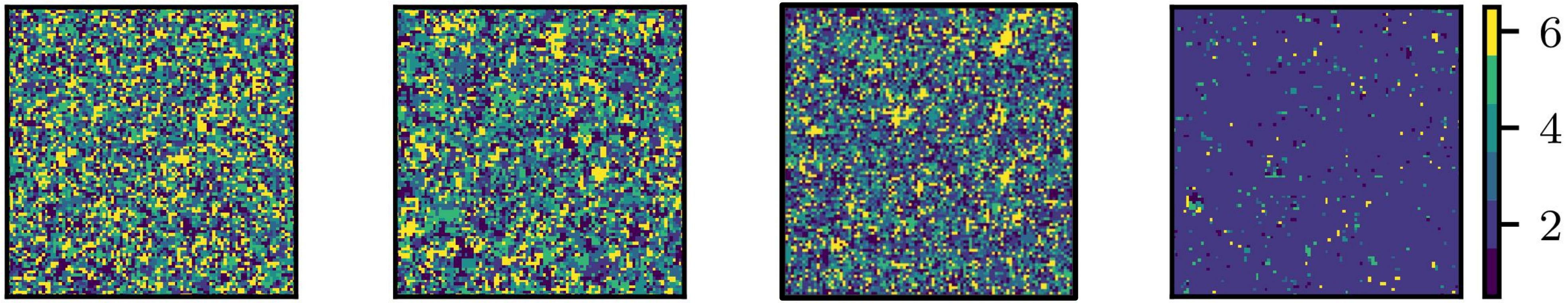
Detecting Phases and Distinguishing Local and Non-Local Order using t-SNE and Monte Carlo Methods



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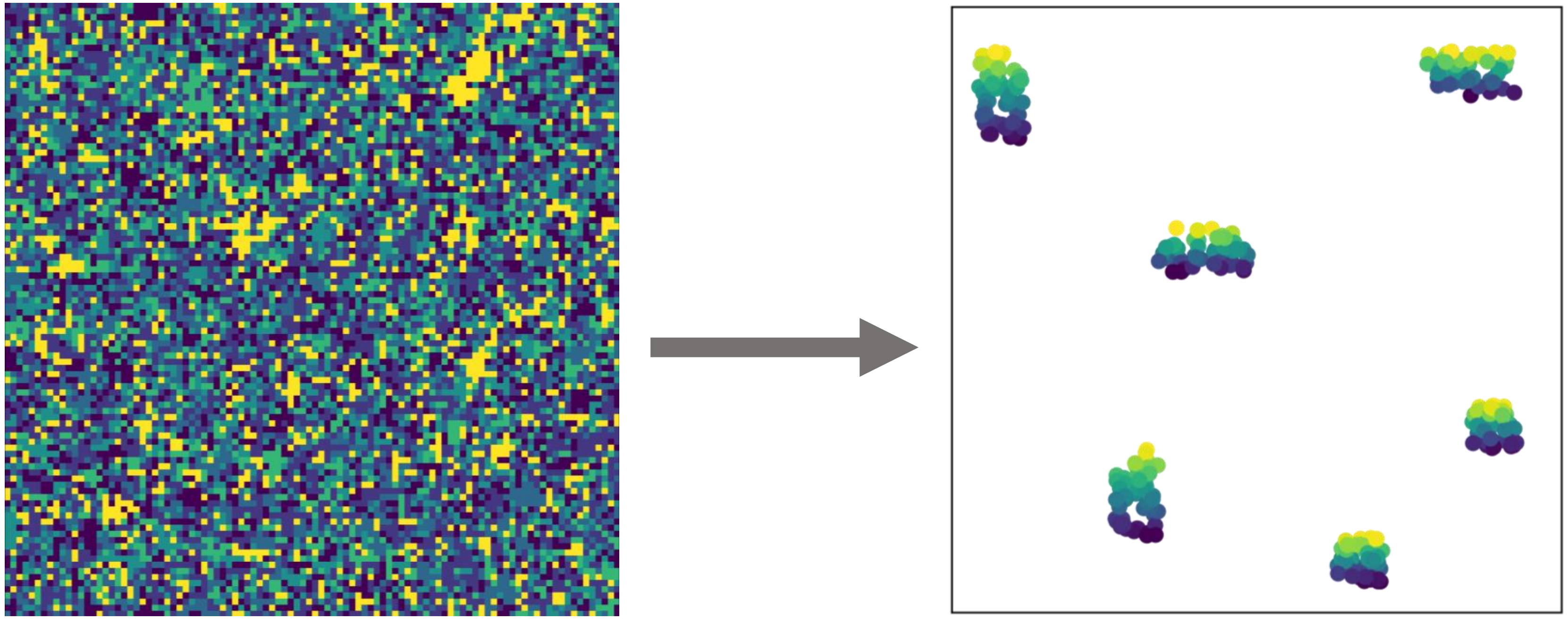
Objectives



