# Characterization of the phase transition phenomenon using minkowski functionals

Mehdi Yousefzadeh  -  Mohammad Khaledi Pour

Supervisor : Prof. Seyed Mohammad Sadegh Movahed

Ph.D. Student, Department of Physics, Shahid Beheshti University (SBU)
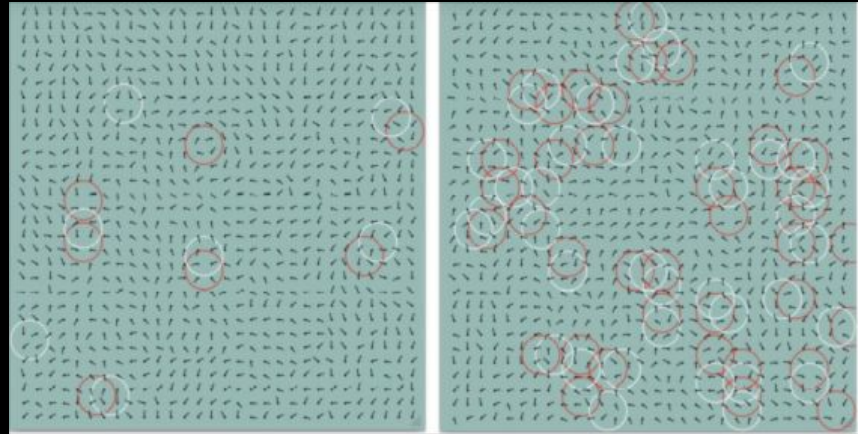
July 2

# Table of Contents
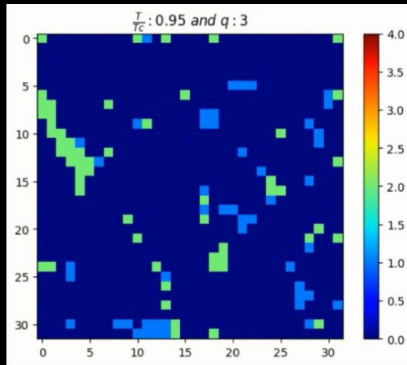
# Phase Transition

- Traditional classification of the phase transition phenomenon:

- First order phase transition:
    - The divergence occurs in the first order derivative of the free energy.
    - The co-existence of different phases is possible.

- Second order phase transition:
    - The divergence occurs in the second order derivative of the free energy.
    - The co-existence of different phases is not possible.
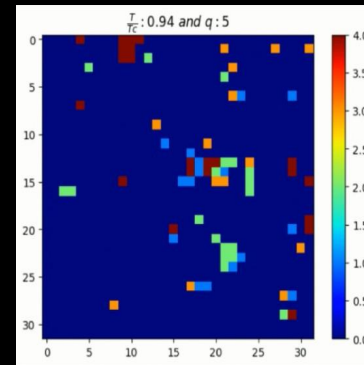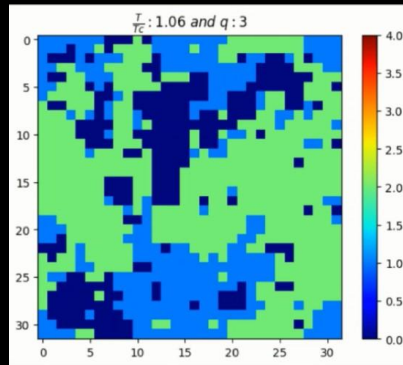
- **Topological Phase Transition**

---

- It was proved that the correlation of spins undergoes major changes with increasing temperature.
- New kind of phase transition was introduced by Kosterlitz which is based on the evolution of topological defects.

4  Kosterlitz, J. M., & Thouless, D. J. (2018). Ordering, metastability and phase transitions in two-dimensional systems. In *Basic Notions Of Condensed Matter Physics* (pp. 493-515). CRC Press.

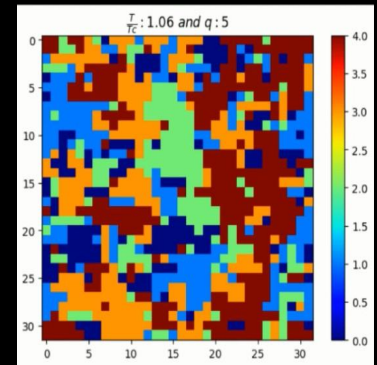# Phase Transition - Potts Model



2nd Order - q=3
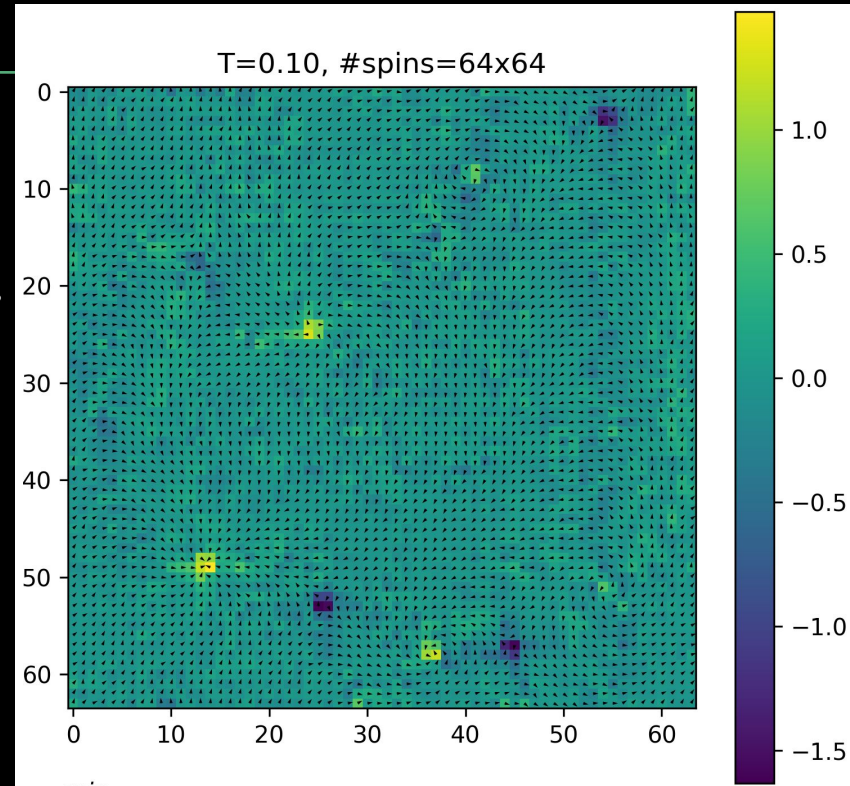
1st Order - q=5

# Simulation

- Modified XY Models Simulation Code

- List T: [0.1, 0.3, 0.5,0.6,0.7,0.75,0.8,0.82,0.84,0.86,0.87,0.88,0.89,0.9, 0.91,0.92,0.94,0.96,1.0,1.1,1.2,1.3,1.5,1.75,2.0,2.5,3.0,4.0,5.0,6.0,8.0,10]

- List size: [32,48,64,96,128,192,256]

