Ising Model for Ferromagnetism

$$E = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i$$

- Spin, σ of each magnetic atom is either 1 (up) or -1 (down)
- Total Energy is controlled by:
  - two bodies interacting strength, *J*
  - external magnetic field strength, *h*
- Value of *J* is system dependent, e.g. lattice structure, species of magnetic atoms, etc.

J.V. Selinger, *Introduction to the Theory of Soft Matter, 2016*

Motivation

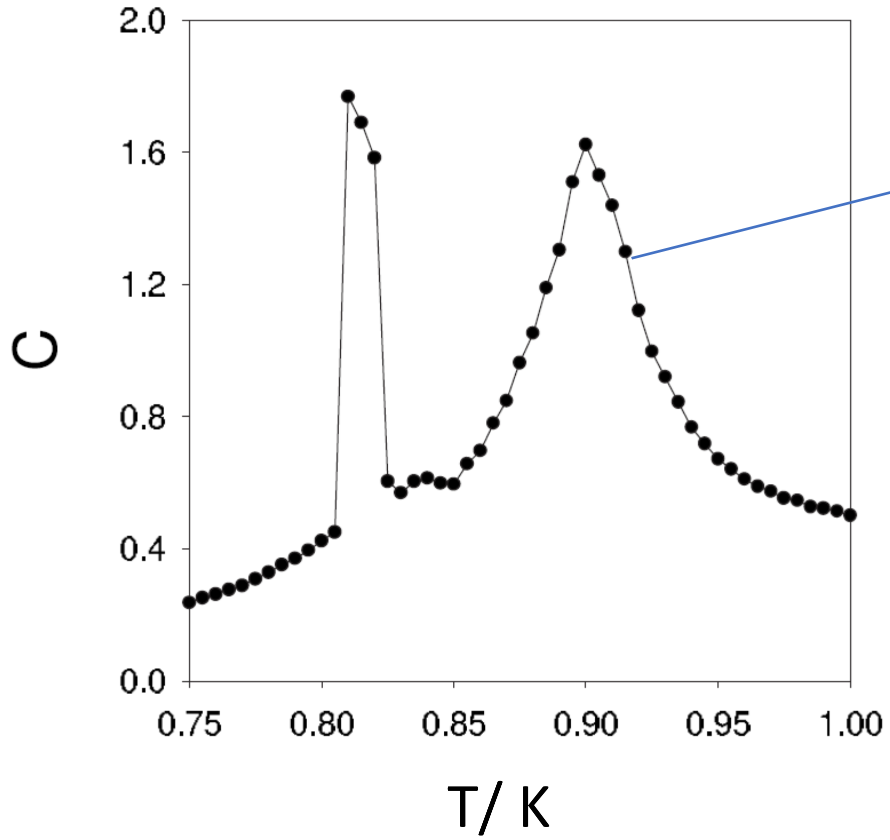
- To determine the temperatures at which magnetic phase transitions happen, e.g. Curie temperature.
- Conventional method (relatively), Monte Carlo simulation (MC) to determine the heat capacity or magnetic susceptibility:

- $$C = \frac{\partial E}{\partial T} = \frac{(\Delta E)^2}{k_b T} = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_b T^2}$$
- $$\chi = \frac{\partial M}{\partial T} = \frac{(\Delta M)^2}{k_b T} = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_b T}$$

J. Kotze*. Introduction to Monte Carlo methods for an Ising Model of a Ferromagnet. ArXiv e-prints, March 2008.*

Motivation

- Conventional method can be time consuming, e.g.



At each T, 10^4 steps (thermalization) + 10^5 steps (calculate heat capacity)

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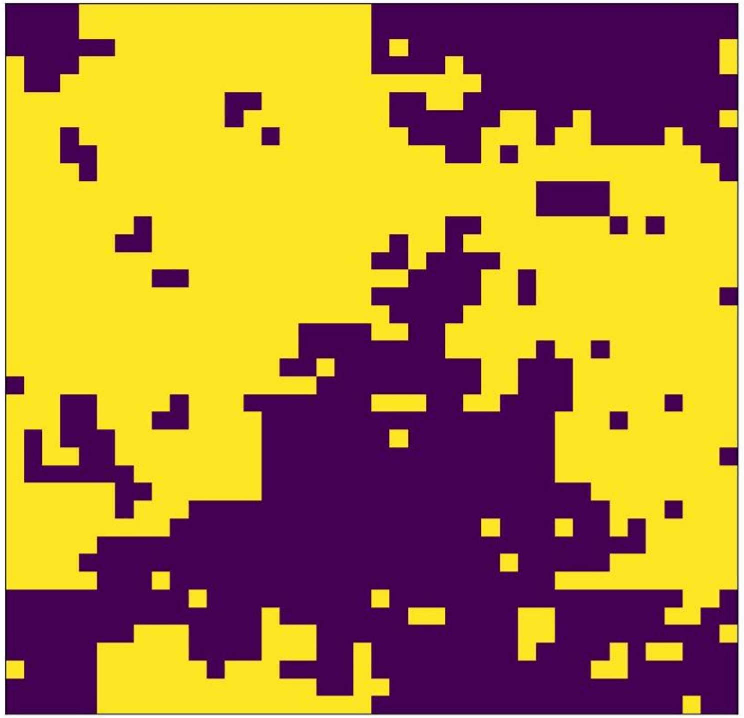
- AI may require only 10^4 steps for thermalization + classification

