Heisenberg model

The Heisenberg model can be seen as a generalization of the Ising model, where a more realistic model of classical magnetization is represented by the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j, \tag{1}$$

where $\vec{S}_i \in \mathbb{S}^2 \subset \mathbb{R}^3$ belongs the surface of a 3-sphere.

While for the XY model (spins in $\mathbb{S}^1$) it is advantageous to use polar coordinates, it is unclear and possibly system dependent if in the 3D spin case the added complexity and FLOP introduced by spherichal coordinates, justifies the memory savings.

Implement a MC simulation of the Heisemberg model with a Metropolis algorithm. Outside a few changes in the update probability computation and the representation of you cluster, you should not need to modify the code from previous exercises much. Remember to normalize your vectors if you use a cartesian representation.

Taks 1: *Compute the critical temperature for $J = 1$. You can use either the binder cumulants, or the magnetic susceptibility. You should find $T_c \approx 1.443$.*

Task 2: *Compute the autocorrelation time, either for E or $|\vec{M}|$, at T_c and find the critical dynamical exponent given by the relation $\tau \propto L^{z_c}$.*

The cluster algorithm can be extended to system with spins of arbitrary dimensions, with the trick of considering reflections around a random plane at each MC step. For each step select a random unit vector $\vec{r}$ which is chosen to be orthogonal to the reflection plane. Decide if you want to implement Swedsen-Wang or Wolff, grow a cluster with bond probability

$$p_{i,j} = 1 - \exp\Big[-2\beta(\vec{S}_i \cdot \vec{r})(\vec{S}_j \cdot \vec{r})\Big] \tag{2}$$

and flip the spins as

$$\vec{S}_i{}' = \vec{S}_i - 2\vec{r}(\vec{S}_i \cdot \vec{r}). \tag{3}$$

Task 3: *Repeat the computation of T_c and z_c using the Swendsen-Wang or Wolff algorithm.*

Unsupervised machine learning

We can use PCA and k-means to investigate condensed matter systems. One of the paradigmatic systems is the two-dimensional ferromagnetic Ising model. It has two phases separated by a well-known critical temperature at $T_c = 2.26$.

Task 1: *Generate $10^3 - 10^4$ samples of L-by-L Ising systems using Metropolis or a cluster Monte Carlo method, with $L = 10$ for smaller systems, and $L = 32$ for larger systems at different temperatures.*

Task 2: *Perform PCA on these data points and find the 2 directions u_1 and u_2 with the largest variance. Make a scatter plot of the configurations in the u_1-u_2 plane. Describe and interpret your results. What is the difference between the small and the large system?*

Hint: Use fit(PCA, X; maxoutdim = 2) of the package MultivariateStats.

We can use k-means to determine the boundary between the three (two) phases, so that when we are given a new data point, we can determine which phase it belongs to.

Task 3: *Find the three stabilized centroids using k-means and divide the u_1-u_2 plane into three phase regions.*

Hint: Use kmeans(X, 3) of the package Clustering.

A very interesting phenomena can be observed for the data points in u_1 and u_2 direction.

Task 4 a): *Plot the mean value of the absolute value of the data points in the u_1 direction as a function of temperature and compare it with the mean magnetization of the corresponding spin configurations.*

Task 4 b): *Plot the mean value of the absolute value of the data points in the u_2 direction as a function of temperature and compare it with the susceptibility of the corresponding spin configurations.*

Solution.

Heisenberg model

In this exercise we implemented the Metropolis and the Wolff algorithm by extending the code from exercise 1 and 3. We choose to represent the spin states in cartesian coordinates. For the Wolff algorithm we still do not have to store the cluster sites if we flip them immediately. Swendsen-Wang should give similar behavior.

Metropolis: The system was thermalized in $500 * L^3$ Metropolis steps. We then did 10^5 measurements with $N = L^3$ subsweeps in between. In Figure 1 we show the energy E/N, the magnetization $|M|/N$, the susceptibility and the heat capacity as a function of inverse temperature. For the critical temperature we find $\beta_c \approx 0.7 \approx 1/1.43$.

The correlation time τ can be found from the correlation series, which decays as $\sim e^{-t/\tau}$. We repeatedly calculate the correlation time for different system size L and obtain the critical dynamical exponent from $\tau \sim L^{z_c}$. At critical temperature T_c we get $z_c \approx 1.8$ for the magnetization (literature: ≈ 2).

