Phase transition detection without order parameters

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Final presentation for CS460 project

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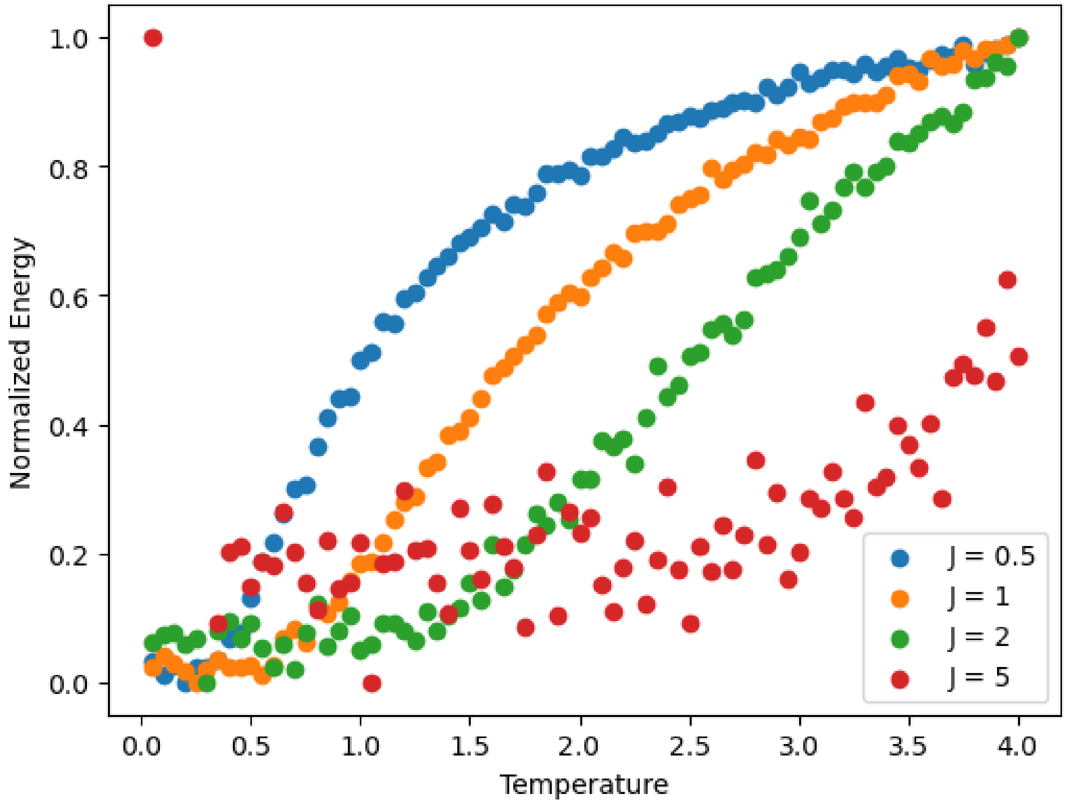
Updates after midway