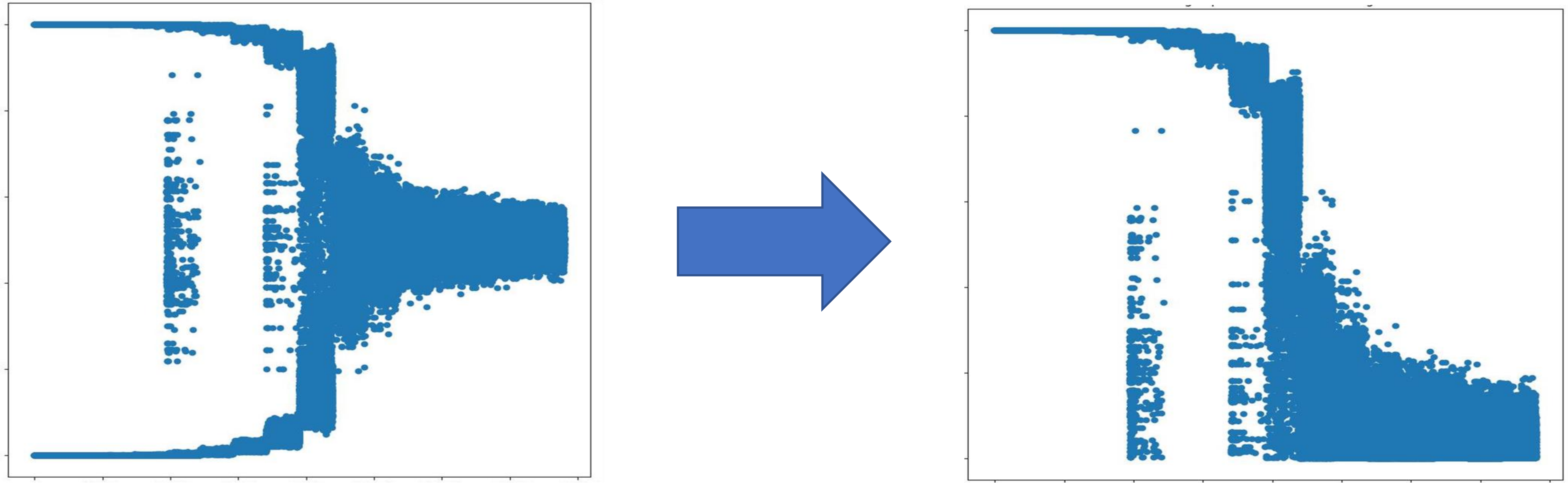
Data Structure/ Visualization

- 156000 training images + 4000 testing images
- Each image = 40 x 40 pixel corresponding to spin up & down, e.g.



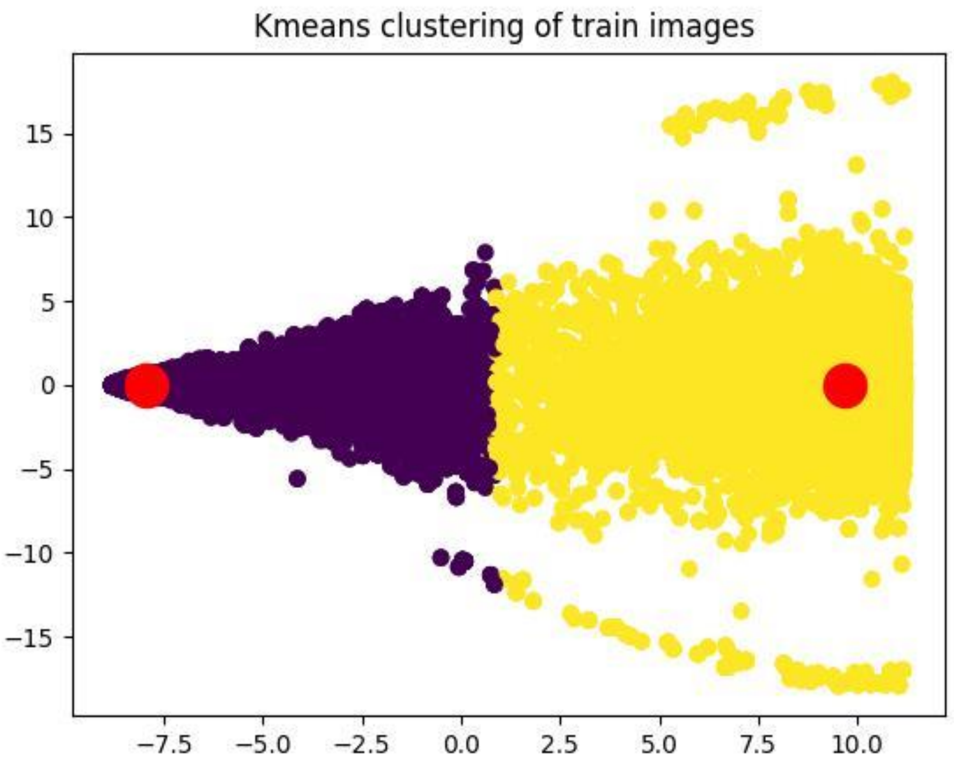
Data Structure/ Visualization

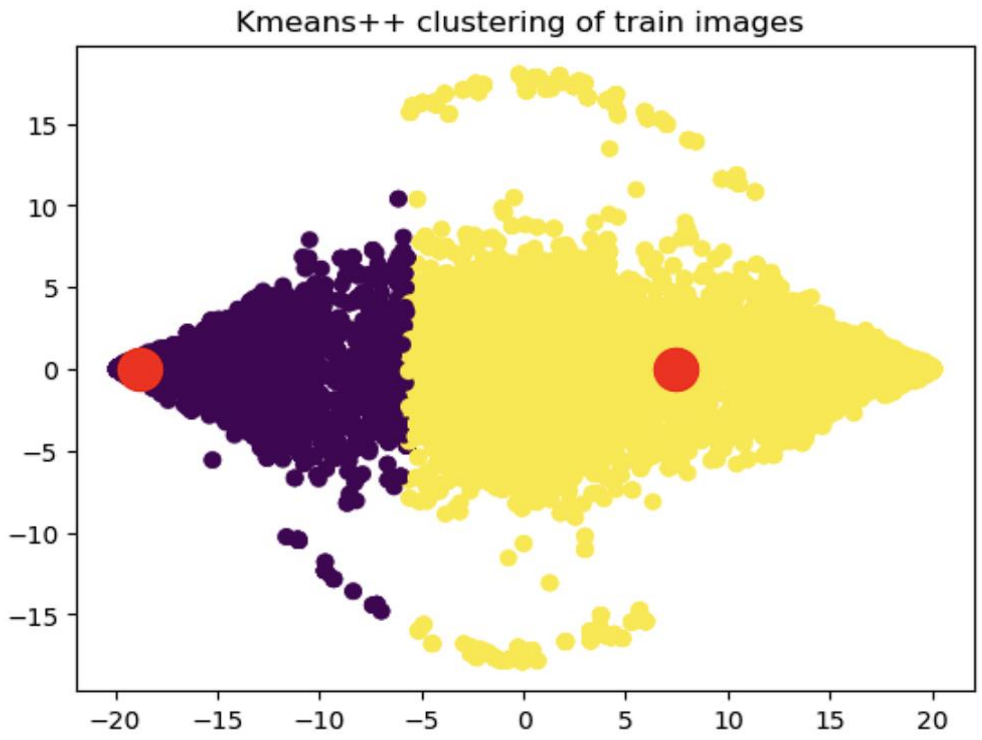
- Standardization: majority spins → 1; minority spins → 0
- Average magnetization vs index of training image:

