# Machine Learning and Histogram Reweighting: Detecting and Studying Phase Transitions

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Joint work with Profs. Gert Aarts and Biagio Lucini.

# What is a neural network, really?

Could it be..

# What is a neural network, really?

Could it be..

# ..an observable in a statistical system?

## Supervised Machine Learning for Phase Identification

In a supervised framework we can train a **machine learning algorithm** on a set of **training data**, to learn a **function f(·)** that separates the **symmetric** and the **broken-symmetry** phases of a system.

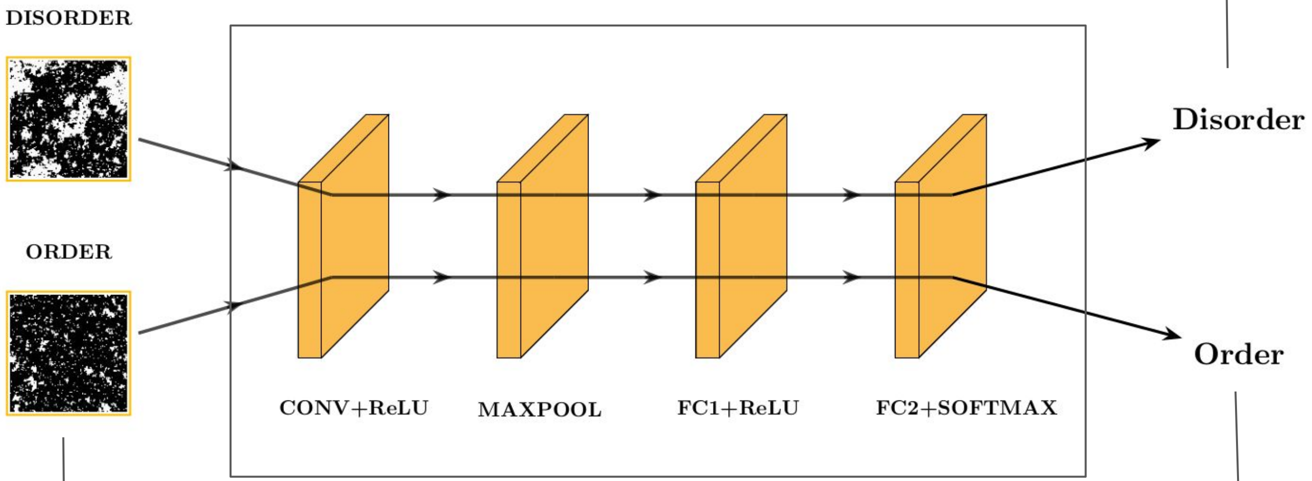
# Machine Learning:

**Training of a convolutional neural network on the Ising model:**

Labeled as 1.

Labeled as 1.

f(x)

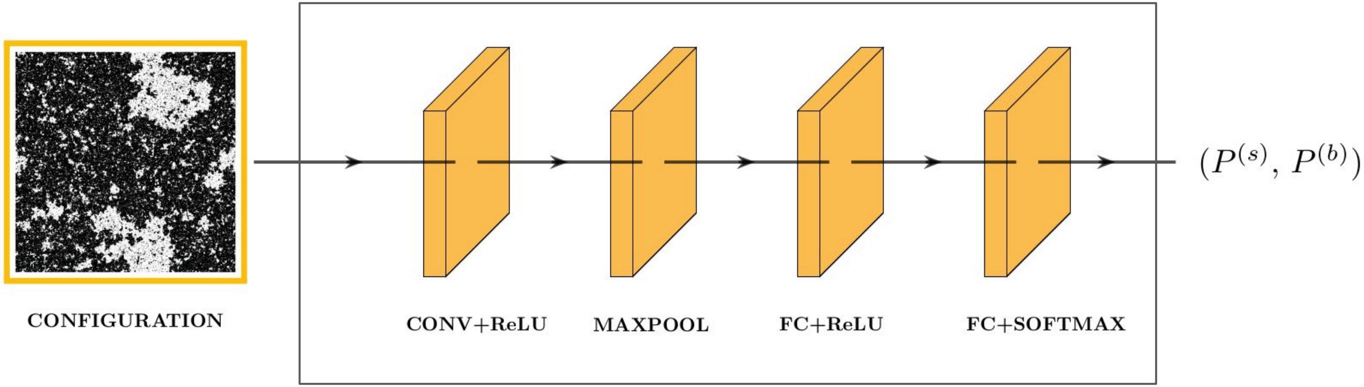



Labeled as 0.