- Modified Curl Algorithm



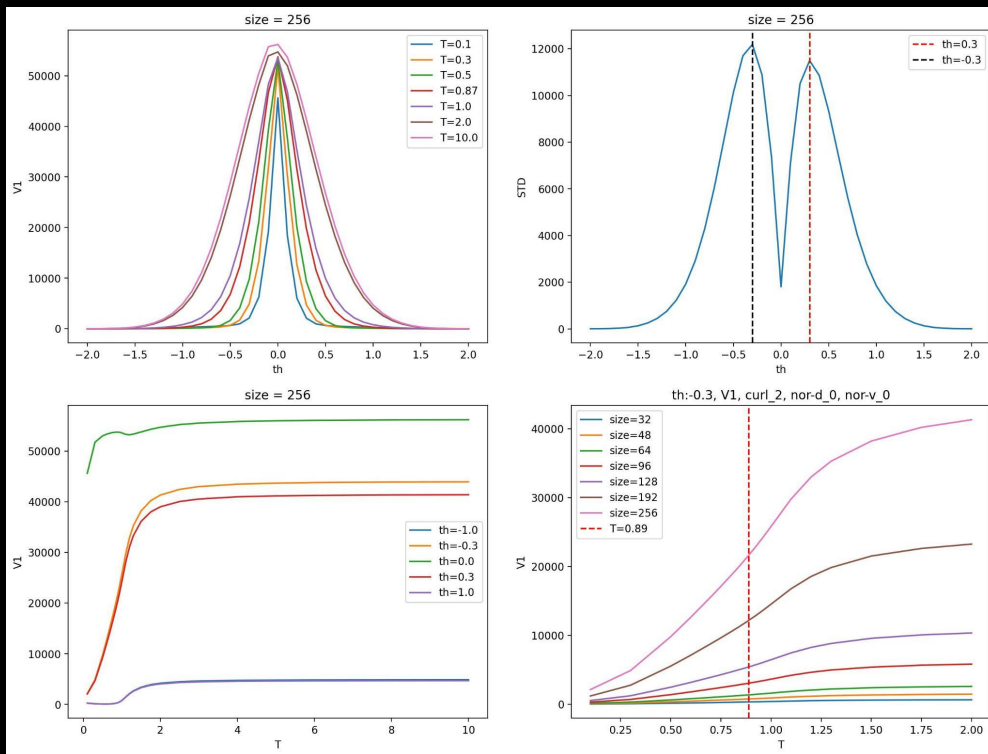T=0.10, #spins=64x64

- Curl of Lattice

# Motivations

- Minkowski functionals extracts morphological features of a system.
- The central idea is that the singular energy dependence displayed by the thermodynamic observables at a phase transition is the shadow of topological change.
- The connection between the topology change and the phase transition was proven to hold true for a certain class of systems with short-range interactions, showing that a topology change is a necessary condition for a phase transition to take place.
- The lack of geometrical measures is evident.
- Potential analytic and numerical analysis, using both topology and geometry, can show hidden orders of this phenomenon.
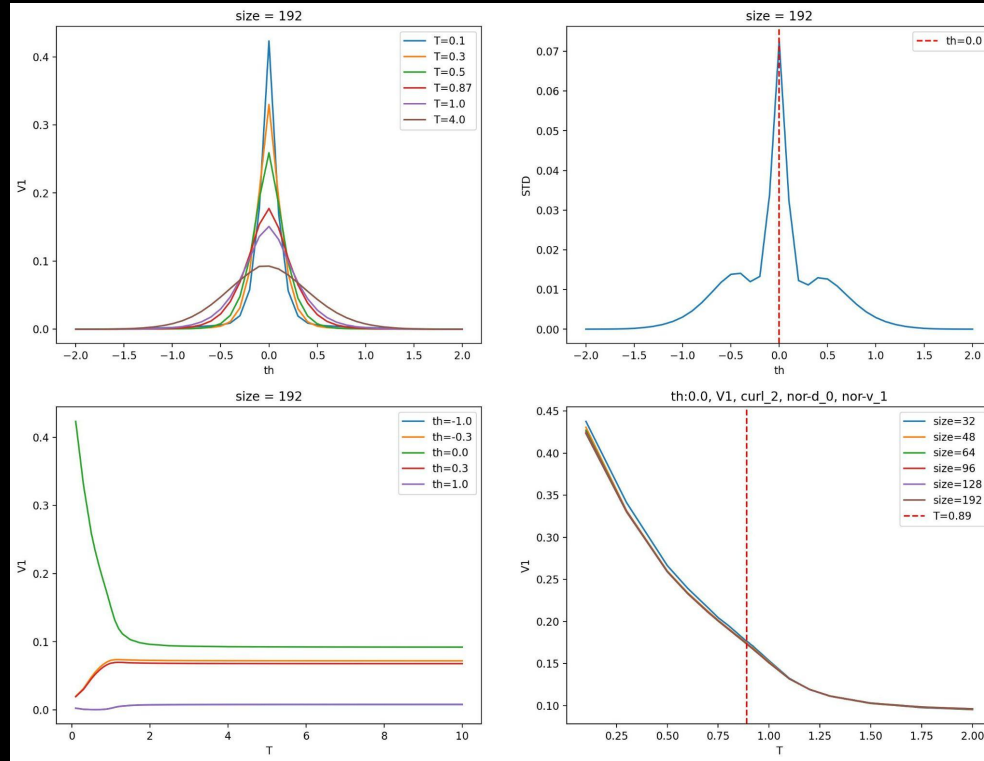
# Motivations
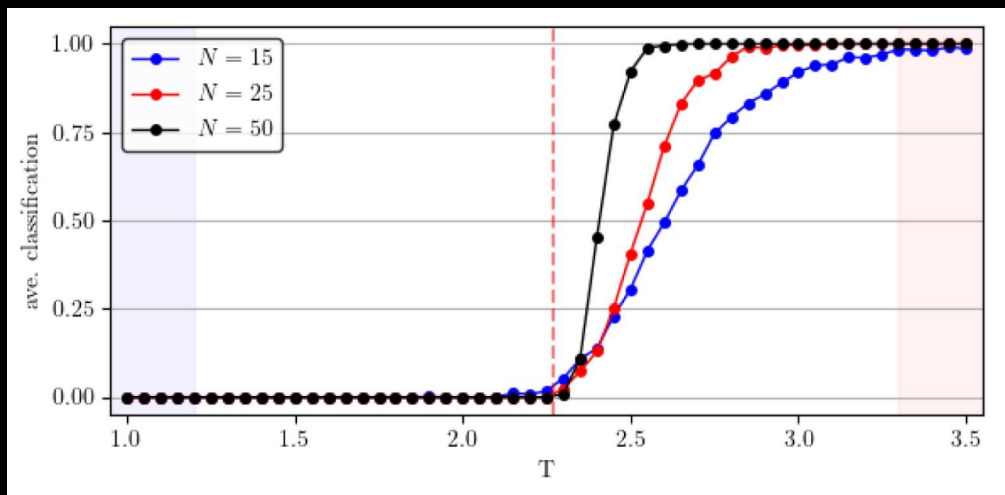


Output of a logistic regression machine which is
trained by topological features of an Ising model

8 | Cole, A., Loges, G. J., & Shiu, G. Quantitative and interpretable order parameters for phase transitions from persistent homology. arXiv 2020. *arXiv preprint arXiv:2009.14231.*
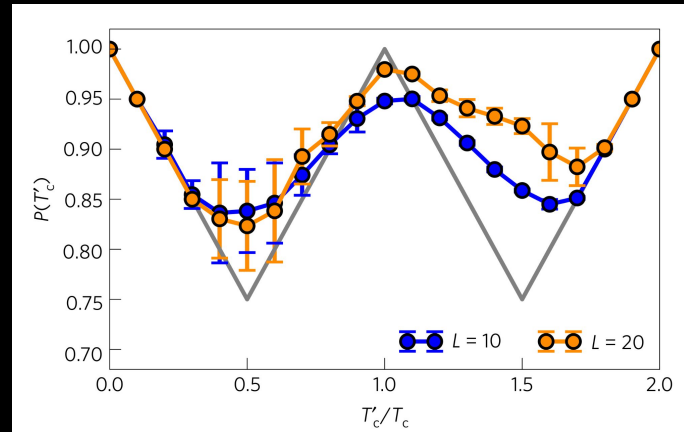
# Minkowski Functionals - V1

# Minkowski Functionals - V1(Normalized)

# Methods - Learning by Confusion (LBC)

- We confuse the machine by milabeling the data around an assumed transition temperature.
- Continuous (2nd order) transitions show high accuracy when the assumed transition temperature is near the real critical temperature.