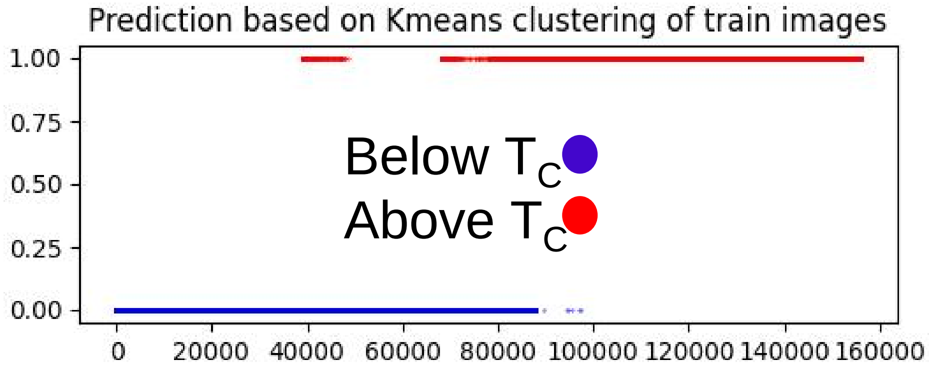


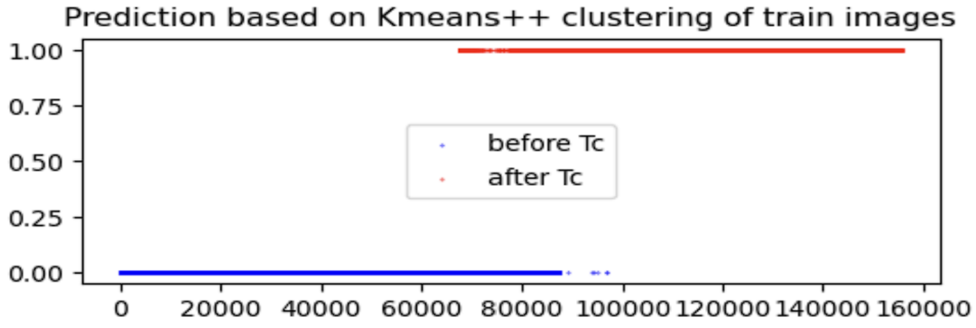
- Indexes of training images are arranged in the order of increasing temperature

Clustering (Kmeans & Kmeans++)

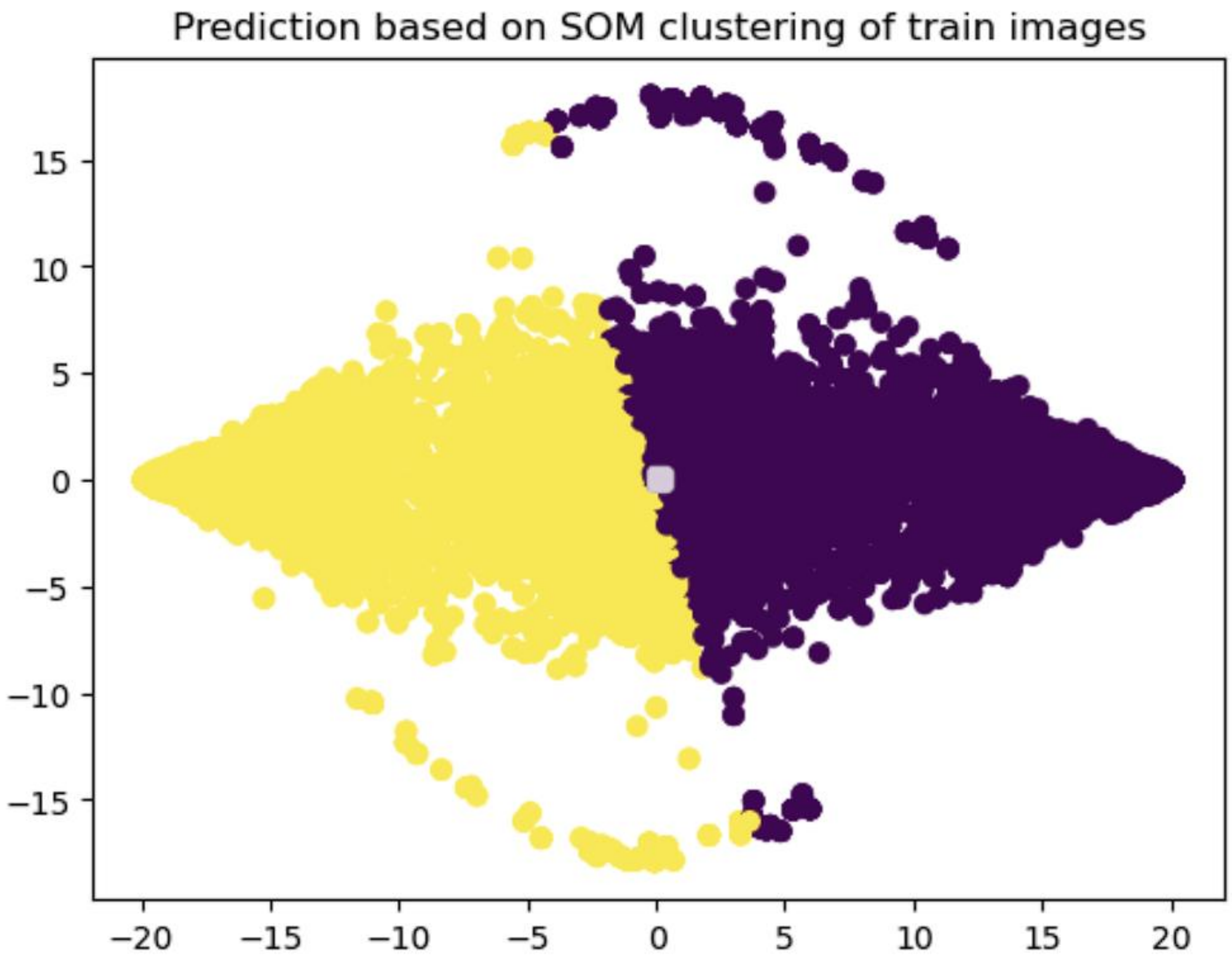








Clustering (SOM)