Labeled as 0.

# Machine Learning:

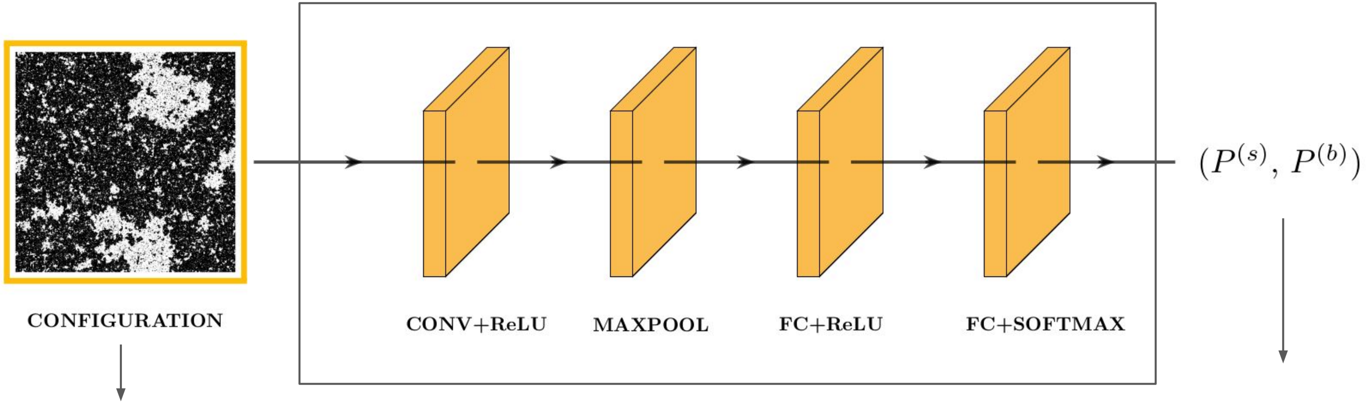
**Predicting the phase of a configuration:**




f(x)

Machine Learning:

**Predicting the phase of a configuration:**




The configuration is **importance-sampled** so it has an **attached Boltzmann weight**.

f(x)

The output is calculated on an **importance-sampled** configuration so it must have the **same Boltzmann weight**.

## Machine Learning:

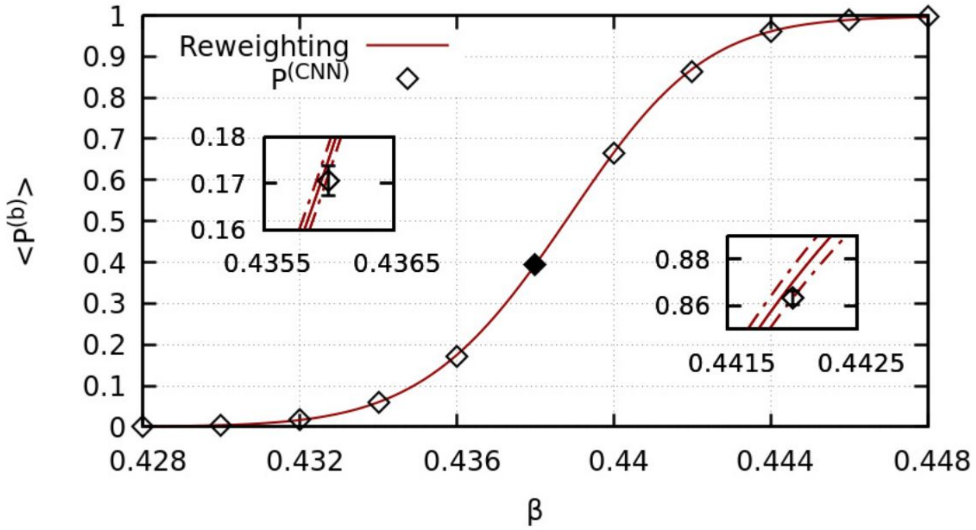
The **output probability** is an **observable** in the system:

$$\langle P \rangle = \frac{\sum_\sigma P_\sigma \exp[-\sum_k g^{(k)} S_\sigma^{(k)}]}{\sum_\sigma \exp[-\sum_k g^{(k)} S_\sigma^{(k)}]}$$