Using LBC for the the Ising model

Van Nieuwenburg, E. P., Liu, Y. H., & Huber, S. D. (2017). Learning phase transitions by confusion. *Nature Physics*, *13*(5), 435-439.

# Previous Results:
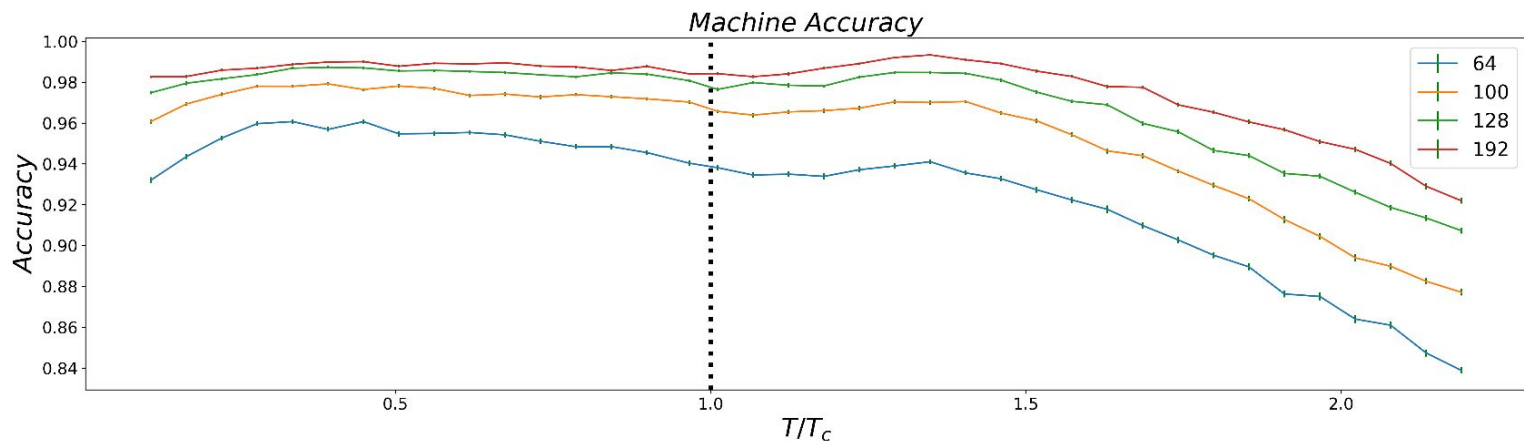
- We trained a K-NN machine using first order minkowski functionals:
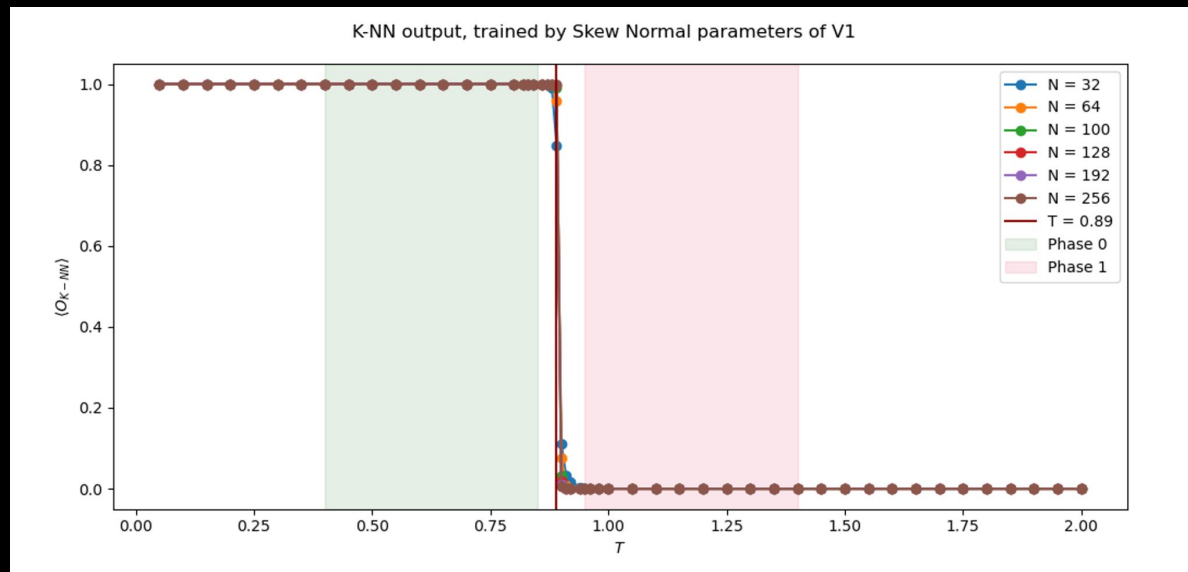
# Previous Results:

- A problem: Different labeling shows wrong transition point.
- To solve this problem, we are going to use LBC.



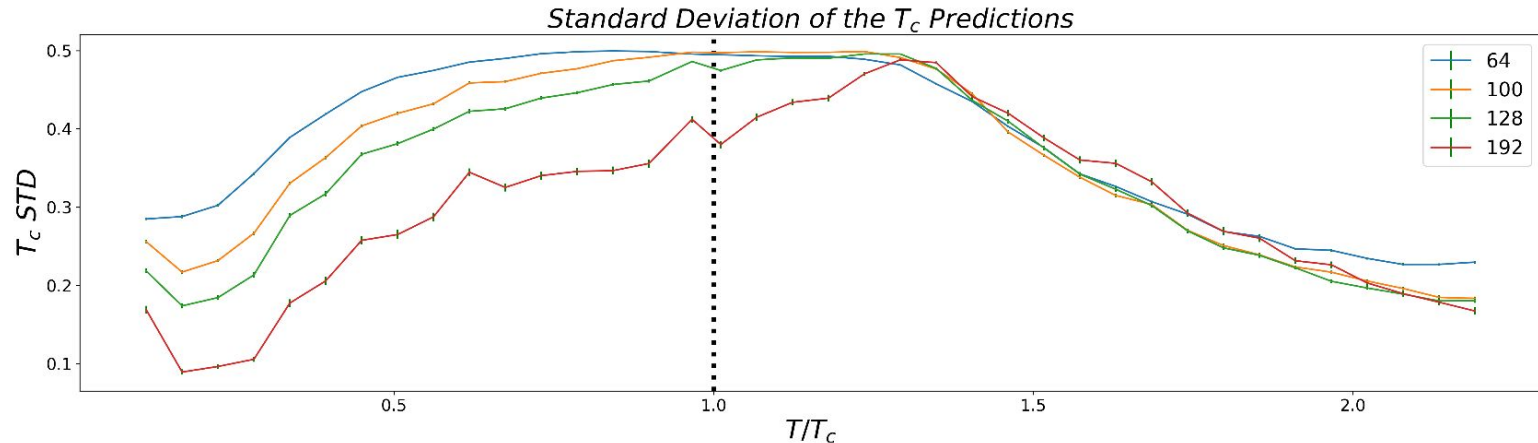K-NN output, trained by Skew Normal parameters of V1

# Results of the LBC:

- Machine accuracy (Performance):

# Results of the LBC:

- Standard deviation of machine prediction on the assumed transition temperature:



Standard Deviation of the $T_c$ Predictions

# Conclusion on the LBC:

- The LBC method works in the matter of BKT transition.

- BKT transition does not show universal W-shaped performance.

- Machine prediction got confused more as it gets near the real transition point but it is not precise as must be.

