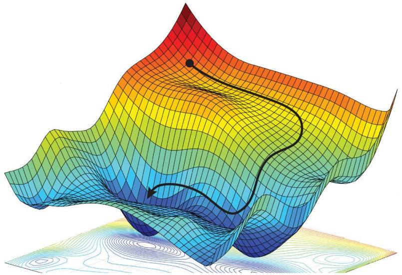
Machine Learning Quantum Matter

Supervised learning of many-body phases

Authors: Juan Carrasquilla, Roger G. Melko

Nikkin Devaraju



DOI: 10.1038/NPHYS4035

Outline

Machine Learning

- Building blocks of neural network
- Underfit and overfit
- Double descent

2D Ferromagnetic Ising model

- Model description
- Machine learning of two phases using Neural networks
- Data collapse + Finite scaling
- Extension to triangular lattice

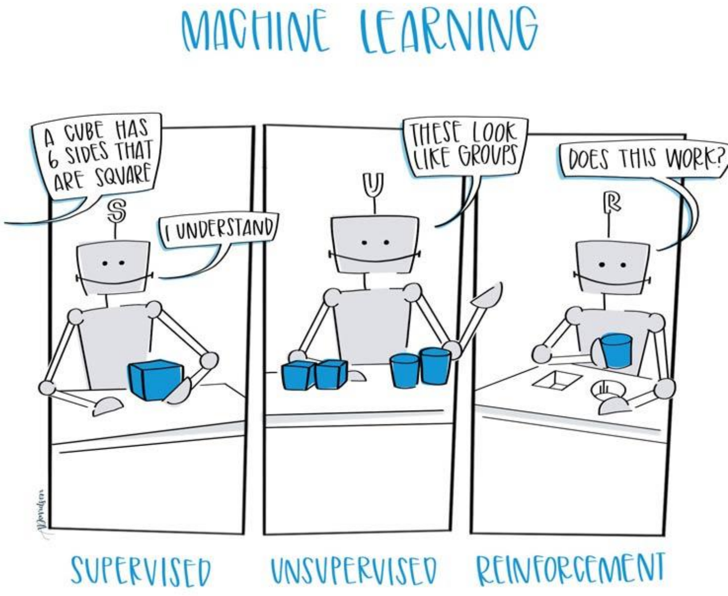
Ising Gauge theory

- Setup
- Results from CNN (Convolutional neural network)

Summary

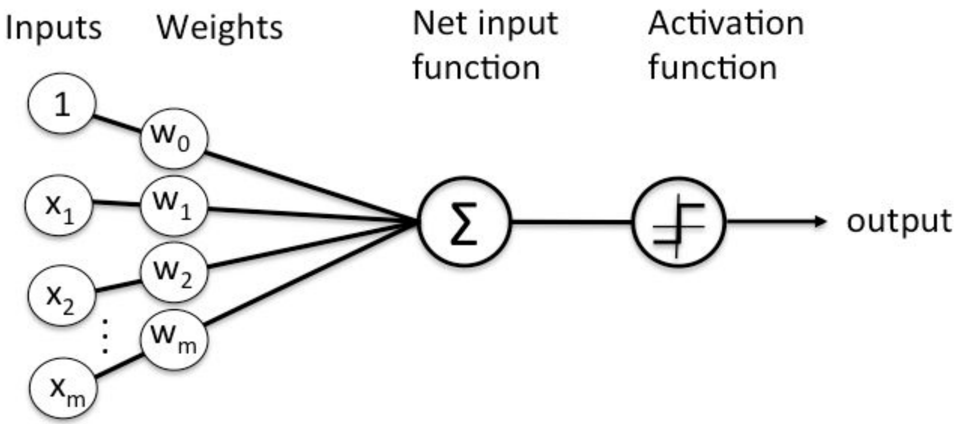
Machine learning

- Subfield of AI to develop algorithms capable of learning from data automatically
- Sustained motivation? - Availability of big data sets
- Applications in physics
- 3 broad paradigms in ML
  - Supervised learning- Classification, Regression
  - Unsupervised learning - Clustering, association, dimensionality reduction
  - Reinforcement learning - Q-Learning, Deep Q
- Neural networks used in all 3

