

Problem set 4: Computational Molecular Physics

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(Please send the solution by e-mail to tahereh.ghane@gmail.com by **Mon. 18.05 (4pm)** at the latest.)

1 Markov Chain

(15 points) Germany is blessed by many things, but not good weather! There are no two nice days in a row. If there is a nice day, the next day is as likely to be a cold day as it is to be a rainy day. If there is cold or rainy day, there is an even chance of having the same weather the next day. If there is a change from a cold day or a rainy day, only half of the time is this a change to a nice day. Using this information:

- Write down the transition probability for the weather in Germany.
- Predict the weather for the next 6 days by performing the transition matrix of each day.

2 Metropolis-Hastings

(15 points) Choose your favorite programming language and using the Metropolis algorithm estimate the integral of problem set 3 (question 2) and compare its value to that of the previous exercise.

3 1D Ising Model

(20 points) Consider a chain of 100 spins, randomized by setting each spin randomly to +1 or -1. The Hamiltonian of the model is given by $H = -J\sum_i S_i S_{i+1}$. For simplicity we set $J=1$. The difference in energy between the old and new configuration is calculated using $\Delta E = 2S_i(S_{i-1} + S_{i+1})$. Using your favorite programming language and by choosing the proper Monte Carlo approach compute the average energy per spin as a function of T . (Note: If the old configuration has spin up, the new one should have spin down and vice versa.)