Detection of phase transition via neural network

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Machine Learning in physics

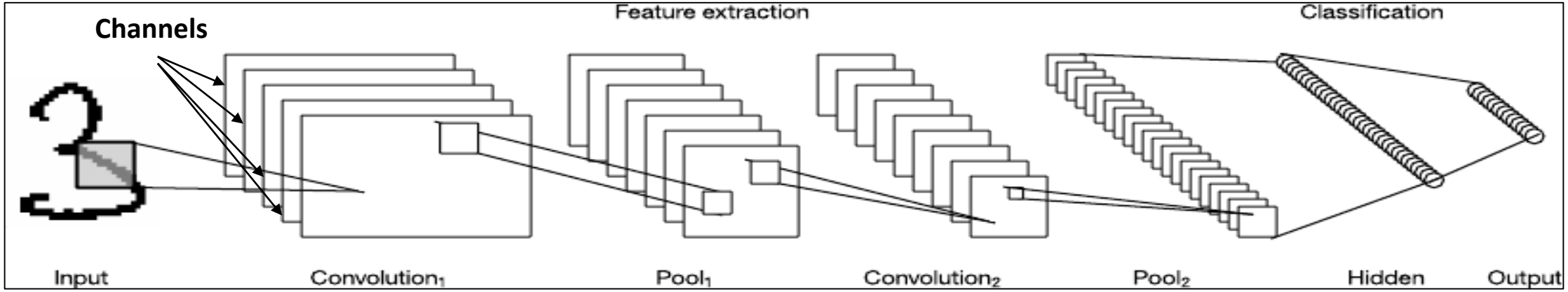
arXive	Title
1606.02318	*Solving the Quantum Many-Body Problem with Artificial Neural Networks*
1612.04262	*An equation-of-state-meter of QCD transition from deep learning*
1705.05582	*Machine Learning of Explicit Order Parameters*
1709.01971	*Deep Learning Beyond Lefschetz Thimbles*
1801.05784	*Machine learning action parameters in lattice quantum chromodynamics*
1807.05971	*Machine Learning Estimators for Lattice QCD Observables*
1812.01522	Phase transition encoded in neural network

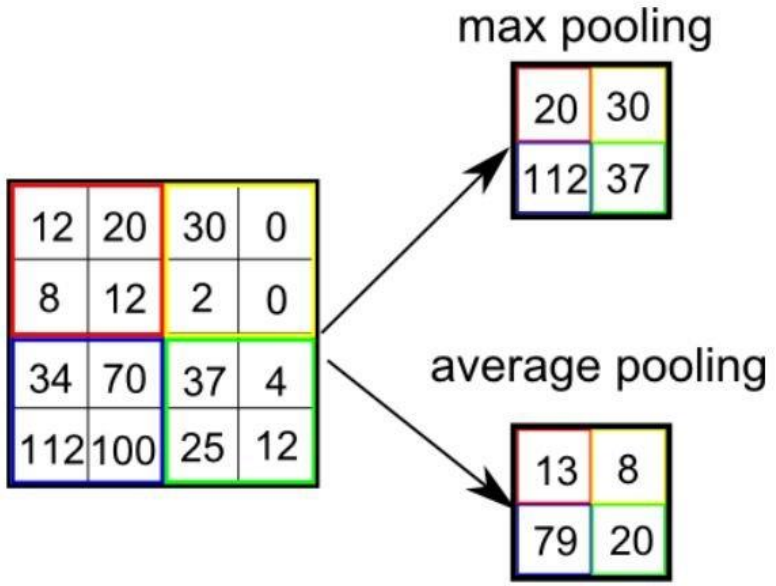
General idea is searching of unknown order parameters.

