Phase transition detection without order parameters

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Mid-semester follow-up for CS460

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Motivation/Previous works

- Rem et al (2019) showed that CNNs can be used to identify phase transitions in ultracold quantum gases, but they can't necessarily point out phase boundaries accurately. So, what exactly leads a CNN to deduce the presence of a phase transition and consequently, phase boundaries?
- Tanaka and Tomiya (2017) that a CNN could be used to identify the phase transition for the 2d Ising model. Along with this, the used the CNN to come up with a weight matrix that could act in the same way as an order parameter. This weight matrix indicated that a phase transition was in fact occurring at the same temperature as calculated analytically.

Ising model

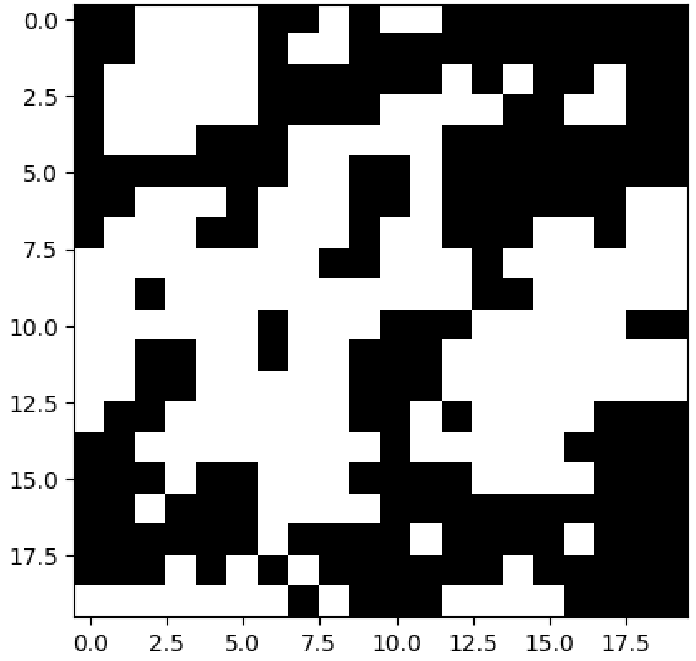
- The Ising model is a toy model used to demonstrate the phenomenon of a phase transition. It demonstrates a 2^{nd} order phase transition
- A phase transition is usually recognised by means of an order parameter (in this case, magnetisation). Above the critical temperature, the model acts as a paramagnet, and below, it acts as a ferromagnet
- However, it's not always feasible or possible to measure the order parameter for a given system (Eg: Bose-Hubbard model, Ultracold gases)
- In the model we are currently interested in, the probability of each spin changing is a function of spins that are the nearest neighbours of a chosen spin (i.e., 4 sites)

