Computational Quantum Physics
Exercise 6

PHYS-463
Prof. G. Carleo

In this exercise we try to find the ground-state to the 1D transverse field Ising model with **periodic boundary conditions** using the stochastic VMC method introduced in this week's lecture. The Hamiltonian is given by

$$\mathcal{H}_{TFI} = J \sum_i \sigma_i^z \sigma_{i+1}^z - \Gamma \sum_i \sigma_i^x \tag{1}$$

The most important ingredient to the VMC method is the variational wave-function Ansatz $\psi_\theta(s_1, ..., s_N) = \langle s_1, ..., s_N | \psi_\theta \rangle$ (θ denotes the set of all variational parameters, and s_i is the spin of the i-th particle) as its expressiveness determines if it can faithfully reproduce the ground-state of the system. To see this more clearly, in this exercise we will use two different Ansätze (mean-field and Jastrow) and compare the obtained results.

The ground-state of the given system is positive and we can therefore use real wave-function Ansätze. Also for stability reasons and simplicity (Eq. (8.12) in the lecture notes), throughout this exercise we will work in **log-space** rather than real-space when working with the wave-function Ansatz.

Problem 6.1 Mean-field Ansatz

The mean-field Ansatz is given by

$$\psi_\theta(s) = \prod_i \phi_i(s_i) \tag{2}$$

and consequently

$$\log(\psi_\theta(s)) = \sum_i \log(\phi_i(s_i)) \tag{3}$$

a) Write a function *logpsi* that implements a mean-field Ansatz (as described in Sec. 8.4.1 in the lecture notes) **in log-space** such that $\psi_\theta(s) = \exp[\text{logpsi}]$ (here $s = (s_1, ..., s_N)$ denotes a *sample* of a spin-configuration). The function should take a batch of samples i.e. in the form $(\text{n}_{\text{samples}}, \text{n}_{\text{dims}})$.

b) Compute the derivative of the the mean-field Ansatz w.r.t. the variational parameters θ analytically by hand and implement it. Again your function should take a batch of samples.

c) Implement a method that samples directly from your mean-field Ansatz.

d) Implement a method that, provided the function logpsi, performs a Markov Chain in configuration space of the given system, as is described in Sec. 8.3.2 in the lecture notes. Be careful to use $p(s) = |\psi(s)|^2$. We recommend to use single spin-flips as update rule to obtain new configurations.
NOTE: Since your initial state can in general not be considered a sample from $p(s)$ it might be necessary to let your chain *thermalize* before you start collecting samples. This means that you should discard the first few hundred states of your Markov chain. You can also use j) as a more reliable heuristic for convergence.

e) Implement a function that, given a sample s, computes all the connected elements s_{conn} and the matrix elements $\langle s| H |s_{conn}\rangle$.
NOTE: For the transverse field Ising model the only connected elements are those which differ by at most one spin from the configuration s.

f) Implement a function, that given a sample s and all connected elements s_{conn} and matrix elements $\langle s_{conn}| H |s\rangle$, computes the local energy of that sample.

g) Using c), directly sample from your mean-field Ansatz and use the obtained samples to compute an estimate of the energy of the system.

h) Using d), sample your mean-field Ansatz using MCMC and compute an estimate of the energy of the system. Do you get the same results as in g)?

i) Finally, also compute the derivative of the local energy (Eq. (8.14) in the lecture notes) and update the variational parameters of your Ansatz according to the gradient descent scheme given in Eq. (8.16) of the lecture notes. Iterate this procedure until you reach convergence. What is the final energy you reach?

j) (Bonus) A widely used quantity to determine the correlations between the samples of your Markov Chain is the auto-correlation time τ (Eq. (8.39) in the lecture notes). Here we want to estimate this quantity. Use Eq. (8.40) - (8.42) to estimate the auto-correlation time for the local energy.

Problem 6.2 Jastrow Ansatz

a) Repeat the above exercise (only the MCMC part without direct sampling) with a nearest neighbour Jastrow Ansatz of the form

$$\psi_\theta(s) = \exp\left[J_1 \sum_i s_i s_{i+1}\right] \tag{4}$$

and consequently

$$\log(\psi_\theta(s)) = J_1 \sum_i s_i s_{i+1} \tag{5}$$

where J_1 is a variational parameter.
How do the results compare to the mean-field and the exact results?

b) Increase the connectivity of your Ansatz by taking into account next-to-nearest neighbours as well i.e.

$$\psi_\theta(s) = \exp\left[J_1 \sum_i s_i s_{i+1} + J_2 \sum_i s_i s_{i+2}\right] \tag{6}$$

Does the energy estimate improve? How many neighbours do you need to get the "exact" ground-state energy?