Fast Detection of Phase Transitions with Multi-Task Learning-by-Confusion

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github.com/multitaskLBC

Abstract

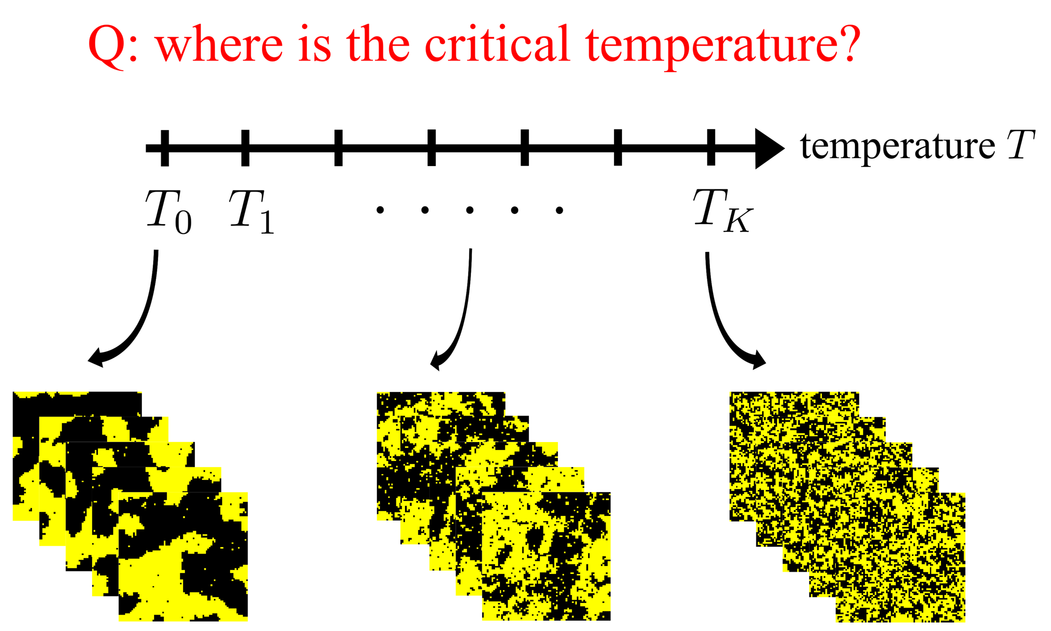
The characterization of phases of matter and the study of critical phenomena are of great importance in physics. One of the most popular machine learning methods for the data-driven detection of phase transitions is *Learning-By-Confusion* [1]. Up to now, for a given system it was necessary to train a binary classifier for each tentative position of the phase transition in parameter space.

In this work [2], we propose a faster implementation based on a multi-tasking approach where only a single classifier must be trained. Moreover, by revealing structure in the output images of the Stable Diffusion model, we demonstrate its application beyond physics.

Detection of Phase Transitions from Data

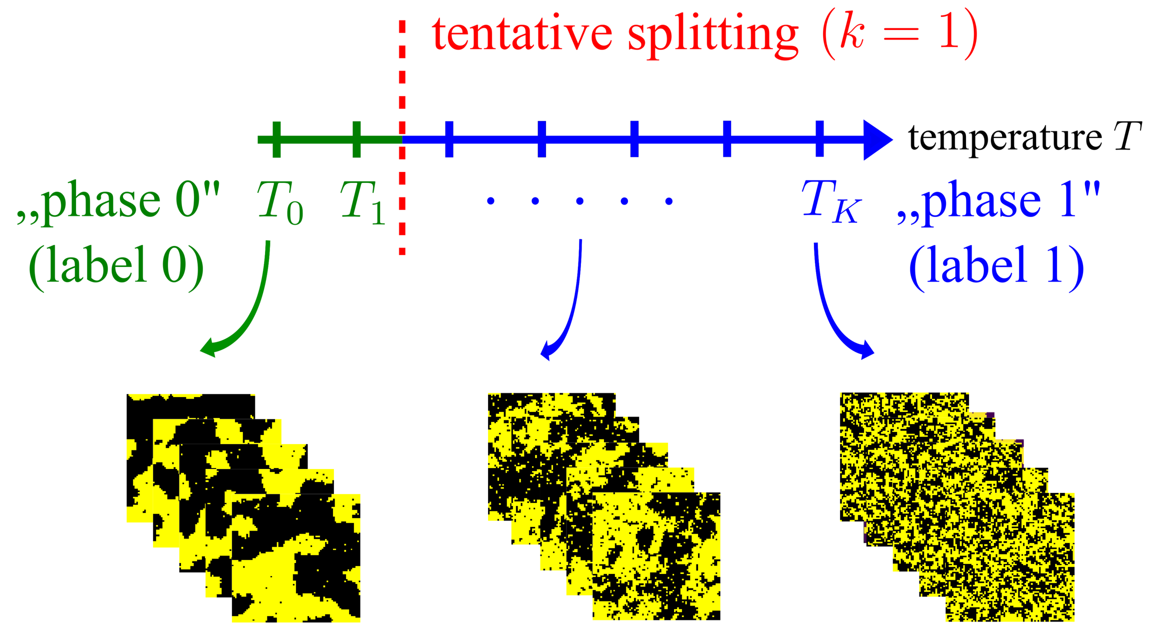
Setup and Task:

- The system can occupy a multitude of states & the probability of each state depends on a parameter such as temperature T. Prototypical example: Ising model.
- Given: Samples $\boldsymbol{x}$ randomly drawn at different temperatures. Task: Find the critical temperature where the system transitions from one state to another.



