Machine learning and the inverse renormalization group

Dimitrios Bachtis

Phase transitions in particle physics

Event at Galileo Galilei Institute

Mar 28, 2022 - Apr 01, 2022

Outline

1) **Interpretation of machine learning functions as physical observables:**
   a) How to construct effective order parameters with machine learning.
   b) How to reweight machine learning functions in parameter space.
   c) How to discover unknown phase transitions with machine learning.
   d) How to include machine learning functions within Hamiltonians to induce phase transitions.
   e) How to utilize the renormalization group to obtain critical exponents using machine learning functions.

Outline

1) **Interpretation of machine learning functions as physical observables:**
   a) How to construct effective order parameters with machine learning.
   b) How to reweight machine learning functions in parameter space.
   c) How to discover unknown phase transitions with machine learning.
   d) How to include machine learning functions within Hamiltonians to induce phase transitions.
   e) How to utilize the renormalization group to obtain critical exponents using machine learning functions.
2) **Inverse renormalization group with machine learning**:
   a) How to generate configurations of systems with larger lattice size without having to simulate these systems and without critical slowing down effect.
   b) How do inverse renormalization group flows emerge.
   c) How to calculate multiple critical exponents with the inverse renormalization group.

Neural Networks as Physical Observables

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.

We require:

1. A set of configurations from distinct phases. Each configuration has been labeled accordingly to the phase it belongs to.
2. A machine learning algorithm (different algorithms provide different benefits or have different limitations).

Machine learning phases of matter, J. Carrasquilla, R. Melko, Nature Phys 13, 431–434 (2017)

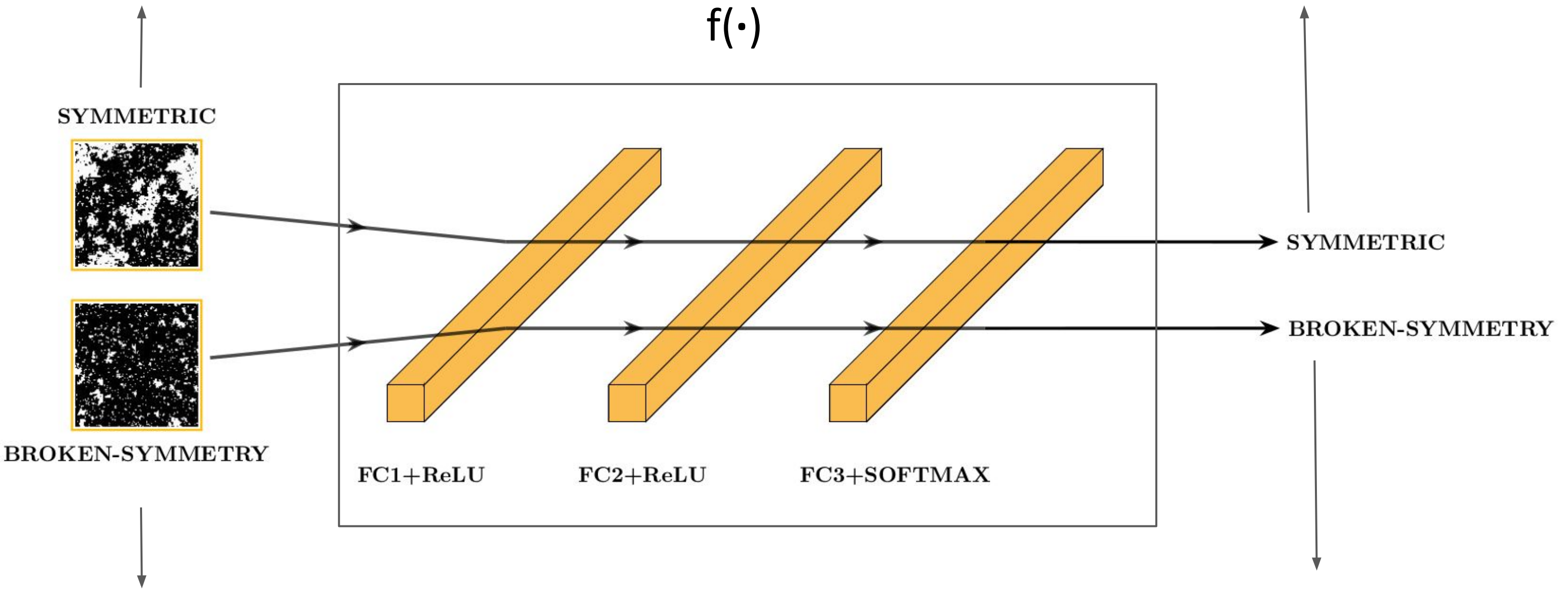
Machine learning and the physical sciences, Carleo et al., Rev. Mod. Phys. 91, 045002 (2019)

