1/2 & \text{if} \quad x = 1 \\ 1/2 & \text{if} \quad x = 0 \\ 0 & \text{if} \quad x \notin R_{X_n} \end{cases}$$

Use the central limit theorem to derive an approximate distribution for the mean of the first 100 terms of the sequence, then plot the distribution.