# Challenges

- Direct analysis of data with large lattice size is not possible with ML models.
- How to calculate our measurement in temperature steps that we did not simulate?
- Can tools like the Minkowski Function replace the raw Lattice itself?
- Considering the lack of prior knowledge about Tc and creating restrictions on the use of supervised models, how do unsupervised methods such as PCA and VAE behave on Potts and XY models?
- In the past unsupervised related works and in the XY model, two direct input methods have been used, using the angular size of the spins or Sin and cos of the spins as a one-dimensional array. Does it help to use Curl of Lattice as pre-processing to calculate Measurement on it?
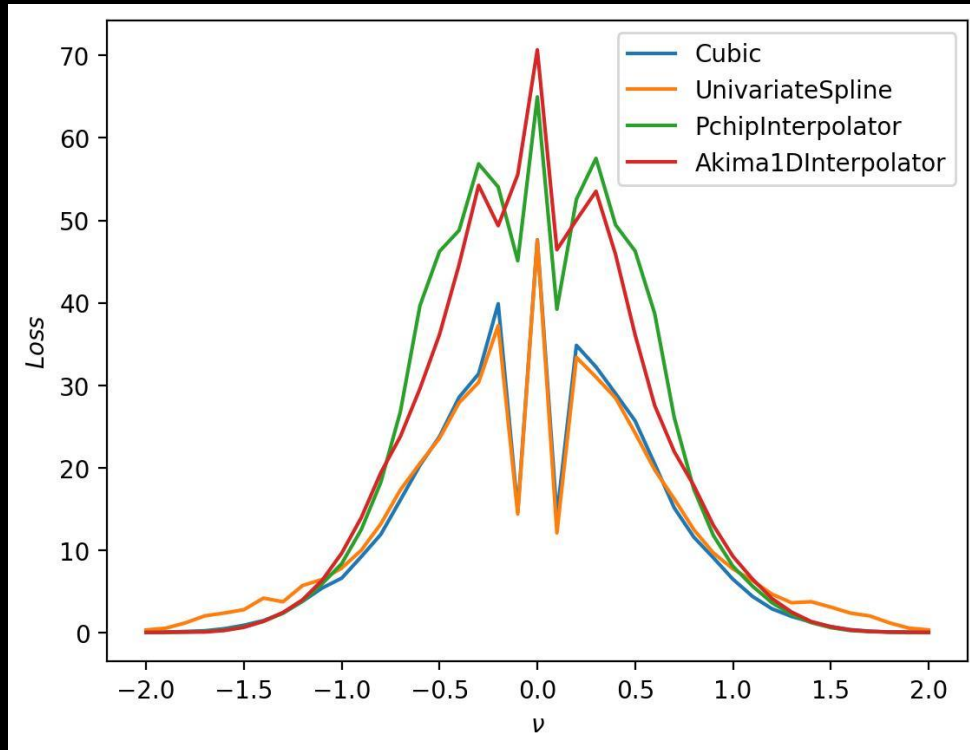
# Method: Interpolation

Interpolation for unavailable  T:

- Simple interpolation: Linear, Cubic, …

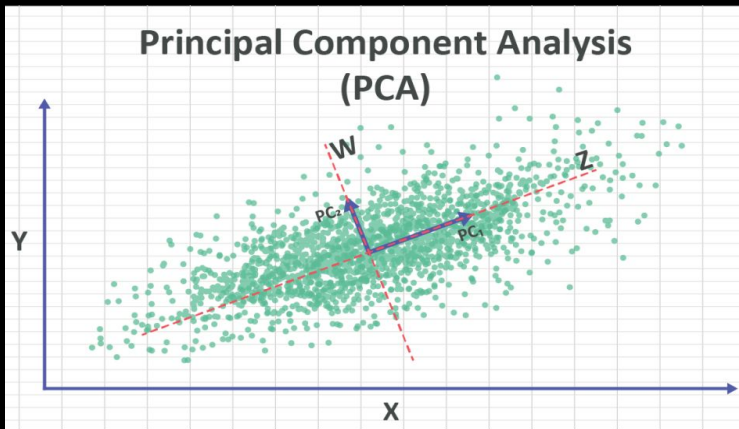- Using Regression ML methods: SVR,LR, GPR, …