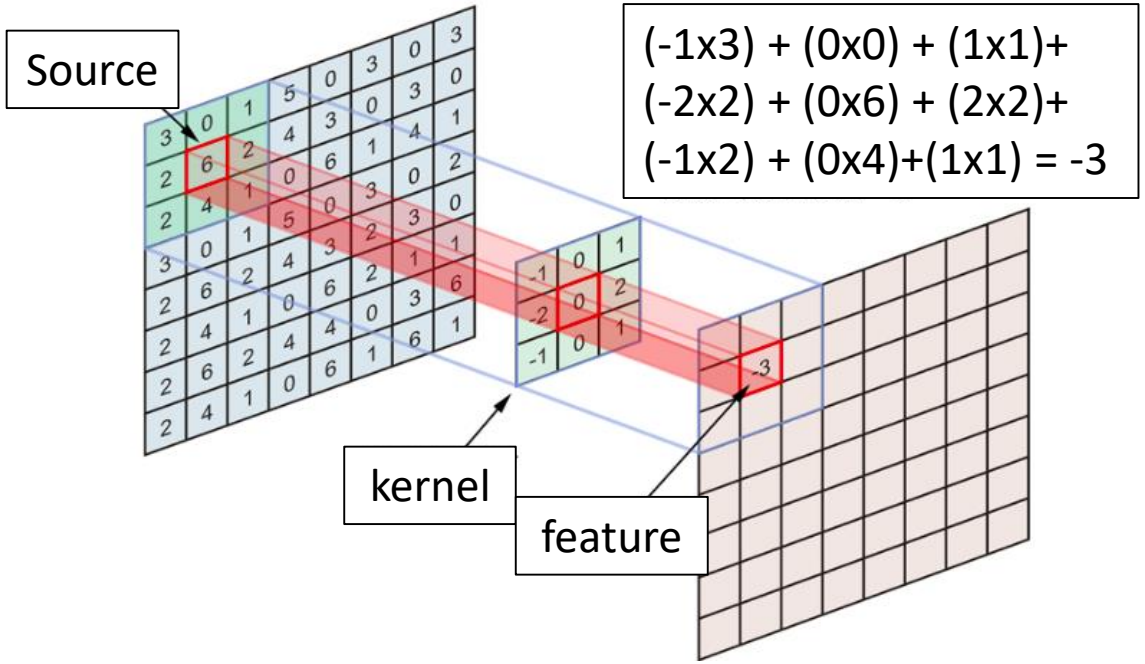
Tasks:

1. Prediction of phase transition or observables.
2. Generation of configurations with Neural Network
3. Prediction of unknown order parameters.

CNN (Convolution Neural Network)







Ising model

Hamiltonian function:

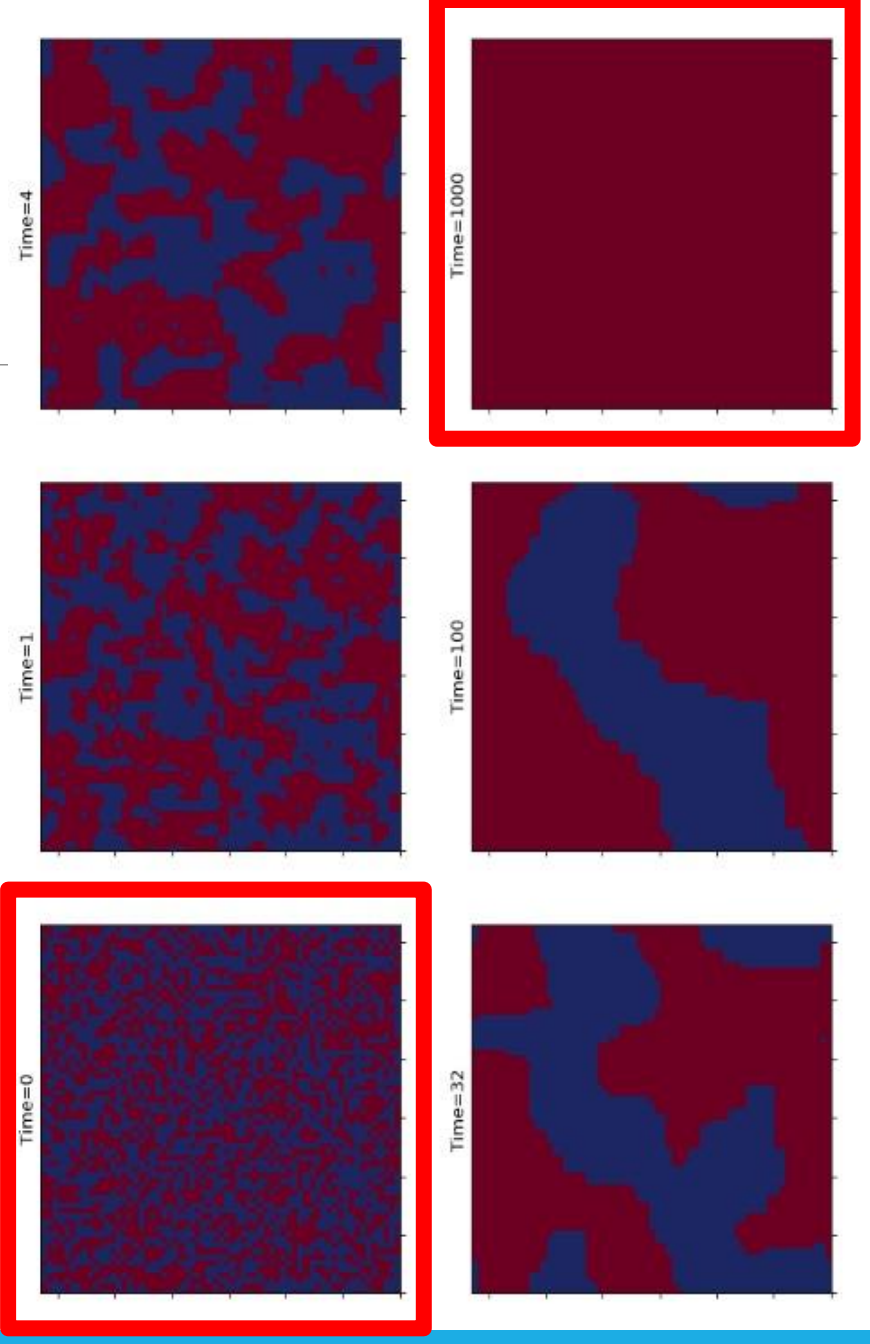
$$\mathrm{H}(\sigma) = -\sum J_{ij}\sigma_i\sigma_j$$