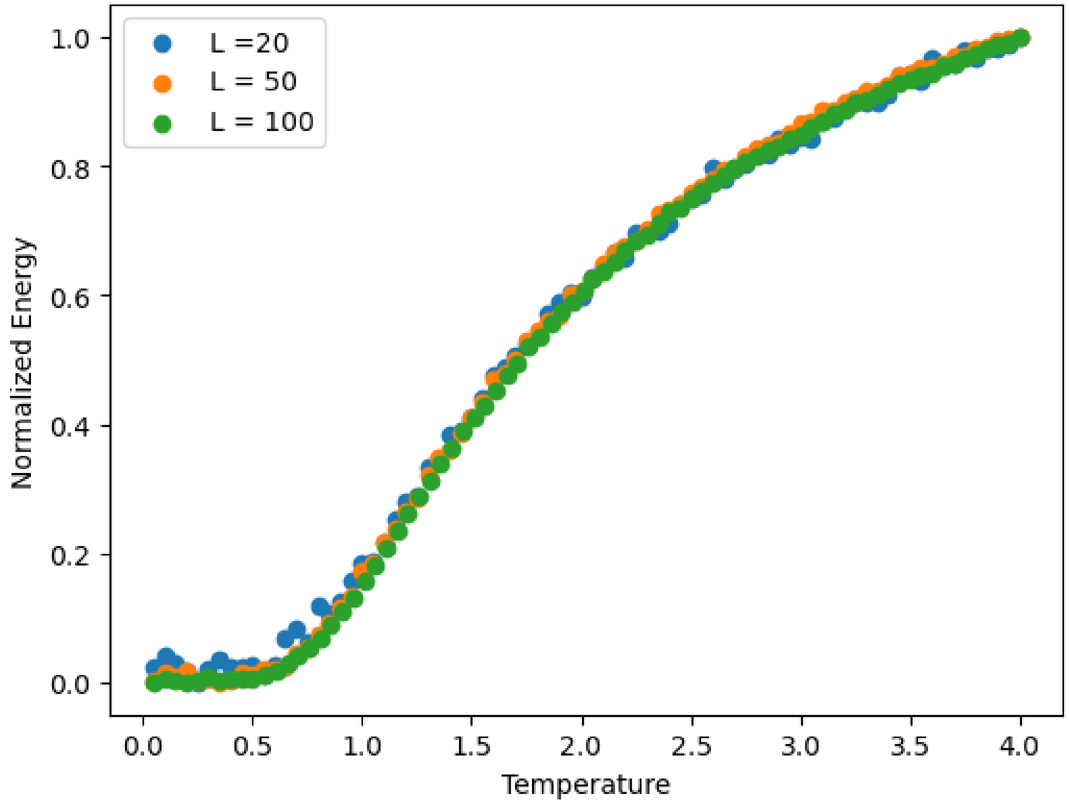
- Tried a regression CNN model with limited success
- Ran the Ising model simulations with multiple coupling constant values and checked how thermodynamic variables vary with temperature for the snapshots – since the critical temperature varies, could not run any models on these datasets
- Ran the Ising model simulations across various lattice sizes – the regression model doesn't directly seem to recognise a phase transition
- Not able to obtain weight matrices (analogous to the order parameter) for each set of simulations while using regression
- Resorted to using testing loss as a new order parameter

New datasets

- In total, 20k snapshots each were produced for 4 different coupling constants (J = 0.5, 1, 2, 5) in case of 20*20 lattices
- 20k snapshots were produced for 20*20, 50*50, and 100*100 lattices
- In these 6 datasets, data was taken from T = 0.05 to T = 4.00
- In order to check if the critical point (T_c) was still present, magnetisation vs temperature and energy vs temperature plots were prepared