q^{L^d} dimensions

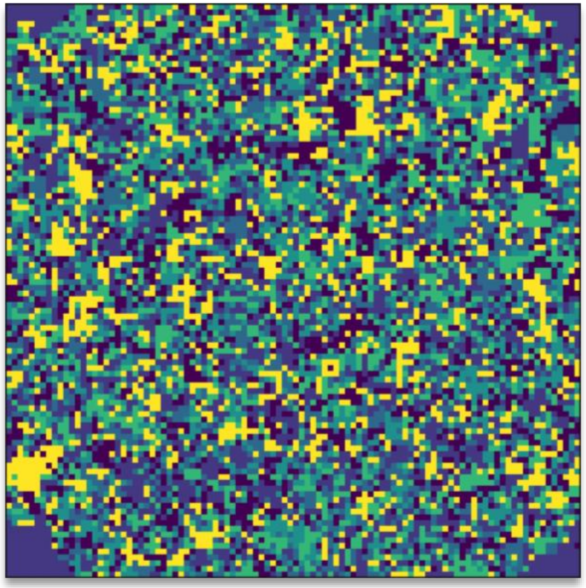
2 dimensions

Overview

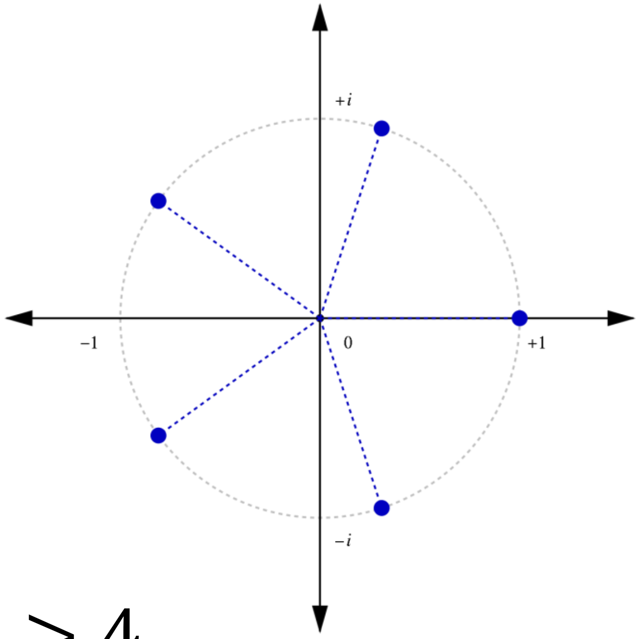
- Spin models and critical behaviour

- Monte Carlo simulations
- Dimensional reduction

- Numerical analysis with PCA and t-SNE
- Future work



Spin Models



- Local order:
  - Ising model: Continuous transition
  - q-state Pott's model: First order transition for $q > 4$.

$$H_{Potts} = -J \sum_{<ij>} \delta_{s_i, s_j} \qquad s_i \in \{1, 2, \dots, q\}$$

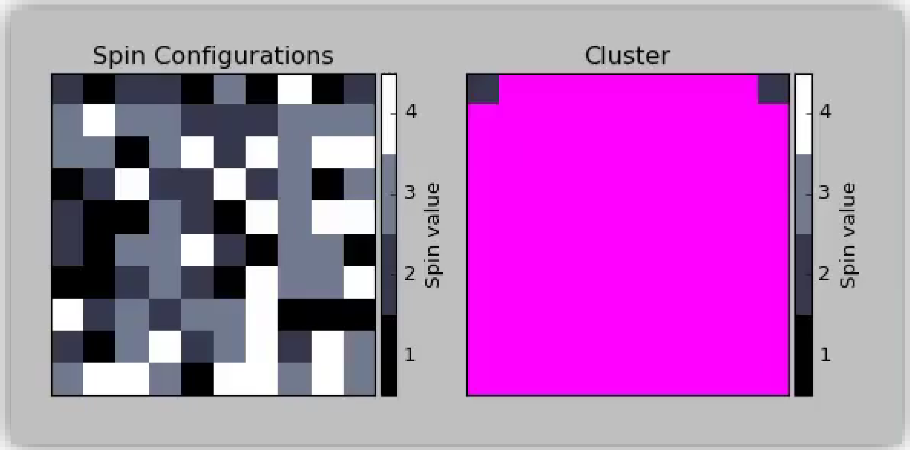
- Non-local order:
  - $\mathbb{Z}_2$ lattice gauge theory: Topological transition

Monte Carlo Simulations

- Process of N steps to estimate observables $\mathcal{O}$:

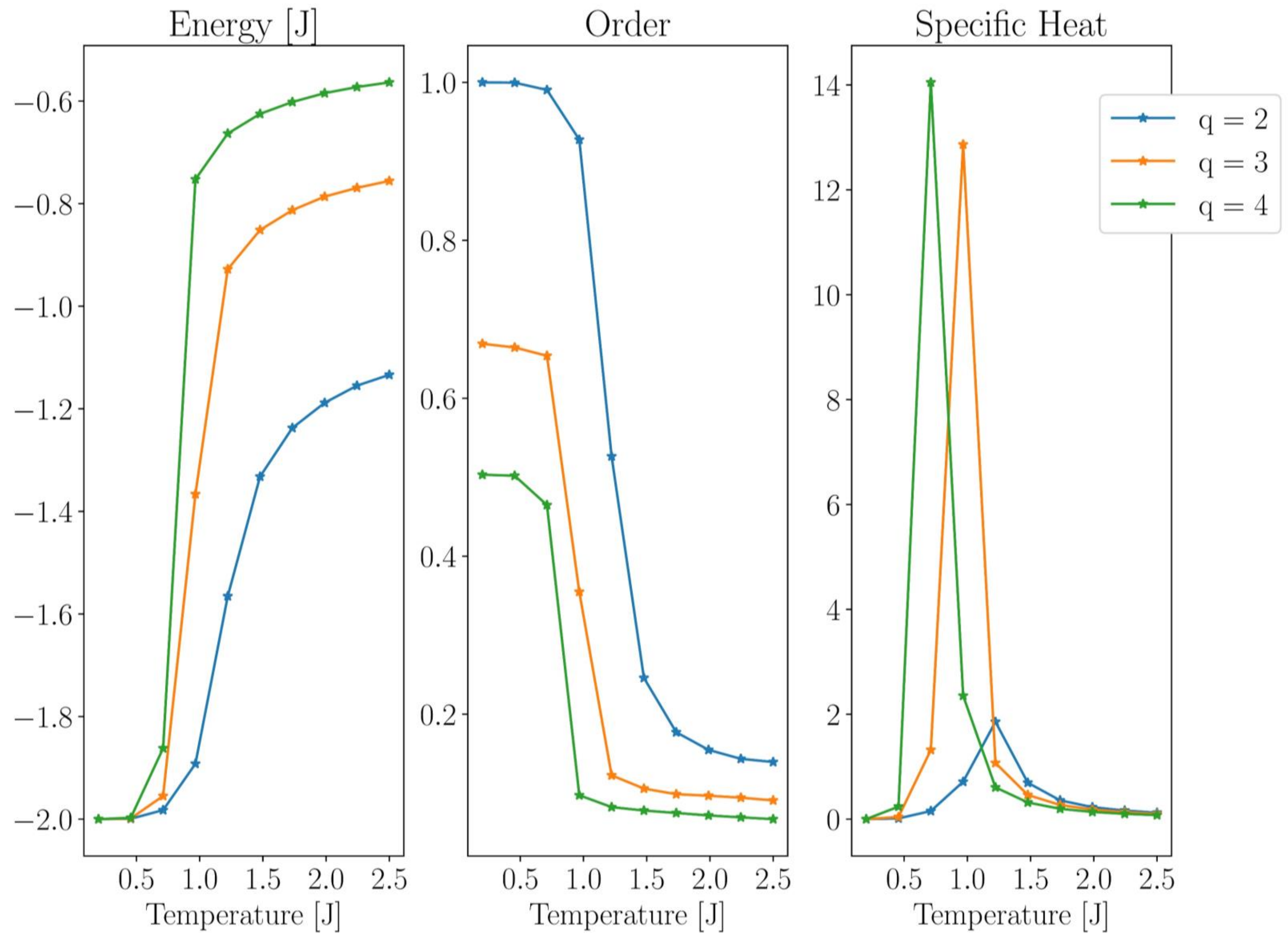
$$\langle \mathcal{O} \rangle \approx \bar{\mathcal{O}} = \frac{1}{N} \sum_t \mathcal{O}_t$$