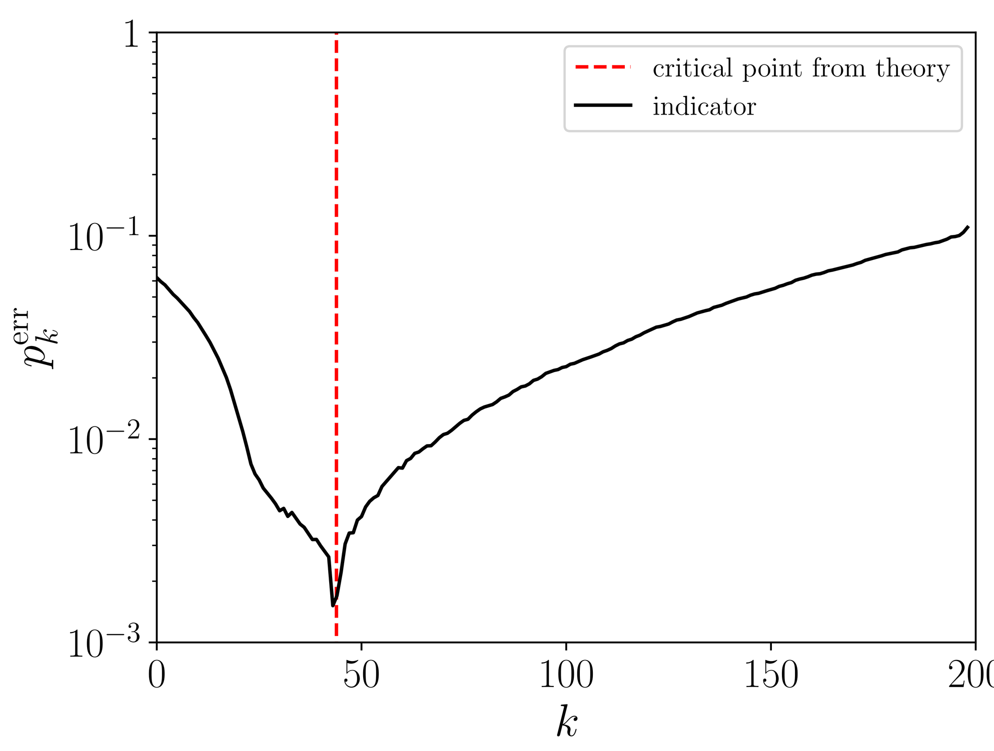
Learning-by-Confusion Algorithm [1]:

- Pick a tentative candidate for the critical temperature T_k and label the samples with the resulting phase.
- Train a binary classifier on this data and evaluate its error rate p_k^{err}.
- Repeat for every possible splitting $k \in [0, K-1]$ of the parameter space.



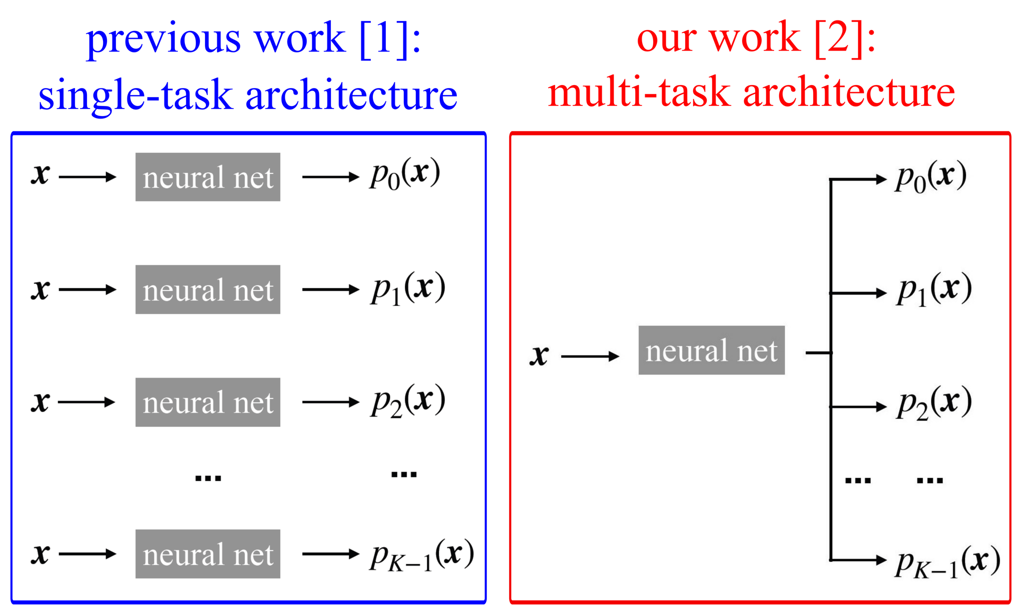
Result:

- The candidate for the critical temperature that resulted in the lowest error rate for the classifier corresponds to a splitting where the two sets are most distinguishable. This is your best guess for the critical temperature.