Neural Networks as Physical Observables

Training of a neural network on the Ising model:

Labeled as 0.

Labeled as 0.

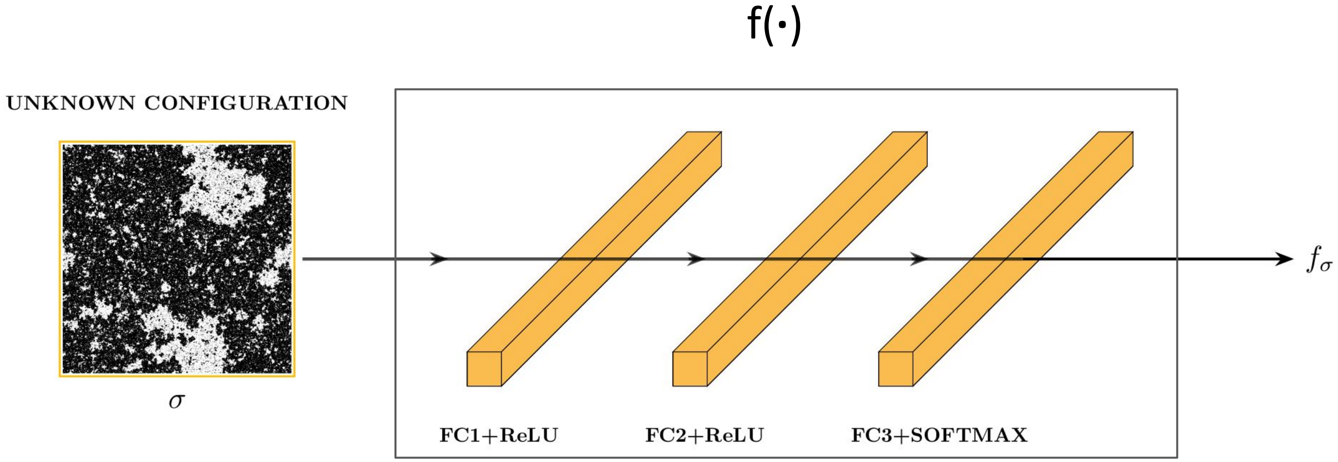


Labeled as 1.

Labeled as 1.

Extending machine learning classification capabilities with histogram reweighting, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E **102** (2020).