- Histogram Reweighting
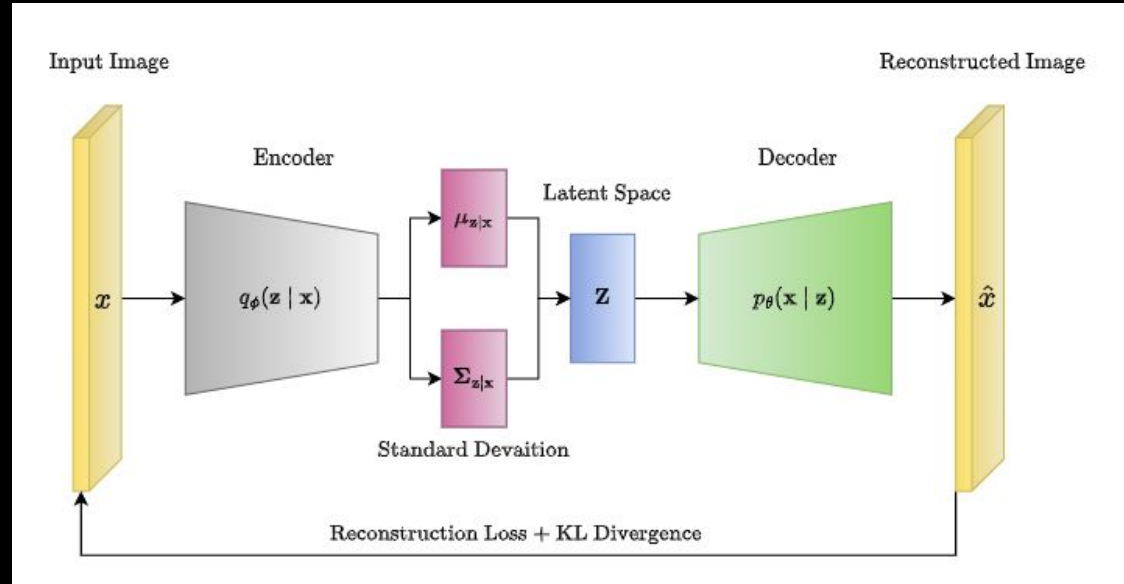
# Result: Interpolation - Cubic
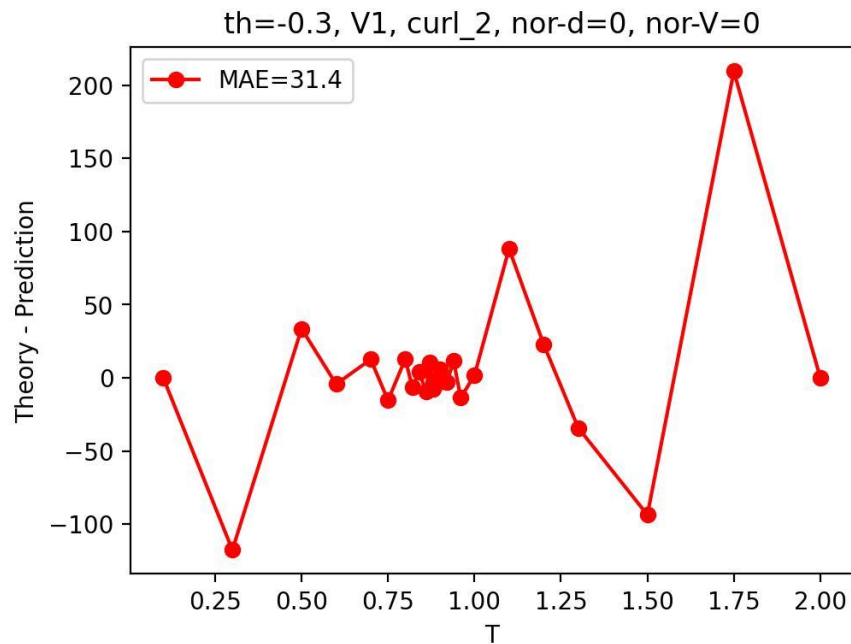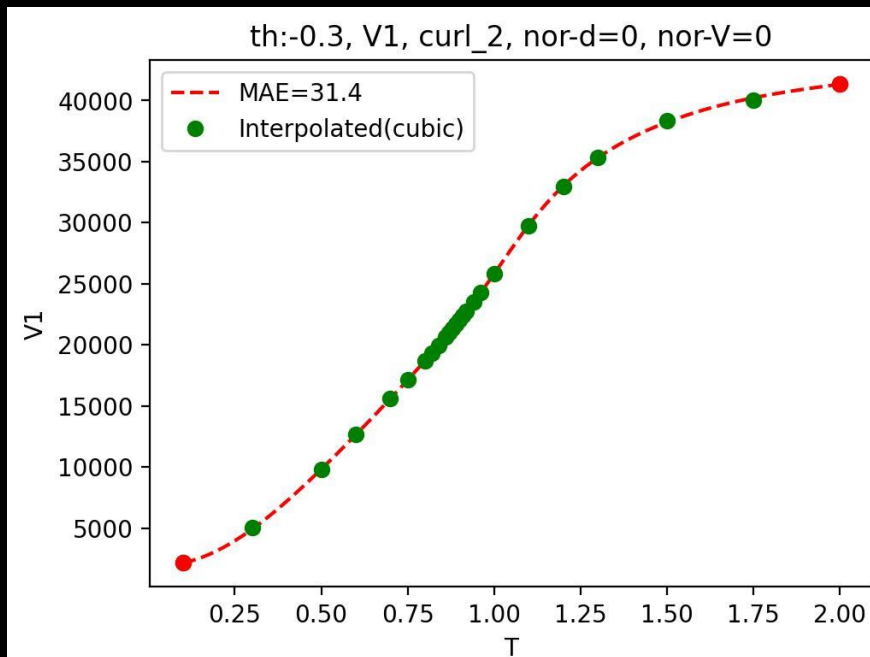
# Result: Interpolation Loss
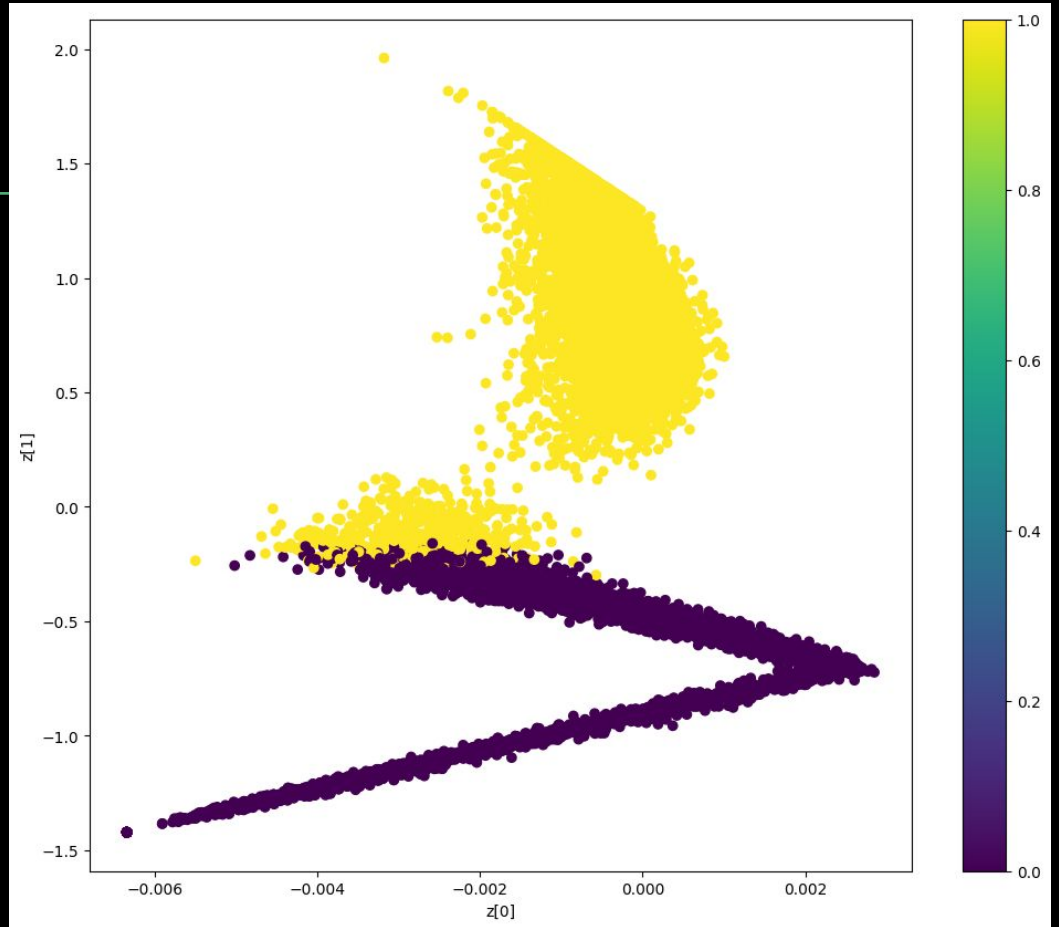
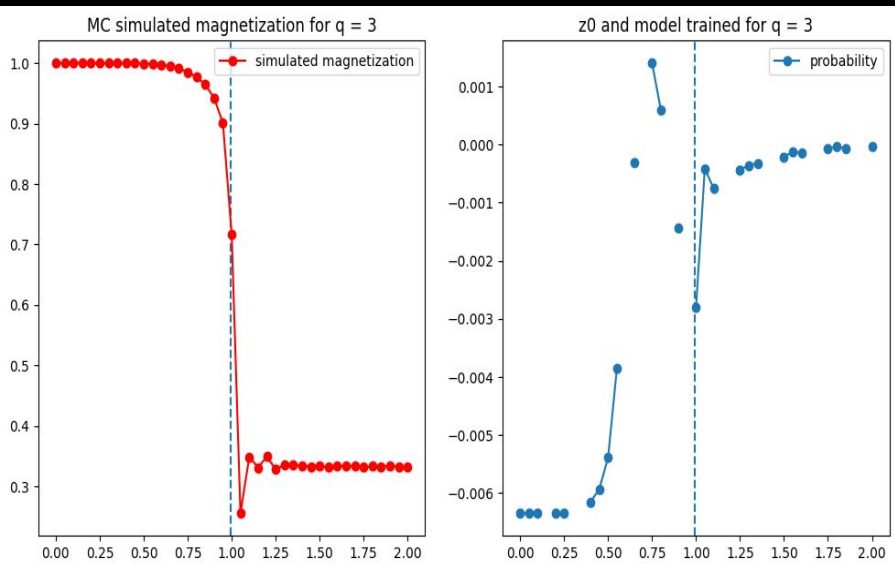# Methods: PCA - VAE