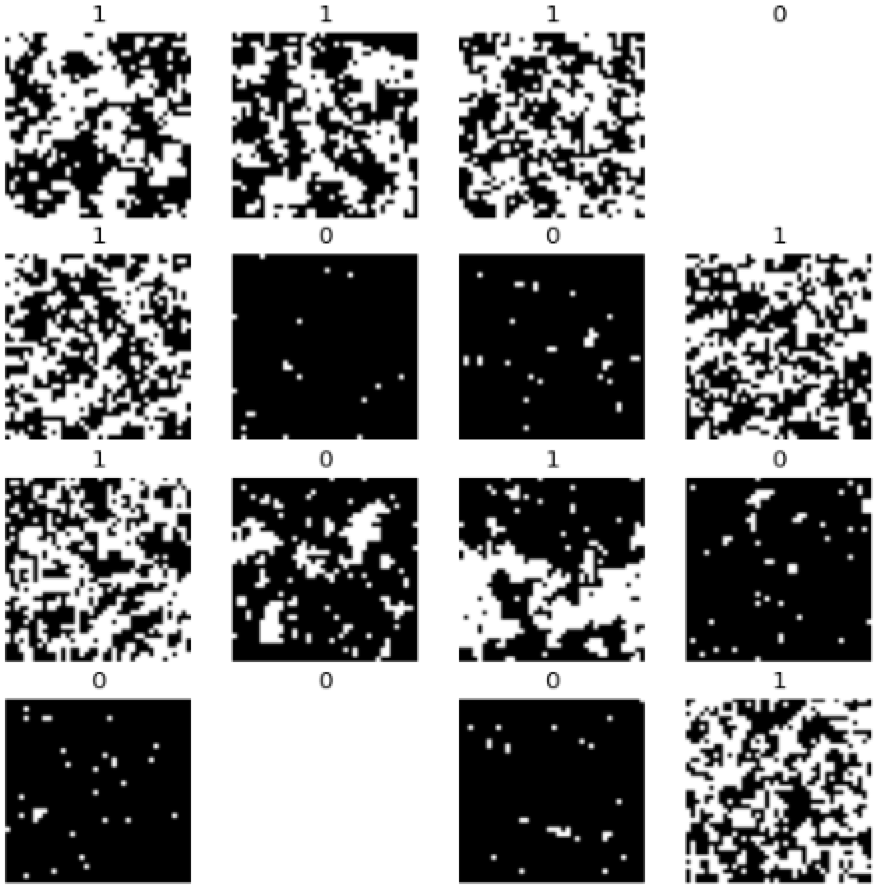
CNN Model

In this case we found that using the 2 labels of [1 0] and [0 1] for below and above the critical temperature (equivalent to 0 and 1) served to have a good accuracy when using a CNN to analyze the images with the labels determined from the K-means clustering.

```
Shape of Training images set (99840, 40, 40)
Shape of Validation images set (99840, 2)
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 reshape (Reshape)           (None, 40, 40, 1)         0

 conv2d (Conv2D)             (None, 36, 36, 16)        416

 max_pooling2d (MaxPooling2D  (None, 18, 18, 16)       0
 )

 flatten (Flatten)           (None, 5184)              0

 dense (Dense)               (None, 2)                 10370

=================================================================
Total params: 10,786
Trainable params: 10,786
Non-trainable params: 0
_________________________________________________________________
```

CNN Prediction

Predicted labels for the images in the testing dataset are 1 for the disordered state and 0 for the ordered state corresponding to above and below Tc respectively.