Order parameter: $M = \frac{1}{N}\sum \sigma_i$

Configurations:

- 6000 confs. in ordered phase with 28x28 size
- 6000 confs. in disorder phase with 28x28 size

***Notice**: Neural networks work with raw configurations and know nothing about the Hamiltonian of the system under study.*



Ising model

Supervised learning is applied here for binary classification problem.

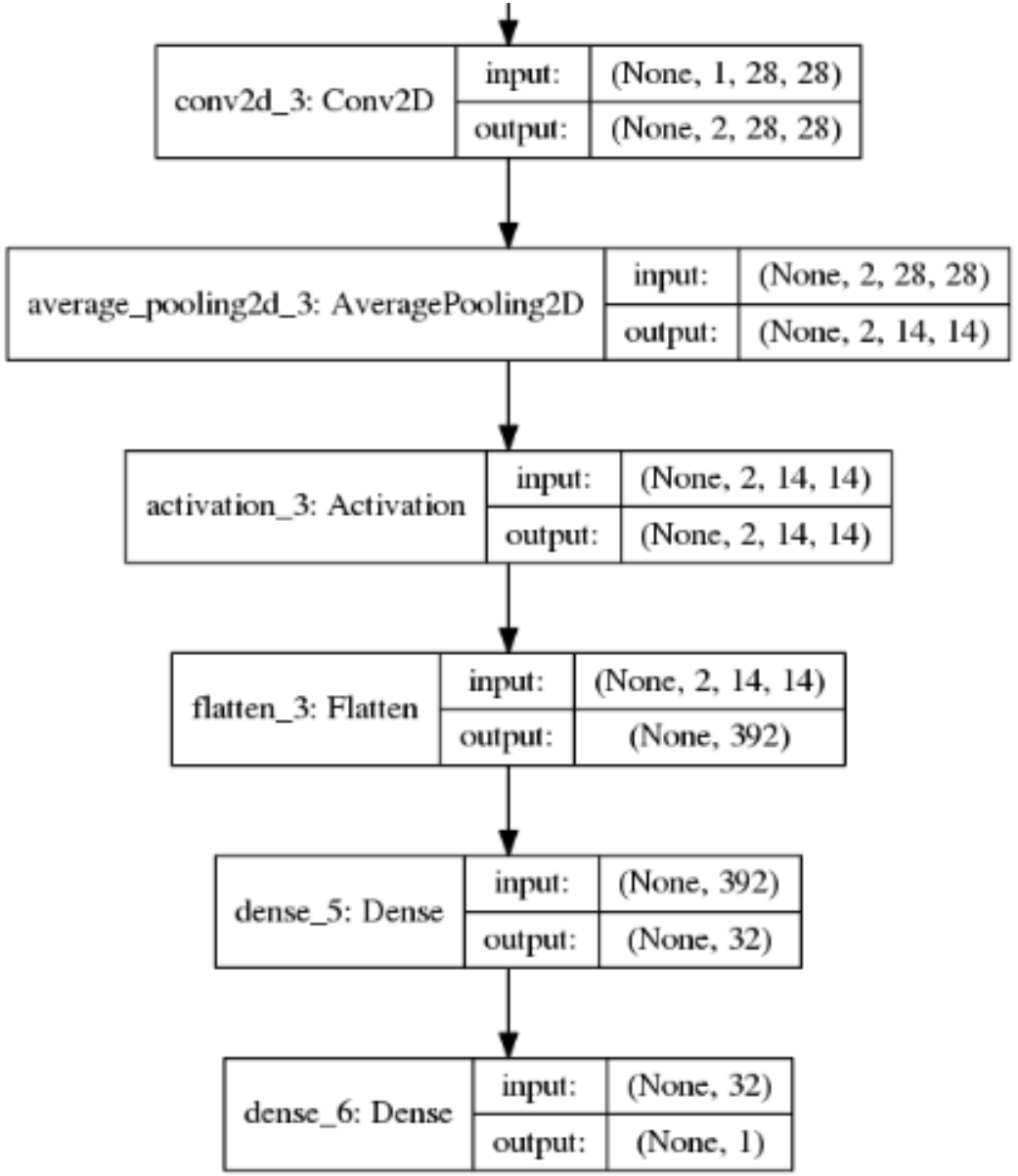
Machine Learning:

- Training data: 10000 configurations (randomly chosen)
- Holdout data: 2000 configurations
- Answers: Phase probability (0; 1)
- Loss functions: Cross Entropy

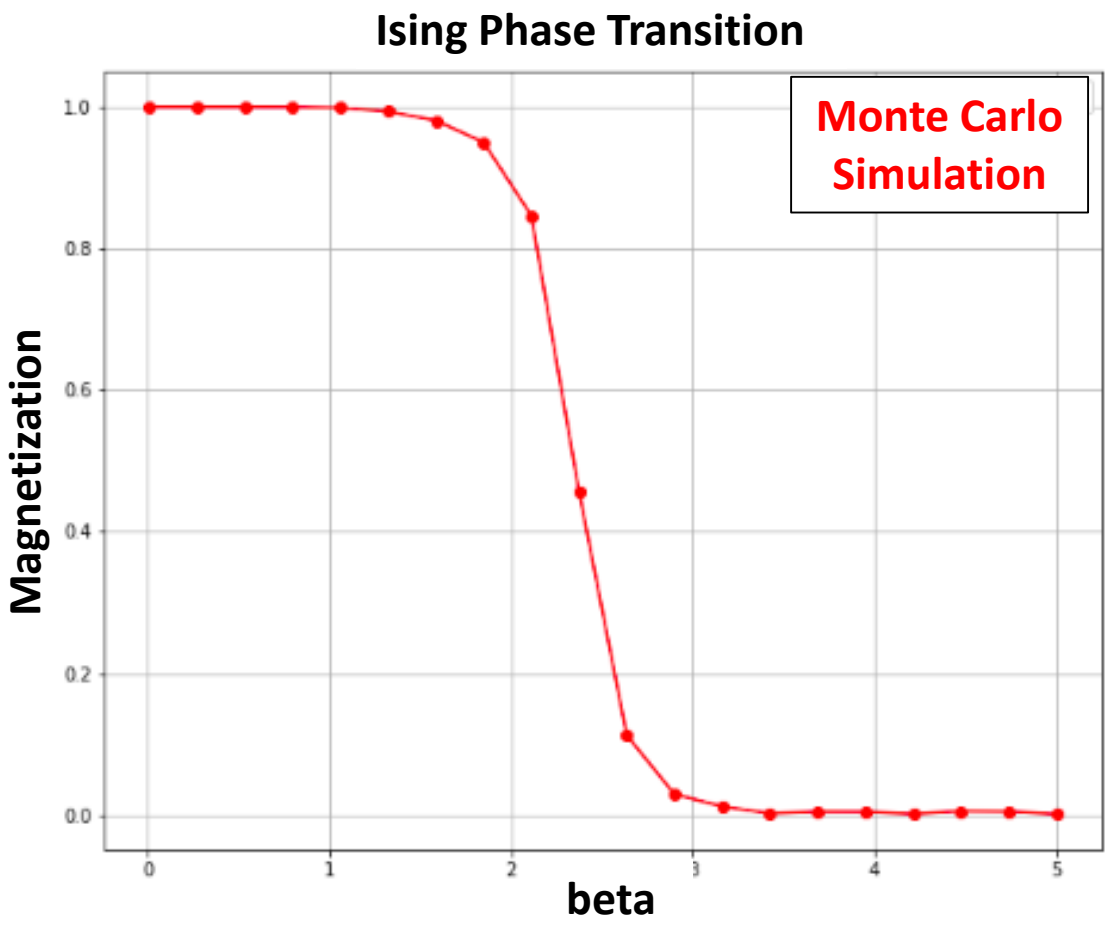
$$CE = -\sum_i p_i log(q_i)$$

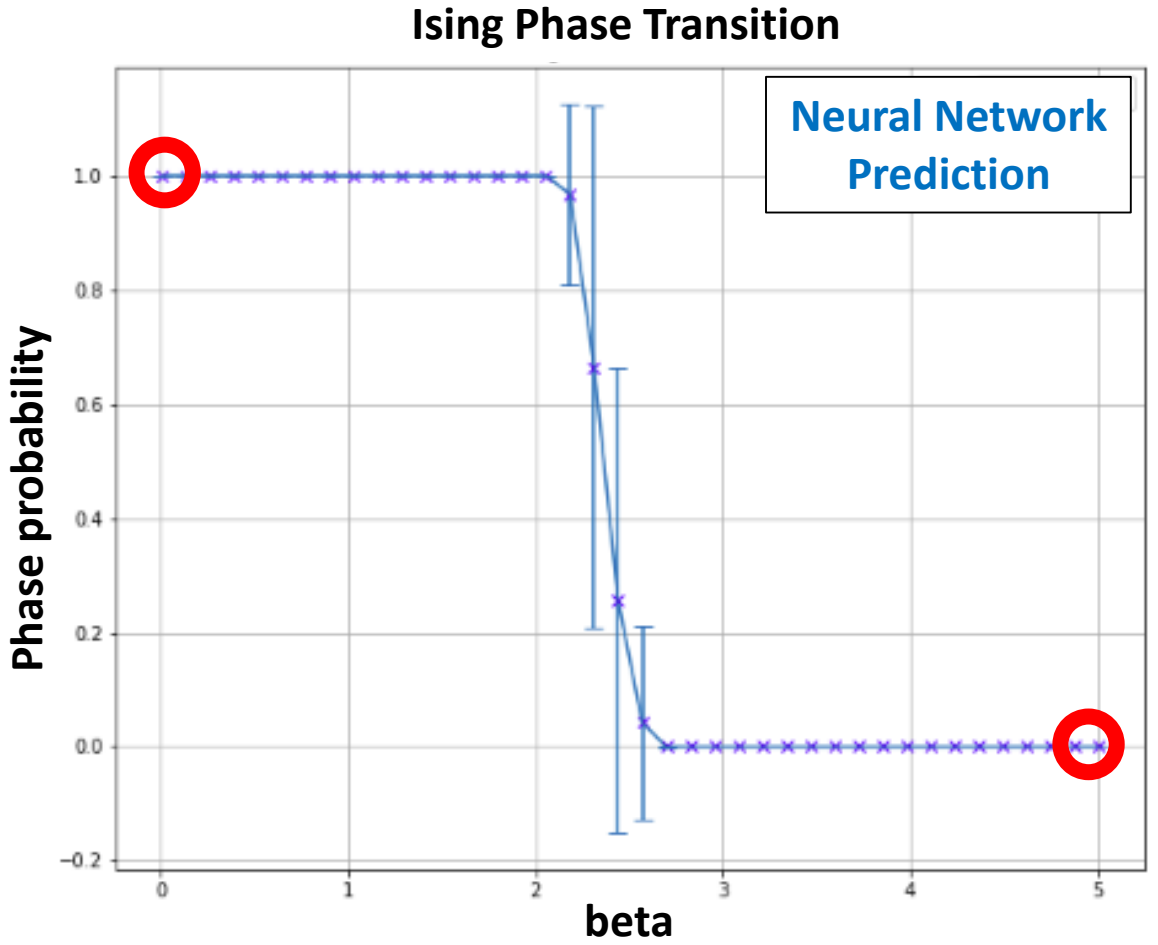
$$p_i - true\ labels,\ q_i\ - model\ predictions$$

- Optimization: RMSprop method



Ising Results





ML for 3+1 SU(2)

