In the name of God

Department of Physics
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COMPUTATIONAL PHYSICS

Exercise Set 11

(Date Due: 1397/03/07)

1. Based on Variational theorem in the quantum mechanics, write a variational Monte-Carlo program to estimate the ground state of 1D harmonic oscillator.

2. Write a MCMC program to compute $\langle E \rangle$, $\langle M \rangle$, C_V and χ as a function of temperature for a 2d Ising model with

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j$$

   suppose you have 400 atoms and $k_B = J = 1$ and for $T \in [1-4]$ with $\Delta T = 0.1$.

3. Fitting formula: Using file which is called *fitinput.txt* and consider $y_{theory} = ax^H$ compute a, H and their errors using MCMC method.

4. Hamiltonian Monte Carlo method for data modeling: Using file which is called *fitinput.txt* and consider $y_{theory} = ax^H$ compute a, H and their errors using HMC method.

Good luck, Movahed

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