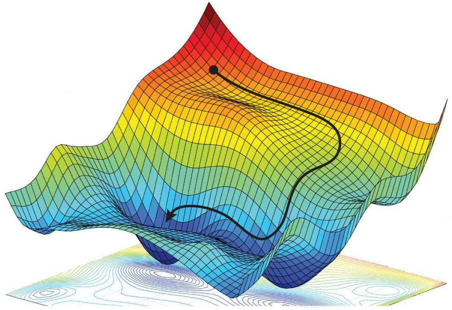


ceralytics

Building blocks of neural network



Basic Perceptron Network



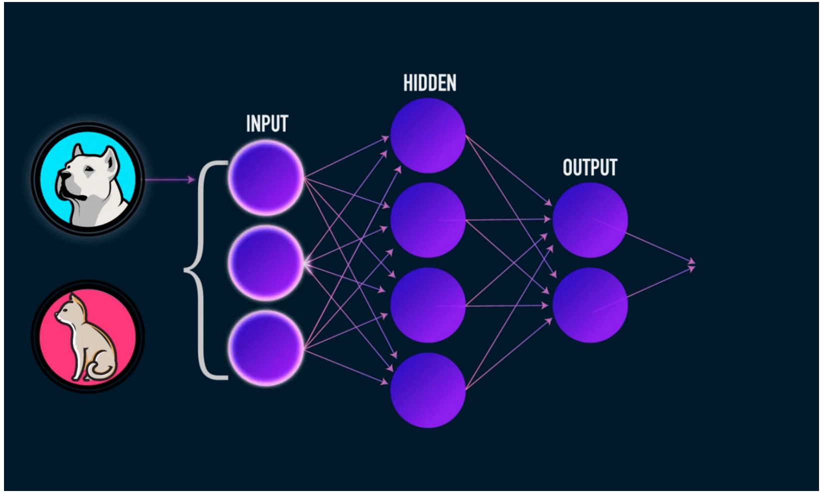
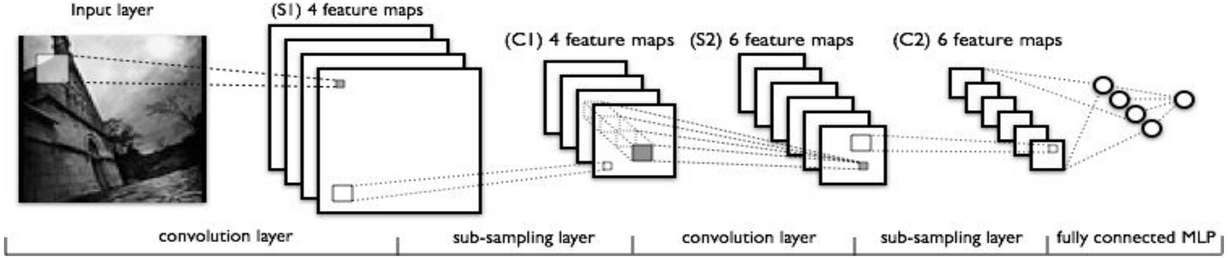


Image Source: https://pathmind.com/wiki/neural-network
https://becominghuman.ai/beginners-guide-cnn-image-classifier-part-1-140c8a1f3c12
https://www.sciencemag.org/news/2018/05/ai-researchers-allege-machine-learning-alchemy