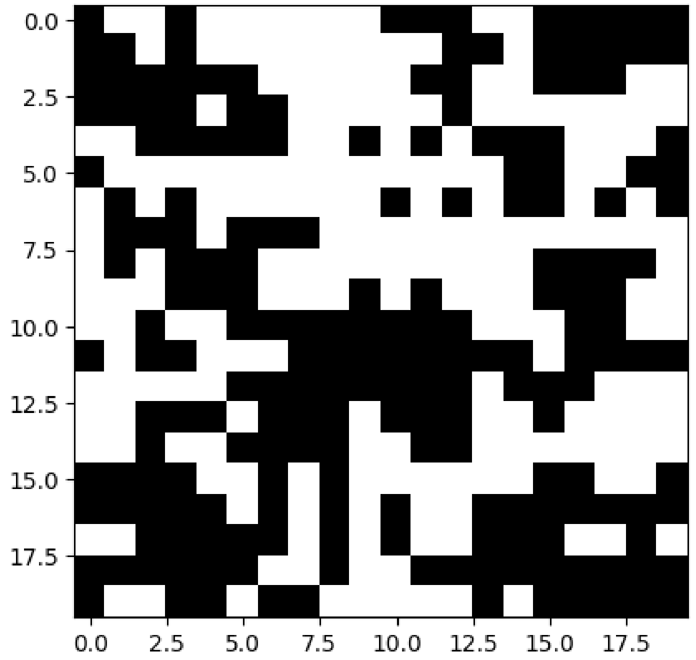
Dataset

- In total, 41k snapshots were produced
- 20k of these were produced below the critical temperature ($T_c \approx 2.27$) between T = 0.05 and T = 1.00. These are snapshots taken in the ordered phase.
- 21k of these were produced above T_c, between T = 3.00 and T = 4.00. These are snapshots taken in the disordered phase.

2d Ising model simulations

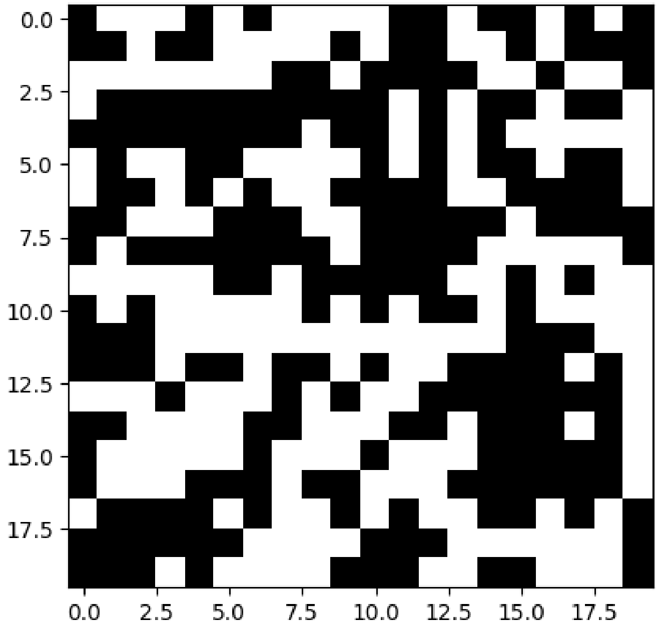
- A few examples out of the dataset we used
- These snapshots were produced using Monte-Carlo simulations
- They can also be produced through other random number-generating algorithms
- On the right – two snapshots taken at T = 0.05 and 1.00 respectively (below T_c)
- For these low temperature cases, in theory, one should be able to see more well-segregated islands in the lattice after the simulation has run for a large amount of time

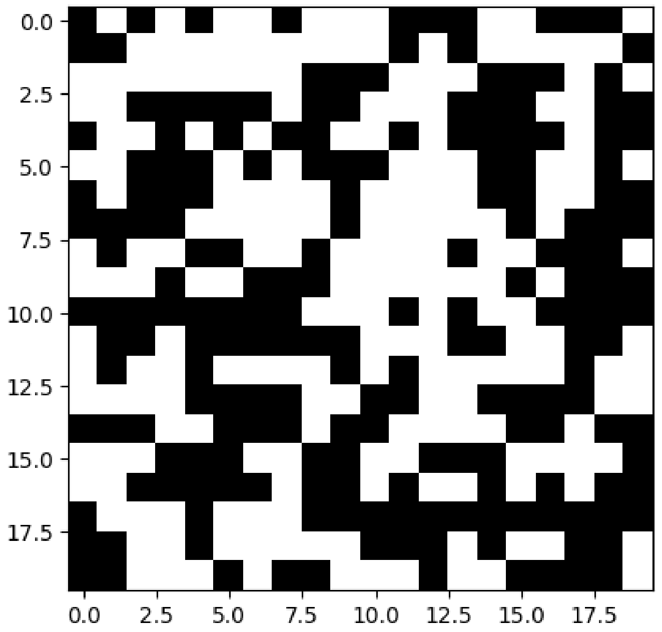




2d Ising model simulations

- For the high temperature cases, no matter how long the simulation has run, disorder tends to dominate
- In this case, we ran our simulations for 1000 steps each
- What you see here is the snapshot after the 1000th step at a given temperature
- On the right – two snapshots taken at T = 3.05 and 4.00 respectively





