Machine learning approaches to the QCD transition

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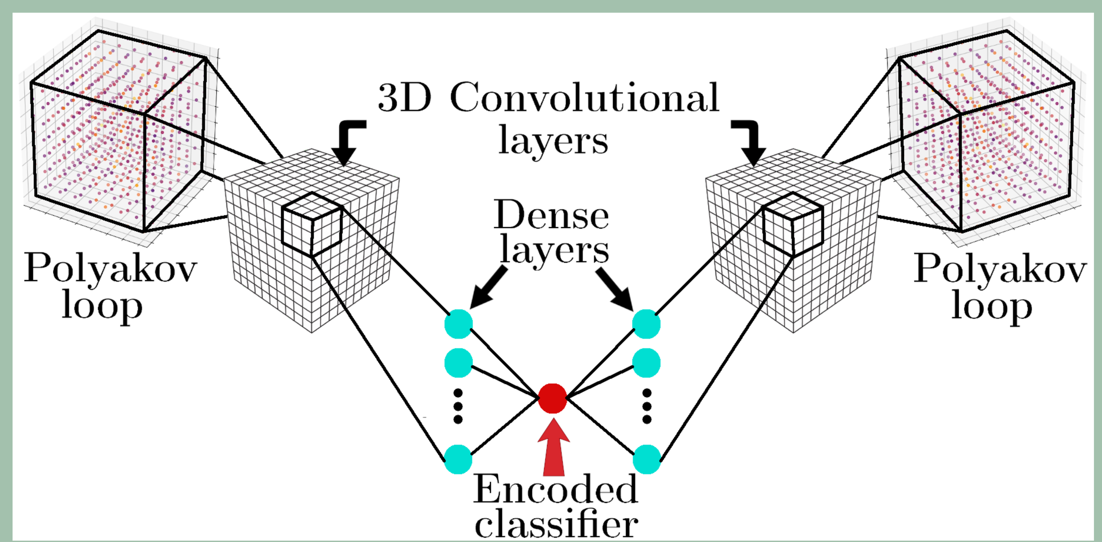
Abstract

We study the high temperature transition in pure SU(3) gauge theory and in full QCD with 3D-convolutional neural networks trained as parts of either unsupervised or semi-supervised learning problems. The code used is available [1].

Method

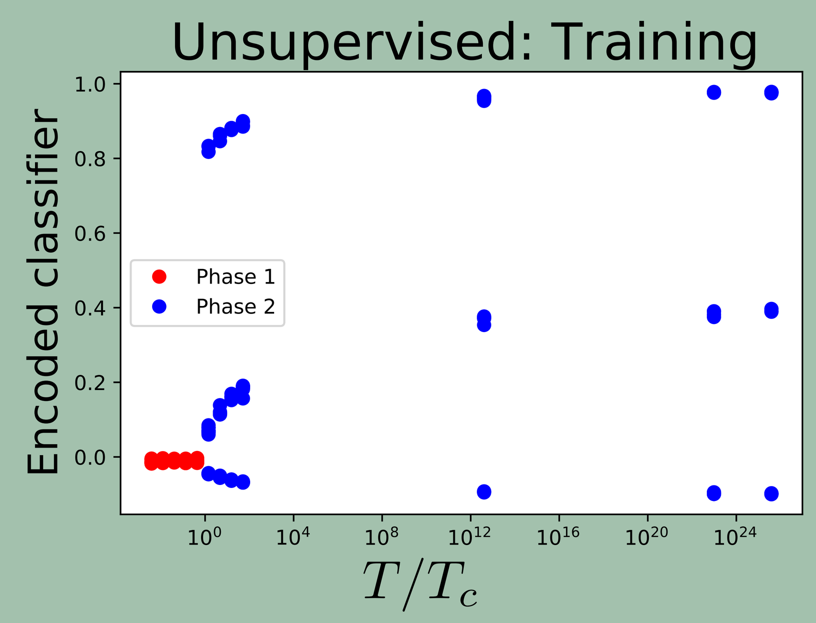
We build 3D-convolutional autoencoders to classify Polyakov loops configurations at different temperatures using TensorFlow and Keras. An autoencoder is a compound of two neural networks: an encoder that reduces the input information, for example to a single number, and a decoder, which reconstructs the input data from the compressed data. Here, the encoder processes the information contained in the Polyakov loops configuration to a single number, named **Encoded classifier** (see Figure below).

