Machine Learning for Model Hamiltonian

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https://github.com/meng-su/Machine-learning-for-Model-Hamiltonian

Contents

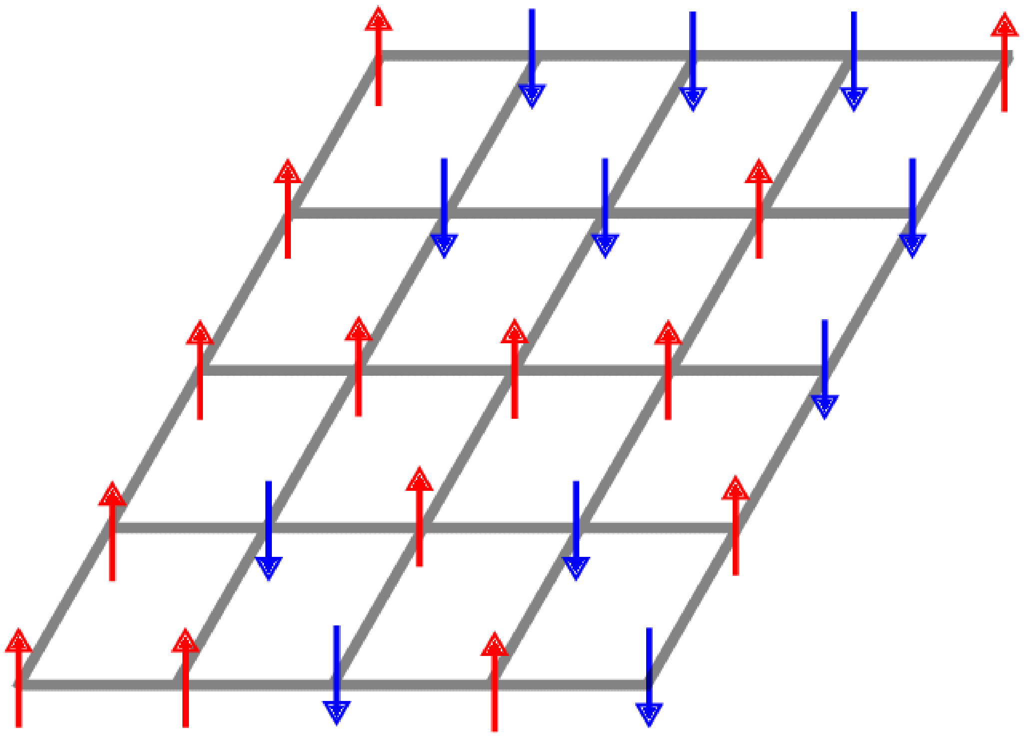
Ising Model

- Ising model:

$$H = -\sum_{<i,j>} J_{ij} S_i^z S_j^z - h \sum_i S_i^z$$

- $J_{ij} > 0$: ferromagnetism,
- $J_{ij} < 0$: antiferromagnetism
- 2D Ising model critical temperature (h=0)[1],[2] :

$$k_B T = \frac{2J}{\ln(1+\sqrt{2})} \approx 2.269J$$



Monte Carlo

- Metropolis Monte Carlo
- Equilibrium condition:

$$\frac{d}{dt}P_a = \sum_b w_{b\to a}P_b - w_{a\to b}P_a = 0$$

- Boltzmann distribution $P_a \propto \mathrm{e}^{-\beta E_n}$:

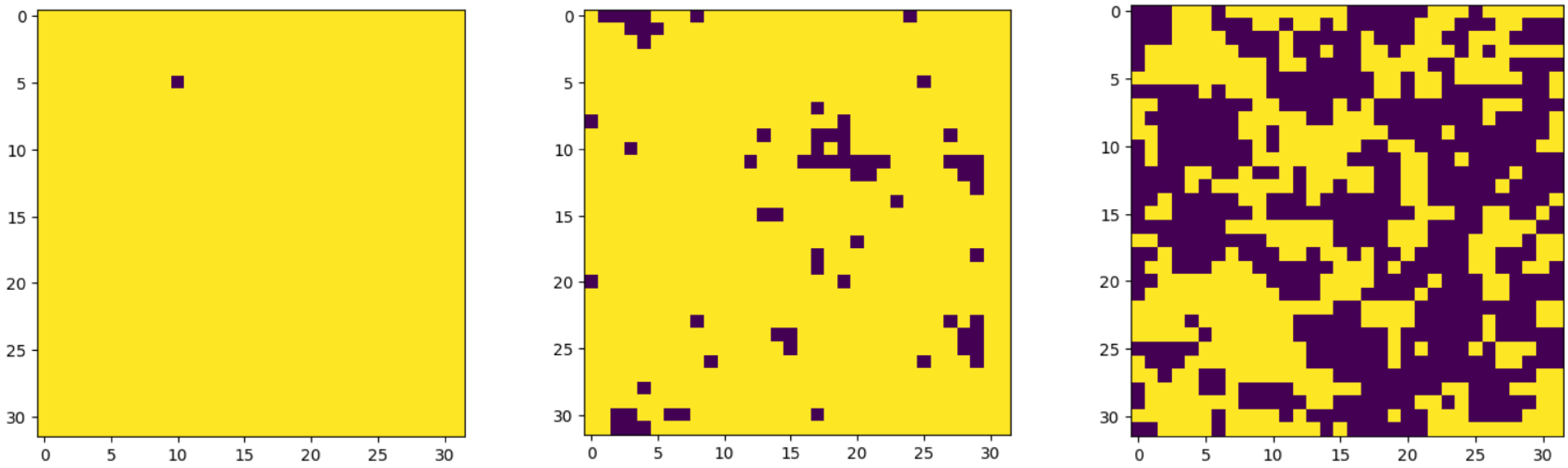
$$w_{a\to b} = \begin{cases} e^{\beta \Delta E_{ab}} & (E_b > E_a) \\ 1 & (E_b \leq E_a) \end{cases}$$

$$w_{b\to a} = \begin{cases} 1 & (E_b > E_a) \\ e^{-\beta \Delta E_{ab}} & (E_b \leq E_a) \end{cases}$$