The **output probability** can therefore be **reweighted** to different parameters through **histogram reweighting** (e.g. inverse temperatures in the Ising model):

$$\langle P \rangle_\beta = \frac{\sum_{i=1}^{N} P_{\sigma_i} \exp\left[-(\beta - \beta_0) E_{\sigma_i})\right]}{\sum_{i=1}^{N} \exp\left[-(\beta - \beta_0) E_{\sigma_i}\right]}$$

# Machine Learning:




Training was conducted below β=0.41 and above β=0.47

**Red line**: obtained using reweighting from a single dataset at β= 0.438 (filled point)

**Empty points**: Actual calculations of the neural network on independent Monte Carlo datasets.

Does it look like an effective order parameter?

# Phase Transitions:

When $\beta \cong \beta_c$ and $\xi \sim L$ **finite size effects** dominate and fluctuations, such as the magnetic susceptibility, have **maximum** values in the critical region:

$$\chi = \beta V(\langle m^2 \rangle - \langle m \rangle^2)$$

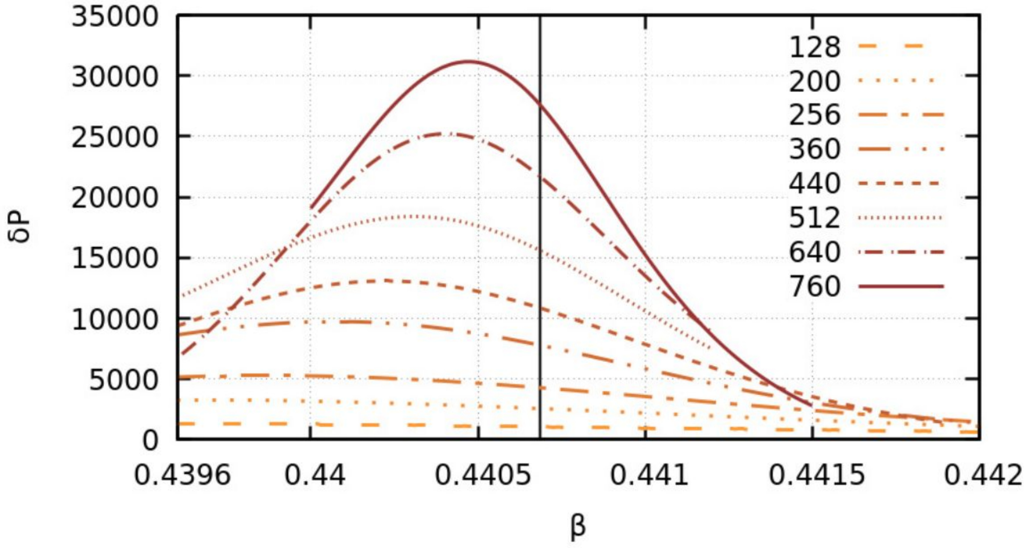
These maximum values converge to the **inverse critical temperature** in the thermodynamic limit:

$$\lim_{L \to \infty} \beta_c^{\chi} = \beta_c$$

**Question**: How do the fluctuations of the neural network output probability behave?

$$\delta P = \beta V(\langle P^2 \rangle - \langle P \rangle^2)$$

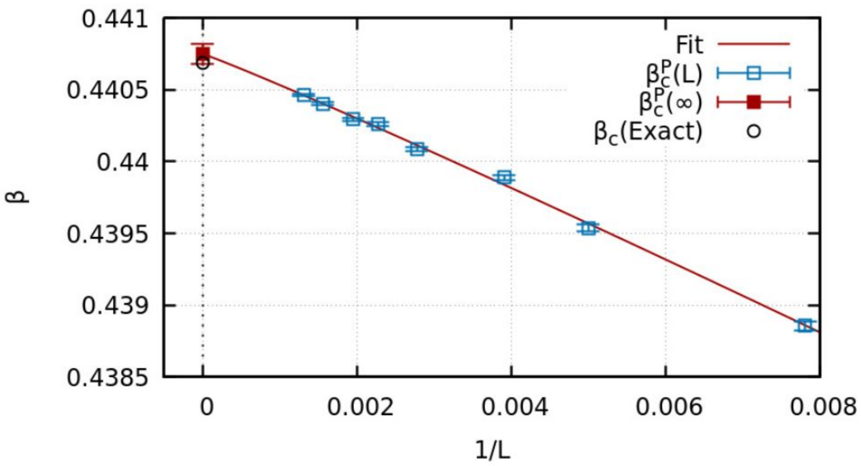
# Phase Transitions:

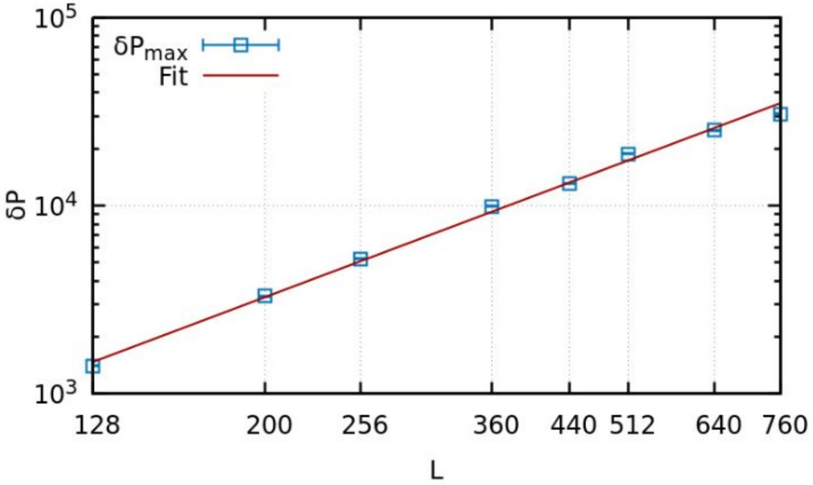



$$\delta P = \beta V(\langle P^2 \rangle - \langle P \rangle^2)$$

# Phase Transitions:

Results obtained by quantities derived entirely from the neural network




$$|t| = \left|\frac{\beta_c - \beta_c(L)}{\beta_c}\right| \sim \xi^{-\frac{1}{\nu}} \sim L^{-\frac{1}{\nu}}$$

$$\delta P \sim L^{\frac{\gamma}{\nu}}$$

| | $\beta_c$ | $\nu$ | $\gamma/\nu$ |
|---|---|---|---|
| CNN+Reweighting | 0.440749(68) | 0.95(9) | 1.78(4) |
| Exact | $\ln(1+\sqrt{2})/2$ | 1 | 7/4 |
| | $\approx 0.440687$ | | =1.75 |

## **Discovering Phase Transitions**

The function f(·) was learned on configurations of the Ising model.

f(x) can successfully predict the phase of Ising configurations x.

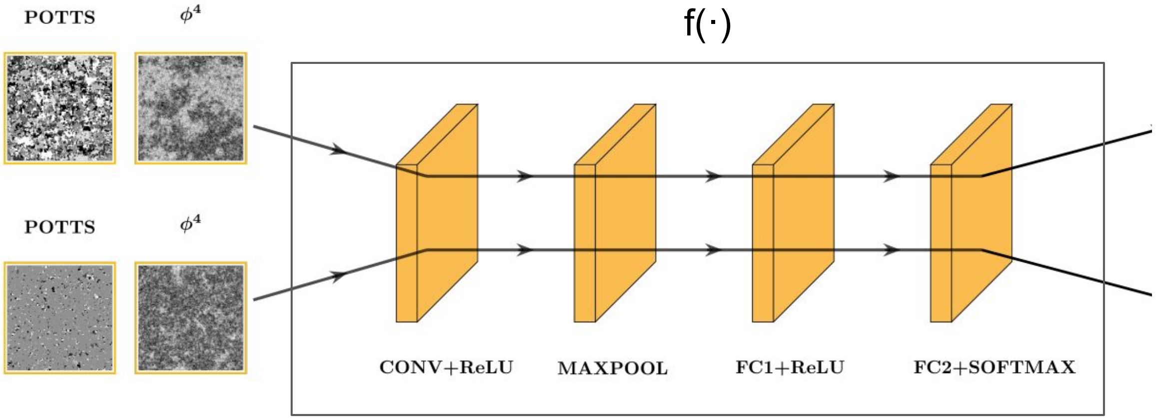
**But what happens if we give configurations x’ of a different system as input to the Ising-learned function f(·)? Can we accurately separate phases in different systems? Can we discover a phase transition through f(x’)?**