Neural Networks as Physical Observables

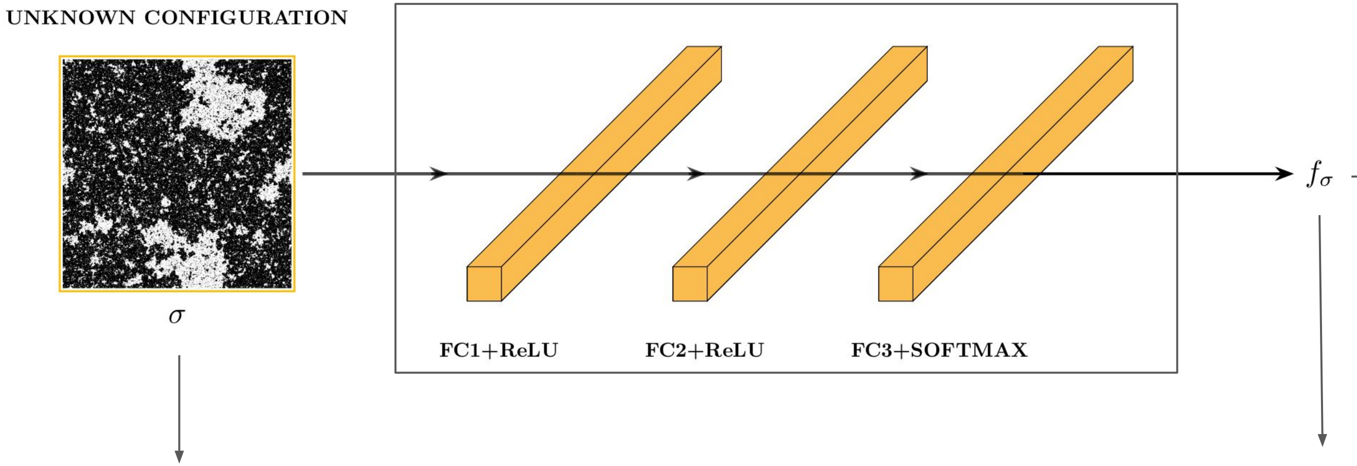


Probability that a configuration is in the broken-symmetry phase

Extending machine learning classification capabilities with histogram reweighting, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E **102** (2020).

Neural Networks as Physical Observables

f(·)



Probability that a configuration is in the broken-symmetry phase

The **configuration** is drawn from an equilibrium distribution and therefore has an **associated Boltzmann weight**.

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

Extending machine learning classification capabilities with histogram reweighting, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E **102** (2020).

Neural Networks as Physical Observables

The neural network function f is an observable in the system:

$$\langle f \rangle = \sum_{\sigma} f_{\sigma} p_{\sigma} = \frac{\sum_{\sigma} f_{\sigma} \exp[-\beta E_{\sigma}]}{\sum_{\sigma} \exp[-\beta E_{\sigma}]}$$

σ : configuration of the system

p_{σ} : Boltzmann probability distribution

β : inverse temperature

Extending machine learning classification capabilities with histogram reweighting, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E **102** (2020).

Neural Networks as Physical Observables

Expectation value of an arbitrary observable <O> as calculated during a Monte Carlo simulation:

$$\langle O \rangle = \frac{\sum_{i=1}^{N} O_{\sigma_i} \tilde{p}_{\sigma_i}^{-1} \exp[-\beta E_{\sigma_i}]}{\sum_{i=1}^{N} \tilde{p}_{\sigma_i}^{-1} \exp[-\beta E_{\sigma_i}]}$$

$\tilde{p}_{\sigma_i}$: probabilities used to sample from the equilibrium distribution

Extending machine learning classification capabilities with histogram reweighting, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E **102** (2020).

Neural Networks as Physical Observables

Expectation value of an arbitrary observable <O> as calculated during a Monte Carlo simulation:

$$\langle O \rangle = \frac{\sum_{i=1}^{N} O_{\sigma_i} \tilde{p}_{\sigma_i}^{-1} \exp[-\beta E_{\sigma_i}]}{\sum_{i=1}^{N} \tilde{p}_{\sigma_i}^{-1} \exp[-\beta E_{\sigma_i}]}$$

$\tilde{p}_{\sigma_i}$: probabilities used to sample from the equilibrium distribution

(Some) possible choices for $\tilde{p}_{\sigma_i}$

$$p_{\sigma_i} = \frac{\exp[-\beta E_{\sigma_i}]}{\sum_{\sigma} \exp[-\beta E_{\sigma_i}]}$$

Importance sampling

$$p_{\sigma_i}^{(0)} = \frac{\exp[-\beta_0 E_{\sigma_i}]}{\sum_{\sigma} \exp[-\beta_0 E_{\sigma_i}]}$$

Reweighting

Extending machine learning classification capabilities with histogram reweighting, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E **102** (2020).