Building blocks of neural network



Convolutional Neural network

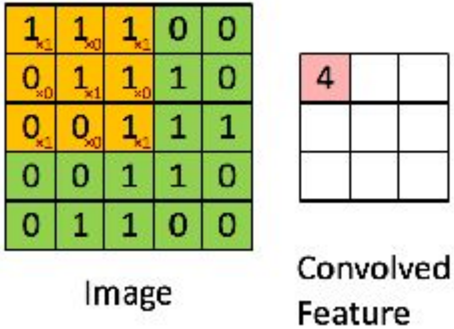
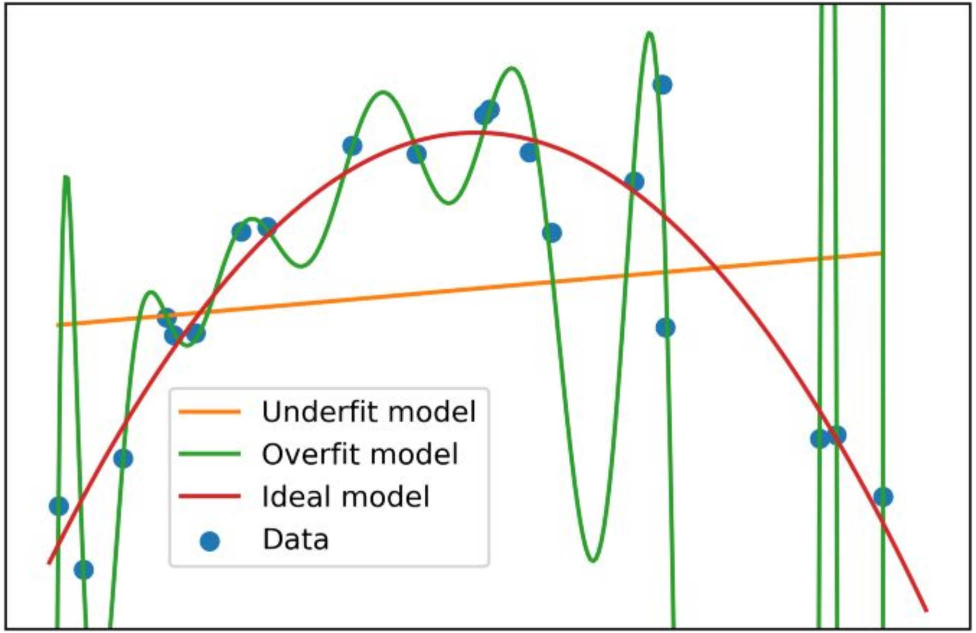


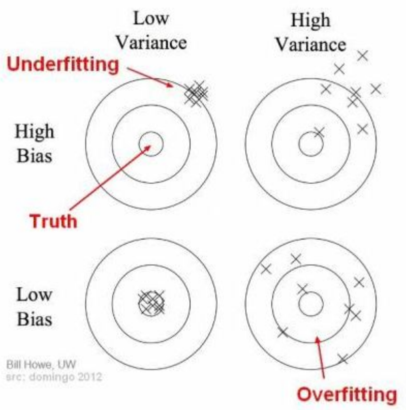
Image Source: https://pathmind.com/wiki/neural-network
https://becominghuman.ai/debunking-convolutional-neural-networks-cnn-with-practical-examples-688284c45b85