- State transitions $\nu \to \eta$ must satisfy:
  - Ergodicity
  - Markov Process
  - Equilibrate



$q = 4$ Pott’s model Wolff cluster updates at $T < T_c$.

Pott’s Model Sampling



Dimensional Reduction

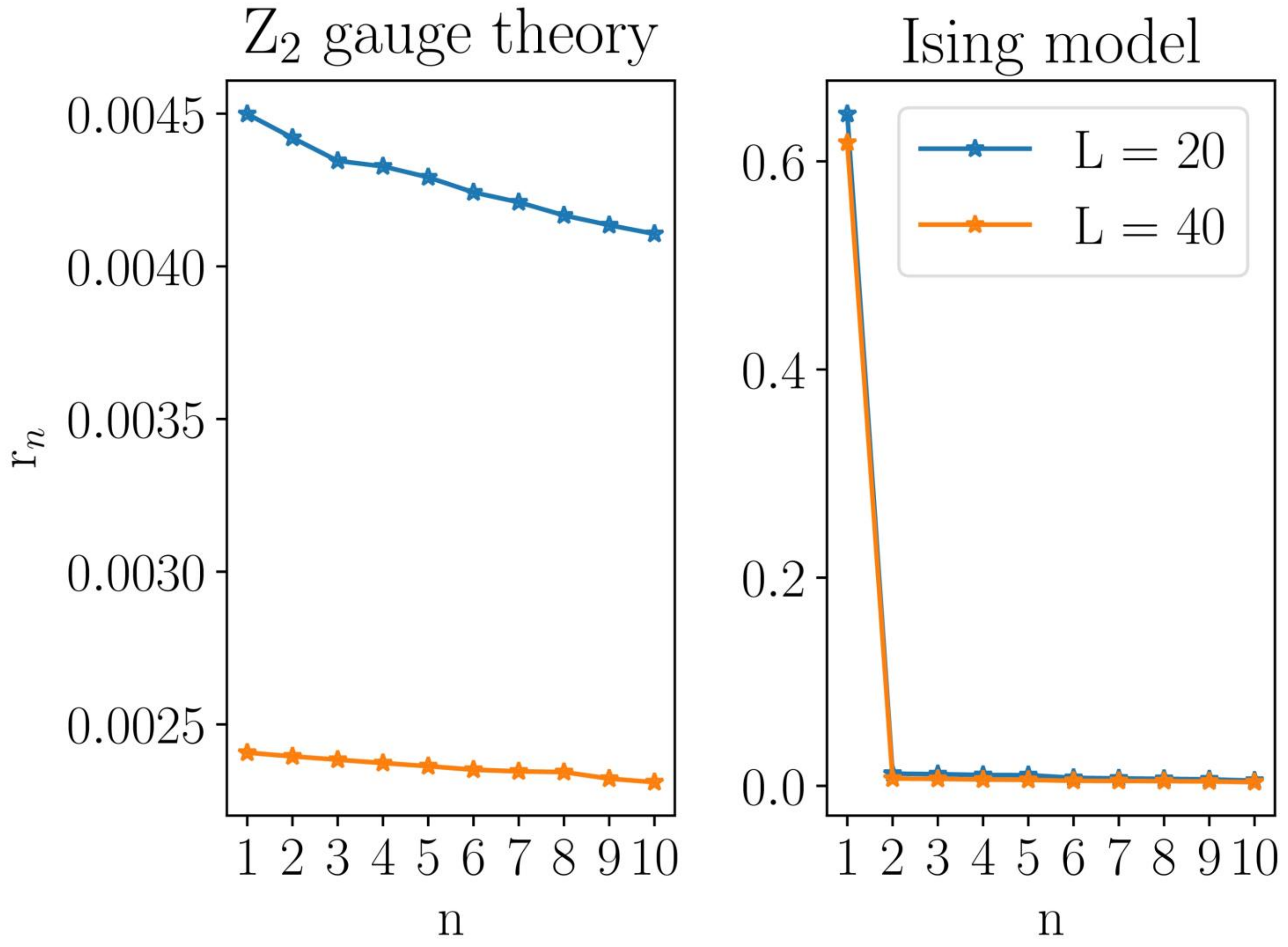
- From higher N dimensional datasets, lower $\tilde{N}$ dimensional representations are learned through training.