Neural Networks as Physical Observables

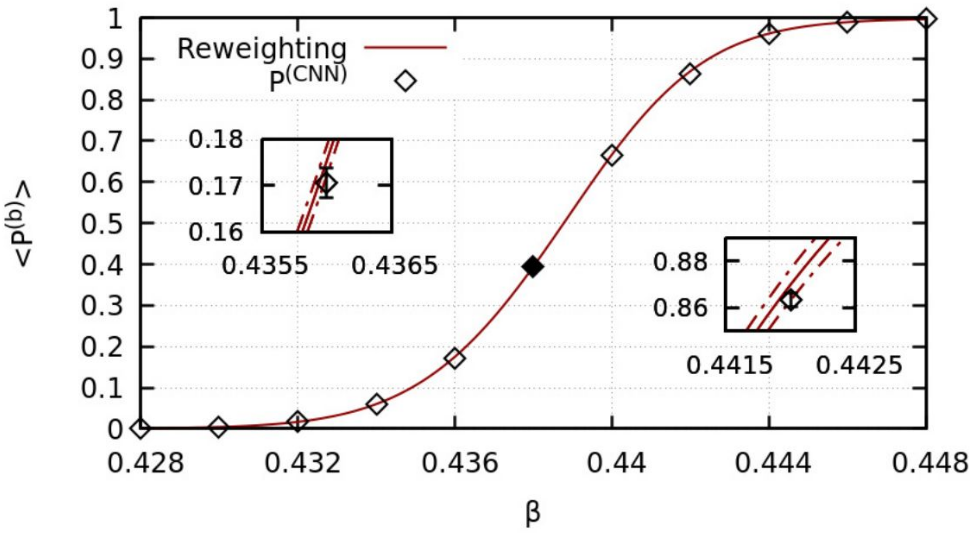
Reweighting equation:

$$\langle O \rangle = \frac{\sum_{i=1}^{N} O_{\sigma_i} \exp[-(\beta - \beta_0) E_{\sigma_i}]}{\sum_{i=1}^{N} \exp[-(\beta - \beta_0) E_{\sigma_i}]}$$

Given configurations sampled at inverse temperature β_0 we can calculate the expectation value of observables at inverse temperature β.

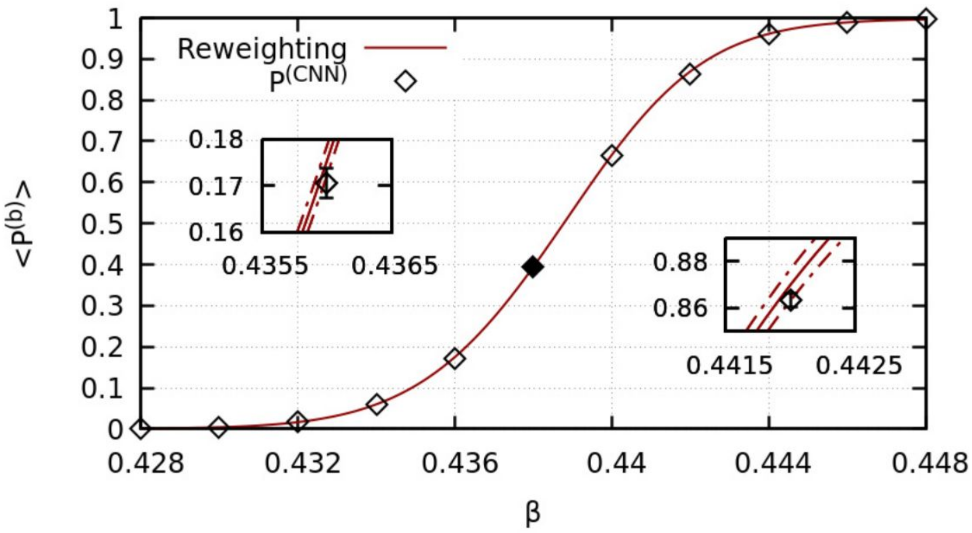
Extending machine learning classification capabilities with histogram reweighting, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E **102** (2020).

Neural Networks as Physical Observables



Extending machine learning classification capabilities with histogram reweighting, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E **102** (2020).