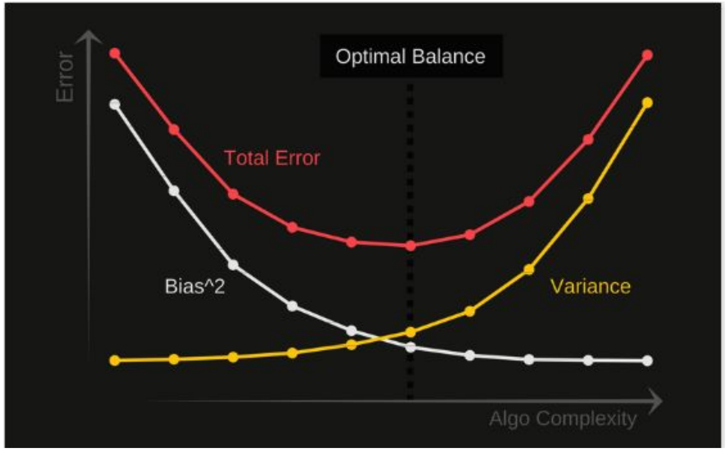
Underfit and overfit

Bias - Deviation from truth
Variance - Sensitivity to small fluctuations



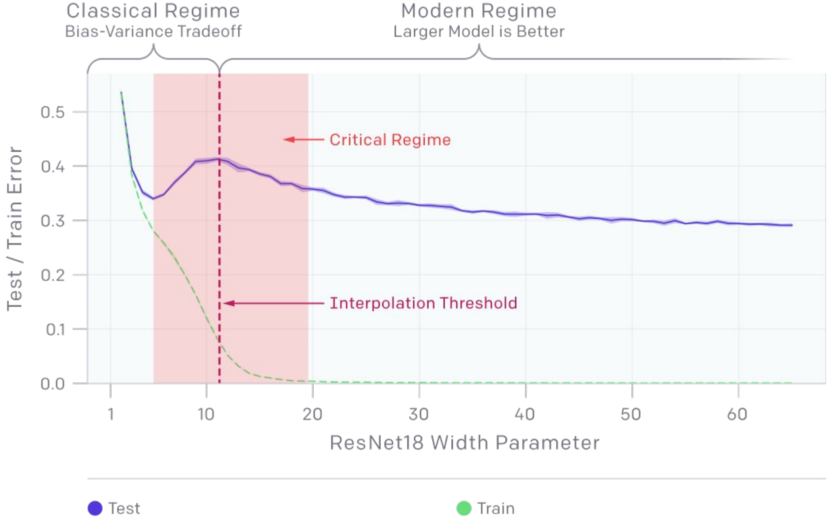
Source

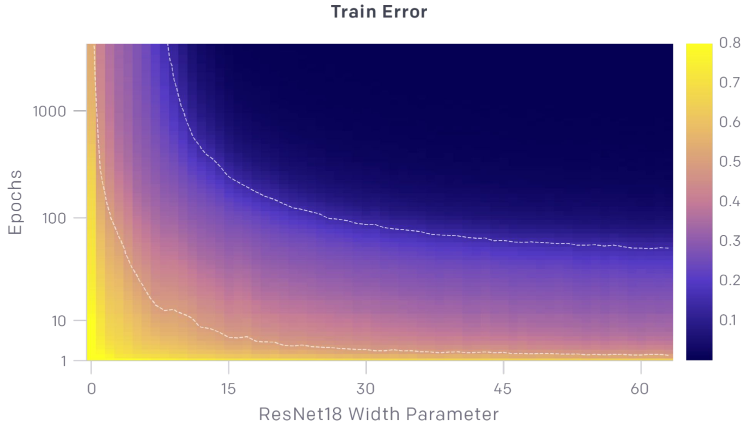


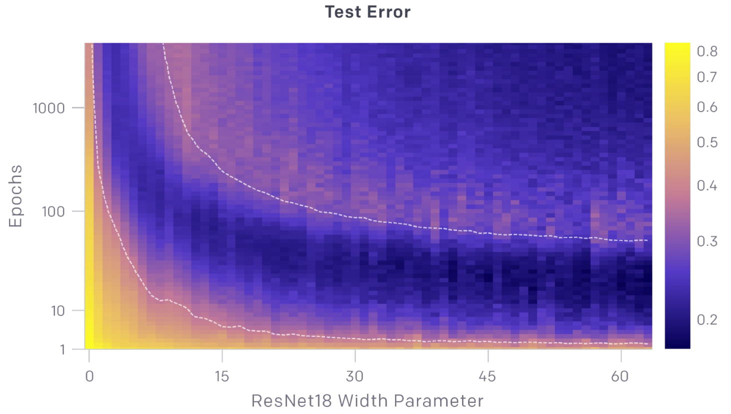


Double Descent

- Universal phenomenon in modern deep learning
- Test error shows double descent







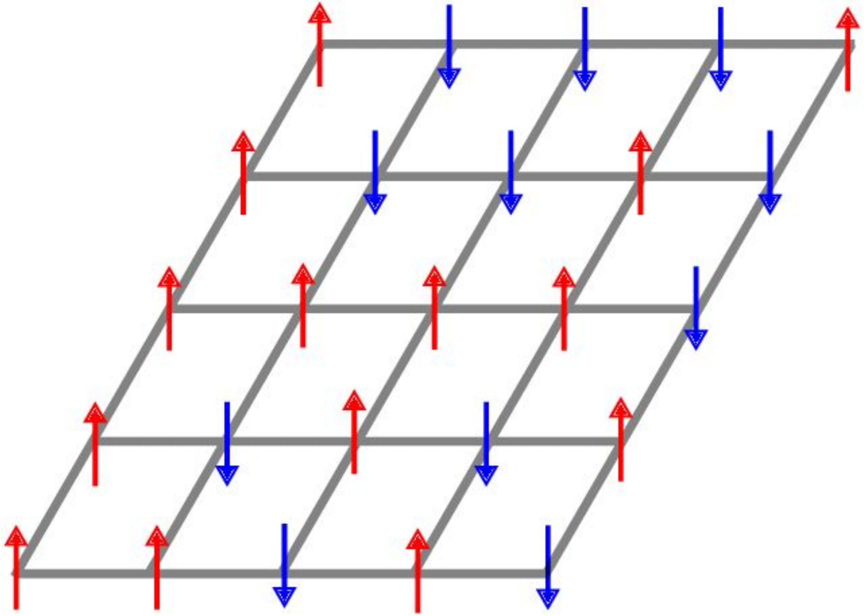
Source: OpenAI

2D Ising model

- Hamiltonian for classical Ising model

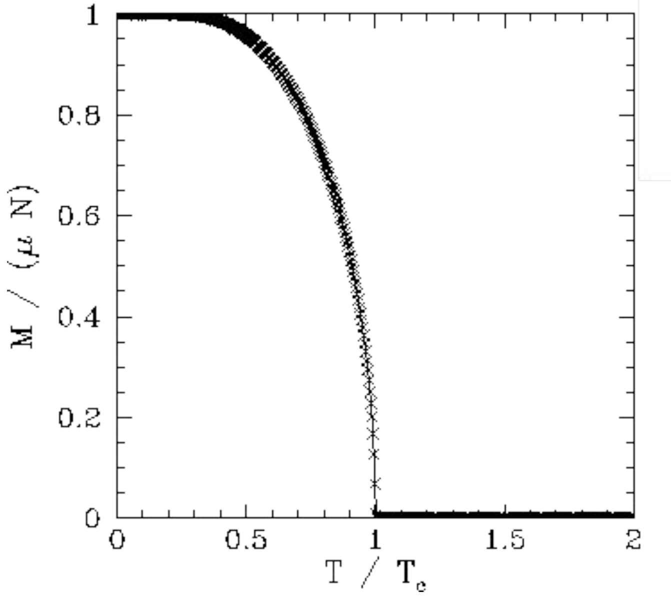
  $H = -J\boldsymbol{\Sigma}S_iS_j$

- Indices i,j run over nearest neighbours on 2D lattice
- Onsager proved the phase transition in the thermodynamic limit from an ordered ferromagnet (with all spins aligned) to a (disordered) paramagnetic phase at the critical temperature $T_c/J = 2/\log(1+\sqrt{2}) \cong 2.26$



Second order phase transition

- Also called "continuous phase transitions". Characterized by a divergent susceptibility, an infinite correlation length, and a power law decay of correlations near criticality.
- X - Temp, Y - order parameter (magnetization)
- Ferromagnetic - 1
- Paramagnetic - 0
- Drops to zero at the critical temp. Scaling ansatz