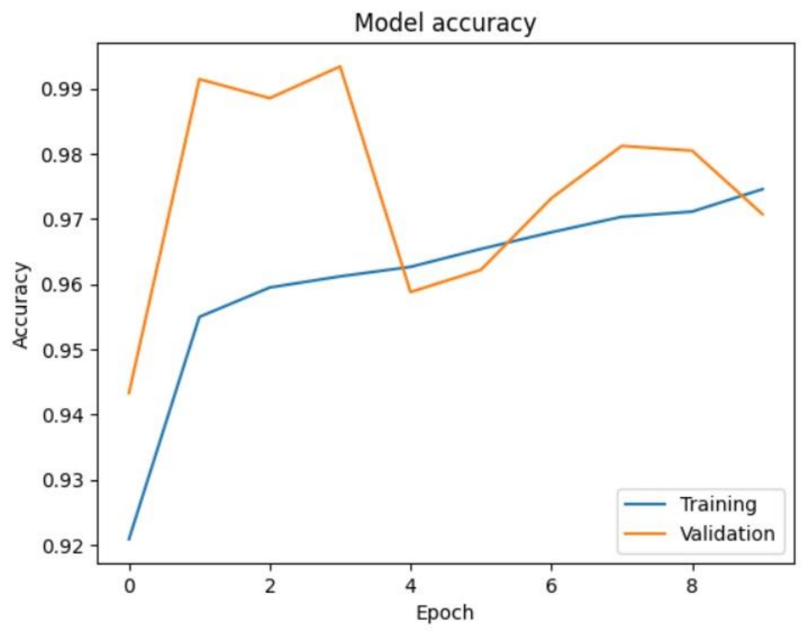
Baseline

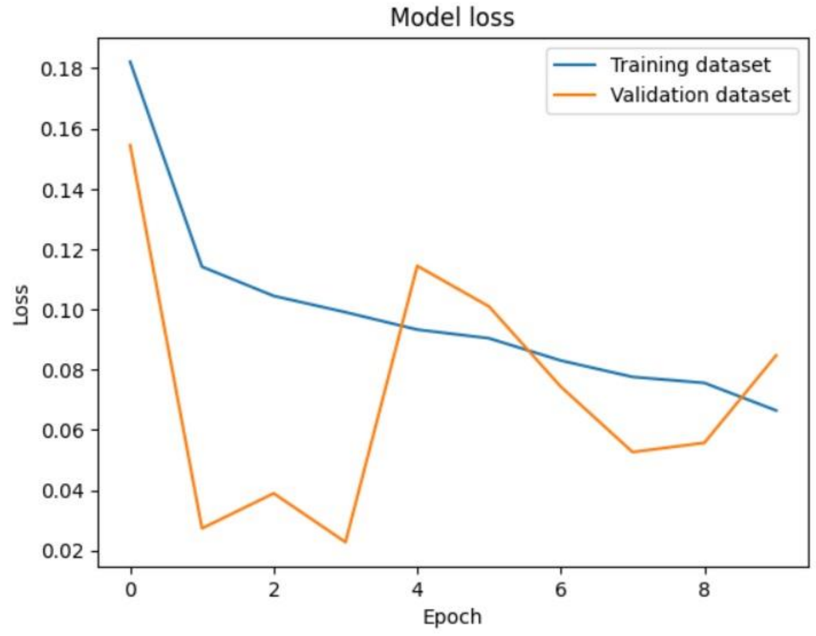
- We trained a sequential CNN on the 41k dataset to distinguish between snapshots taken in ordered and disordered phases
- On the right – layers in our Sequential CNN model

```
In [55]: model.summary()

Model: "sequential_5"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 conv2d_10 (Conv2D)          (None, 18, 18, 32)        320

 max_pooling2d_10 (MaxPoolin  (None, 9, 9, 32)         0
 g2D)

 conv2d_11 (Conv2D)          (None, 7, 7, 64)          18496

 max_pooling2d_11 (MaxPoolin  (None, 3, 3, 64)         0
 g2D)

 flatten_5 (Flatten)         (None, 576)               0

 dense_10 (Dense)            (None, 64)                36928

 dense_11 (Dense)            (None, 1)                 65

=================================================================
Total params: 55,809
Trainable params: 55,809
Non-trainable params: 0
_________________________________________________________________
```