New datasets

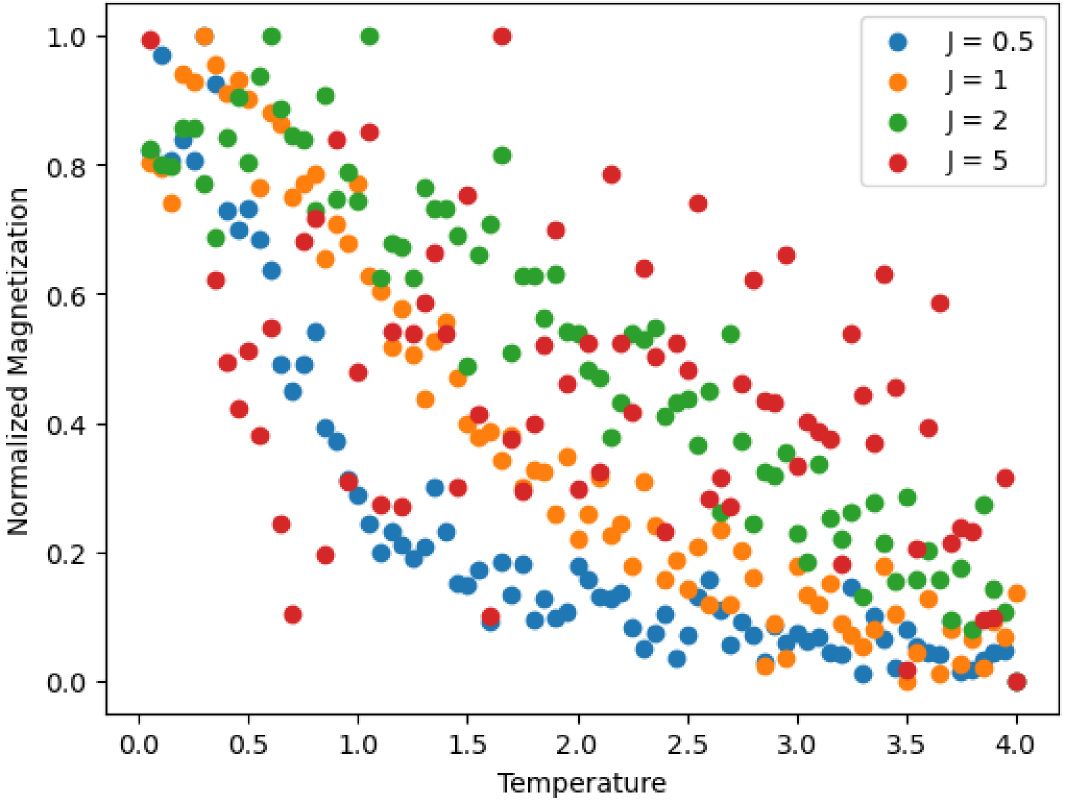




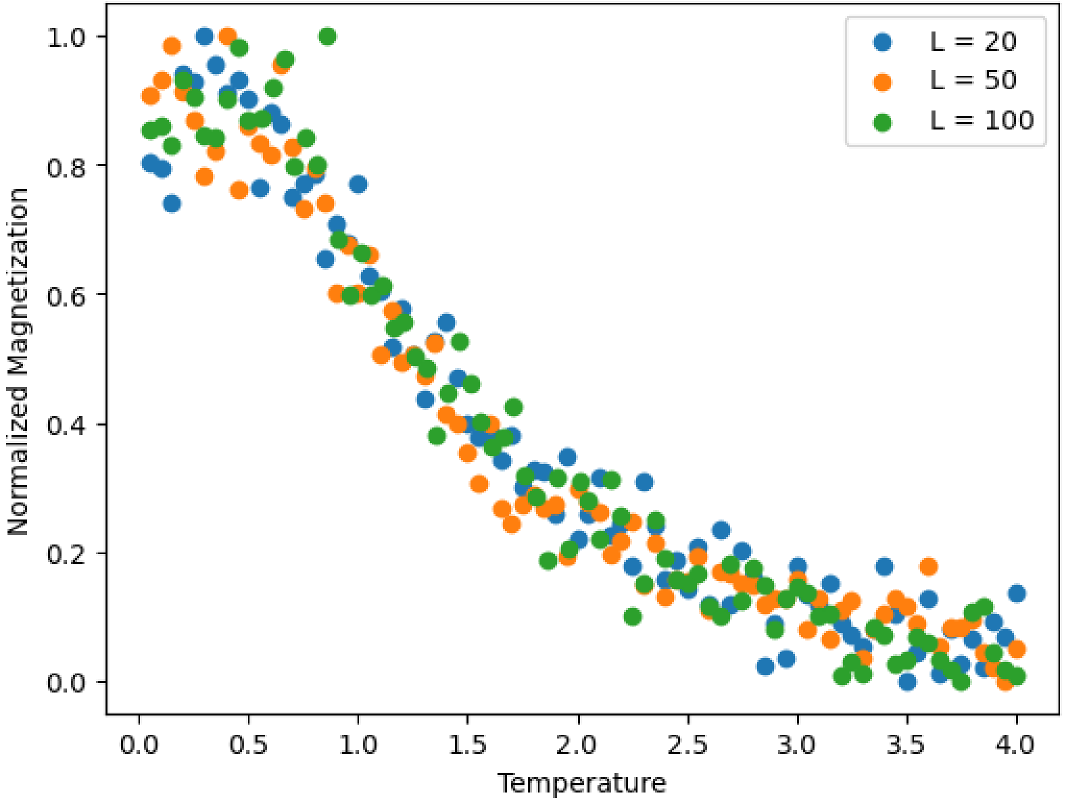
- Normalised energy for simulations at different J's