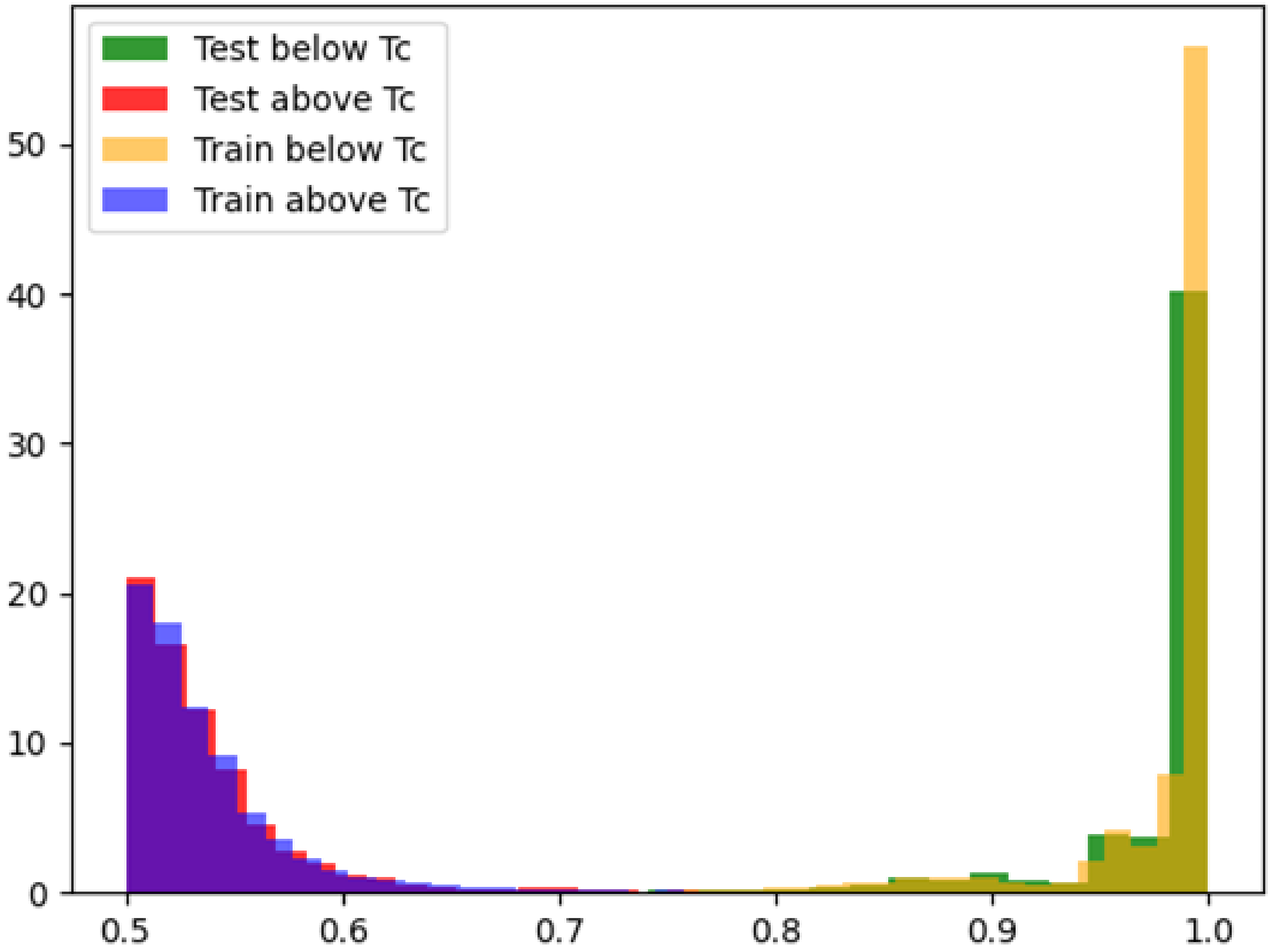


CNN Model (Transfer Learning)

- Employs the pre-trained MobileNetV2 model to capture image characteristics.
- Includes fully connected layers for high-level feature learning.
- Applies dropout layers to prevent overfitting and enhance model robustness.

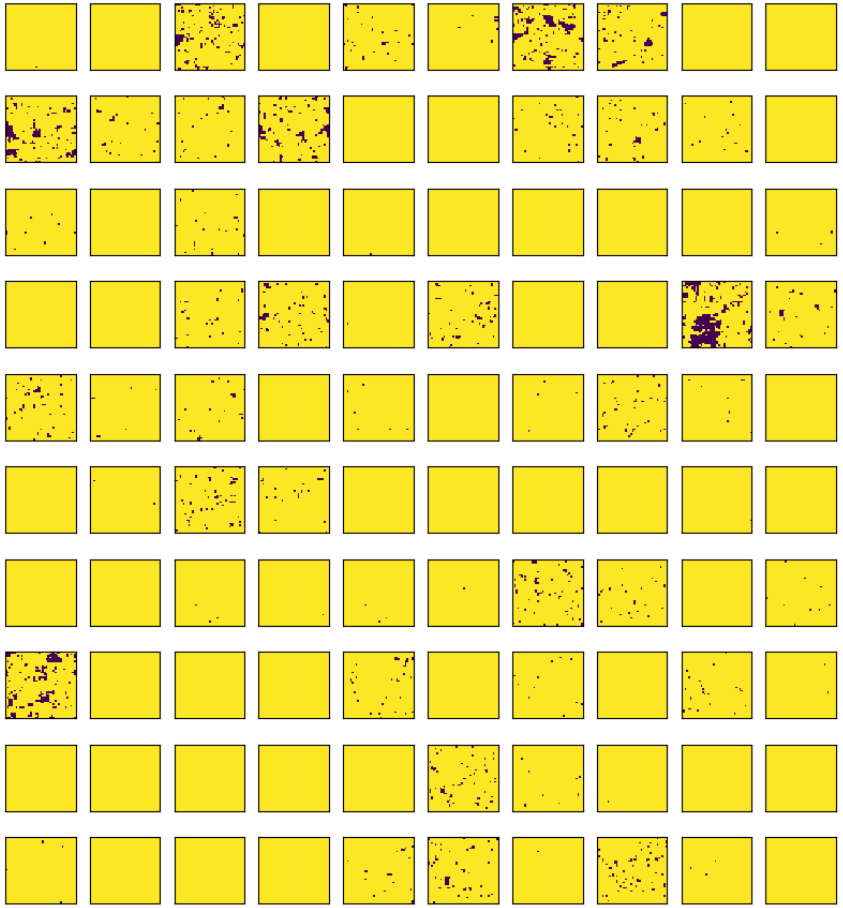
```
Model: "sequential_10"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 mobilenetv2_1.00_224 (Funct  (None, 2, 2, 1280)       2257984
 ional)

 flatten_10 (Flatten)        (None, 5120)              0

 dense_40 (Dense)            (None, 1024)              5243904

 dropout_18 (Dropout)        (None, 1024)              0

 dense_41 (Dense)            (None, 512)               524800

 dropout_19 (Dropout)        (None, 512)               0

 dense_42 (Dense)            (None, 64)                32832

 dense_43 (Dense)            (None, 2)                 130

=================================================================
Total params: 8,059,650
Trainable params: 5,801,666
Non-trainable params: 2,257,984
_________________________________________________________________
```

Results of CNN (Histogram)