Neural Networks as Physical Observables

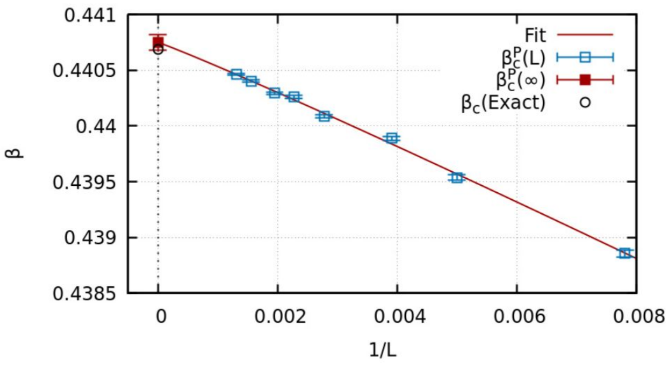


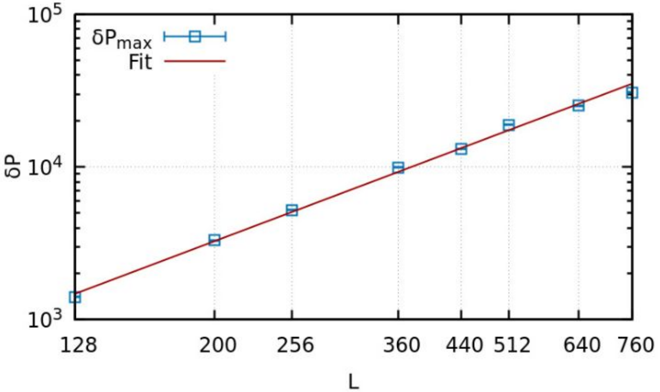
Does it look like an effective order parameter?

Extending machine learning classification capabilities with histogram reweighting, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E **102** (2020).

Neural Networks as Physical Observables

Results obtained by quantities derived entirely from the neural network





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

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

	β_c	ν	γ/ν
CNN+Reweighting	0.440749(68)	0.95(9)	1.78(4)
Exact	$\ln(1+\sqrt{2})/2$	1	7/4
	≈ 0.440687		=1.75

Extending machine learning classification capabilities with histogram reweighting, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E **102** (2020).

Neural Networks as Physical Observables

We have answered these questions:

- ➔ How to construct effective order parameters with machine learning.
- ➔ How to reweight machine learning functions in parameter space.

Summary:

1. No knowledge about the symmetries or the Hamiltonian was explicitly introduced during the training of the machine learning algorithm.
2. Neural network functions are statistical-mechanical observables: they are associated to a Boltzmann weight and can hence be reweighted in parameter space.
3. Using only the neural network function f and its susceptibility χ we were able to obtain multiple critical exponents and the critical inverse temperature of the 2D Ising model.

Extending machine learning classification capabilities with histogram reweighting, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E **102** (2020).

Neural Networks as Physical Observables

We saw that the neural network function f is (for all practical reasons) an observable in the system.

What else can we achieve with f?

Mapping distinct phase transitions to a neural network, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E 102, 053306 (2020).

Neural Networks as Physical Observables

The function f(·) was learned on configurations of the Ising model and 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’)?

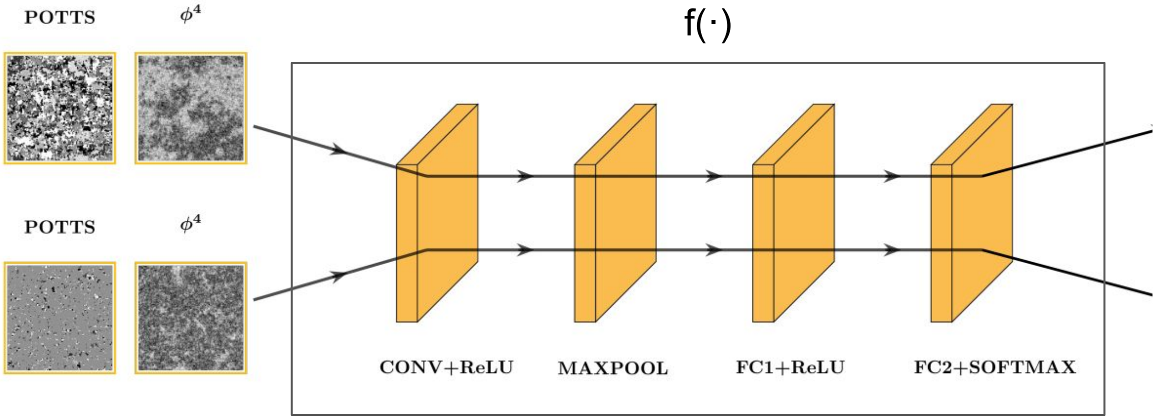
Mapping distinct phase transitions to a neural network, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E 102, 053306 (2020).