- Patterns and symmetries in datasets are recognized and taken advantage of during optimization (Carrasquilla and Melko, 2017).

Principal Component Analysis (PCA)

- Linear transformation to matrix similar to diagonalized eigenvalues λ_n.
- First $\widetilde{N} \ll N$ components are analysed.
- Explained variance ratio $r_n = \frac{\lambda_n}{\sum_m \lambda_m}$ depicts relative magnitude of new components (Wang, 2016).

Variance Ratio of Principal Components



t-distributed Stochastic Neighbour Embedding (t-SNE)

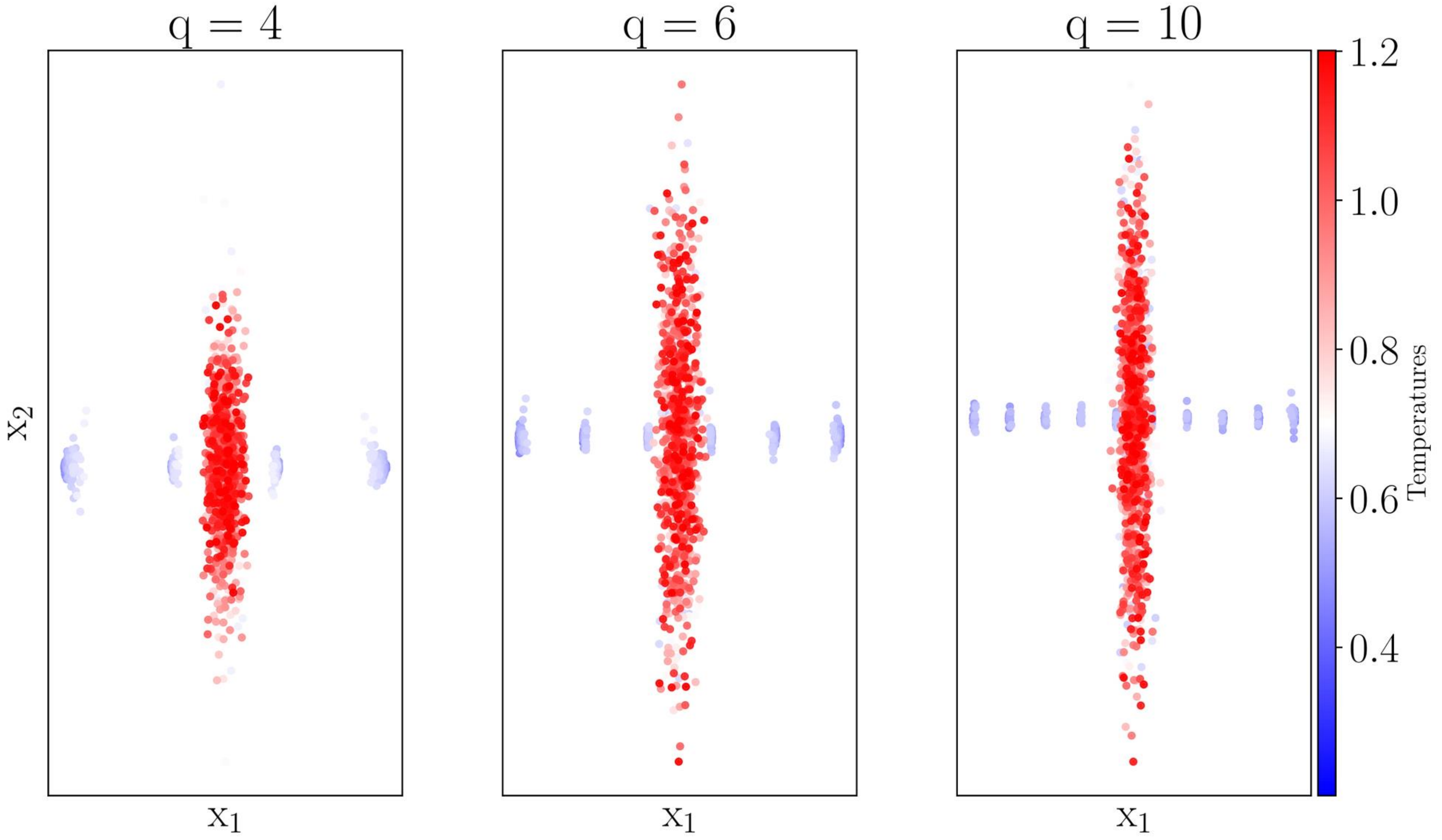
- Non-linear transformation (van der Maaten and Hinton, 2008).
- Higher N dimensional $x_i \longmapsto$ Lower $\widetilde{N}$ dimensional y_j .

$$p_{ij} \sim e^{-\frac{\left|x_i - x_j\right|^2}{\sigma_i^2}} \quad \longmapsto \quad q_{ij} \sim \frac{1}{1 + \left|y_i - y_j\right|^2}$$