Multi-Task Architecture

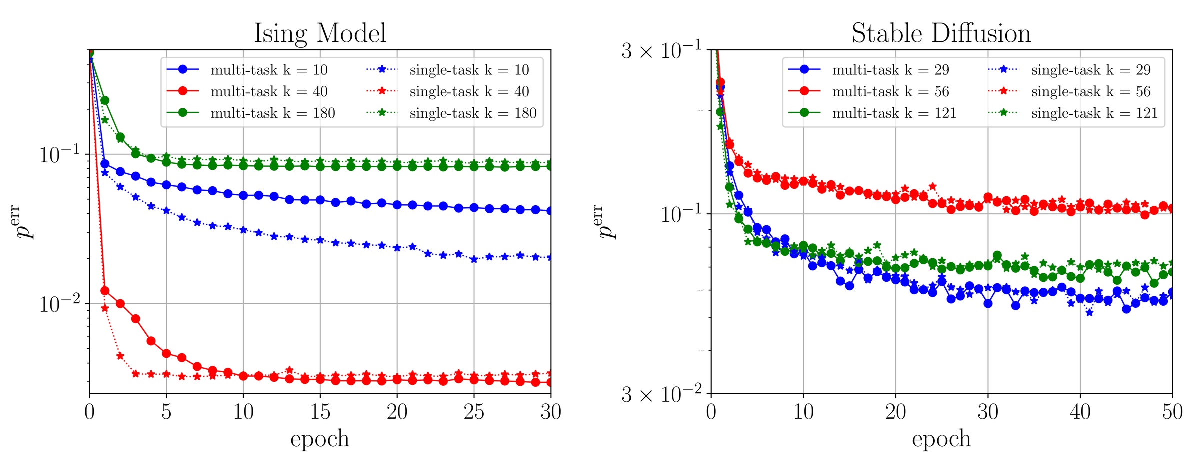
Multi-Task Approach: Train a *single* multi-class classifier on all possible splittings simultaneously instead of a distinct binary classifier for each possibility, which would correspond to the single-task approach.



- Multi-tasking is efficient because the K classification tasks are very similar:
- They only differ in the tentative splitting of parameter space making the learned features highly transferable between tasks.
- Implementation at **github.com/multitaskLBC**.

Benchmark

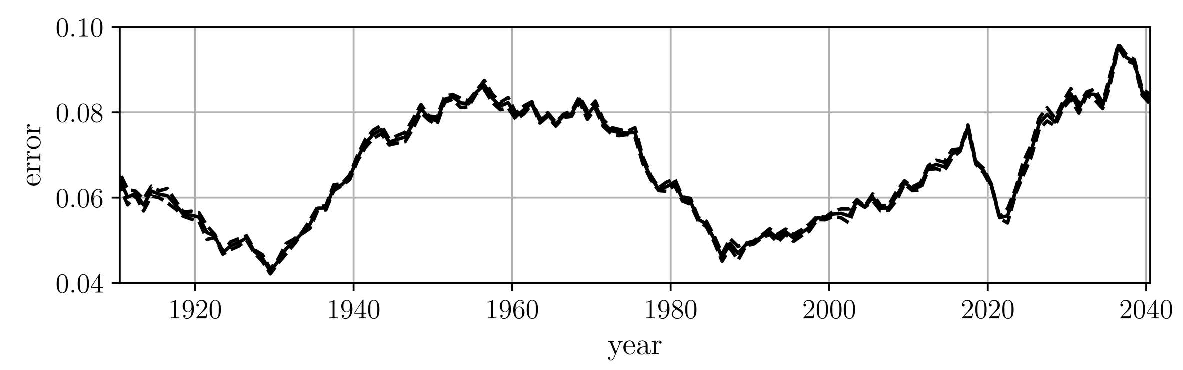
The overhead in the number of training epochs of multi-task approach compared to single-task approach is mostly negligible.



Result on Stable Diffusion Dataset

Change point detection in Stable Diffusion dataset. Here, no prior theory is available to predict the location of transition points.

Prompt with variable T:
"Technology of the year T"



References

[1] E.P.L. Van Nieuwenburg, Y.-H. Liu, and S.D. Huber, Nat. Phys. **13**, 435–439 (2017)

[2] J. Arnold, F. Schäfer, and N. Lörch, arXiv:2311.09128 (2023) and github.com/multitaskLBC

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