Monte Carlo Result

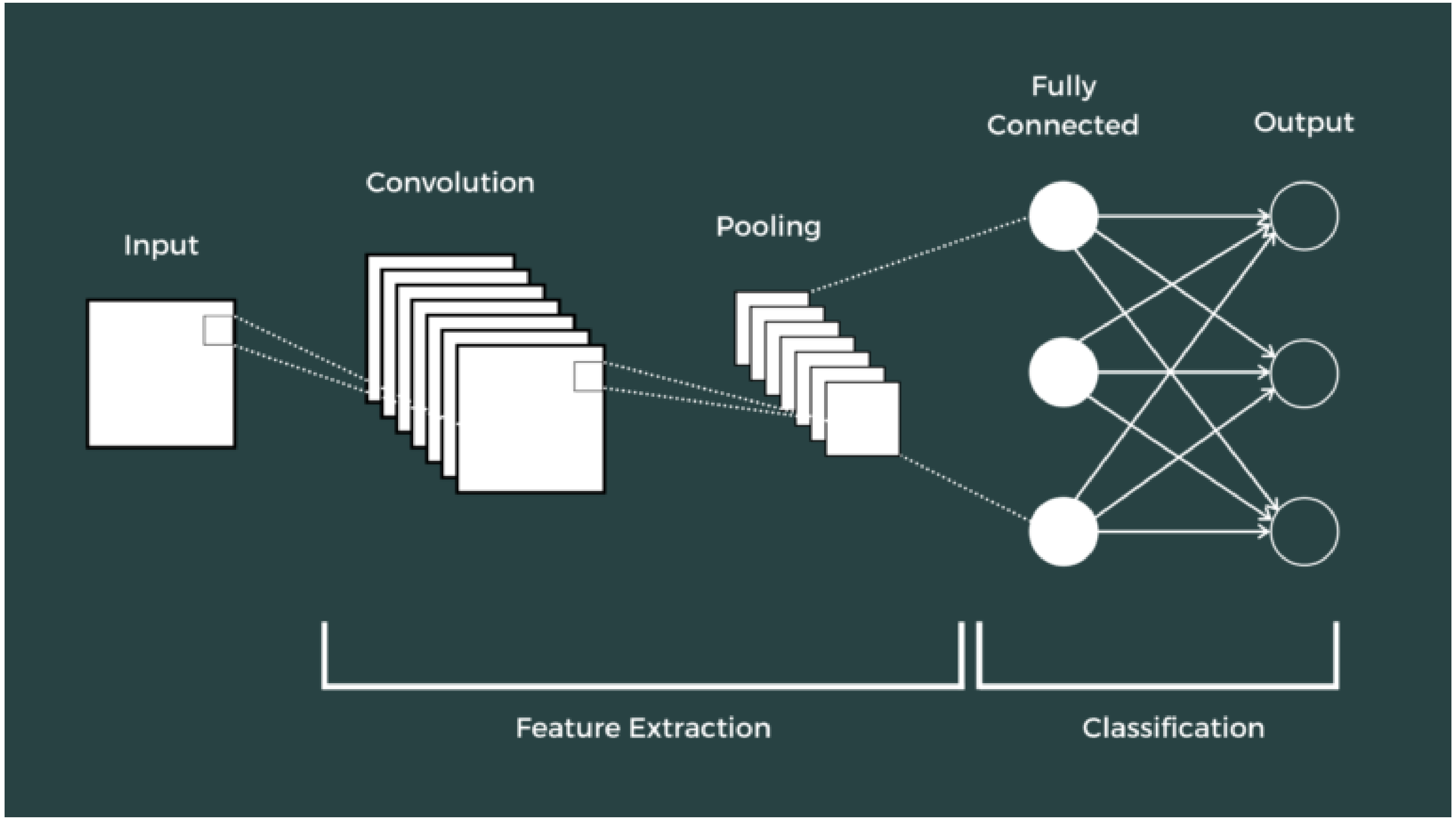
Size = 32×32, J = 1.0, h = 0.0

T = 1.0 T = 2.0 T = 3.0



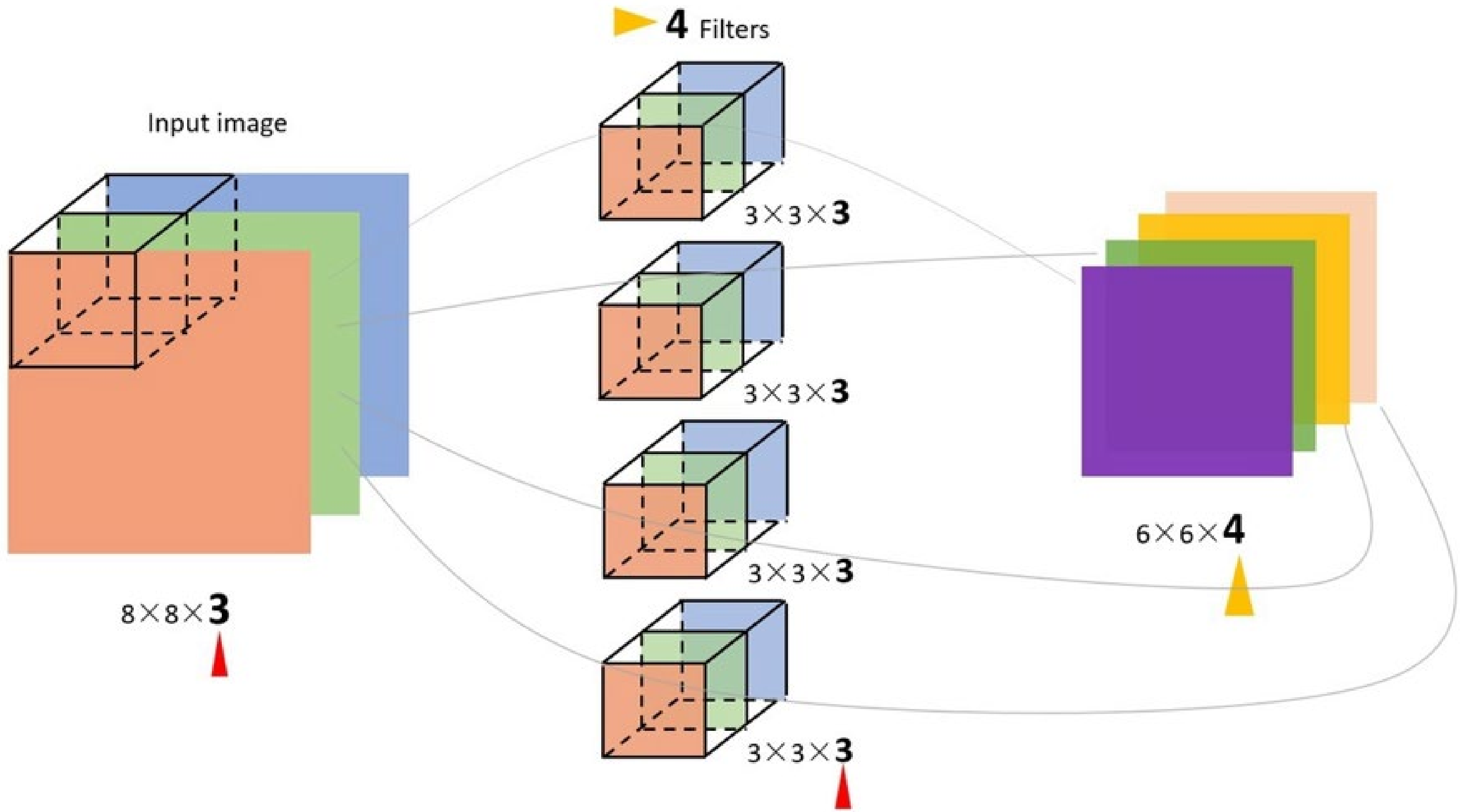
Convolution Neural Networks

- $input \rightarrow Feature\ Extraction \rightarrow Classification\ (Regression)$



