Applying machine learning methods to prediction problems of lattice observables

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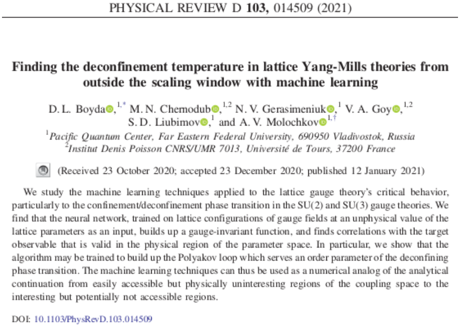
Introduction

In this project, we investigate the ability of a neural network to reconstruct gauge-invariant observables based on the analysis of a limited set of lattice configurations.

Outline:

- Introduction
- Machine learning tools
- Problems
- Realization of neural network
- Training process
- Results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Finding the deconfinement temperature in lattice Yang-Mills theories from outside the scaling window with machine learning

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We study the machine learning techniques applied to the lattice gauge theory's critical behavior, particularly to the confinement/deconfinement phase transition in the SU(2) and SU(3) gauge theories. We find that the neural network, trained on lattice configurations of gauge fields at an unphysical value of the lattice parameters as an input, builds up a gauge-invariant function, and finds correlations with the target observable that is valid in the physical region of the parameter space. In particular, we show that the algorithm may be trained to build up the Polyakov loop which serves an order parameter of the deconfining phase transition. The machine learning techniques can thus be used as a numerical analog of the analytical continuation from easily accessible but physically uninteresting regions of the coupling space to the interesting but potentially not accessible regions.

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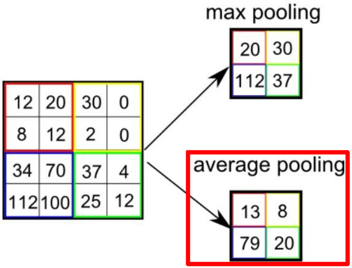
Introduction

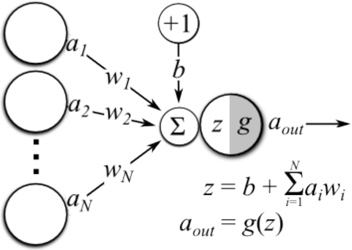
arXive	Title
1606.02318	Solving the Quantum Many-Body Problem with Artificial Neural Networks
1612.04262	An equation-of-state-meter of QCD transition from deep learning
1705.05582	Machine Learning of Explicit Order Parameters
1709.01971	Deep Learning Beyond Lefschetz Thimbles
1801.05784	Machine learning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

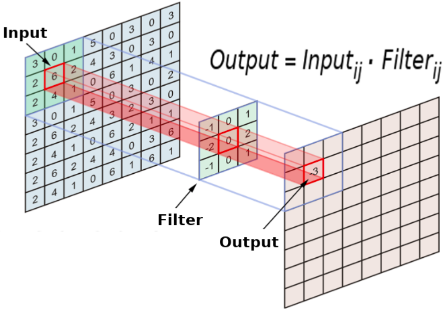
Main ideas:

- Speeding up calculation
- Searches of underline physics
- Applications where standard methods do not work

Machine learning tools

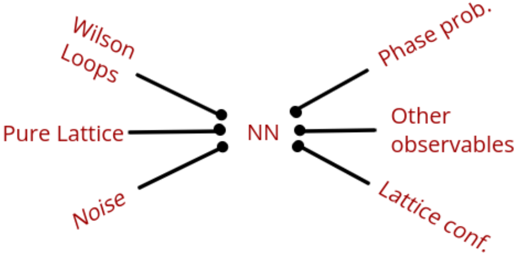


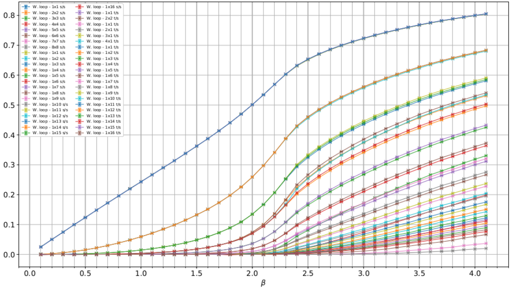




Machine learning tasks

- Prediction of phases
  (Classification task)
- Prediction of lattice observables
  (Regression task)
- Simulation of lattice configurations
  (Generation task)





Problems

Neural network problems:

- Matrices
- Gauge-invariant behavior of obsevables
- Interpretation of results

Explanation:

- $\begin{bmatrix} M \\ M \end{bmatrix} \rightarrow N.Network \rightarrow M + \Delta$
- $(\infty) \rightarrow N.Network \rightarrow Number$
- $Input \rightarrow (???) \rightarrow Output$

What to do?: Build a new type of gauge invariant neural network that itself can work in terms of matrices.
Another question: Will this neural network guarantee any approximation? (Universal approximation theorem)
BUT:
Is it possible to estimate behavior of observables?