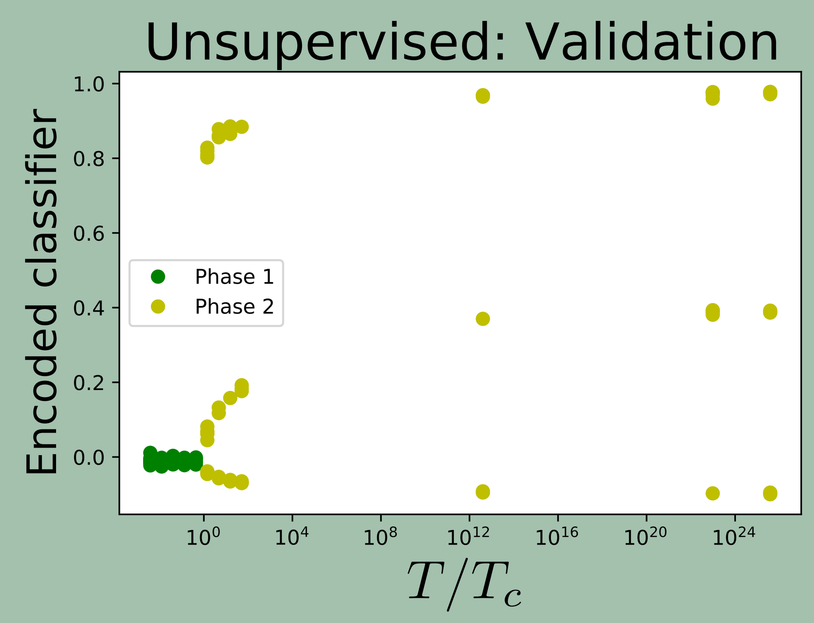


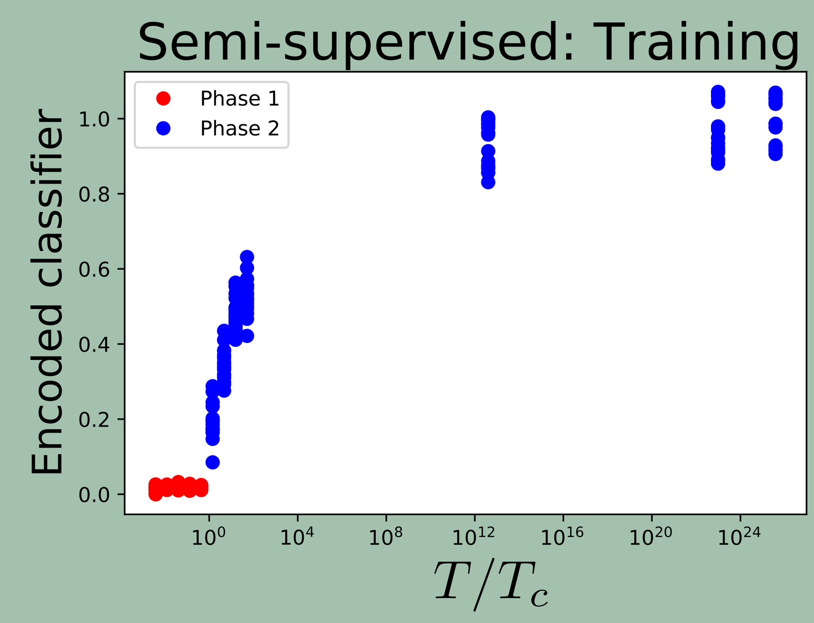
The autoencoder is trained, as a whole, to reproduce as output its own input. When this is achieved, the encoded classifier effectively "encodes" the most important feature(s) describing the variety of the input. The mapping of the input to the encoded classifier, however, can be arbitrarily complicated and impossible to read for humans. To address this problem, one can perform a "semi-supervised" training by pinning some of the input configurations at extreme temperatures to predefined labels. In such a scheme, the unlabelled configurations similar to those pinned somewhere in the latent space, are clustered together, defining a human-understandable "meaning" for the encoded space. Assuming lattice configurations simulated at different temperatures are mainly distinguished by their degree of disorder, an autoencoder may provide an effective order parameter for an arbitrary lattice configuration, independently of the underlying theory.