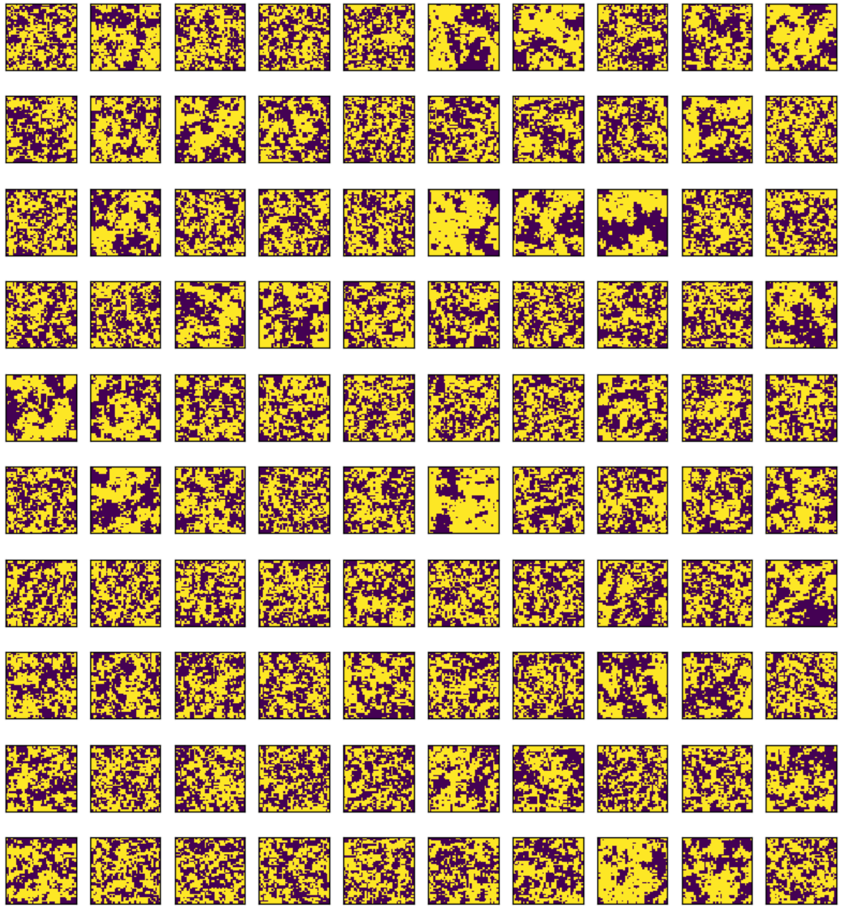


Results of CNN with Transfer Learning (Images with labels)

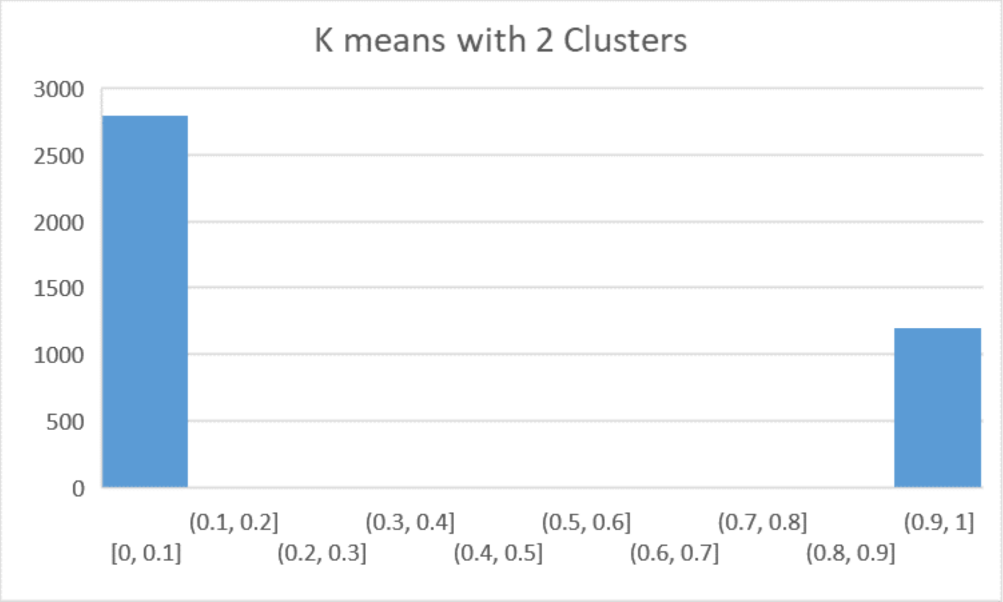
Samples of Test images predicted as below Tc