CNN: Convolution

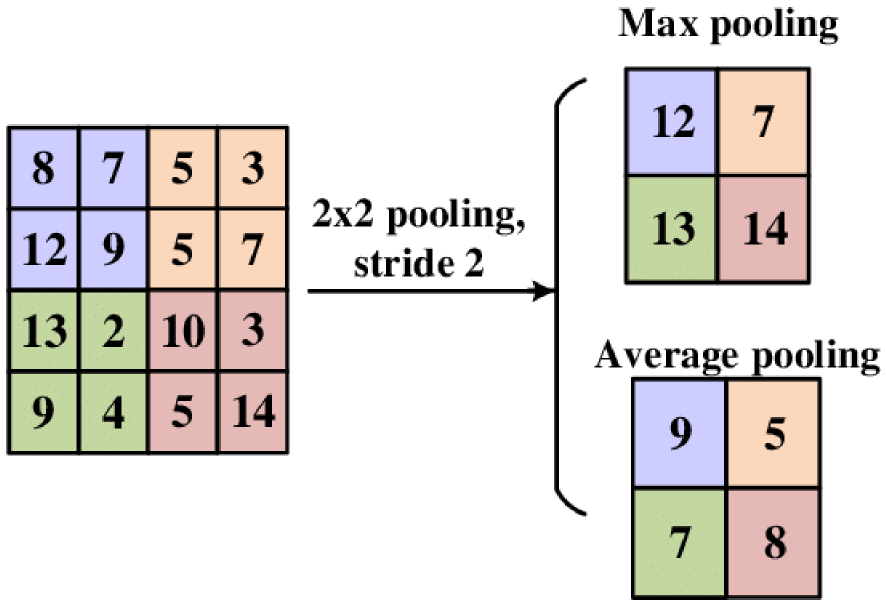
- Input: Usually, input data are $n1 \times n1 \times n2$, 3D array.
- In our case, n1=32(size of lattice), n2 = 29 (selected from 1000 micro states)



A convolution with multi-channel

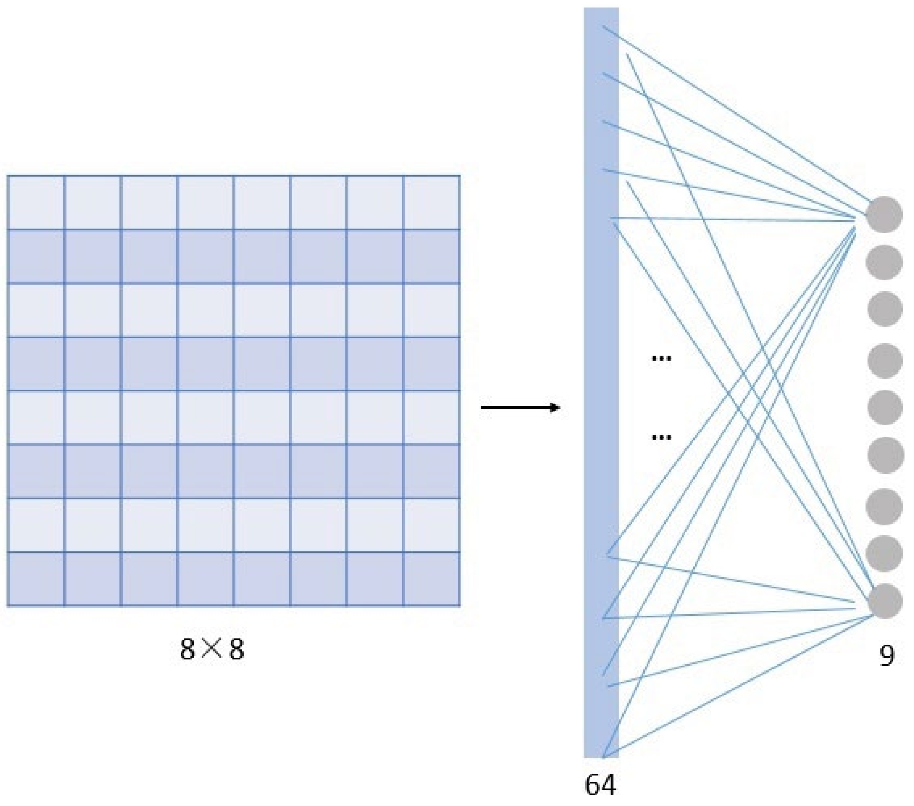
CNN: Pooling

- Pooling: reduce dimension, extract feature



CNN: Classification or Regression

- Flatten and MLP



Results

- Data set D: 30000
- Training data T: 22500
- Testing data S: 7500
- $D = \mathrm{T} \cup S, \mathrm{T} \cap S = \emptyset$