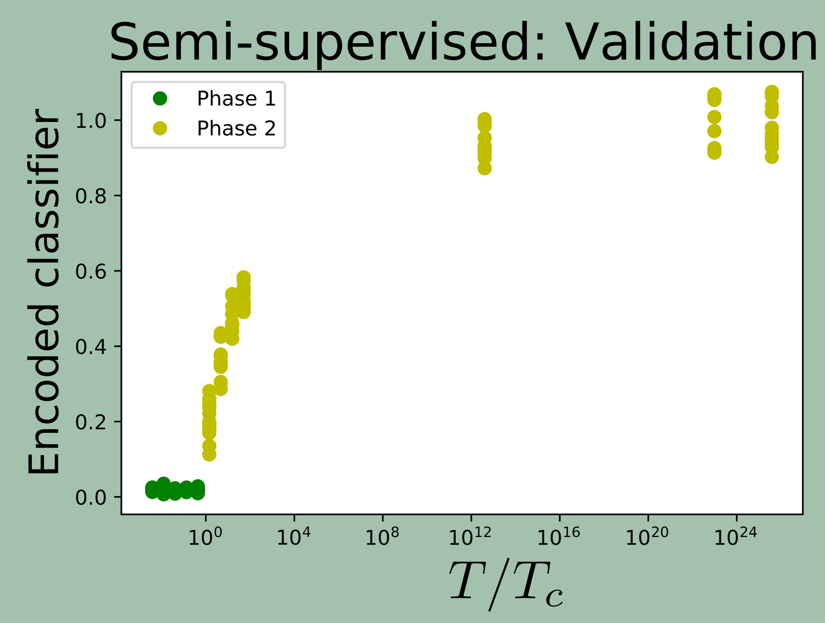
Pure $SU(3)$ gauge theory

In the case of pure $SU(3)$ gauge theory, the mean Polyakov loop is an exact order parameter for confinement. We study $8^3 \times 4$ lattice configurations generated using the MILC public code [2]. Training the autoencoder as an unsupervised and semi-supervised classification problem we obtain an encoded classifier clearly related to the order parameter. Indeed, two classes are identified by the encoded classifier below and above T_c. The unsupervised scheme highlights the $\mathbb{Z}_3$ symmetry breaking, while the semi-supervised training strengthens the correlation of the encoded classifier with the order parameter.