- Normalised energy for simulations at different L's

New datasets



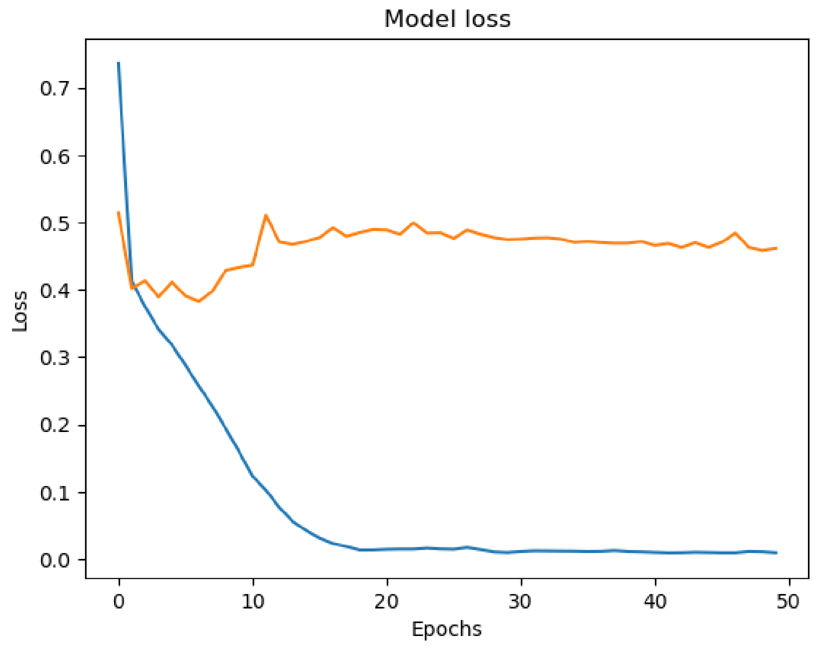
- Normalised magnetisation for simulations at different J's

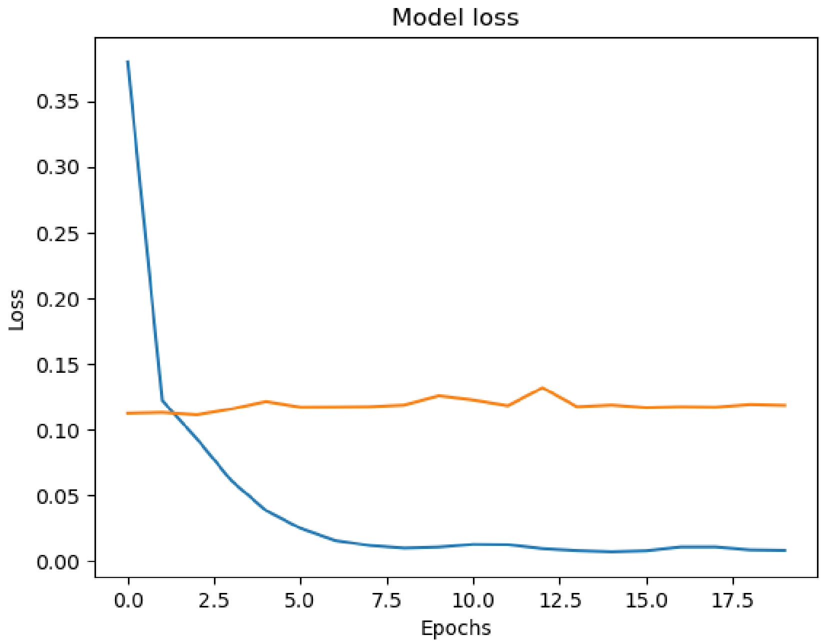


- Normalised magnetisation for simulations at different L's

Regression algorithm

- Our current regression algorithm does not perform very well due to having a rather low number of parameters
- Upper right – loss for training L=20
- Lower right – loss for training L=50
- In the Tanaka (2017) paper, the authors actually performed classification using DenseNet (dividing the dataset using each β (inverse of T) as a class), and then did a best fit of the model weights for the tan hyperbolic function that relates magnetism to temperature