Principal Component Analysis



Variational AutoEncoder

# Result - VAE - Potts

# Methods - VAE - Potts
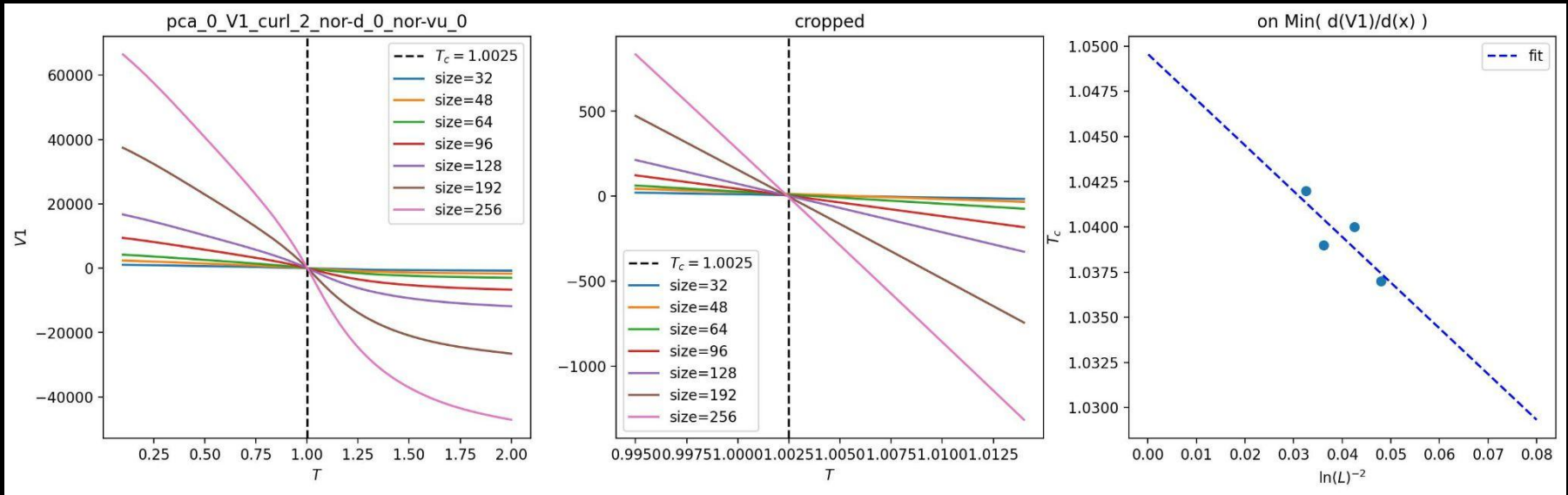


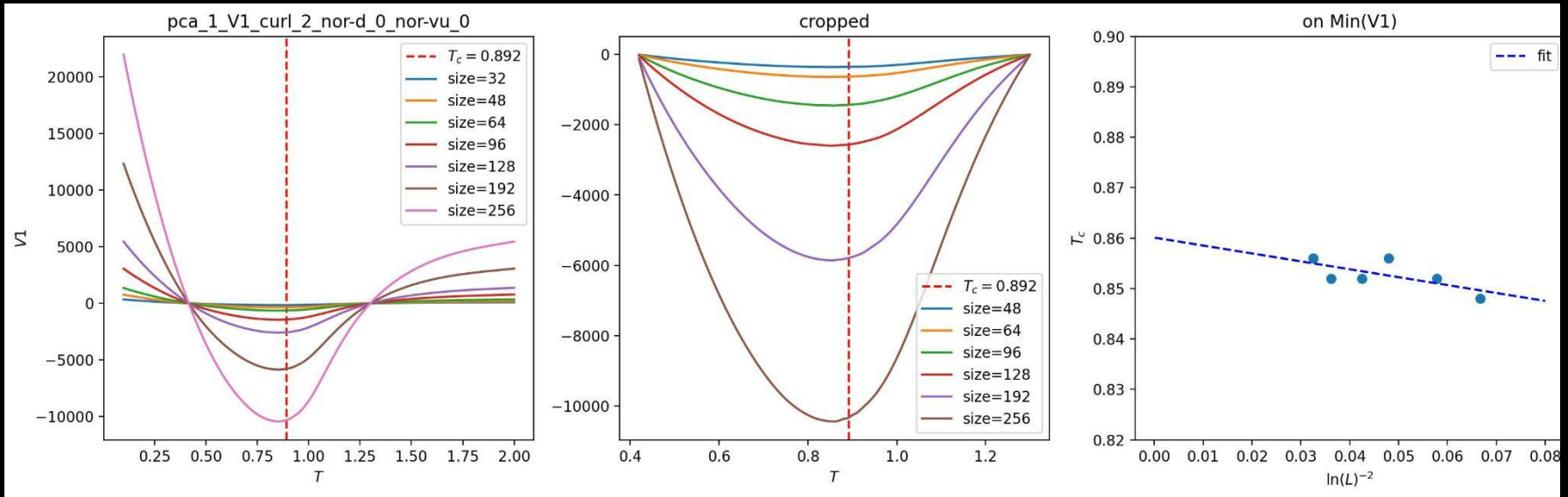z0                                                                z1
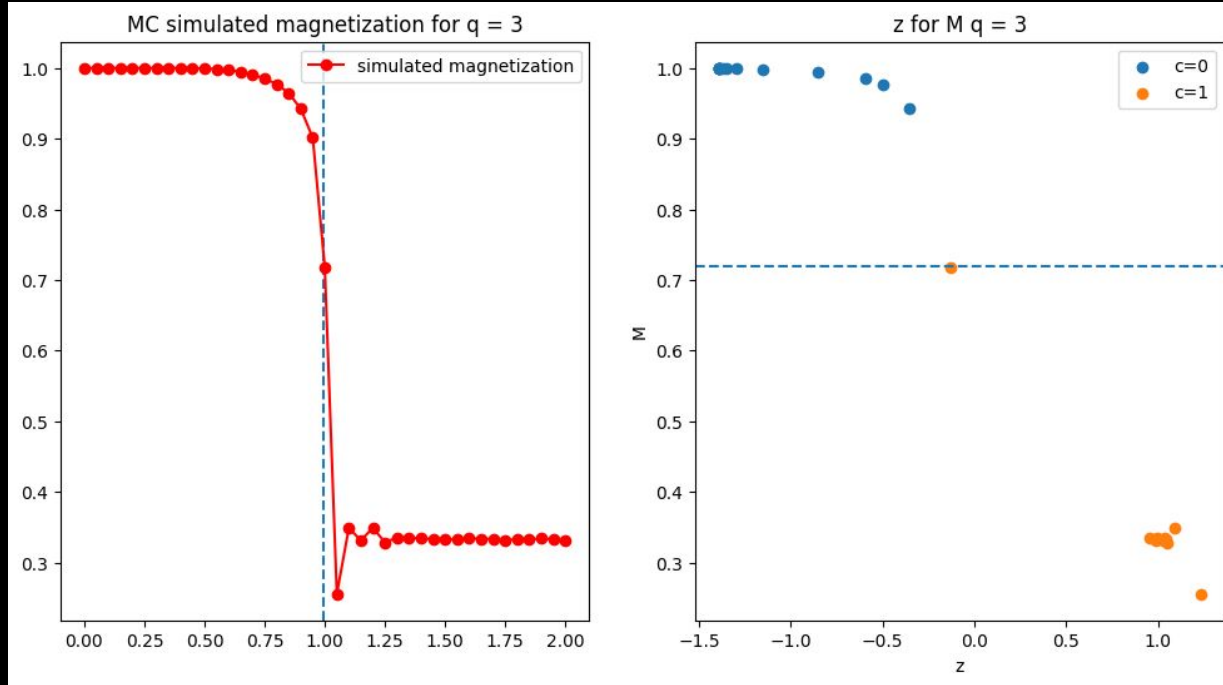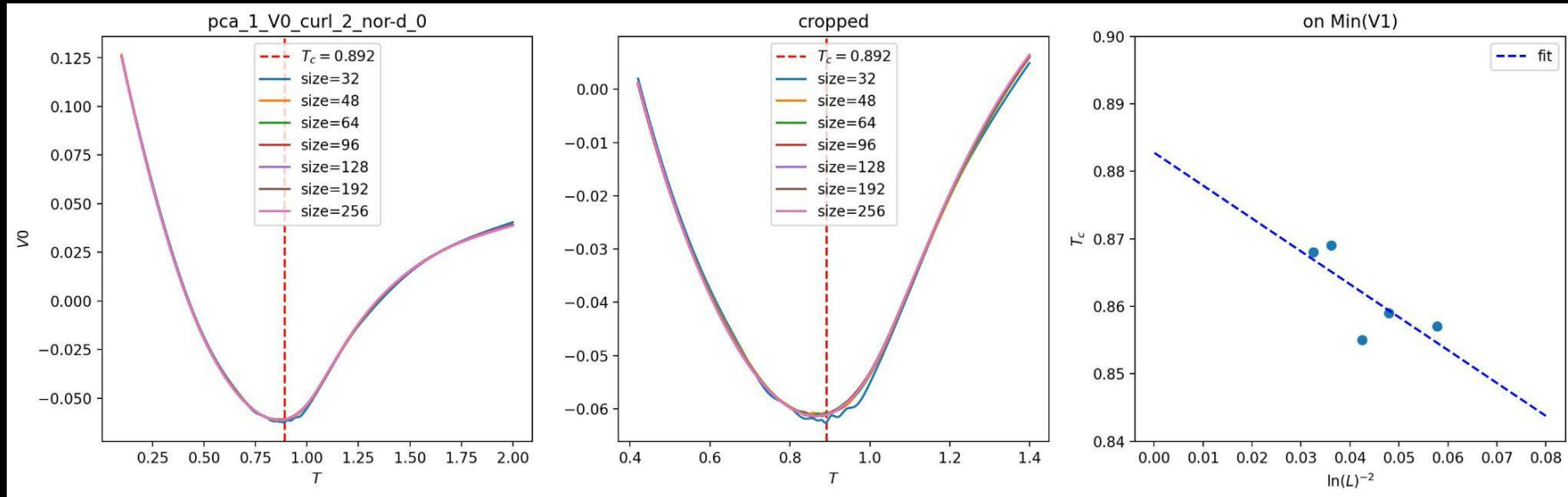
z1 and q=3