Neural Networks as Physical Observables

Equivalently:

Learned on Ising configurations

f(·)

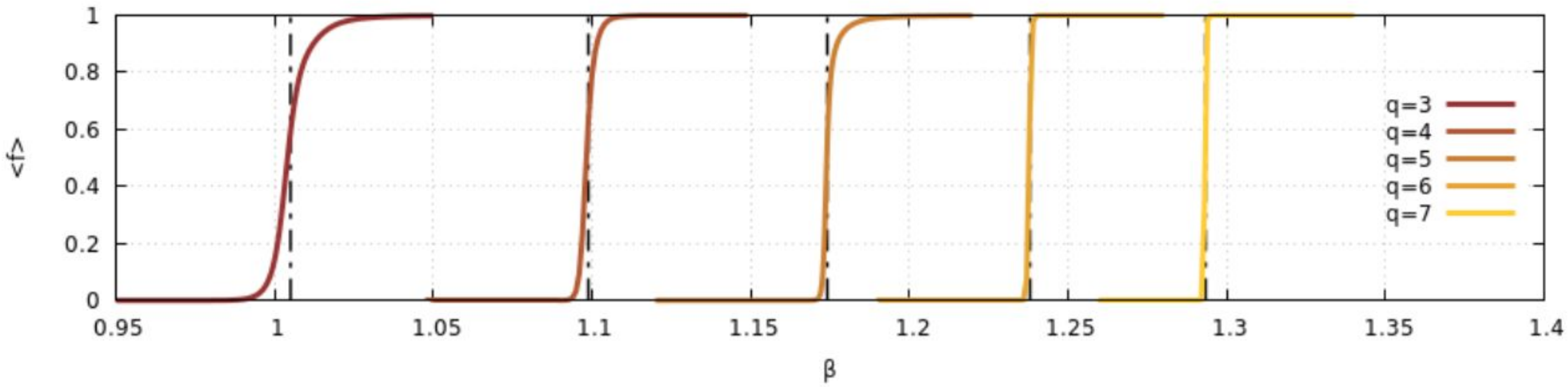


?

Mapping distinct phase transitions to a neural network, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E 102, 053306 (2020).

Neural Networks as Physical Observables

Potts models:

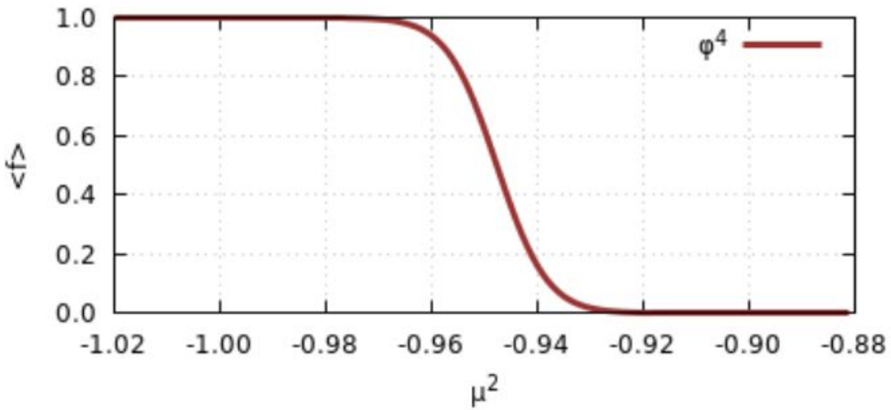


Results obtained through a function f learned exclusively on the Ising model.