Wolff: The system was thermalized in 500 steps. We then measured teh magnetization and energy 10^5 times. In Figure 1 we show the energy E/N, the magnetization $|M|/N$, the susceptibility and the heat capacity as a function of inverse temperature. For the critical temperature we find $\beta_c \approx 0.7 \approx 1/1.43$.

The autocorrelation time can be calculated in the same way as described above. At critical temperature T_c we obtain for the critical dynamical exponent $z_c \approx 0.8$ for the magnetization. The literature value is $z_c \approx 0$, but they take into account, that the relative cluster size (wrt. L^3) decreases with L. For this reason they define one MC time step when L^3 spins have been flipped.

Unsupervised machine learning

In this exercise we used unsupervised machine learning to identify order parameters of the 2D Ising model. We generated Ising spin configurations at temperatures from 0.2 to 4 for systemsize $L = 10$ and $L = 32$. In a first step we apply PCA to find the two most relevant directions.

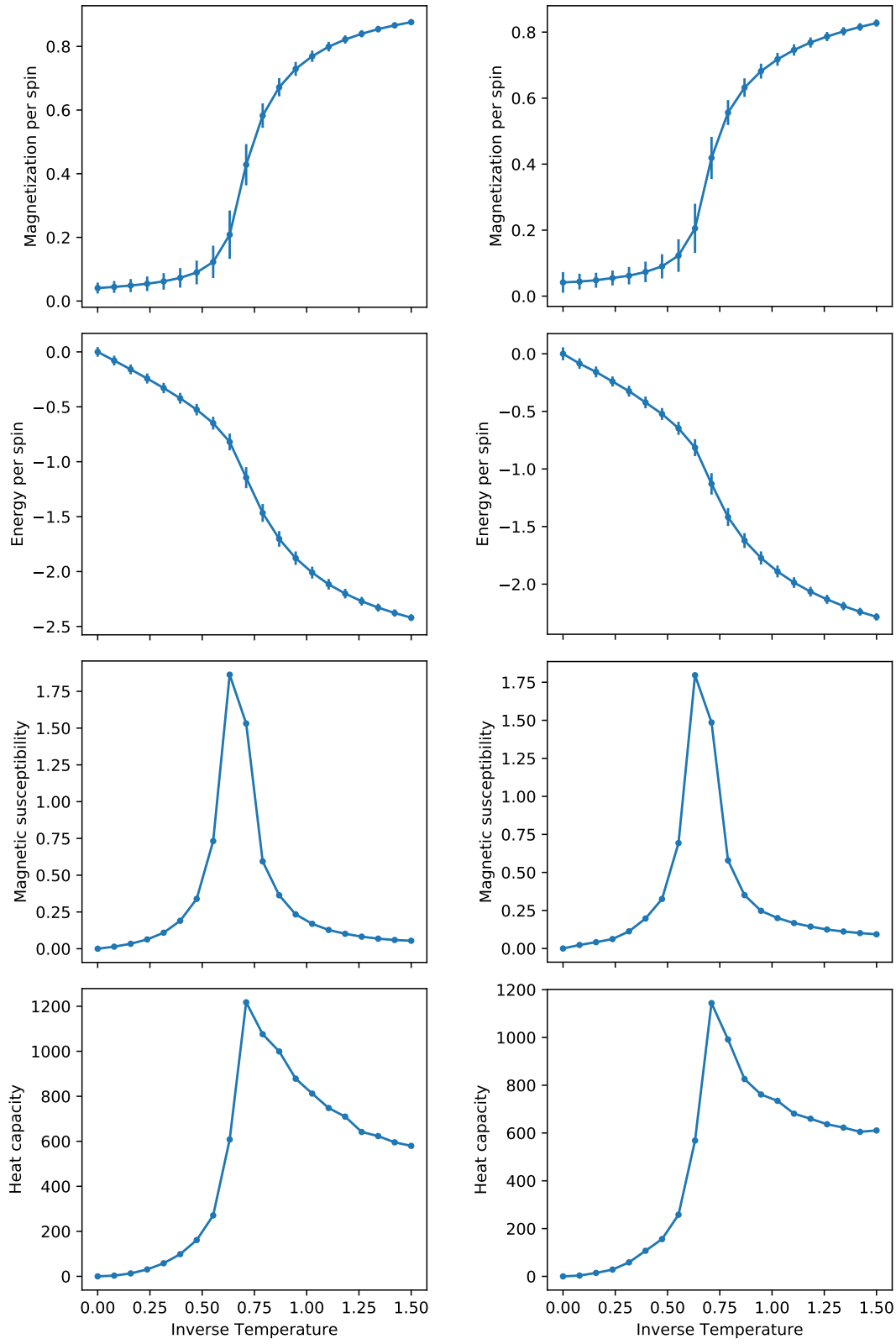

Figure 1: Magnetization, energy, magnetic susceptibility and heat capacity for different temperatures and $L = 8$ (left: Metropolis, right: Wolff).