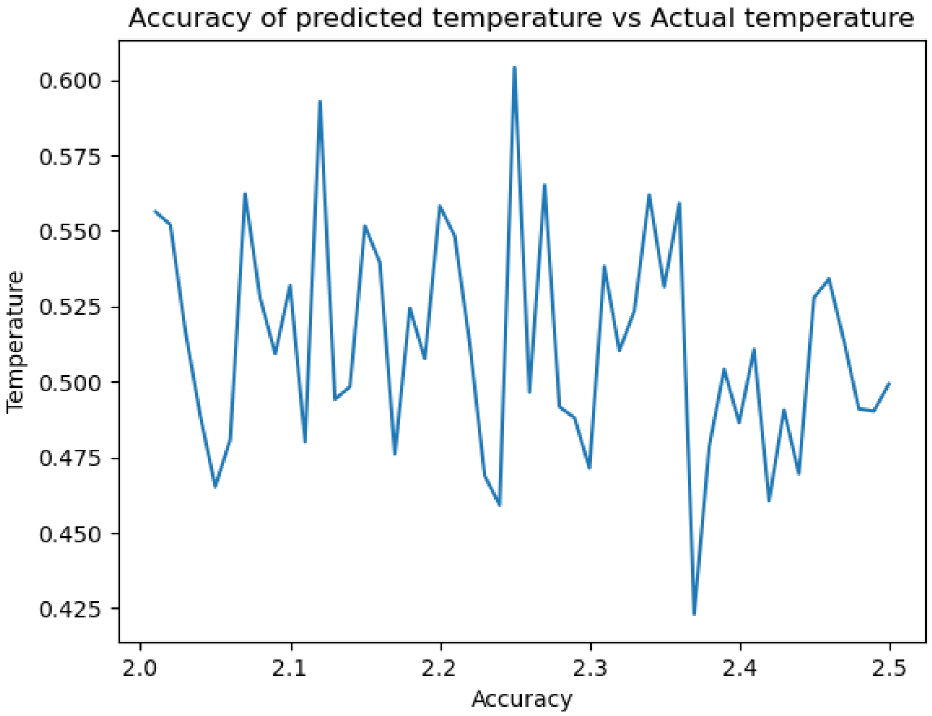


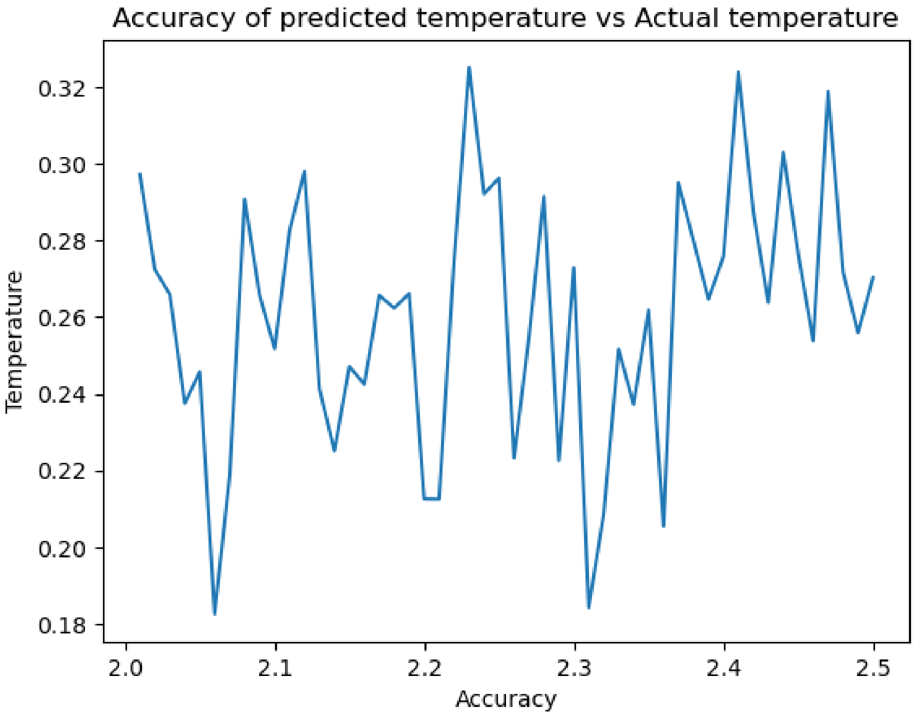
Regression algorithm

- Loss vs epochs is seen to saturate fairly quickly for the model
- Mean absolute error was seen to reach close to the resolution at which the snapshots were taken (0.05) during training, which implies that the algorithm was overfitting
- Another sign of overfitting that we observed – fluctuation in validation loss while training loss continuous to drop

Regression algorithm

- Sequential CNN on both 20*20 and 50*50 datasets
- Not clear where critical point is present





An alternate order parameter

- One can make use of loss as an order parameter
- For the Ising model, it is known that entropy is a derivative of the free energy of the system

$$S = -\partial F / \partial T$$

- Here, the free energy is given as:

$$F = -kTln(Z)$$

where, T is the temperature and Z is the partition function (sum over states)

- It can be shown that:

$$S = k \sum_i \rho_i ln(\rho_i)$$

An alternate order parameter

- In our case, where we make use of the cross-entropy loss function in training our classifier, we have the loss calculated as

$$L_{CE} = \sum_{j=1}^{n} \mathrm{y}_\mathrm{i}^{*} . \log(\mathrm{y}_\mathrm{i})$$