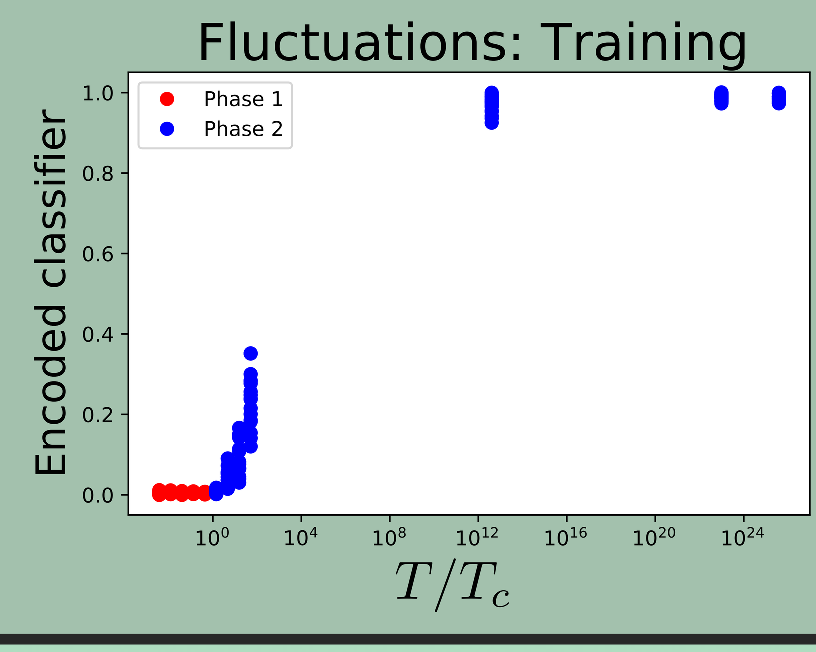


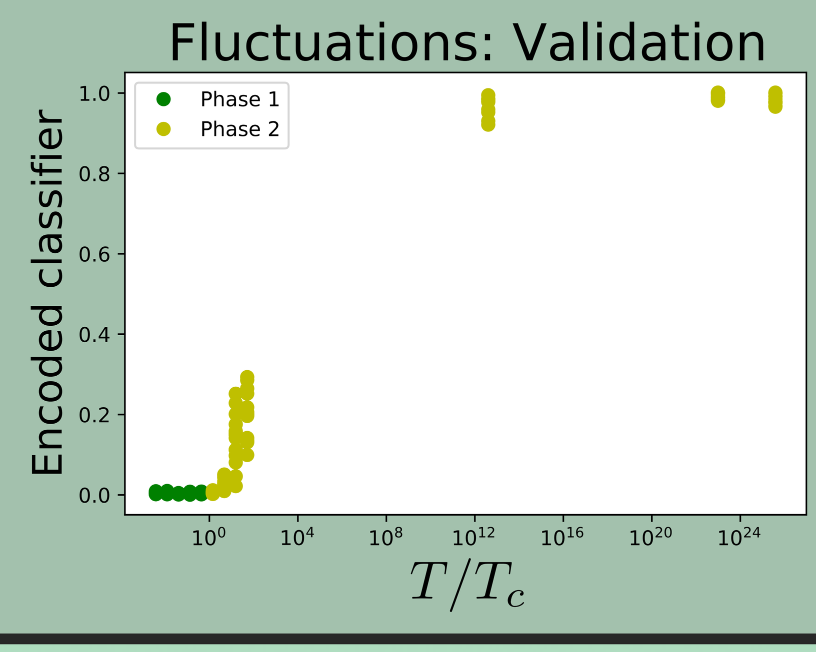




Standardized Polyakov loop

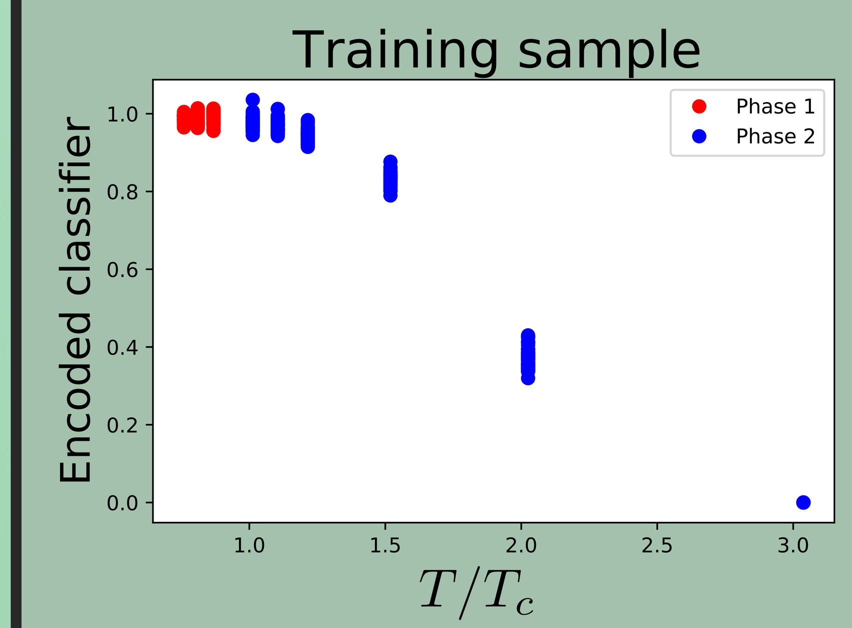
In order to ensure that the network is learning from the texture on the lattice rather than simply averaging the Polyakov loops on each simulation, we define a standardized Polyakov loop. Being μ_i the mean value of the i-th Polyakov loop configuration $P^{(i)}$, $\sigma_i = \sqrt{\sum_{abc} |P^{(i)}{}_{abc} - \mu_i|^2 / 2 \times 8^3}$ the components of the i-th standardized configuration are: $\tilde{P}^{(i)}_{abc} = (P^{(i)}_{abc} - \mu_i)/\sigma_i$.
Despite a slight loss in precision, the network is still perfectly able to identify the presence of a phase transition at $T \sim T_c$.