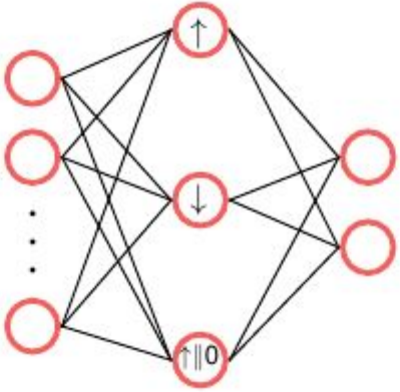


Source: http://farside.ph.utexas.edu/teaching/329/lectures/node110.html

Using NN

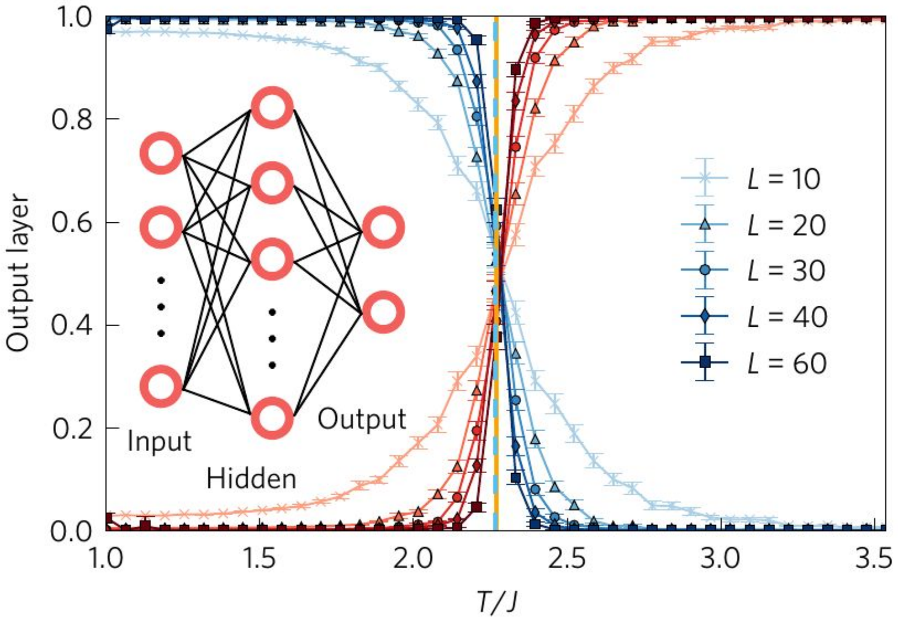
- Employ logistic regression to classify the states of the 2D Ising model according to their phase of matter
- If successful, this can be used to locate the position of the critical point in more complicated models where an exact analytical solution has so far remained elusive

Setup - Demo!



Machine learning of two phases

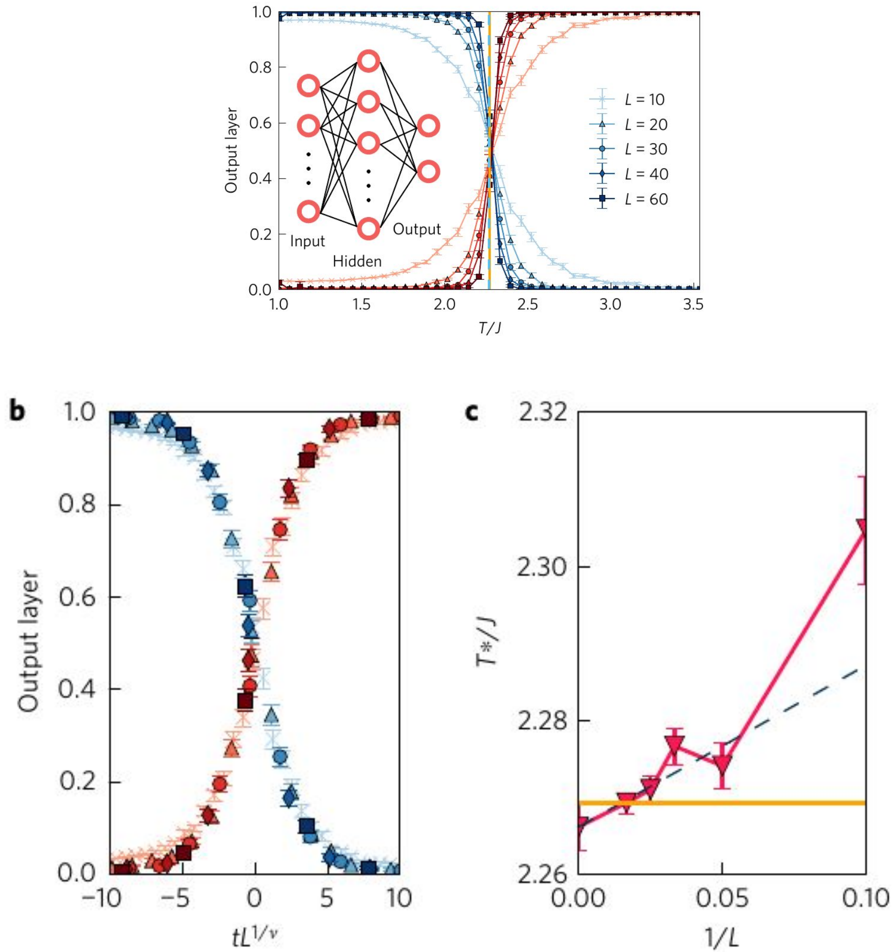
- 100 neurons in hidden layer
- For each T, Monte Carlo sampling is followed by thermalization
- Output gives the probability that the state is one of the 2
- Results on test data already shows finite sized effects