Baseline

- Training accuracy and loss follows a clear trend (increasing and decreasing respectively)
- Final training accuracy was 97.46%
- Final training loss was 0.0665
- However, validation accuracy and loss are not as consistent in terms of showing a trend





Testing

- The baseline model was able to distinguish between ordered and disordered phase snapshots with an accuracy of 100% when tested on snapshots within the temperature ranges the CNN was trained on (50 samples)
- For temperature ranges much closer to T_c, the model was accurate 76% of the time (50 samples)
- For a second order transition, there is a bit of smoothness to the change in magnetisation with respect to temperature, hence the confusion of the algorithm is expected

```
In [9]: # Test the model
test_ordered_files = glob('Under Tc test/*.txt')
test_disordered_files = glob('Above Tc test/*.txt')

test_data = []
for file in test_ordered_files:
    test_data.append(np.loadtxt(file).reshape((20, 20)))
for file in test_disordered_files:
    test_data.append(np.loadtxt(file).reshape((20, 20)))

np_test_data = np.array(test_data)

test_labels = np.concatenate((np.ones(len(test_ordered_files)), np.zeros(len(test_disordered_files))))

test_loss, test_acc = model.evaluate(np_test_data, test_labels, batch_size=10)
print('Test accuracy:', test_acc)

5/5 [==============================] - 0s 2ms/step - loss: 0.0158 - accuracy: 1.0000
Test accuracy: 1.0
```

```
In [10]: # Test the model close to Tc
close_test_ordered_files = glob('Under Tc close test/*.txt')
close_test_disordered_files = glob('Above Tc close test/*.txt')

close_test_data = []
for file in close_test_ordered_files:
    close_test_data.append(np.loadtxt(file).reshape((20, 20)))
for file in close_test_disordered_files:
    close_test_data.append(np.loadtxt(file).reshape((20, 20)))

np_close_test_data = np.array(close_test_data)

close_test_labels = np.concatenate((np.ones(len(close_test_ordered_files)), np.zeros(len(close_test_disordered_files))))

close_test_loss, close_test_acc = model.evaluate(np_close_test_data, close_test_labels, batch_size=10)
print('Test accuracy:', close_test_acc)

5/5 [==============================] - 0s 2ms/step - loss: 0.6683 - accuracy: 0.7600
Test accuracy: 0.7599999904632568
```

Further plans

- To obtain the weight matrix for various temperatures as seen in *Tanaka and Tomiya (2017)*, which essentially acts as an order parameter
- To see the difference in results in case of long-range spin interaction. As per Prof Anamitra (SPS), in such a case, a phase transition is NOT supposed to happen, so a CNN should do poorly
- To see how accuracy of the model varies with lattice size
- To check if equilibrium snapshots can be differentiated from non-equilibrium snapshots for the model
- To run the model for other variations of the Ising model (Eg: the Potts model, triangular matrices, etc)

Work division thus far

- Mihir – Reports
- Ratul – Codes

References

- B. S. Rem, N. Käming, M. Tarnowski, L. Asteria, N. Fläschner, C. Becker, K. Sengstock, and C. Weitenberg. Identifying quantum phase transitions using artificial neural networks on experimental data. Nature Physics, 15(9):917–920, Sept. 2019. Number: 9 Publisher: Nature Publishing Group.
- 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.
- Phase transitions in magnetics - https://www.ibiblio.org/e-notes/Perc/ising.htm