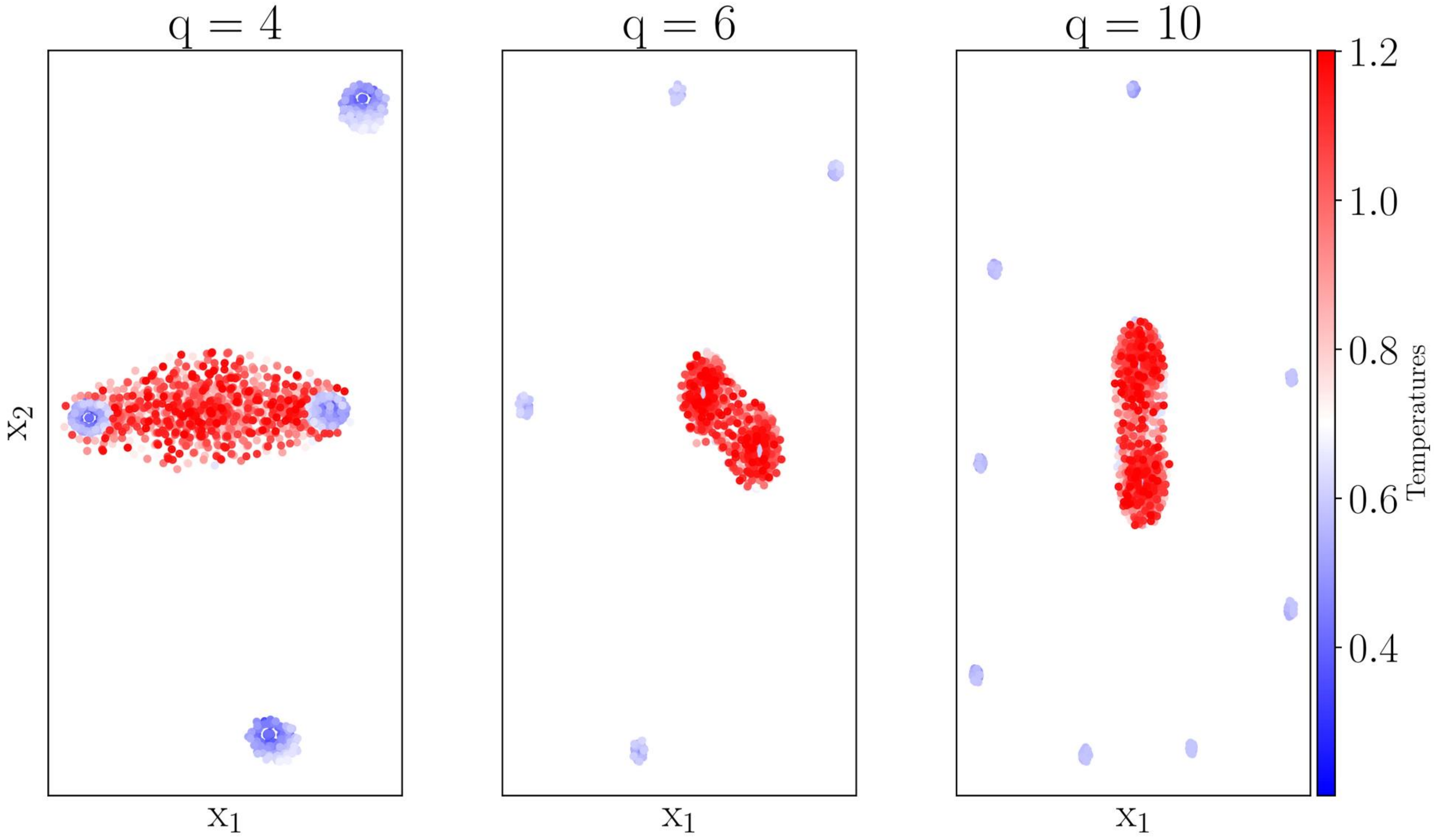
- Minimization of KL divergence aims to preserve distances:

$$KL(p,q) \equiv \sum_{i,j} p_{ij} \log \frac{q_{ij}}{p_{ij}}$$

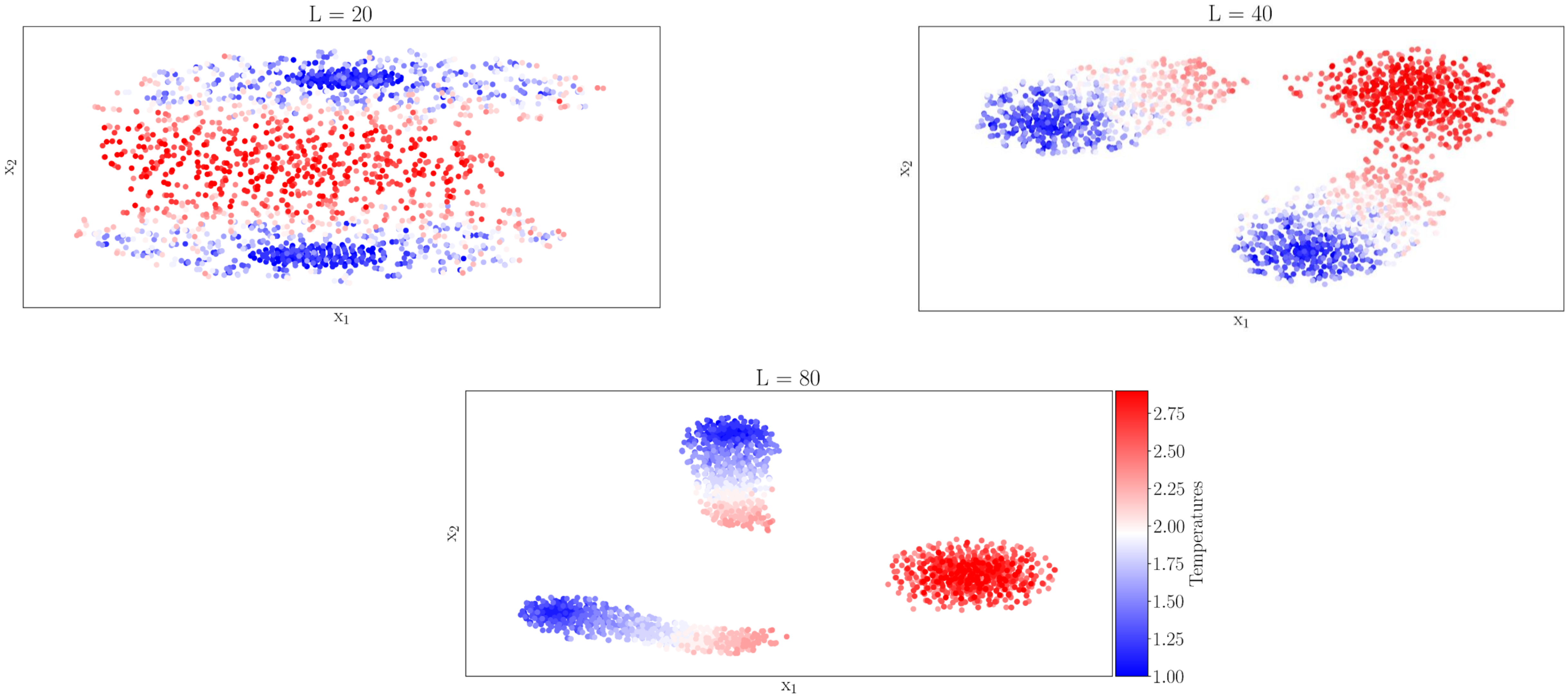
PCA of Pott's model



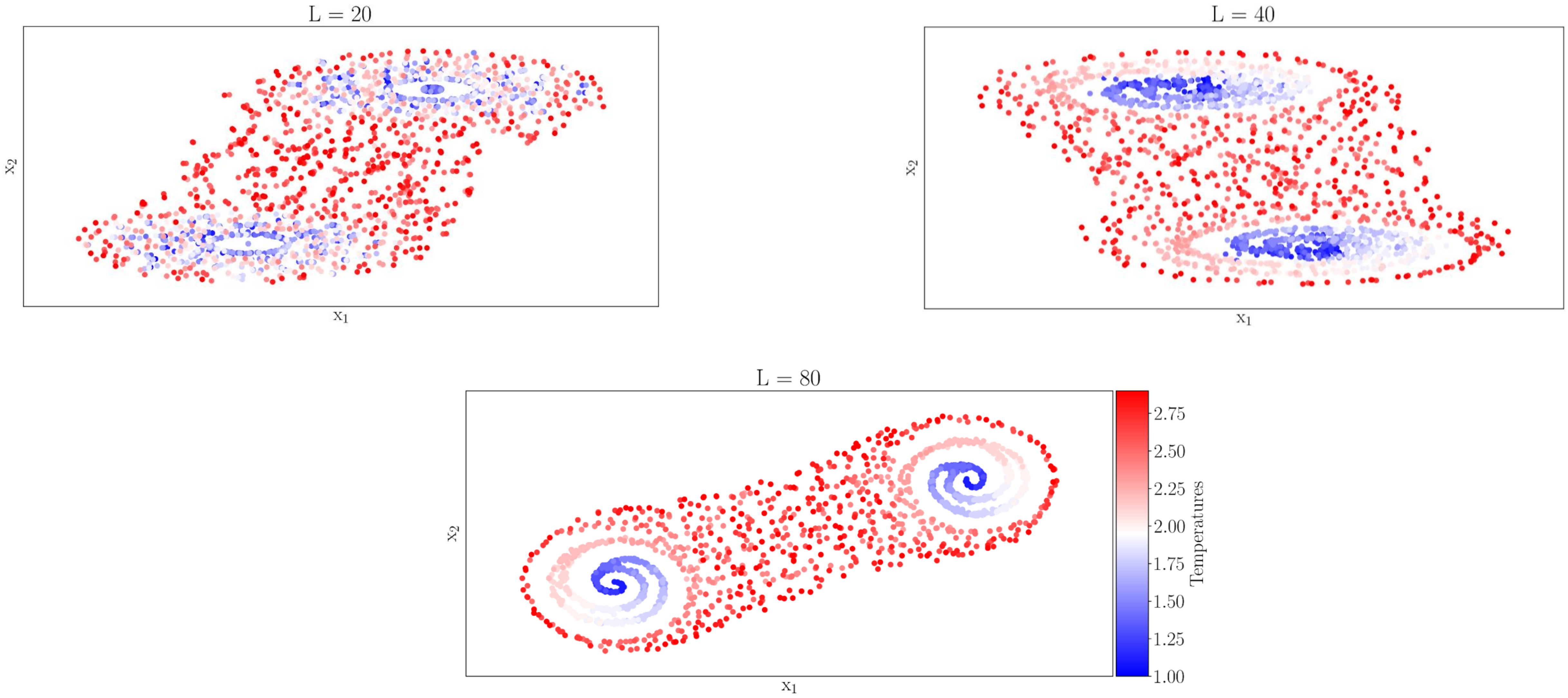
t-SNE (with PCA) of Pott's model



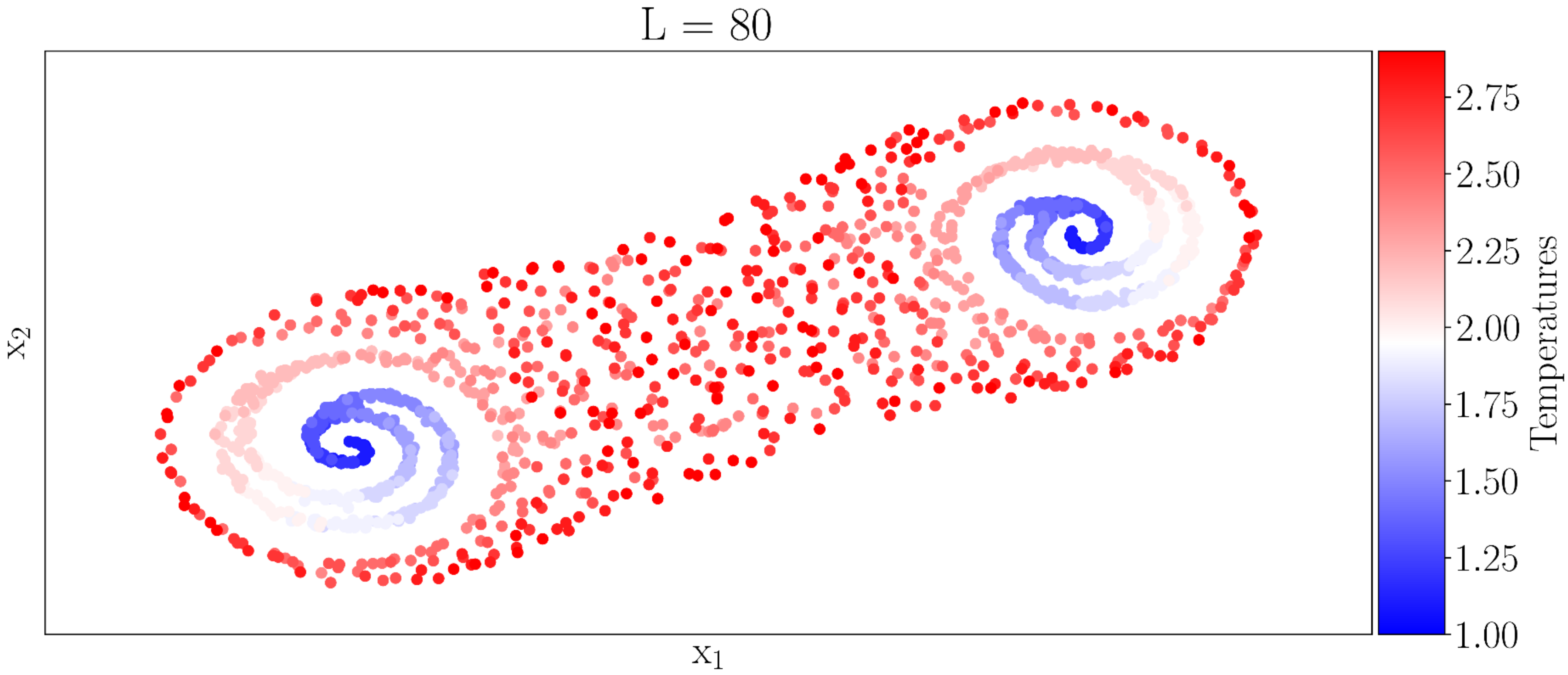
t-SNE (with PCA) of Ising model



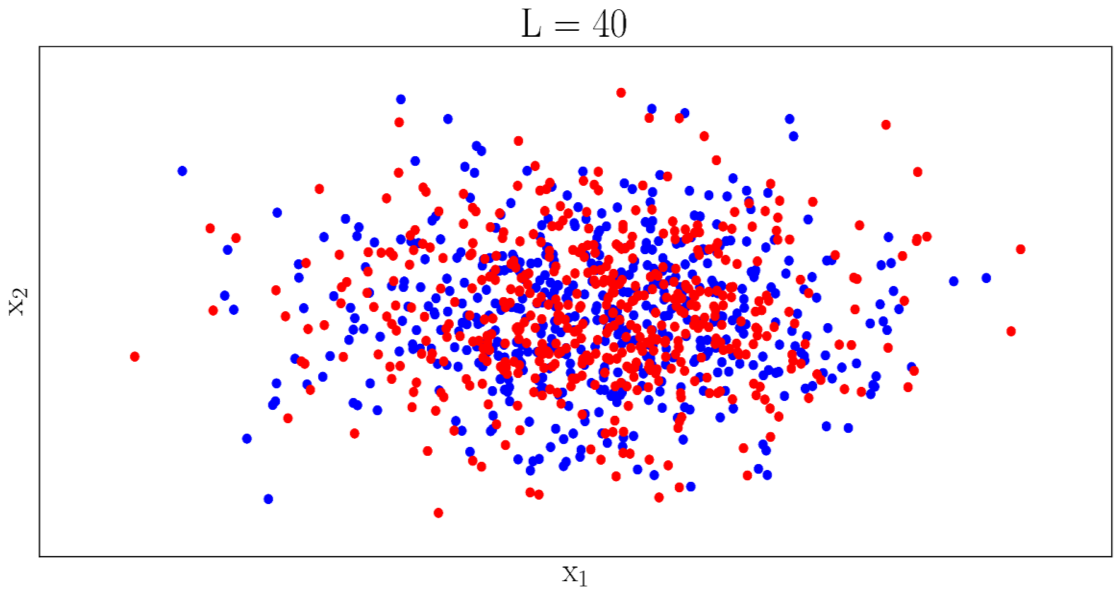
t-SNE (without PCA) of Ising model



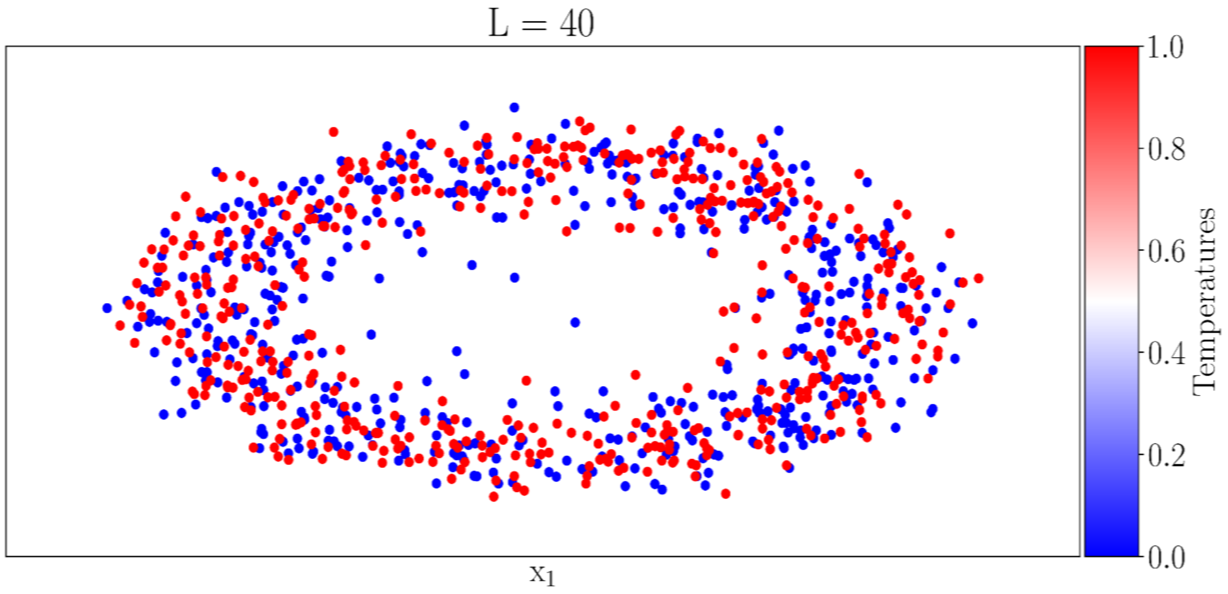
t-SNE (without PCA) of Ising model