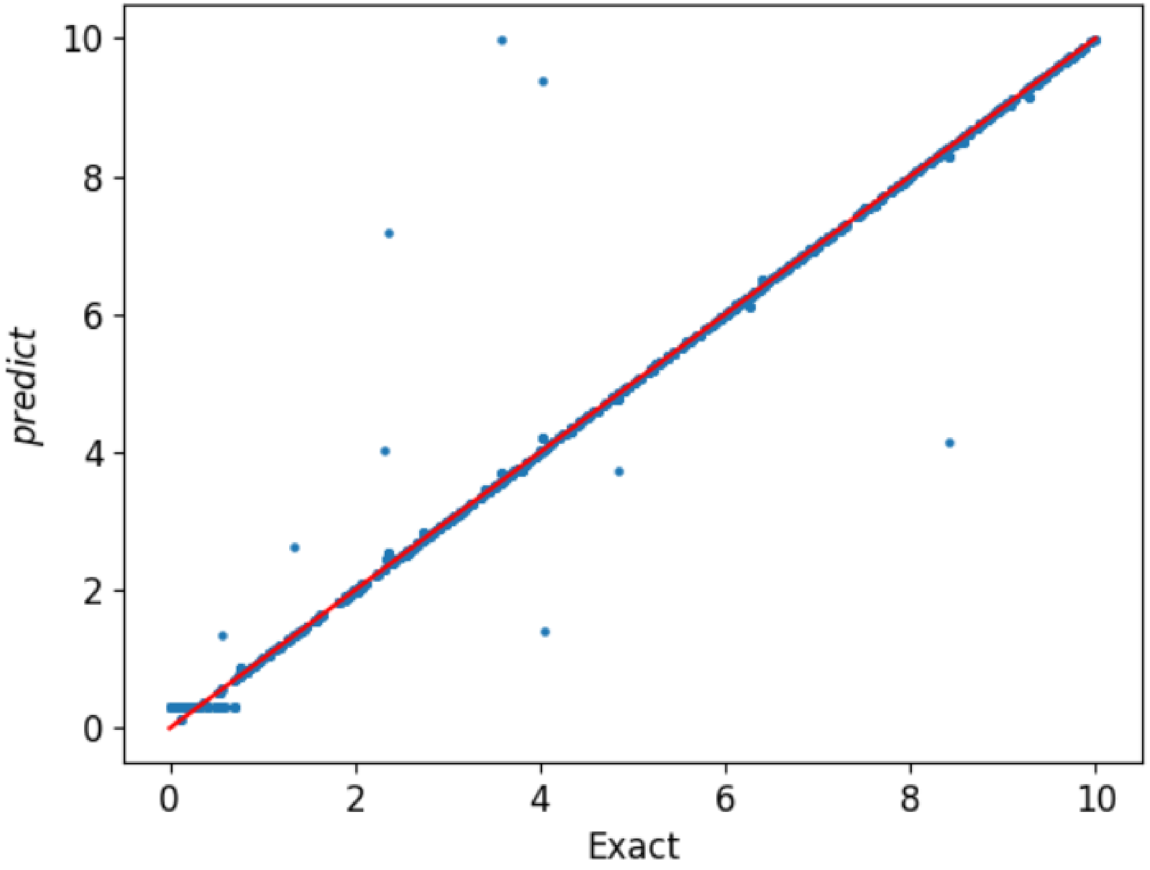
Results

- Input: Ensemble sampling, Label: phase, accuracy=0.994, J = 1.0
- Label: $1 \rightarrow ferromagnetism, 0 \rightarrow paramagnetic$

Testing set	Label	Number in testing set	Number of prediction	Accuracy
$ferromagnetism$	1	1377	1361	0.9887
$paramagnetic$	0	6123	6122	0.9998

Results

- Input: Ensemble sampling, Label: T, accuracy=0.901



Reference

- [1] Introduction to Statistical Mechanics – Wei Cai – Stanford University – Win 2011
- [2] Phys. Rev. 65, 117, 1943

Thanks!