

Problem set 2: Computational Molecular Physics

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Please send the solution by email to kkarathanou@zedat.fu-

1. Markov Chain Monte-Carlo with Barker and Metropolis-Hastings (20 points)

(i) Choose your favorite programming language and using (a) the Barker and (b) the Metropolis acceptance criterion estimate the integral of problem set 1 (question 3) and compare its value to that of the previous exercise.

(ii) What are the main differences between MCMC (Markov Chain Monte Carlo) and "Brute-force" Monte-Carlo?

(iii) What is the importance of choosing an appropriate step size when you propose a new position for MCMC? Give an example.

2. Transition Probabilities (30 points)

The files data1.txt, data2.txt, and data3.txt each contain a series of states, sampled by Markov Chain Monte Carlo.

(i) Plot the histograms of the three series to visualize the distribution of the states. How do they differ for the three series?

(ii) Determine the transition probabilities between the states in the three series

(iii) Do the data series obey detailed balance, i. e. $\pi(i)P(i \rightarrow j) = \pi(j)P(j \rightarrow i)$?