$$S[U] = \beta_{latt} \sum_x \sum_{\mu<v} Re\left(Tr\left(1 - U^x_{\mu v}\right)\right)$$

$$U^x_{\mu v} = U^x_\mu \, U^{x-\hat{\mu}}_v \, U^{x+\hat{\mu}+\hat{v}}_{-\mu} \, U^{x+\hat{v}}_{-\mu}$$

Order parameter: Polyakov Loop for $2x8^3$

$$L = \frac{1}{N} \sum_x \left| Tr\left(U^{0,\vec{x}}_\tau U^{1,\vec{x}}_\tau\right)\right|$$

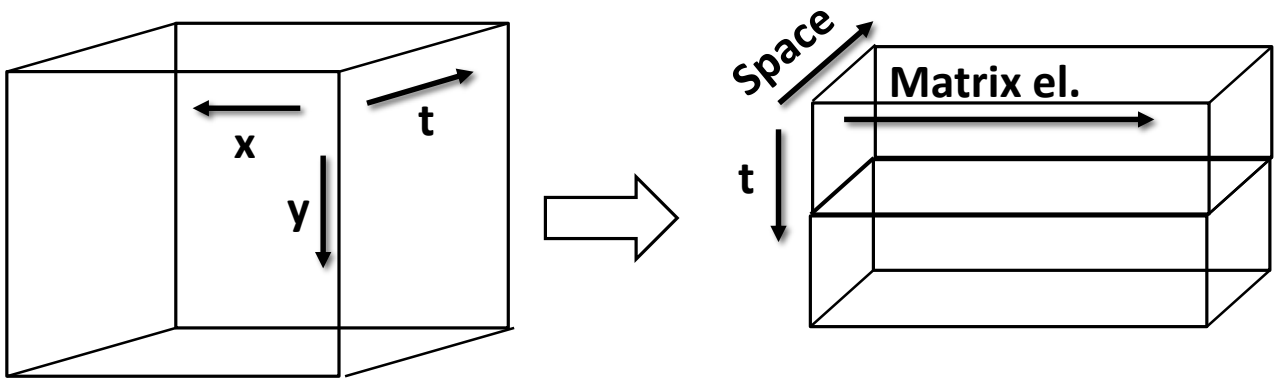
SU(2) matrix presentation:

$$\mathrm{U} = \begin{pmatrix} a+ib & k+iq \\ -k+iq & a-ib \end{pmatrix} \rightarrow (a,b,k,q)$$

Phase transition problems:

1. Trace of matrices is not trivial function.
2. Neural Network doesn't know matrix operations.
3. Separately the matrix elements do not feel the phase transition, only together.

To solve these problems we reshape our configurations and add internal matrix dimension.



Learning

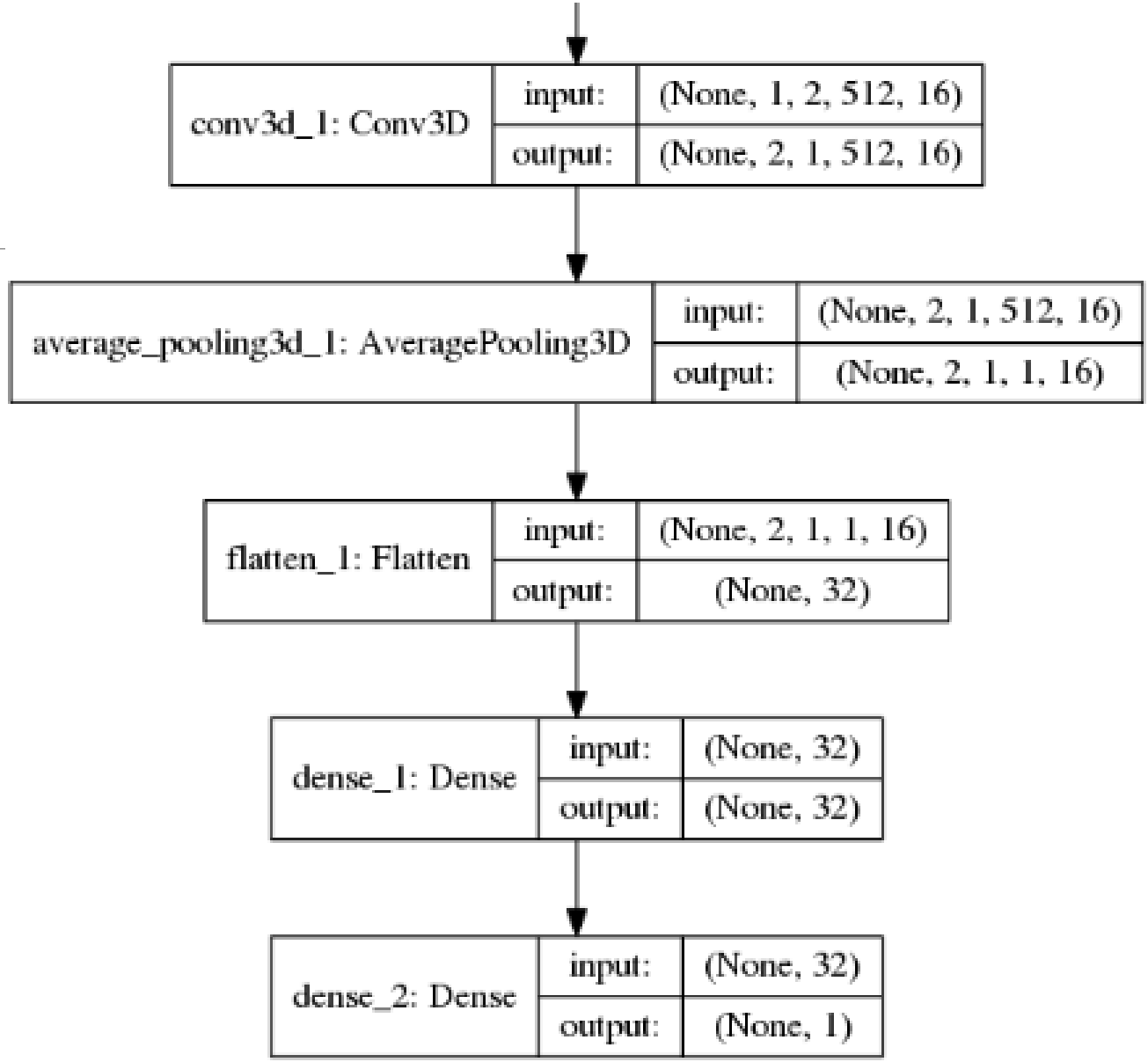
We solve binary classification problem to predict confinement and deconfinement phase.