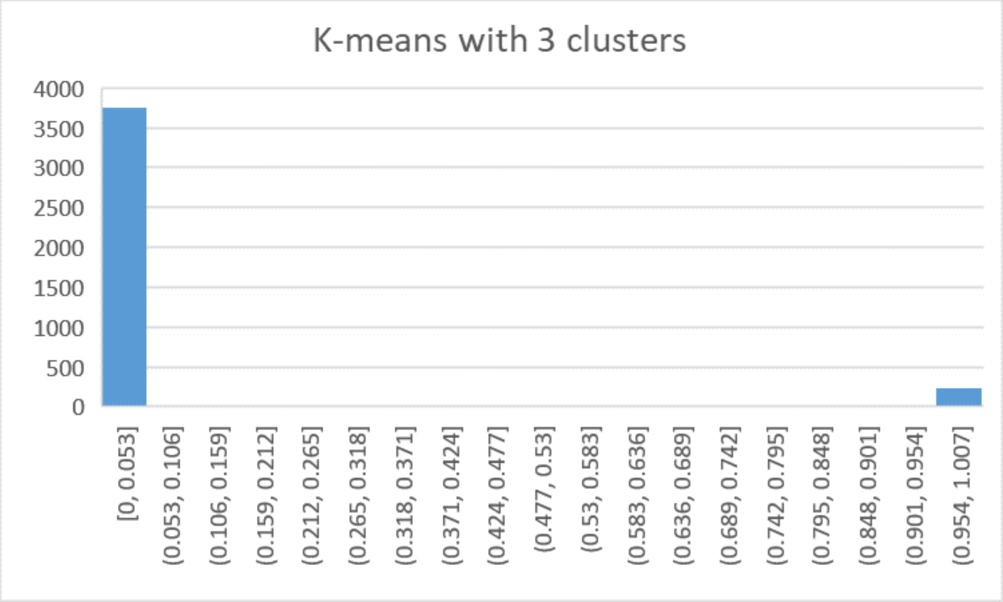


Samples of Test images predicted as above Tc

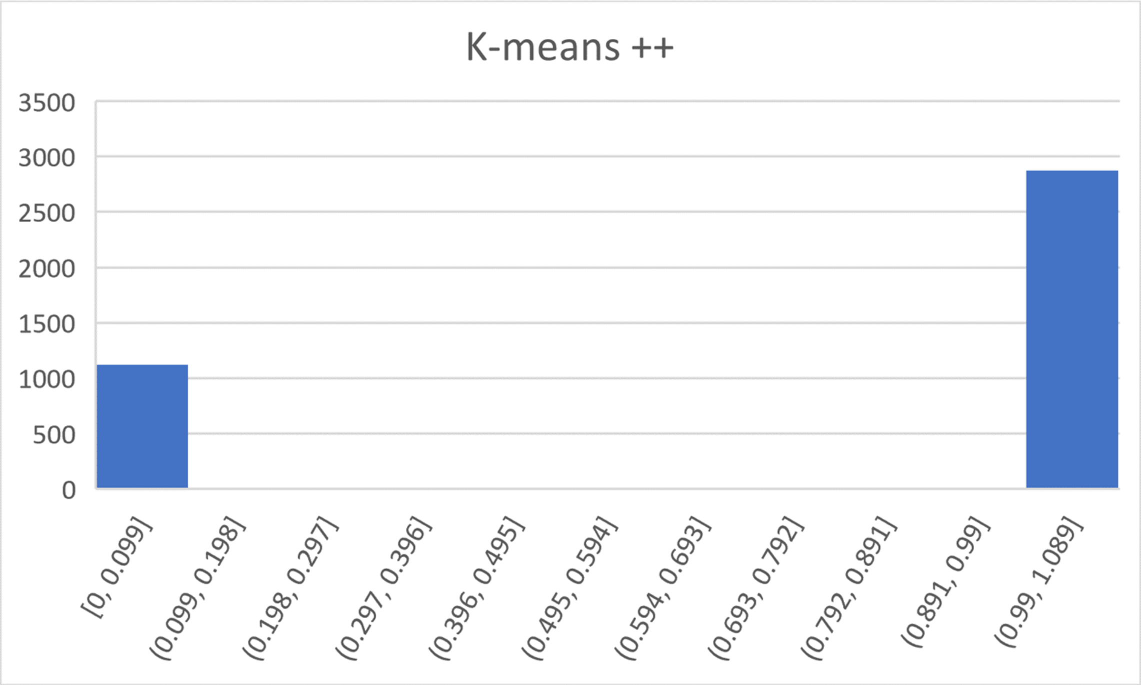


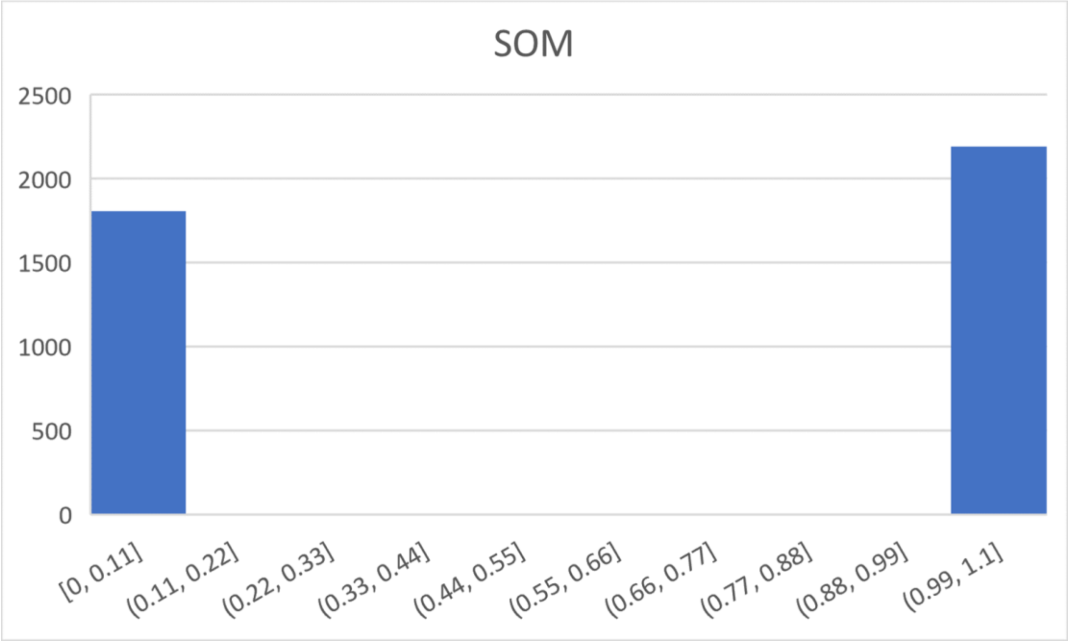
Results of CNN (Images with labels from K-means)