# Result: PCA - XY - V1

First Component

# Result: PCA - XY - V1



Second Component

# Result: PCA - XY - V0



Second Component
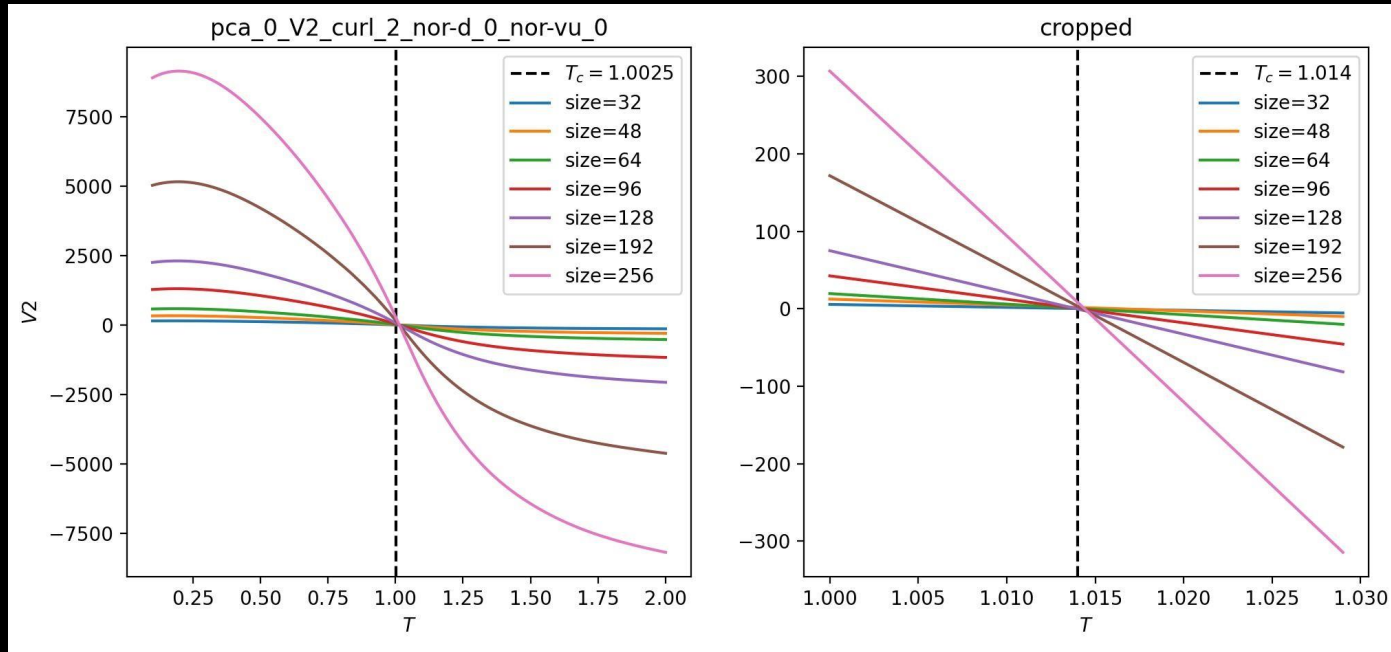
# Result: PCA - XY - V2