Mapping distinct phase transitions to a neural network, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E 102, 053306 (2020).

Neural Networks as Physical Observables

φ^4 scalar field theory:



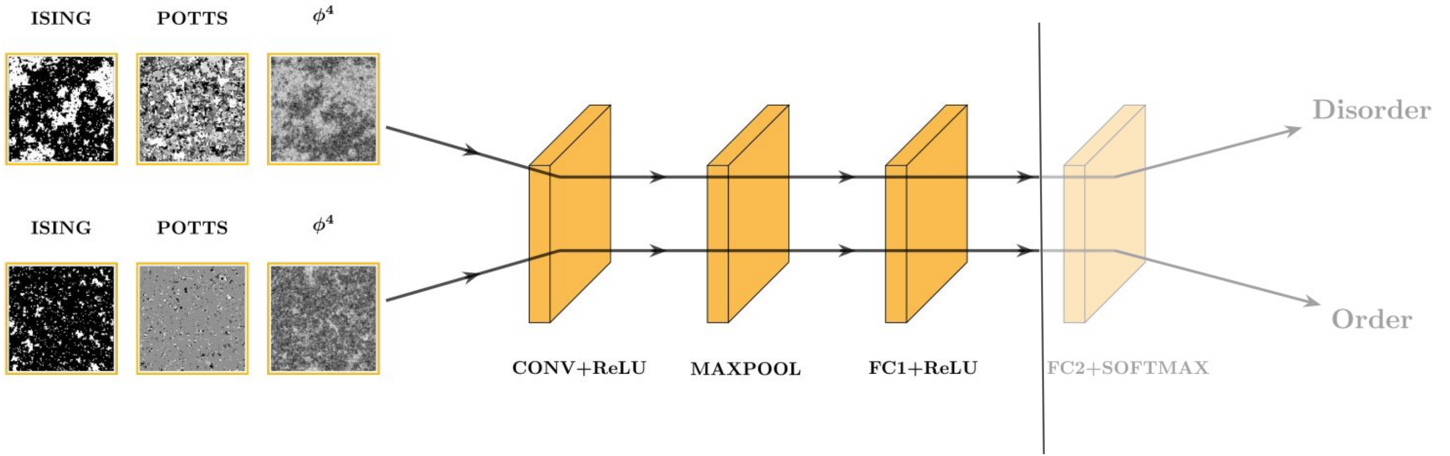
Fixed dimensionless λ=0.7 and varied the dimensionless mass μ^2

Results obtained through a function f learned exclusively on the Ising model.

Mapping distinct phase transitions to a neural network, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E 102, 053306 (2020).

Neural Networks as Physical Observables

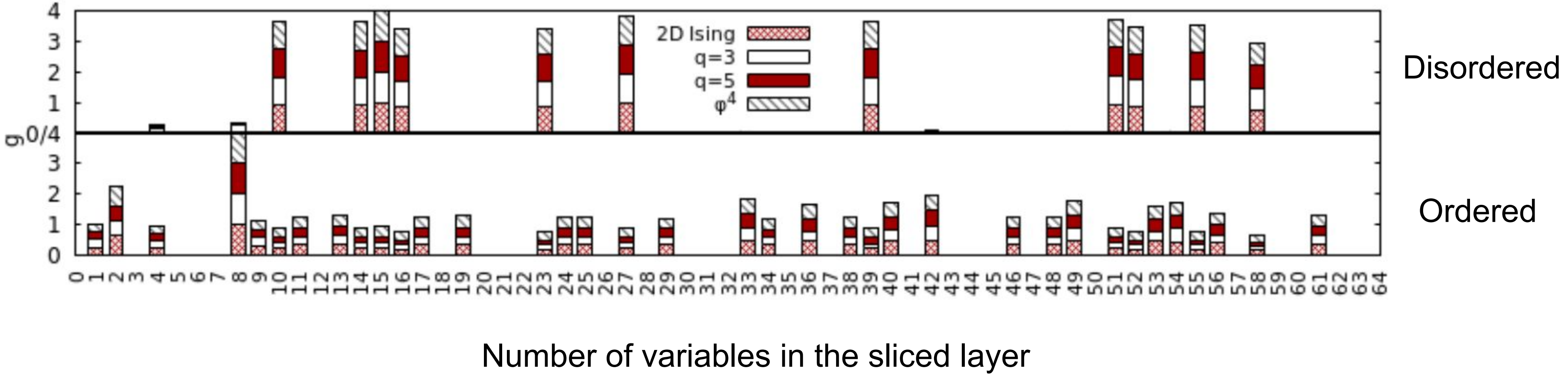
Insights on the results:



Mapping distinct phase transitions to a neural network, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E 102, 053306 (2020).