Learning at:

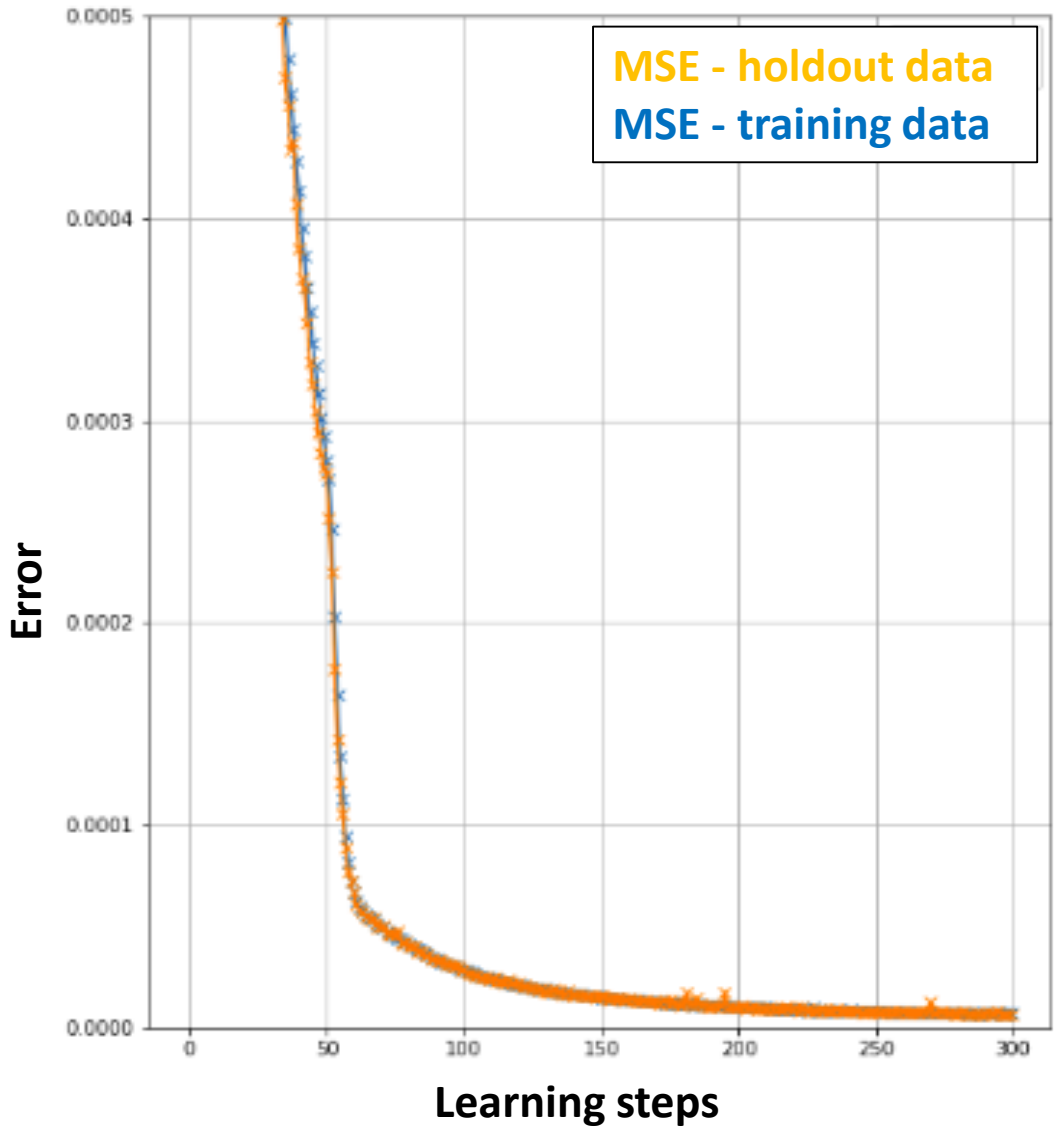
- 2x8x8x8 – lattice size
- 50000 conf. – confinement phase
- 50000 conf. – deconfinement phase

Prediction is the probability of one of the phases.

