

## Assignment 4

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Course: *Machine Learning in Physics (PHYS3151)* – Prof. Zi Yang Meng

Tutor: Mr. Tim Lok Chau

Due date: 15th April, 2025

### 1. PCA and Clustering on 2D ferromagnetic Ising model

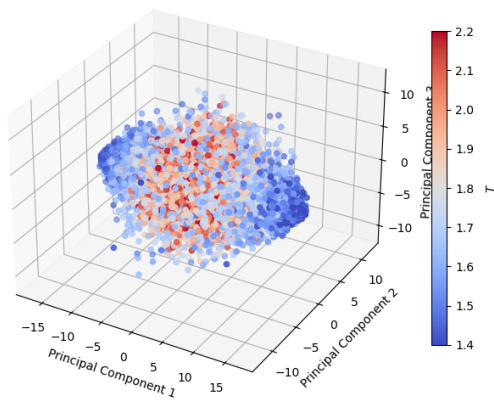
For this question, please load the  $12 \times 24$  2D honeycomb lattice Ising data files [Ising\\_config\\_L12.csv](#) and [T\\_data\\_L12.csv](#).

The Hamiltonian of Ising model is,

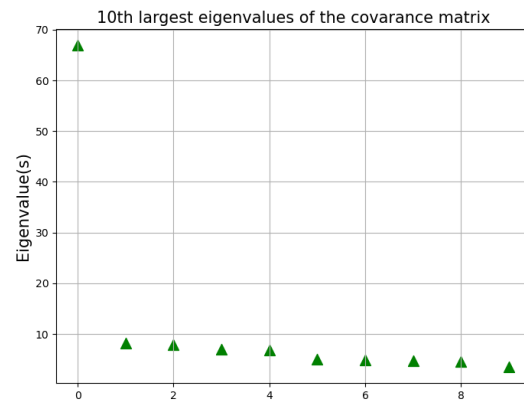
$$H = -J \sum_{i,j} \sigma_i \sigma_j$$

where  $J = 1$  stands for the ferromagnetic case, which means to minimize the total energy, the neighbouring spins point in the same direction at low temperature and point to the opposite direction at high temperature. The data file [Ising\\_config\\_L12.csv](#) contains 8500 configurations of the ferromagnetic Ising model, where **most of them have the temperature above the critical temperature** and each configuration is arranged in a row with 288 columns.

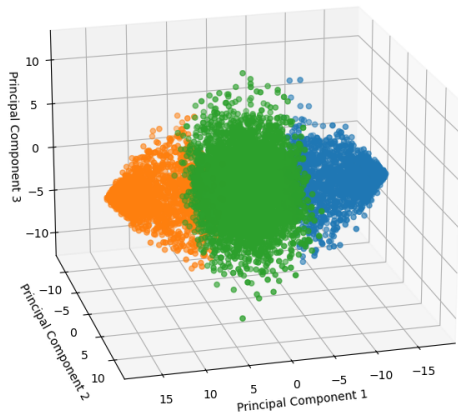
- (a) Perform PCA on the data, plot the sample points against their first **three** principal components. You can refer to graph (1a).
- (b) Plot the values of the first 10th largest eigenvalues you obtain from performing PCA on the covariance matrix in part a). You can refer to graph (1b).
- (c) Perform K-means clustering with 3 centroids, plot the resulting clusters in different colors. You can refer to the plot (1c).
- (d) Plot the distribution of eigenvectors for the first two components as heatmaps on a  $12 \times 24$  lattice. Discuss the physical meaning of the 2 heatmaps. You can refer to the example in (1d) and (1e).



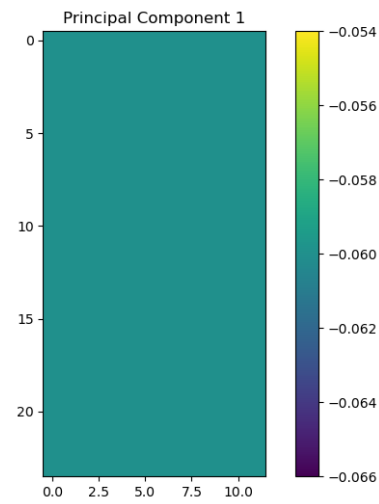
(a) The result of PCA.



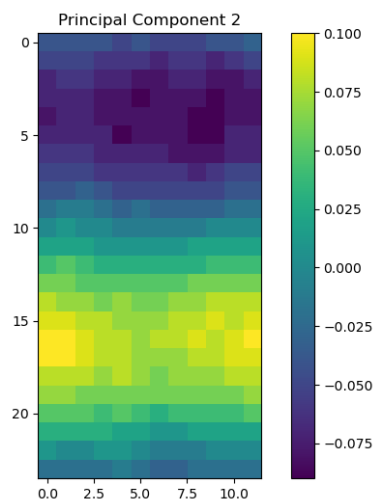
(b) Plot of first 10th largest eigenvalues.



(c) Clustering with 3 centroids.



(d) Principal component with the largest eigenvalue on 12x24 lattice.



(e) Principal component with the 2nd largest eigenvalue on 12x24 lattice.