Source: https://www.nature.com/articles/nphys4035

Data collapse + Finite scaling

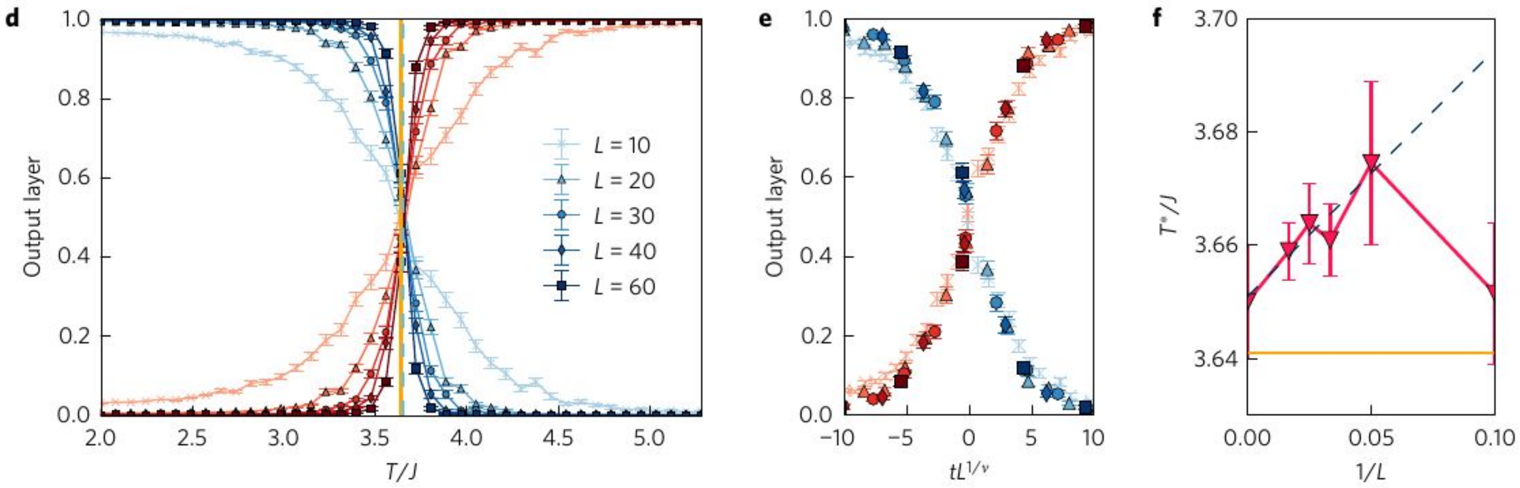
- Scaling ansatz is a power law close to the critical temperature
- Scaling X values by t = (T-Tc) and the L raised to a power (scaling ansatz) results in data collapse
- Exponents are known
- To calculate Tc, T*/J vs. 1/L is used where T* is the crossing temperature
- **NN is able to identify a finite scaling behaviour of a physical observable**



Source: https://www.nature.com/articles/nphys4035

Extension to triangular lattice

- Neural network generalises problems to other lattice structures without being trained.
- Correct prediction of critical values in triangular lattice ising spin model