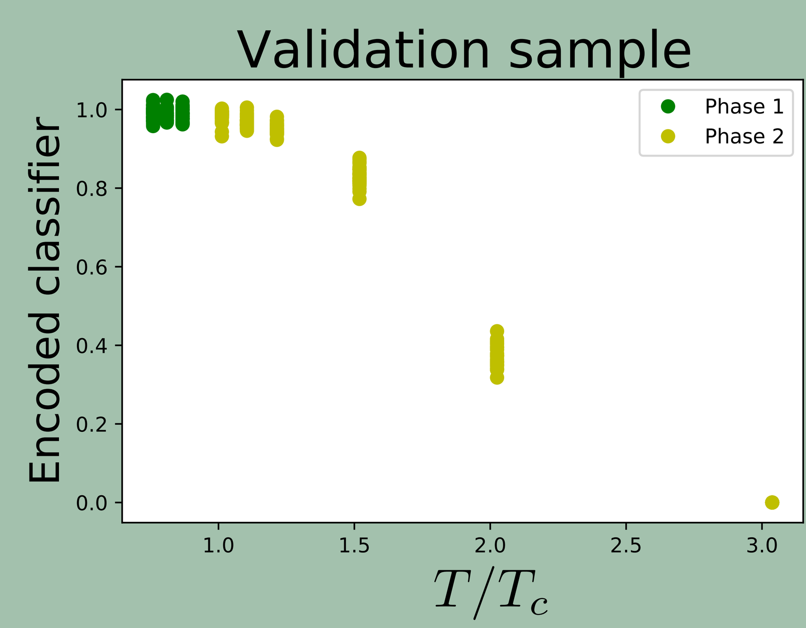


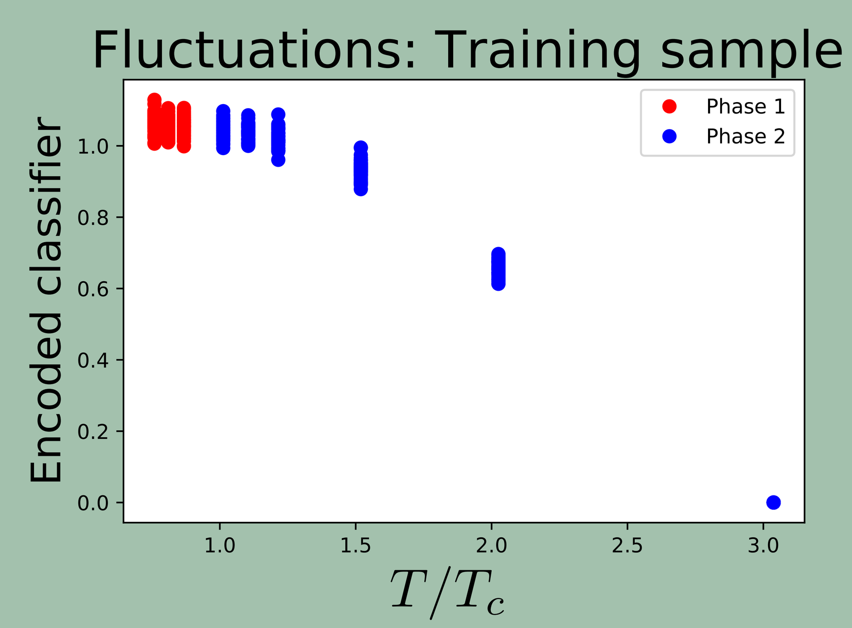


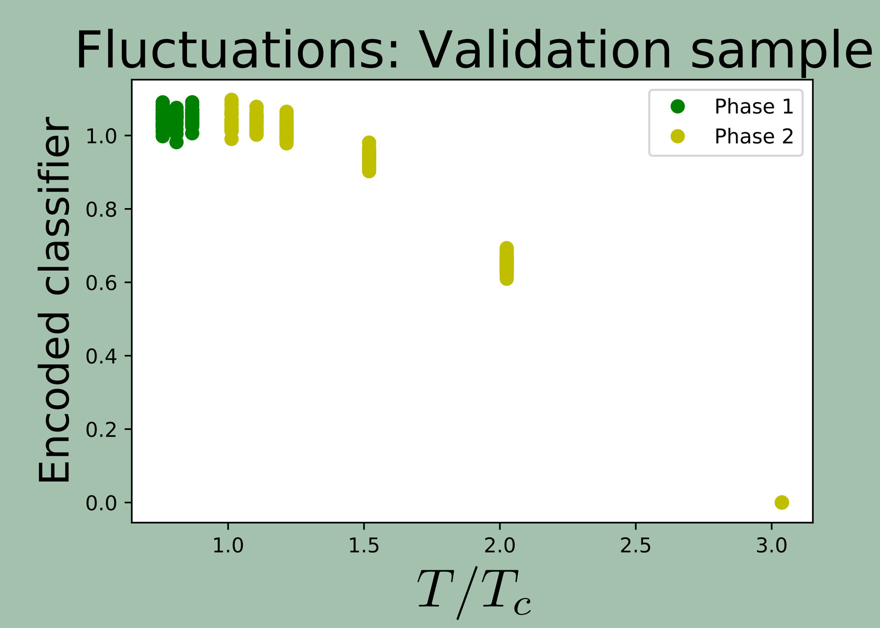
Quantum Chromodynamics

In the case of QCD, the Polyakov loop is no longer an order parameter. The full QCD configurations are from simulations of $N_f = 2+1+1$ Wilson fermions at maximal twist on a lattice of 32^3 space dimension [3]. We study the semi-supervised problem with the Polyakov loop and its standardized version. The distinction of the two classes appears close to the critical temperature.









Conclusion

We probed the capability of Convolutional Neural Networks trained as either unsupervised or semi-semisupervised classifiers to identify different phases of gauge theories. We observe a crossover between the two phases at the expected temperature in a pure gauge theory and a qualitatively similar behavior in full QCD. A finer temperature scan, finite-size scaling and continuum limit will improve the performance of the autoencoder, providing further insight into ML approaches to the study of phase transitions.

References

[1] Repository github.com/AndrePalermo/ML-lattice doi.org/10.5281/zenodo.5082561

[2] MILC collaboration's public lattice gauge theory code. *http://physics.utah.edu/ detar/milc.html.*

[3] F. Burger, E. M. Ilgenfritz, M. P. Lombardo and A. Trunin, Phys. Rev. D **98** (2018) no.9, 094501