PCA and t-SNE (with PCA) of $\mathbb{Z}_2$ Gauge Theory

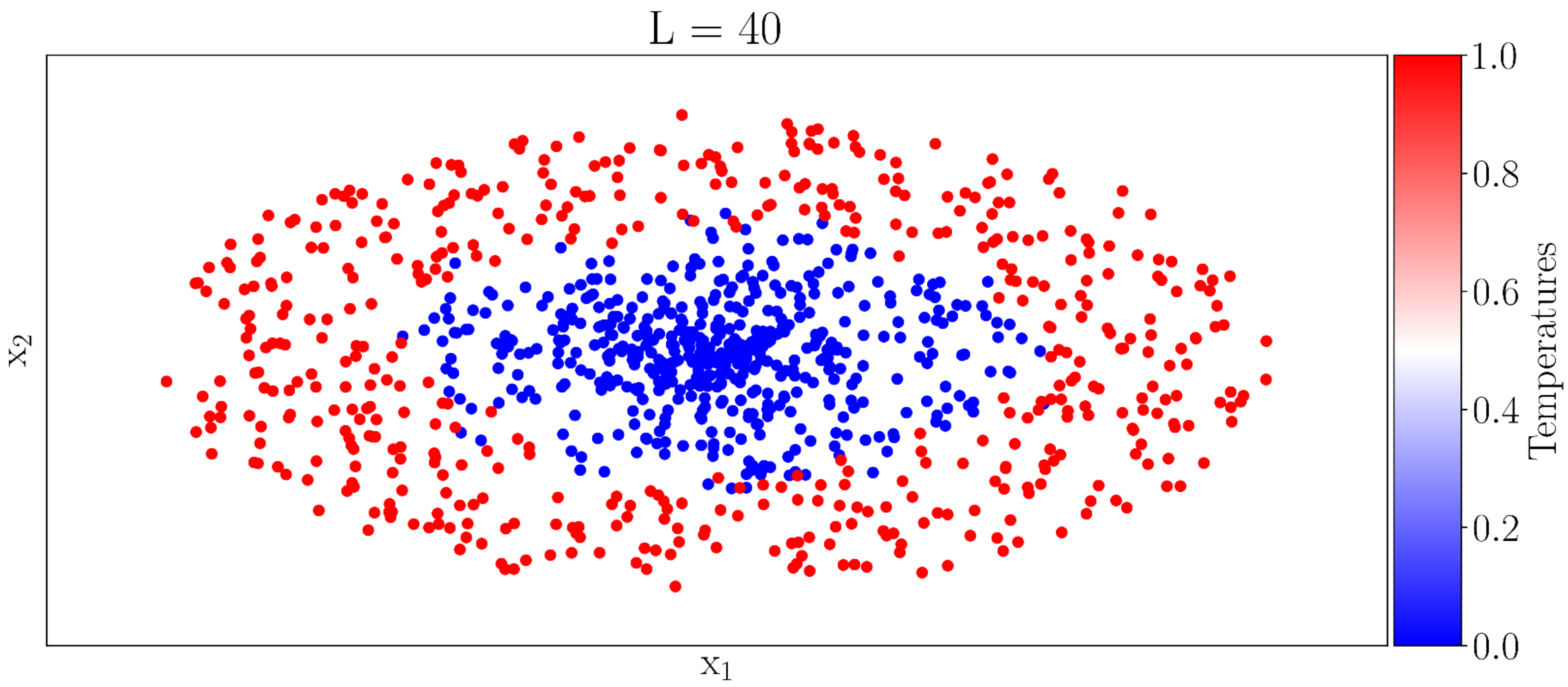


PCA



t-SNE (with PCA)

t-SNE (without PCA) of $\mathbb{Z}_2$ Gauge Theory



Learning of Features versus Interpretability

- PCA and t-SNE are capable of distinguishing phases in:
  - Local systems with first-order and continuous transitions.

- t-SNE is further capable of identifying phases in:
  - Non-local systems with topological transitions.

- Trade-off between ability of methods to distinguish features, and ease of interpretation of such features.

Future Work

- Physical features being learned during training:
  - PCA - Order parameter (Wang, 2016).

- Coexistence of phases at first order transitions (Landau and Binder, 2009).

- Local minima effects
- Sampling effects
- Training and optimization procedures