We can then use k-means to find the three centroids. In Fig. 2 we see the results for $L = 10$ and $L = 32$. We can observe that the data points form clear clusters, where the centroids are located in the center. However, for the smaller system the clustering is less clear because of finite size effects. We can divide the plane into three regions corresponding to the state with all spins aligned ($\approx \pm 1$) or with 0 magnetization.

We can also look at the mean value of the data points in each direction. In Fig. 3 we compare $\langle |p_1| \rangle / L$ and the magnetization. We find that the magnetization is matched very well, showing that the PCA is capable to find the order parameter. Additionally we can also look at the second direction. In Fig. 4 we compare $\langle |p_2| \rangle$ and the susceptibility. The PCA does not return exactly the susceptibility but their behavior is very similar. Comparing $\langle |p_2| \rangle$ for $L = 10$ and $L = 32$ we can also see finite size effects.

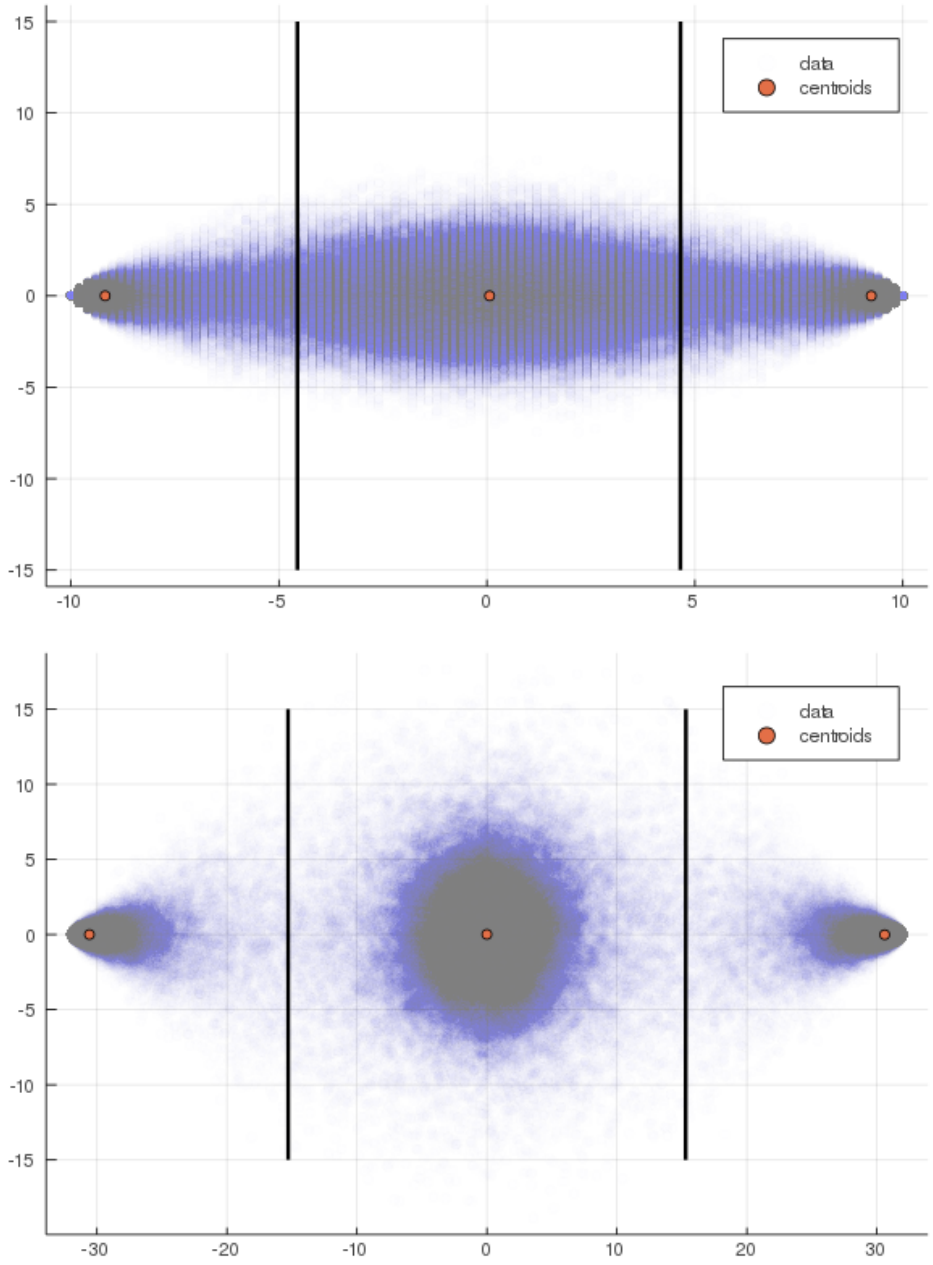

Figure 2: Scatter plot of the data points and the centroids for $L = 10$ (left) and $L = 32$ (right). The black lines divide the plane into three regions belonging to the corresponding to the centroids.

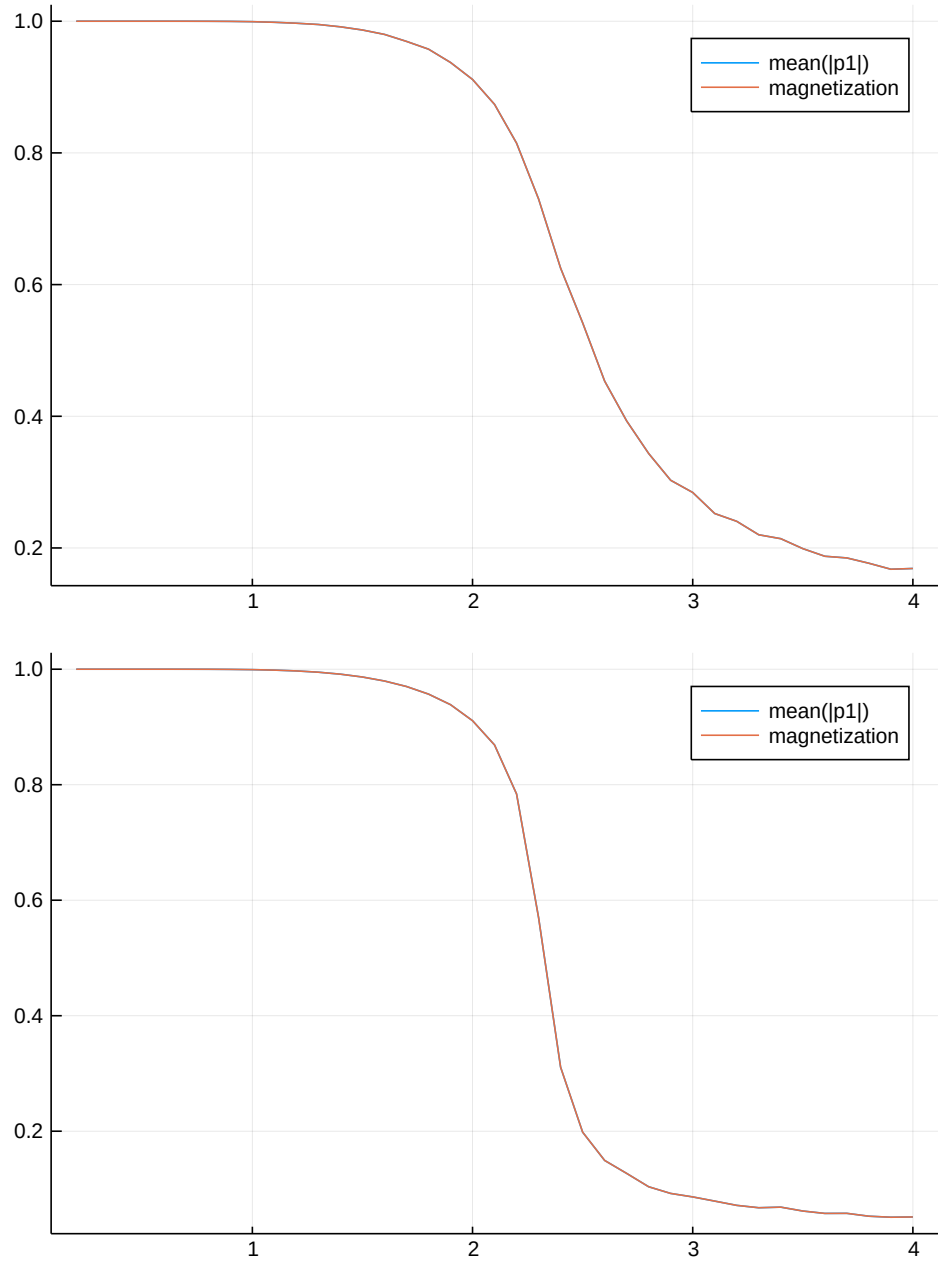

Figure 3: $\langle |p_1| \rangle / L$ and the magnetization as a function of temperature T for $L = 10$ (left) and $L = 32$ (right).