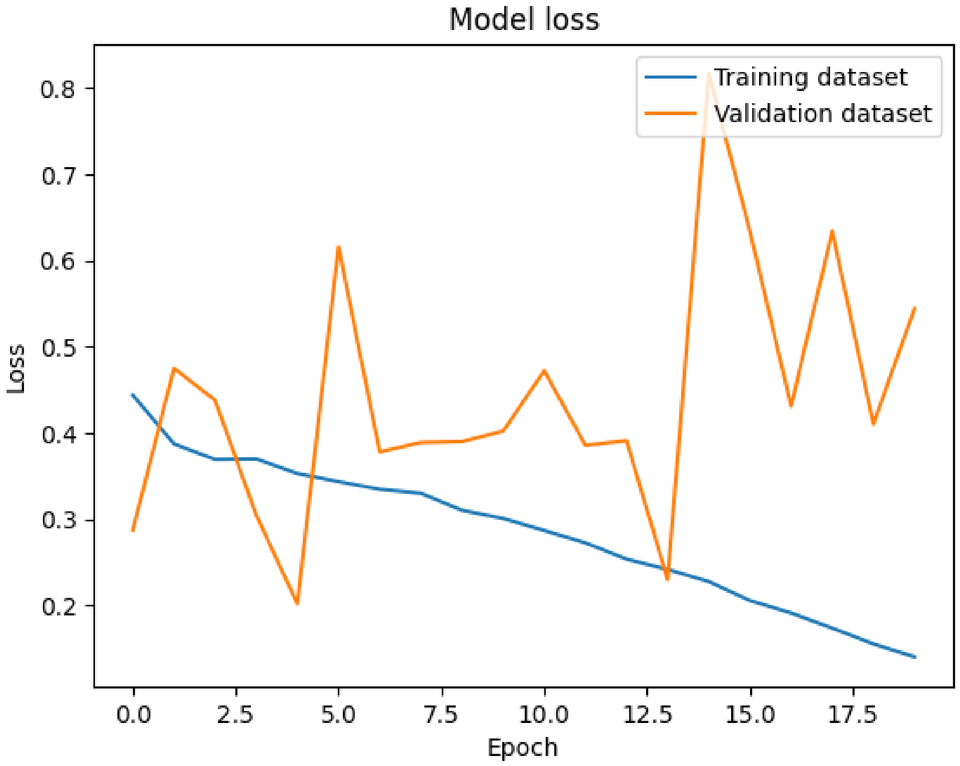
here, y* refers to the true probability distribution

and y refers to the predicted class distribution

- We now examine how the loss varies across the critical point for a test set

Misclassification loss

- For both L=20 (left) and L=50 (right) lattices, we observed that the training loss and accuracy decreased and increased respectively, but the validation trends seem to indicate undertraining

