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FB Mathematik und Informatik

Computational Molecular Physics **Winter 2017/18**

Problem set 3 **20 November 2017**

Problem 3.1 *Monte-Carlo Sampling*

a) Choose your favorite programming language and implement a Monte-Carlo (MC) algorithm to approximate the following integral:

$$\int_0^{\pi} \frac{1}{x^2+cos^2(x)} dx$$

b) Using the uniform distribution function, explore what happens with N=100, 1000, 10000 generating points and plot the results of each case.

c) Using the function $P(x) = exp[-x]$, explore what happens with N=100, 1000, 10000 generating points and plot the results of each case.
Also compute the corresponding variance for every MC calculation.

d*) Estimate the integral using (a) the Barker and (b) the Metropolis acceptance criterion.

Problem 3.2 *Markov Chain Monte-Carlo*

a) Implement a Markov Chain Monte-Carlo algorithm. Generate a Markov chain of N=10000 points (x,y) as a "walk" in the following 2D-potentials

$$\text{V(x,y)} = -(\frac{x^2}{2}+\frac{y^2}{2}) + 5$$

$$\text{V(x,y)} = (\frac{x^2}{2}+\frac{y^2}{2}) - 5$$

The potentials has periodic boundary conditions such that V(x,5.0)=V(x,-5.0) and V(5.0,y)=V(-5.0,y). You can model this by setting e.g. (x,y)=(-6.0,1.0) to (x,y)=(4.0,1.0) or (x,y)=(3.0,7.5) to (x,y)=(3.0,-2.5) etc.

b) Choose a random initial point q_0=(x_0,y_0) from the distributions and propose a new point q_1=(x_1,y_1) by chosing it uniform randomly from an interval [-0.5,0.5] around q_0. Accept/Reject the newly proposed position q_i according to the Metropolis-Hastings acceptance criterion using a Boltzmann distribution with kT=0.5 .

c) Plot the sampled points as a 2D histogramm and explain the different distribution of points in each case.

d*) Consider the asymmetric double well potential (in units of nm, kJ/mol)

$$V(x) = 100x^4 - 100x^2 - 10x$$

Set up a computer code for the Markov Chain Monte-Carlo (Metropolis acceptance criterion) scheme. Try to efficiently sample the Boltzmann distributions for $300K$ temperature by varying the proposal step.

Due date: ***26 November, 12 p.m.***