First Component

# Result: PCA - XY - V2
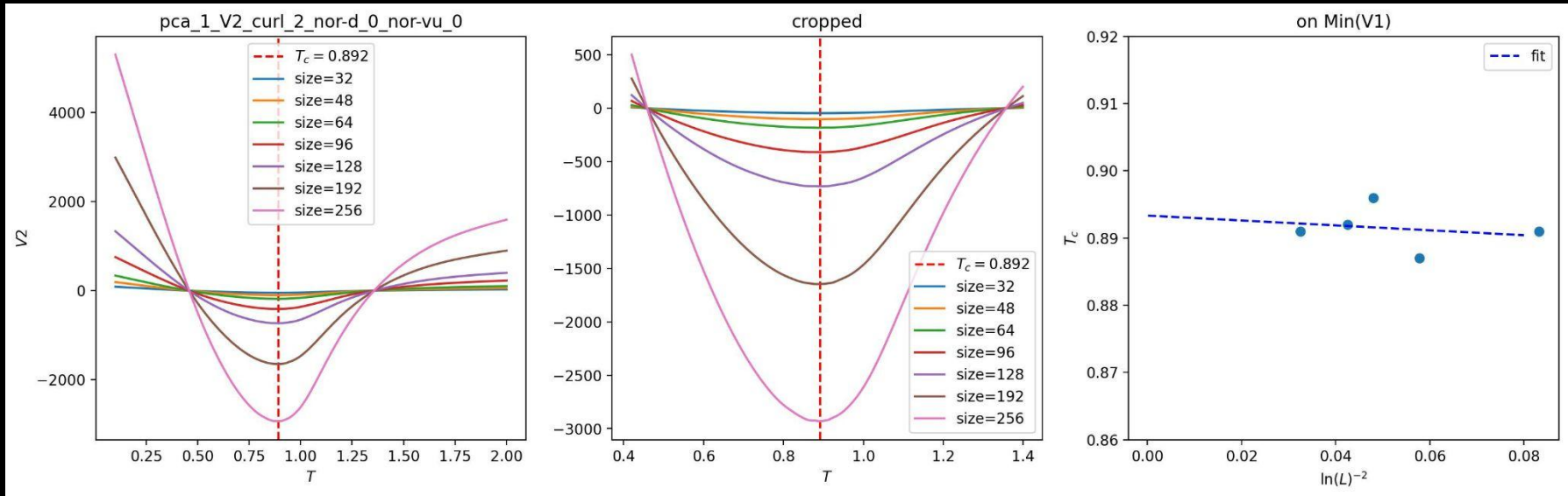


Second Component

# Result: PCA - XY - Normalized V
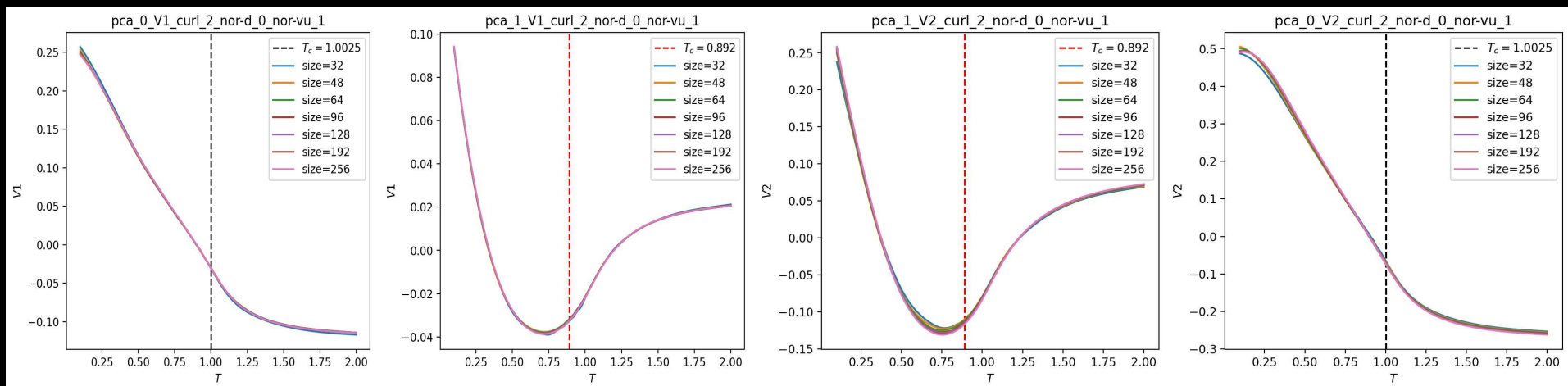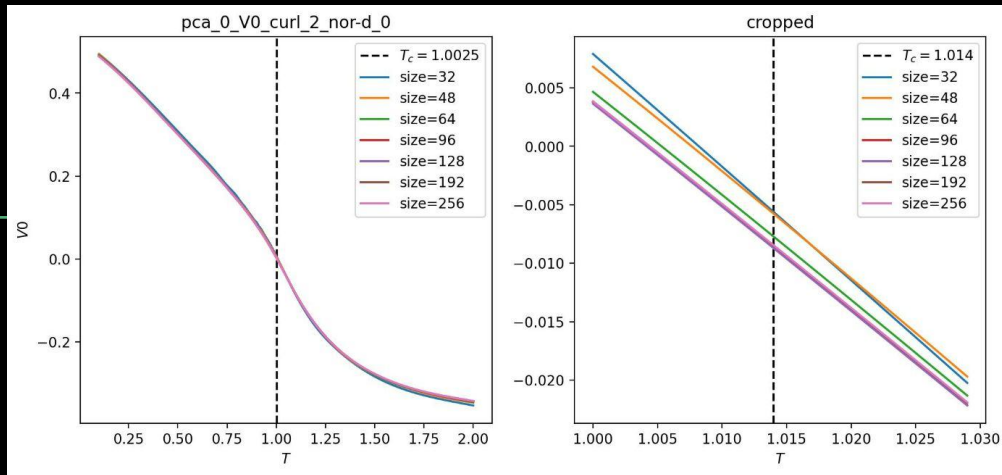
# Future Works



- Improved Result on XY model and report last version in draft of paper
- Using VAE directly on Curl of XY lattice

- Using Semi-Supervised Method and SuperResolution ANN

- Focused MultiFractal Analysis

- Future works for LBC:
  - This method must be examined with different kinds of machine learning algorithms like neural networks.
  - Different types of metrics like TDA can be used instead of Minkowski Functionals to check for the effects of the feature vectors.
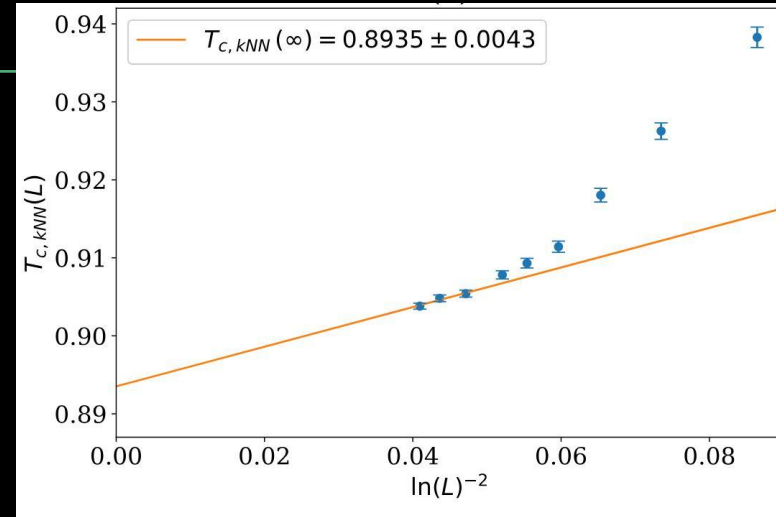
# Khaledi's Gantt Chart

| Activity | Farvardin | Ordibehesht | Khordad | Tir | Mordad | Shahrivar |
|---|---|---|---|---|---|---|
| Early Warning Signals | * | * | | | | |
| Generating Minkowski Functionals with different methods | | * | * | * | | |
| LBC | | | * | * | | |
| Cleaning and regenerating the results | | | | * | * | |
| Paper | | | | * | * | * |

# Yousefzadeh's Gantt Chart

| تابستان۴۰ | بهار۴۰ | زمستان۳۰ | پاييز۳۰ | تابستان۳۰ | بهار۳۰ | زمستان۲۰ | پاييز۲۰ | تابستان۲۰ | فعاليت |
|---|---|---|---|---|---|---|---|---|---|
|  |  |  |  |  |  |  | * | * | تعيين اهداف |
|  |  |  |  |  | * | * | * | * | بررسی NN |
|  |  |  |  |  |  | * | * | * | جمع آوری داده |
|  |  |  |  |  |  | * | * |  | شبیه سازی داده |
|  |  |  |  | * | * | * | * |  | بكارگیری ابزار آماری |
|  |  |  |  | * | * | * |  |  | بكارگیری ابزار توپولوژی |
|  |  |  |  |  | * | * |  |  | بررسی نتایج |
|  |  |  |  | * | * |  |  |  | بهبود نتایج |
|  |  | * | * | * |  |  |  |  | نگارش مقاله |
| * | * |  |  |  |  |  |  |  | نگارش رساله دكتری |

# References

1. Horgan, R. R. Lectures on phase transitions and the renormalization group, 2017.
2. Vogt, Katharina, Höldrich, Robert, Pirrös, David, and Gattringer, Christof. Spin quartets. sonification of the xy model. Georgia Institute of Technology, 2010.
3. Wysin, GM, Pereira, AR, Marques, IA, et al. Extinction of the berezinskii-kosterlitz-Thouless phase transition by nonmagnetic disorder in planar symmetry spin models. Physical Review B, 72(9):094418, 2005.
4. Saberi, Abbas Ali. Recent advances in percolation theory and its applications. Physics Reports, 578:1–32, 2015.
5. Yu, Wei and Lyu, Pin. Unsupervised machine learning of phase transition in percolation. Physica A: Statistical Mechanics and its Applications, 559:125065, 2020.
6. Giannetti, Cinzia, Lucini, Biagio, and Vadacchino, Davide. Machine learning as a universal tool for quantitative investigations of phase transitions. Nuclear Physics B, 944:114639, 2019.

# Thank you!

Question?