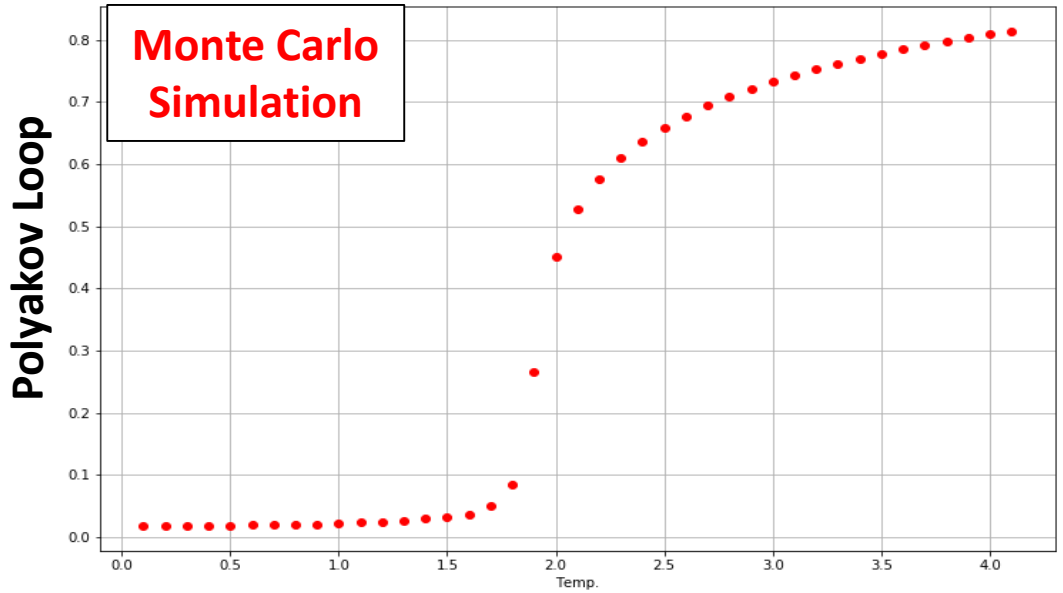
The mean squared error as loss function.

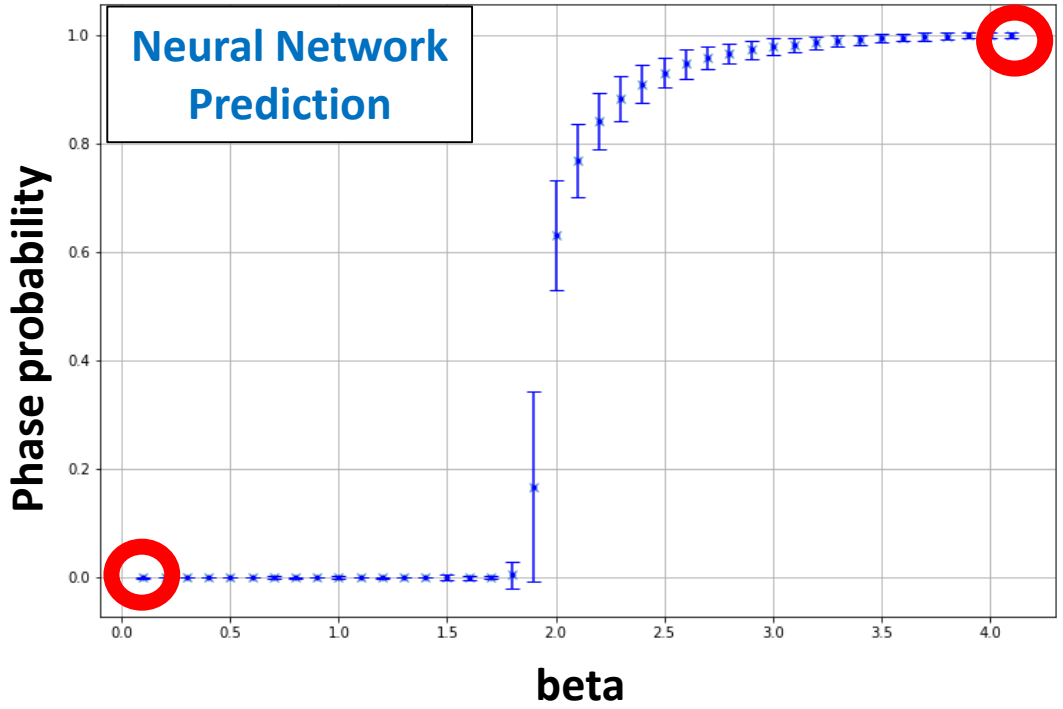


Learning process



SU(2) phase transition





Tasks for the future

1. Prediction of observables.
2. Other models where it is difficult to distinguish phases.
3. Unsupervised learning (the network itself predicts the number of phases).
4. Generation of Monte Carlo configurations with Machine Learning.
5. Application for SU(3).