# Machine Learning

**Equivalently:**

Learned on Ising configurations

f(·)

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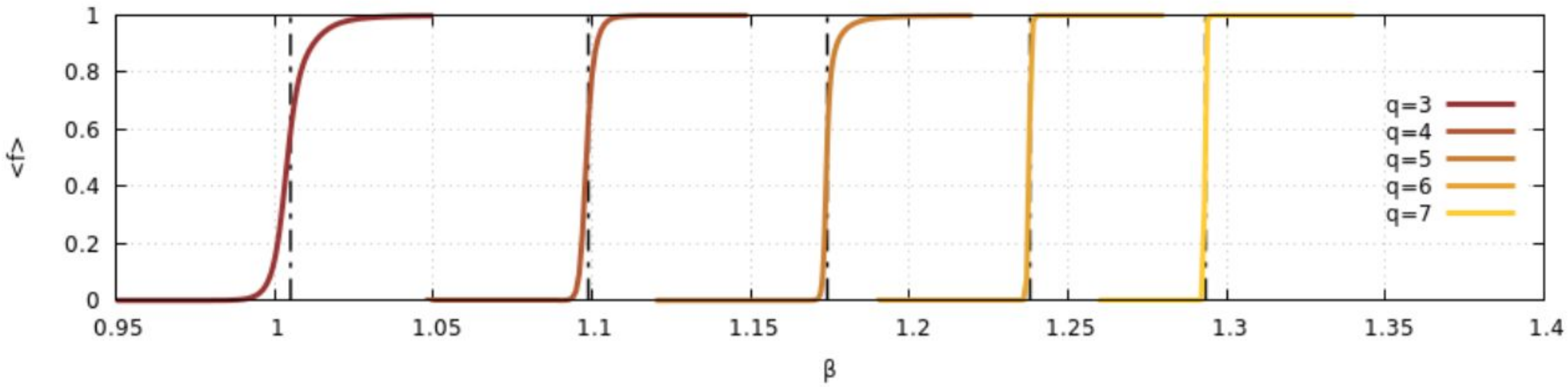
# Machine Learning

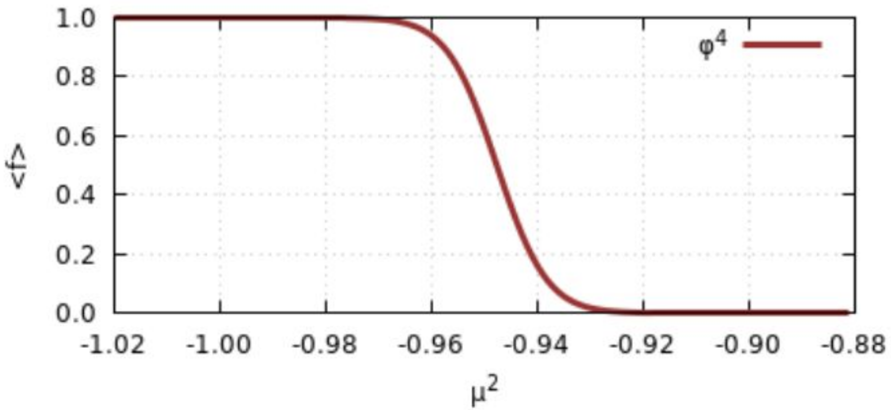
**Potts models:**




**Results obtained through a function f learned exclusively on the Ising model.**
**No knowledge about the presence of a phase transition in the new system is required.**