Realization

We consider SU(2) and SU(3) gauge theories on lattice with Wilson action

$$S[U] = \beta \sum_{n,\mu>\nu} \left(1 - \frac{1}{N_c} Re\left[Tr\ U_{\mu\nu}(n)\right]\right)$$

Deconfinement order parameter

$$L = \frac{1}{N_s^3 N_c} \sum_n Tr \prod_{\mu_t=0}^{N_t-1} U_4(n+\hat{\mu}_t)$$

Transformation of SU(2) lattice elements

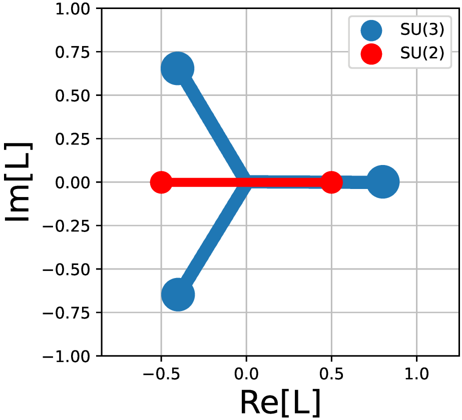
$$U = \begin{pmatrix} a_1 + ia_2 & a_3 + ia_4 \\ -a_3 + ia_4 & a_1 - ia_2 \end{pmatrix} \rightarrow \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix}$$

Layer		Structure
InputLayer	In	$(N_t = 2,\ N_s \times N_s,\ N_s,\ \text{Dim} \times \text{U})$
	Out	$(N_t = 2,\ N_s \times N_s,\ N_s,\ \text{Dim} \times \text{U})$
Conv3D	In	$(2,\ N_s \times N_s,\ N_s,\ \text{Dim} \times \text{U})$
	Out	$(1,\ N_s \times N_s,\ N_s,\ 16)$
Av.Pool.3D + Flatten	In	$(1,\ N_s \times N_s,\ N_s,\ 16)$
	Out	(16)
Dense	In	(16)
	Out	(1)

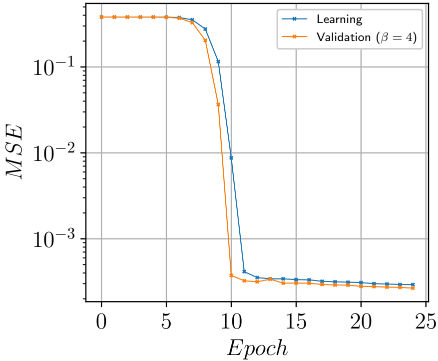
InputLayer	In	$(N_t = 4,\ N_s \times N_s,\ N_s,\ \text{Dim} \times \text{U})$
	Out	$(N_t = 4,\ N_s \times N_s,\ N_s,\ \text{Dim} \times \text{U})$
Conv3D	In	$(4,\ N_s \times N_s,\ N_s,\ \text{Dim} \times \text{U})$
	Out	$(2,\ N_s \times N_s,\ N_s,\ 256)$
Conv3D	In	$(2,\ N_s \times N_s,\ N_s,\ 256)$
	Out	$(1,\ N_s \times N_s,\ N_s,\ 32)$
Av.Pool.3D + Flatten	In	$(1,\ N_s \times N_s,\ N_s,\ 32)$
	Out	(32)
Dense	In	(32)
	Out	(1)

Training process

An important feature of neural network training is the use of data from all vacuums!

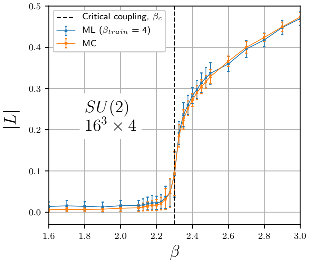


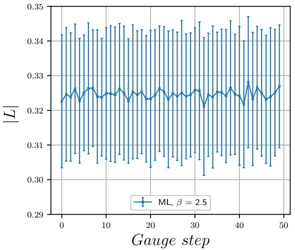
Number of epoch depend on theory and lattice size.

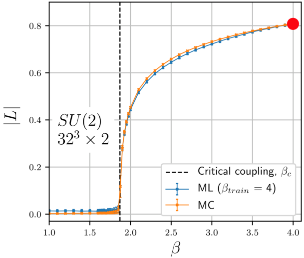


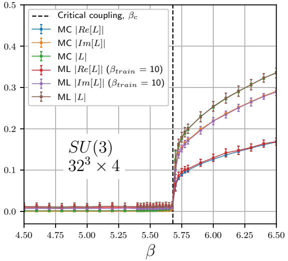
Learning curve for SU(2) 4×16^3

Results









Lattice sizes:

$N_s = 8, 16, 32$

$N_t = 2, 4$

Training:

9000 conf., $\beta_{SU(2)} = 4$

9000 conf., $\beta_{SU(3)} = 10$

Prediction:

100 conf., $\beta_{SU(2)} < 4$

100 conf., $\beta_{SU(3)} < 10$

Conclusion

Summarizing:

- We have chosen the training point far away from the critical region at a very weak coupling in the SU(2) and SU(3) lattice gauge theories.
- We show that numerically constructed order parameter recovers the critical behavior of the system in the physical region.
- After training process, we check that machine-learning algorithm restore a gauge-invariant order parameter.