Principal component analysis (PCA)

The process of PCA involves data standardization, resulting in the matrix $\mathbf{Z} = \mathbf{X} - \bar{\mathbf{X}}$, where $\bar{\mathbf{X}}$ denotes the mean matrix. Next, we perform eigenvalue decomposition on the covariance matrix $\mathbf{C} = \frac{1}{\mathfrak{M}-1}\mathbf{Z}^T\mathbf{Z}$ to obtain eigenvalues λ_i and their corresponding eigenvectors ω_i by solving the equation $\mathbf{C}\,\omega_i = \lambda_i\,\omega_i$. We then select the top k largest eigenvectors to construct the matrix $\mathbf{W}$, leading to the projection $\mathbf{Y} = \mathbf{Z}\mathbf{W}$, where $\mathbf{Y} \in \mathbb{R}^{\mathfrak{M}\times k}$. In this case, we set $k = 2$ to choose the two principal components with the largest eigenvalues, represented by the eigenvectors $y_1 = \mathbf{Z}\,w_1$ and $y_2 = \mathbf{Z}\,w_2$, respectively.

Ising Model

The Hamiltonian of the Ising model without external field is given by:

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

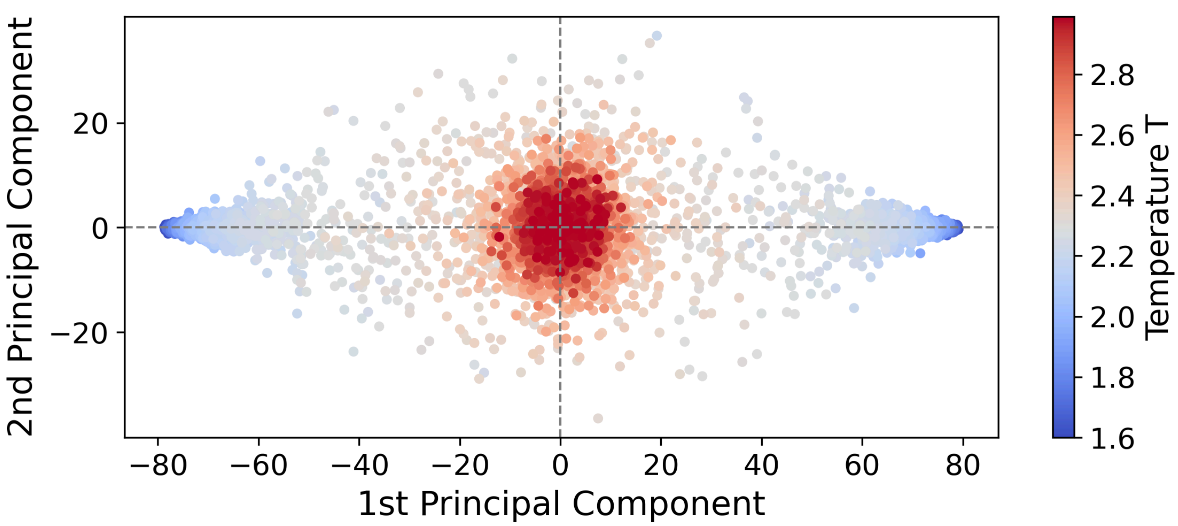
where $\sigma_i = \pm 1$ denotes the spin at site i, $J > 0$ is the coupling constant, and the sum is taken over all nearest-neighbor pairs $\langle i, j\rangle$. The model is defined on a square lattice of size $L \times L$ with periodic boundary conditions. The total magnetization of the system is defined as $M = \sum_i \sigma_i$, and the average magnetization is calculated by $m = M/N$, where $N = L^2$ is the total number of sites. Both the mean and variance of m serve as criteria for thermal equilibration during sampling.

Here, MCMC simulations were performed to generate the configurations of the Ising model. The lattice size was set to $L = 80$, and spin configurations were sampled at $n_{\text{temp}} = 140$ distinct temperatures in the range $T \in [1.6, 3.0)$, using a step size of 0.01. For each temperature, $n_{\text{samp}} = 80$ independent spin configurations were collected, each initialized from a random spin state from $\{-1, 1\}$. To efficiently mitigate critical slowing down, the Wolff cluster algorithm was adopted for spin updates.

At each temperature T, the simulation protocol consisted of system equilibration followed by statistically independent sampling. Equilibrium states were assessed using a dual sliding window approach: two consecutive windows of length $W = 100$ were monitored, and equilibrium was deemed reached when the difference in magnetization means was less than $\varepsilon_m = N \times 10^{-3}$ and the difference in variances was less than $\varepsilon_v = N^2 \times 10^{-4}$. After equilibration, the autocorrelation time τ of the magnetization time series was estimated, and the sampling interval was set to $\delta = \lceil 10 \times \tau \rceil$ to ensure statistical independence among configurations.

PCA on data matrix of Ising configurations

All collected spin configurations were flattened into vectors of length N and assembled into a data matrix $\mathbf{X} \in \mathbb{R}^{V \times N}$, where $V = n_{\mathrm{temp}} \times n_{\mathrm{samp}} = 11,200$ is the total number of samples. The matrix was subjected to PCA, from which the first principal component y_1 and the second principal component y_2 were extracted for further analysis. The scatter plot of (y_1, y_2) for all samples, colored by T, is shown in the following figure. At low temperatures, the data points (shown in blue) are symmetrically distributed at both ends of the y_1 axis, corresponding to the two symmetry-broken ferromagnetic phases. At high temperatures, the data points (shown in red) cluster around the origin, indicating the disordered paramagnetic phase. Moreover, the data points near T_c are scattered in the intermediate region. At low temperatures, the data points (shown in blue) are symmetrically distributed at both ends of the y_1 axis, corresponding to the two symmetry-broken ferromagnetic phases. At high temperatures, the data points (shown in red) cluster around the origin, indicating the disordered paramagnetic phase. Moreover, the data points near T_c are scattered in the intermediate region.



In addition, the variation of the projection of each configuration onto the first principal component y_1 was examined as a function of T. As demonstrated in the following figure, plotting y_1 versus T reveals a distinct bimodal distribution in the low-temperature regime, corresponding to the two symmetry-broken ferromagnetic phases (ordered), while at high temperatures, y_1 converges toward zero, indicating the paramagnetic phase (disordered). A pronounced transition in the distribution of y_1 is observed near the exact critical temperature $T_c = 2/\ln(1+\sqrt{2}) \approx 2.269$ proved by Onsager, clearly distinguishing the ordered and disordered phases of the Ising model.