# Machine Learning

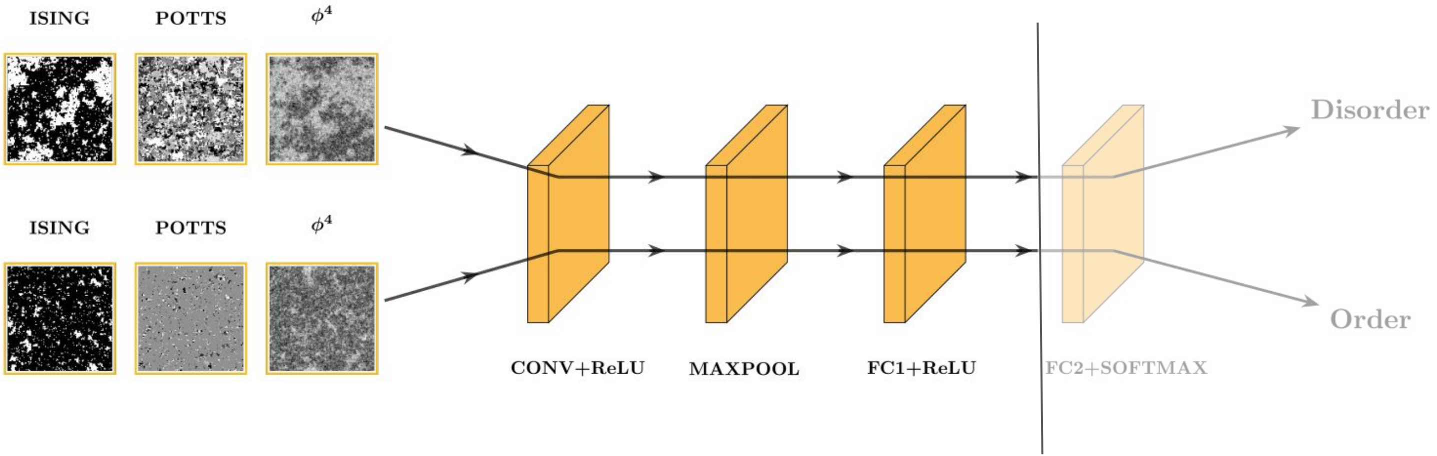
## $\varphi^4$ scalar field theory:




**Fixed dimensionless λ=0.7 and varied the dimensionless mass $\mu^2$**

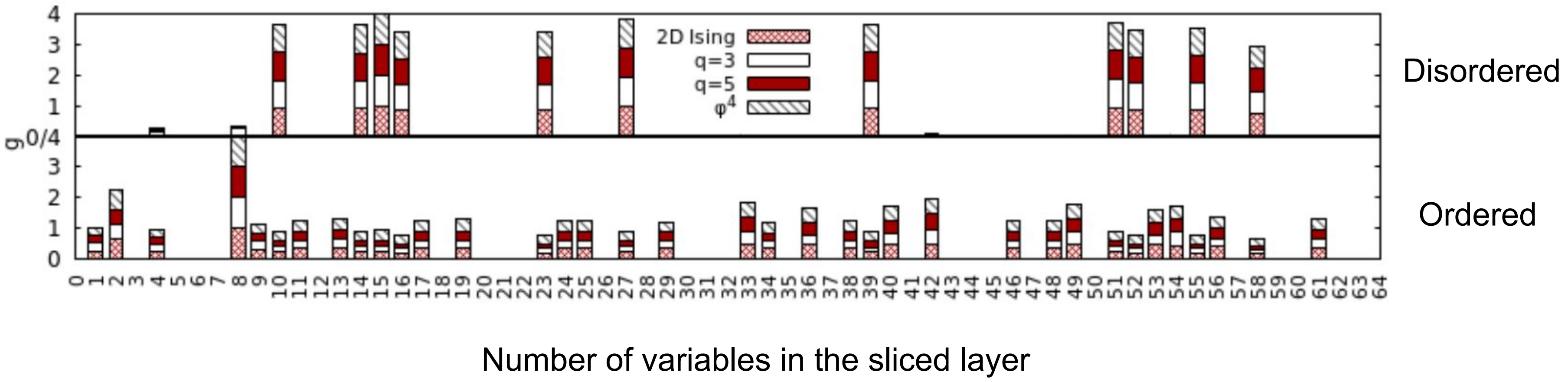
**Results obtained through a function f learned exclusively on the Ising model.**
**No knowledge about the presence of a phase transition in the new system is required.**

