Prometheus: Unsupervised Discovery of Phase Transitions and Order Parameters in the 2D Ising Model Using Variational Autoencoders (Student Abstract)

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Abstract

Phase transitions in condensed matter systems traditionally require prior knowledge of order parameters for identification. We present Prometheus, a variational autoencoder framework for unsupervised discovery of phase transitions and order parameters in the two-dimensional Ising model without prior physical knowledge. Our approach combines convolutional neural networks with beta-variational autoencoders to learn compressed representations that naturally separate ordered and disordered phases. Experimental validation demonstrates automatic discovery of the order parameter with 0.85 correlation to theoretical magnetization and critical temperature detection within 0.27% of the theoretical value, achieving 89% improvement over principal component analysis while requiring no supervision.

Code — https://github.com/YCRG-Labs/prometheus

Introduction and Motivation

Phase transitions represent fundamental phenomena in condensed matter physics where systems undergo qualitative changes in their macroscopic properties (Landau and Lifshitz 1980). The Ising model exhibits a continuous phase transition at $T_c = 2/\ln(1+\sqrt{2}) \approx 2.269$ with spontaneous magnetization as the order parameter (Ising 1925; Onsager 1944).

Traditional approaches require prior knowledge of order parameters and manual identification of critical phenomena (Goldenfeld 1992). Machine learning offers new possibilities: supervised methods classify phases using labeled data (Carrasquilla and Melko 2017), while unsupervised methods identify boundaries through dimensionality reduction (Wang 2016). Variational autoencoders combine deep networks with probabilistic modeling (Kingma and Welling 2013), with beta-VAE extensions controlling reconstruction-disentanglement trade-offs (Higgins et al. 2017; Wetzel 2017).

However, existing approaches require manual feature engineering, lack physics-informed training, and provide limited theoretical validation. This work presents Prometheus, a comprehensive framework for unsupervised phase transition discovery using convolutional beta-variational autoencoders with physics-informed training and comprehensive validation.

Technical Approach

Ising Model Simulation

We simulate the two-dimensional Ising model on square lattices with periodic boundary conditions. The Hamiltonian is:

$$H = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i \tag{1}$$

where $s_i \in \{-1, +1\}$ represents spins, J is the coupling constant, and h is the external field. We use Metropolis-Hastings algorithm for Monte Carlo sampling with proper equilibration (Metropolis et al. 1953).

Physics-Informed VAE Framework

Our framework employs a convolutional beta-VAE with three encoder layers (ReLU, batch normalization, downsampling) mapping to latent parameters, and a mirrored decoder with transposed convolutions. The objective function is:

$$\mathcal{L} = \mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)] - \beta \cdot D_{KL}(q_\phi(z|x)||p(z)) \tag{2}$$

where β controls regularization strength.

Key Innovations

We implement physics-informed training with symmetry-preserving augmentation, cosine annealing schedules, and progressive training from high temperatures. Automated order parameter discovery analyzes correlations between latent dimensions and physical quantities, identifying dimensions with strongest temperature dependence.

Experimental Results

We evaluate on 50,000 Monte Carlo Ising configurations across $T \in [1.5, 3.5]$ with lattice sizes $L \in \{16, 32, 64\}$. Training uses 80/10/10 splits. We compare against PCA, t-SNE, and supervised baselines with $\alpha = 0.05$ significance.

Prometheus achieved 0.85 order parameter correlation (95% CI [0.82, 0.88]) vs. 0.45 for PCA (p < 0.001, Cohen d = 2.8), representing 89% improvement. Critical temperature

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Method	Corr.	Error (%)
PCA	0.45	12.3
t-SNE	0.38	15.7
Supervised	0.72	3.2
Prometheus	**0.85**	**0.27**

Table 1. Phase transition discovery results.

detection within 0.27% of theoretical value demonstrates exceptional precision without supervision. The method maintains consistent performance across lattice sizes with proper finite-size scaling.

The automated order parameter discovery successfully identified key physical relationships: magnetization correlation (85% ± 4%), critical temperature detection (99.7% ± 0.1%), phase boundary identification (91% ± 3%), and symmetry preservation (94% ± 2%). The system generates interpretable descriptions of discovered relationships.

Detailed Analysis

Ablation Study: Each component contributes significantly: full framework (0.85 ± 0.04), without physics constraints (0.72 ± 0.08, $p < 0.001$), without progressive training (0.78 ± 0.06, p = 0.012), without symmetry augmentation (0.81 ± 0.05, p = 0.031). Physics constraints provide the largest improvement (Cohen d = 1.6).

Beta Parameter Optimization: Systematic analysis reveals optimal performance at $\beta = 1.0$ with 0.85 order parameter correlation. Lower values (0.1-0.5) prioritize reconstruction, achieving 0.78 ± 0.06 correlation. Higher values (2.0-10.0) over-regularize, reducing correlation to 0.71 ± 0.09.

Finite-Size Scaling: Performance improves with lattice size: L=16 (0.82 ± 0.05), L=32 (0.85 ± 0.04), L=64 (0.87 ± 0.03), demonstrating proper scaling behavior consistent with theoretical expectations.

Discussion and Future Work

Our experimental results demonstrate significant advances in unsupervised discovery of phase transitions. The 89% improvement in order parameter correlation over PCA (Cohen d = 2.8) shows substantial practical significance beyond statistical significance. The physics-informed training procedures provide strong inductive bias for learning physically meaningful representations.

The automated order parameter discovery achieves 0.85 correlation with theoretical magnetization while requiring no prior knowledge of the underlying physics. Critical temperature detection within 0.27% accuracy demonstrates the precision of the unsupervised approach. The learned latent representations naturally separate ordered and disordered phases, suggesting the framework captures fundamental aspects of the phase transition.

Theoretical Implications

The success of beta-VAE in physics discovery suggests that disentangled representations naturally align with physical order parameters. The optimal $\beta = 1.0$ indicates that standard VAE regularization provides sufficient disentanglement for physics tasks without over-constraining the latent space. The learned representations exhibit proper critical scaling behavior consistent with theoretical predictions.

Implementation Details

All experiments use PyTorch 1.12.0 with 8-dimensional latent space, Adam optimizer, and batch size 128. Training converges within 100 epochs with gradient clipping. Statistical analysis uses bootstrap resampling with 1000 iterations for confidence intervals.

Key contributions include: (1) novel physics-informed variational autoencoder incorporating symmetry constraints and progressive training, (2) automated order parameter discovery achieving 0.85 correlation with theoretical magnetization without supervision, (3) comprehensive experimental validation with rigorous statistical analysis showing significant improvements over traditional dimensionality reduction methods, and (4) open-source implementation enabling reproducible research in computational physics.

Future Work: Extensions to quantum many-body systems, frustrated magnets, and topological phases will advance this interdisciplinary approach. The framework's ability to discover order parameters without supervision makes it particularly valuable for exploring novel phases of matter where theoretical understanding is limited.

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