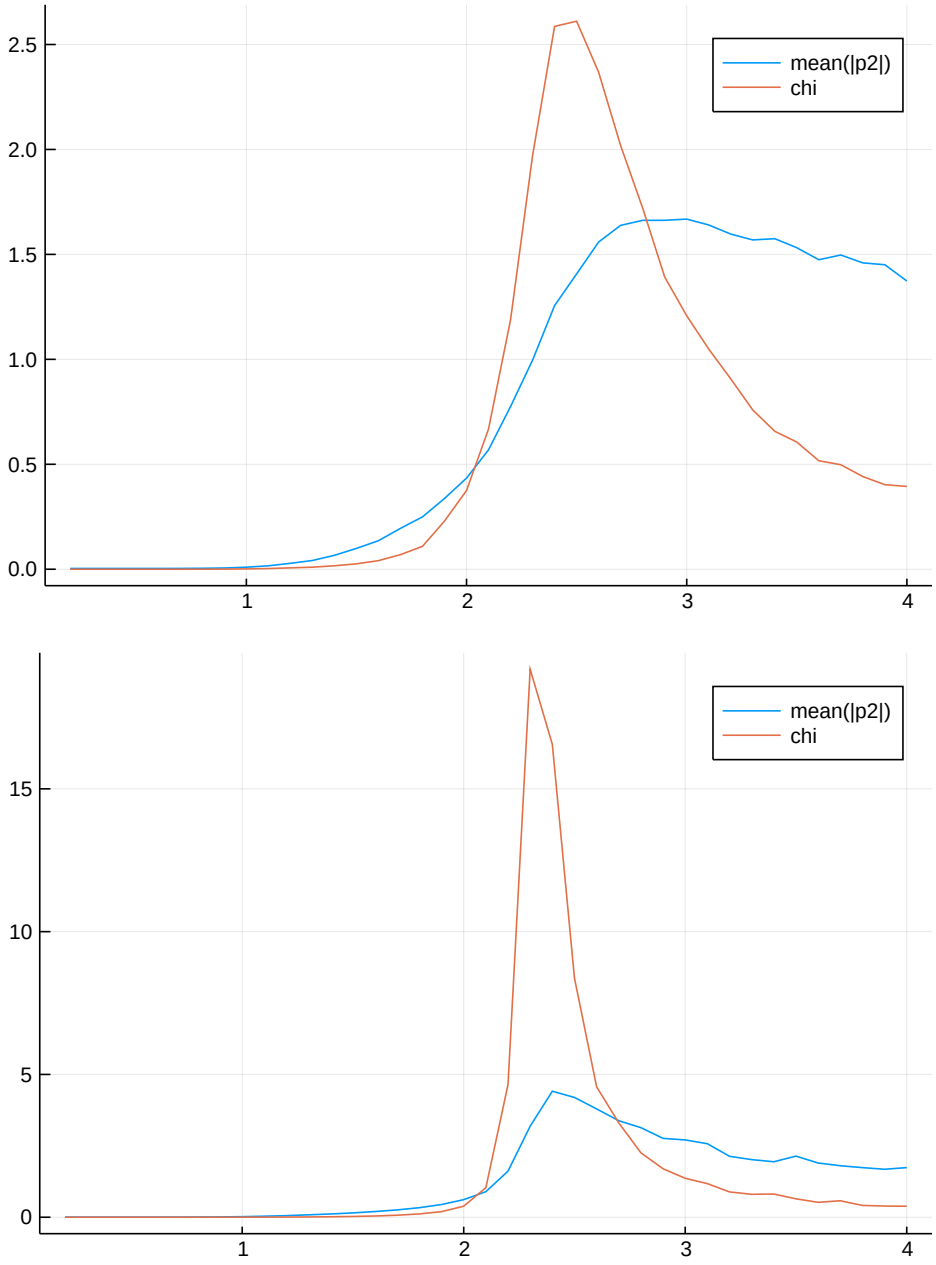

Figure 4: $\langle |p_2| \rangle$ and the susceptibility as a function of temperature T for $L = 10$ (left) and $L = 32$ (right).