**Further insights on the results:**



# Machine Learning

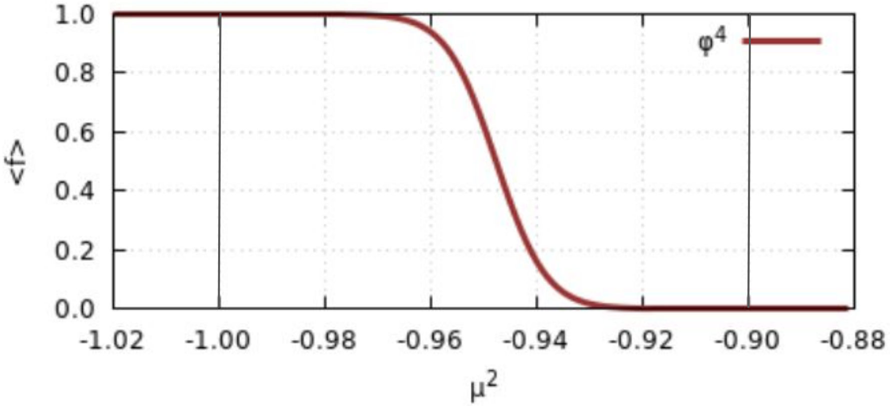
**Further insights on the results:**



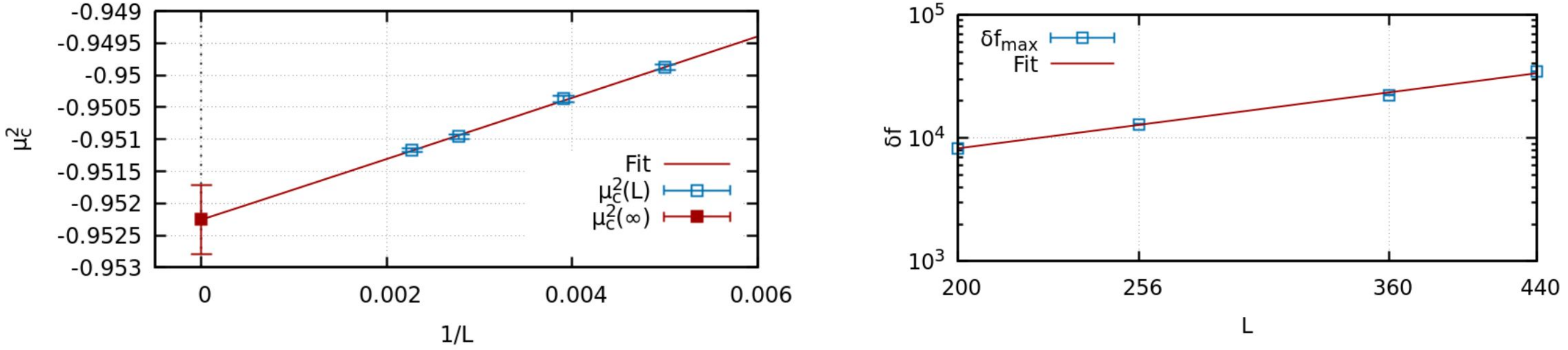

**Similar variables get spiked for configurations in disordered phase (top) and ordered phase (bottom), irrespective of the system.**

**$\varphi^4$ scalar field theory:**

**We didn't include any knowledge about the presence of a phase transition in this system so we have now obtained the knowledge of its critical region. We can therefore study it.**



# Machine Learning




| | $\mu_c^2$ | $\nu$ | $\gamma/\nu$ |
|---|---|---|---|
| CNN+Reweighting | -0.95225(54) | 0.99(34) | 1.78(7) |

TABLE II. Critical $\mu_c^2$ for fixed $\lambda_L = 0.7$ and critical exponents of the $\phi^4$ scalar field theory.

# Discussion

1. We can discover phase transitions using functions learned on simple well-studied systems.
2. We can build effective order parameters with no explicit information introduced about the Hamiltonian during the training of the neural network. The approach can be used when an order parameter isn't known.
3. We can use reweighting on machine-learning devised observables to explore the parameter space and increase precision during infinite-volume limit calculations.

## Presentation based on:


- D. Bachtis, G. Aarts, and B. Lucini, Extending Machine Learning Classification Capabilities with Histogram Reweighting, arXiv:2004.14341.
- D. Bachtis, G. Aarts, and B. Lucini, A Mapping of Distinct Phase Transitions to a Neural Network, arXiv:2007.00355.



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Thank you for your attention!