Classifying Phase Transitions Using Machine Learning

Ising and Potts Models with PCA and Variational Autoencoders

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Outline

What is a Phase Transition?

- Macroscopic changes in a system due to small variations in parameters like temperature or field.
- Example: Ferromagnetic to paramagnetic transition in the Ising model.
- Key concept: **Order parameter** (e.g. magnetization M).

- Spins $s_i = \pm 1$ on a 2D lattice.
- Hamiltonian: $H = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i$
- Phase transition at $T_c \approx 2.269$ (2D, zero field).
- Critical behavior: diverging correlation length, power-law scaling.

The Potts Model

- Generalization: q-state spins $s_i \in \{1, ..., q\}$.
- Hamiltonian: $H = -J \sum_{\langle i,j \rangle} \delta_{s_i,s_j}$
- $q = 2$ is Ising model; $q > 4$ shows first-order transitions.
- Used in modeling multi-phase materials, image segmentation.

Monte Carlo Simulation

- Use Metropolis or Wolff algorithm to sample configurations.
- Input: temperature grid around T_c.
- Output: $N \times L^2$ binary configurations for Ising, categorical for Potts.

Preprocessing

- Normalize configurations (mean 0, std 1).
- Flatten $L \times L$ grid to 1D vector.
- Split into training/testing sets with labels (for supervised).

Neural Network Classifier (PyTorch)

- Input: lattice configuration vector.
- Output: classification (e.g. low vs. high T).
- Loss: cross-entropy; Optimizer: Adam.

Key Idea

Learn to distinguish phases by training on labeled data.

PCA: Principal Component Analysis

- Linear method: projects data onto orthogonal axes of max variance.
- Useful for visualizing structure in data without labels.

pca_latent_plot.png

Clustering and Phase Separation

- Apply k-means or DBSCAN in PCA space.
- Phases form clusters below and above T_c.
- Cluster centers shift with temperature.

What is a VAE?

- Probabilistic autoencoder with latent variables.
- Learns $q(z|x)$ encoder and $p(x|z)$ decoder.
- Loss: ELBO = reconstruction + KL divergence.

$$\mathcal{L}_{\text{VAE}} = \mathbb{E}_{q(z|x)}[\log p(x|z)] - \text{KL}(q(z|x)\|p(z))$$

VAE Architecture (PyTorch)

- Input: configuration vector x.
- Latent space: $z \in \mathbb{R}^2$ or $\mathbb{R}^d$.
- Decoder reconstructs x from z.

vae_architecture.png

Latent Space Comparison

PCA

- Linear projection
- Orthogonal axes
- Fast, interpretable

VAE

- Nonlinear manifold
- Captures higher-order correlations
- Learns generative model

Detecting Criticality via Latent Variance

- VAE latent variables cluster in temperature space.
- Variance in z increases near T_c.
- Can be used as an indicator of phase transition.

latent_variance_plot.png

Key Takeaways

- Machine learning models can classify and detect phase transitions.
- PCA gives interpretable linear structure; VAEs provide generative power.
- Latent representations are effective probes of critical phenomena.
- Future: use diffusion models or normalizing flows.

References

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