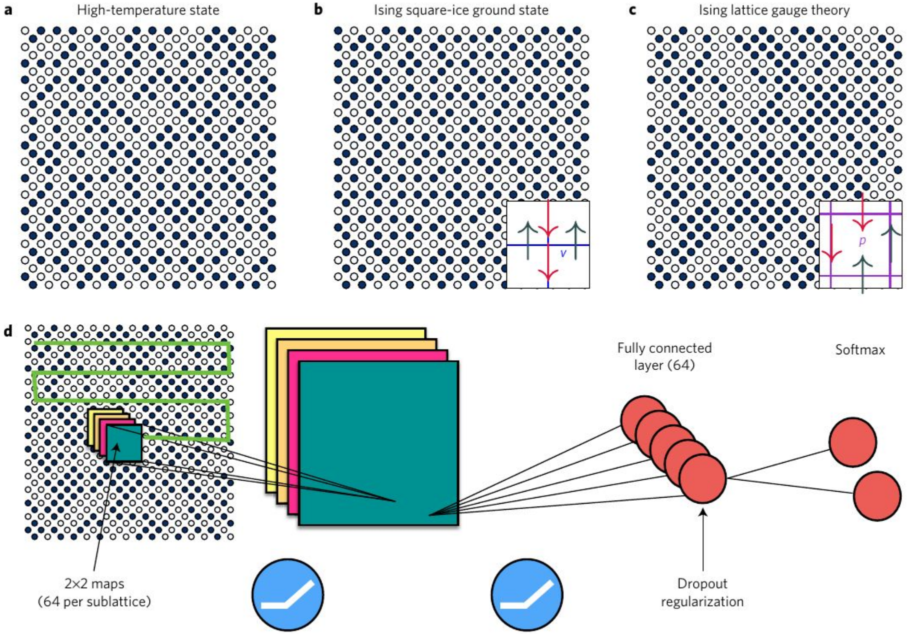


Source: https://www.nature.com/articles/nphys4035

Ising gauge theory

$H = J\sum_v Q_v^2$, where the charge $Q_v = \sum_{i\in v} \sigma_i^z$ is the sum over the Ising variables located in the lattice bonds incident on vertex v,

- Conventional order parameters do not exist in disordered/topological phases
- Using CNN to train Monte Carlo configurations from Ising Gauge theory at T=0 and T=infinity
- NN still discriminates in-spite of the lack of order parameter



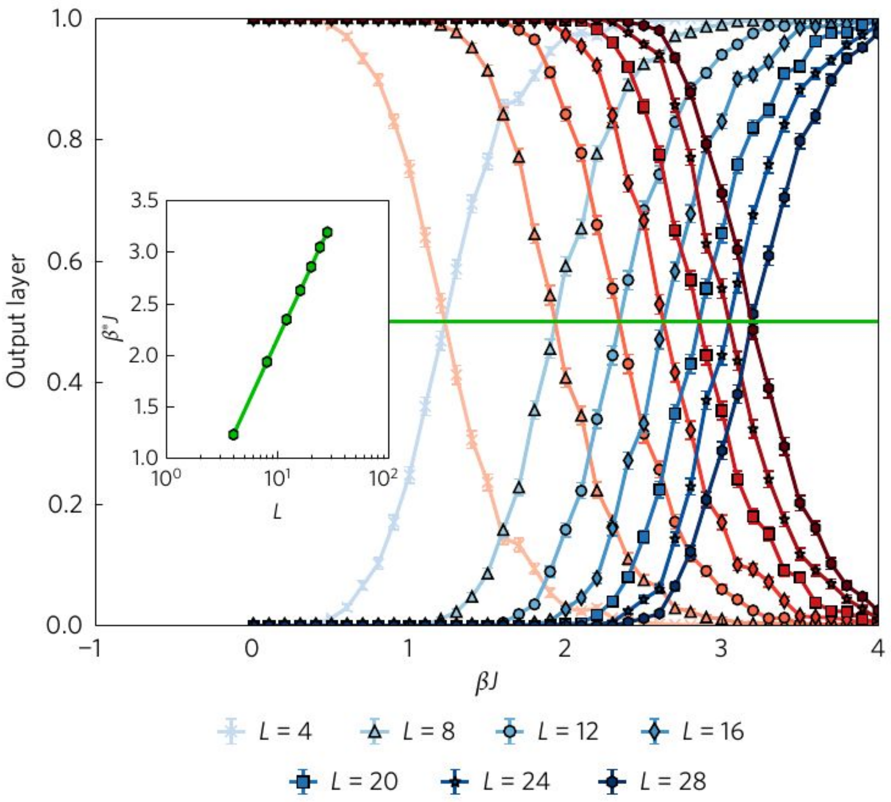
$$H = -J\sum_p \prod_{i\in p} \sigma_i^z$$

Source: https://www.nature.com/articles/nphys4035

Ising gauge theory

- No finite temperature phase transition. So, sampling from T=0 and T=infinity
- But in finite systems, system expected to slowly cross-over to high temperature phase
- $T^* \sim N \exp(2J\beta)$

$$T^*/J \sim 1/\ln\sqrt{N}$$



Source: https://www.nature.com/articles/nphys4035

Summary

- Understanding models with overfit/underfit cases
- NN used to encode phases of matter, discriminate phase transitions in correlated many-body systems
- Learns order parameter without knowledge of energy, locality conditions
- Extends to different lattice structures