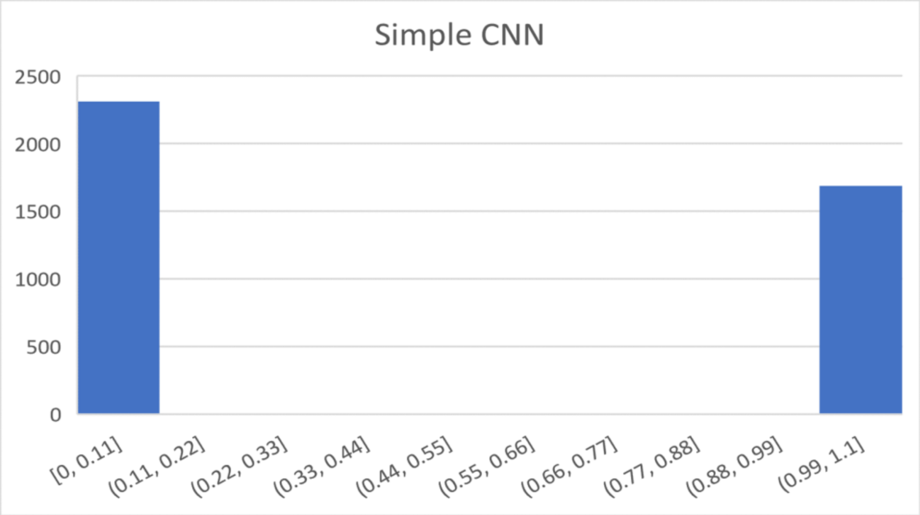


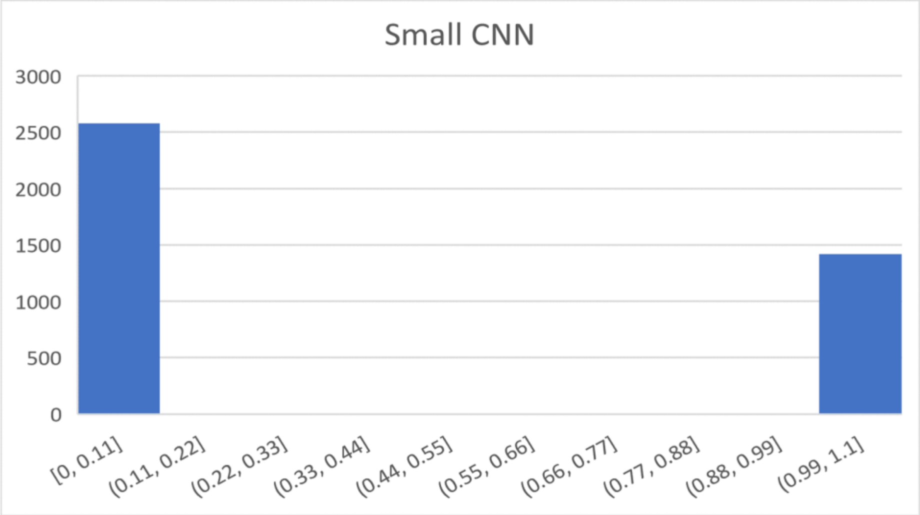
Results of K-means ++ and SOM

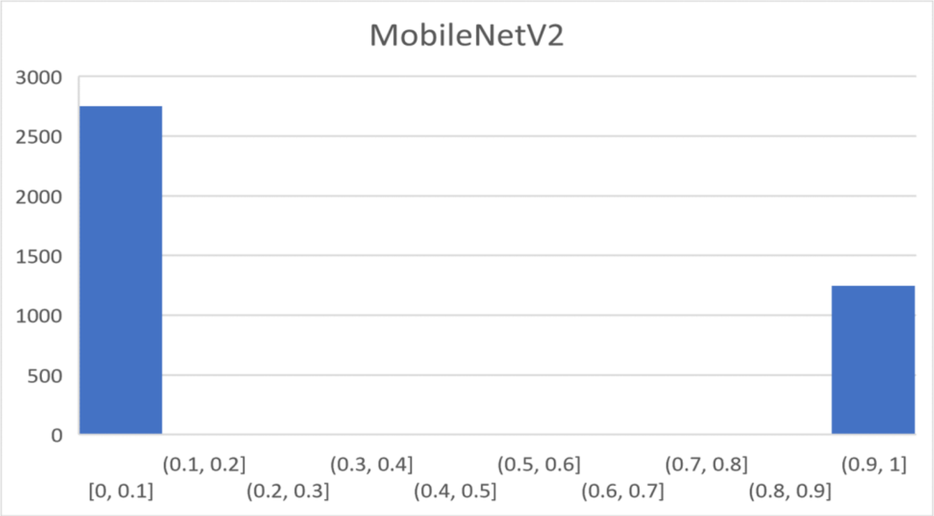




Results of CNN



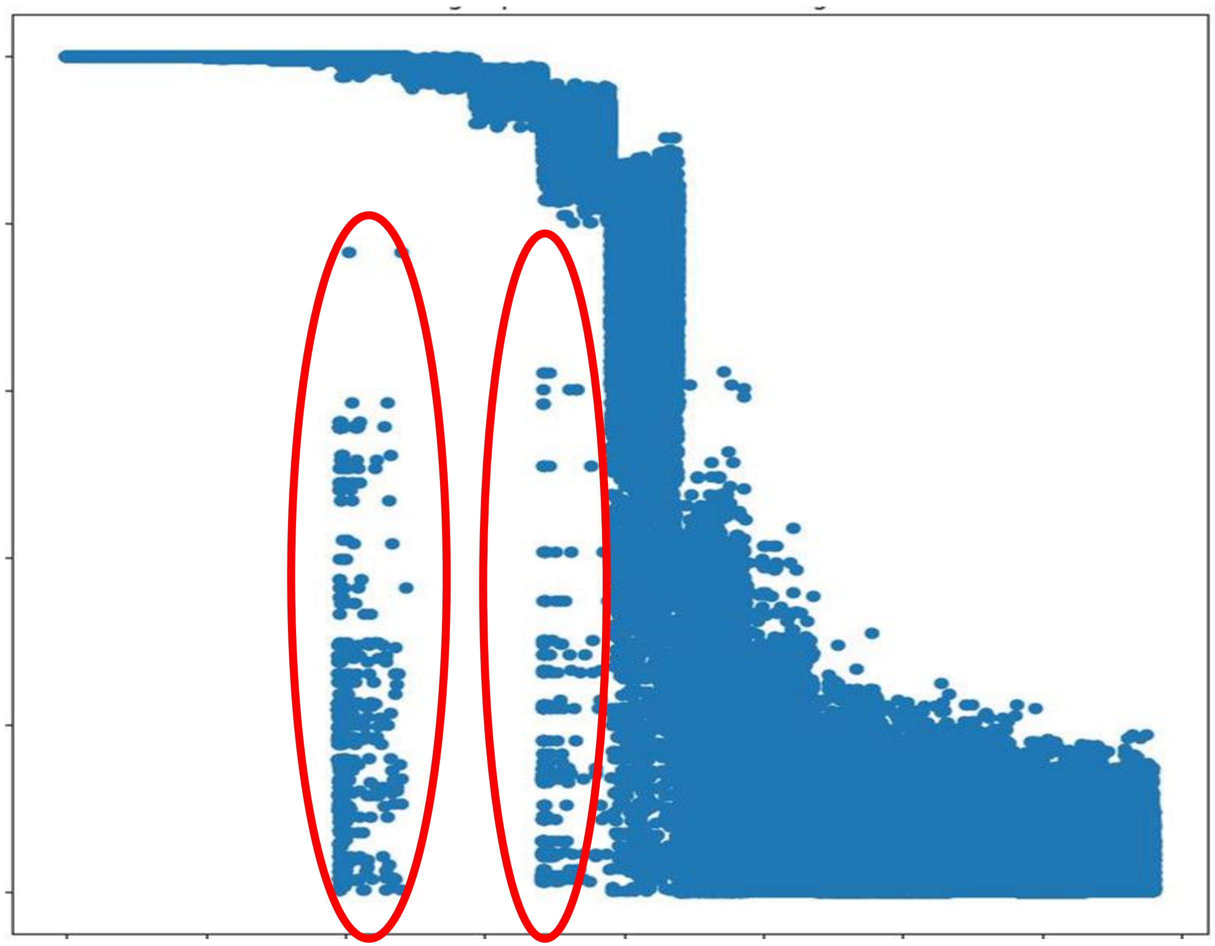




Appendix

Data Structure/ Visualization

- Removal of anomalous data in training images



Justification:
anomalies are caused by non-thermalized samples during simulation

Clustering (removing Outliers)

We use the K-Means method to perform the clustering on the data which then gives us the labels to be able to predict whether an image will be above or below the critical temperature