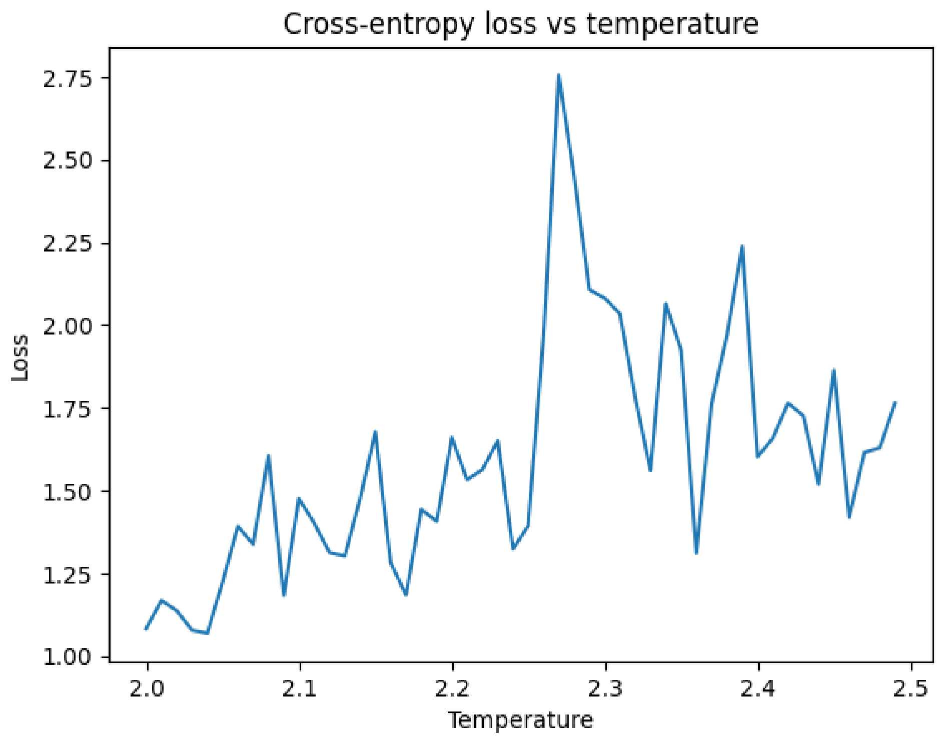


Misclassification loss

- We produced two test sets:
  - For L = 20 : 5k snapshots for T = 2.01 to T = 2.50 with an interval of 0.01, with 100 snapshots for each of the temperatures
  - For L = 50 : 2.5k snapshots for T = 2.01 to T = 2.50 with an interval of 0.01, with 50 snapshots for each of the temperatures
- The model was evaluated for each temperature in this interval to observe the variation in cross-entropy loss with temperature

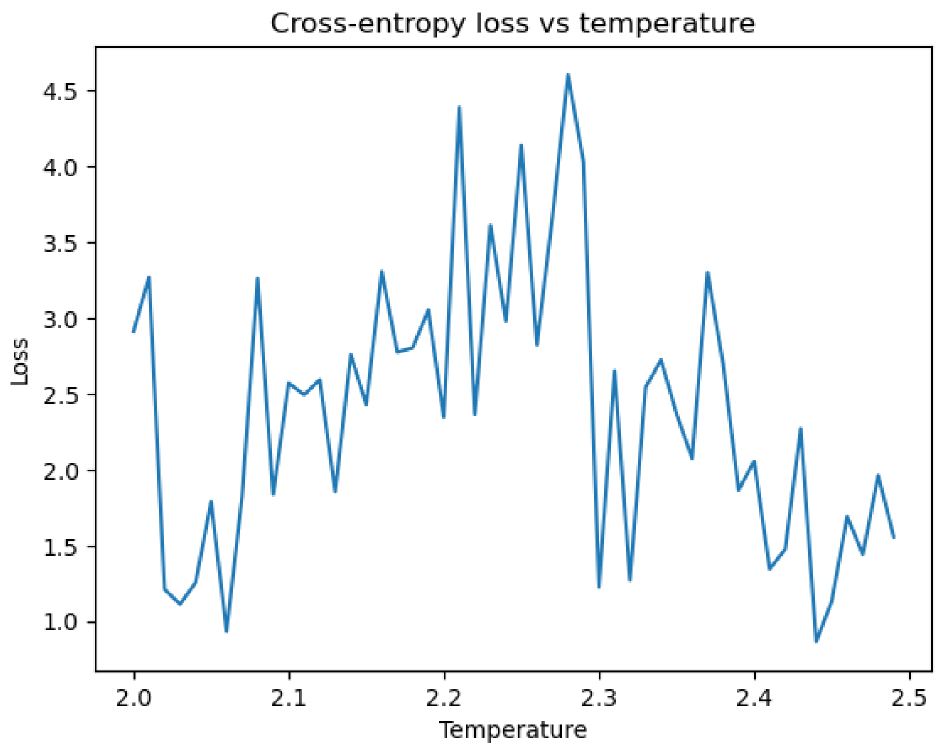
Misclassification loss

- Peaks were observed near the critical point in both the cases
- Qualitatively, it can be said that cross-entropy loss can act as an order parameter



<= L = 20

L = 50 =>



Further plans

- To run the model for larger lattice sizes to confirm that the observed trends in our order parameter can be extended for lattice sizes
- To obtain the weight matrices for various temperatures using a classification algorithm as seen in *Tanaka and Tomiya (2017)* after clearing up bugs faced while running the algorithm
- Repeating the above for multiple lattice sizes and for longer range interactions

Path to publication

- Begegnungszone: Statistical Physics and Machine Learning (2023) : Deadline – May 15 (30 days from today)
- ICCPA 2023 – May 1 (14 days from today)
- ICSPM 2023 – May 1 (14 days from today)

References

- A. Tanaka and A. Tomiya. Detection of Phase Transition via Convolutional Neural Networks. Journal of the Physical Society of Japan, 86(6):063001, June 2017. Publisher: The Physical Society of Japan.