Neural Networks as Physical Observables

Insights on the results:

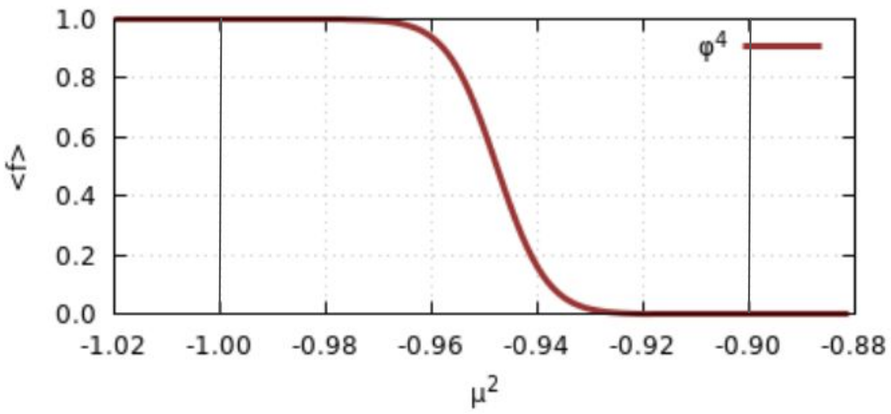


Similar variables get spiked for configurations in disordered phase (top) and ordered phase (bottom), irrespective of the system.

Mapping distinct phase transitions to a neural network, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E 102, 053306 (2020).

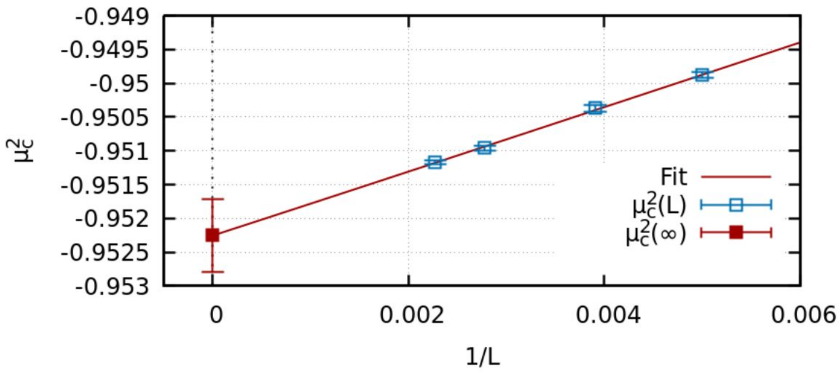
Neural Networks as Physical Observables

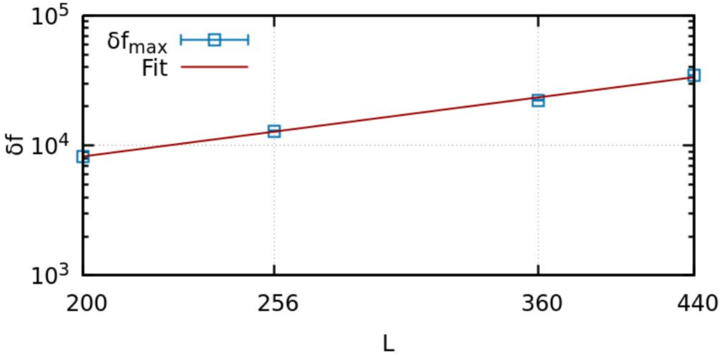
We didn't include any knowledge about the presence of a phase transition in the system so we have now obtained the knowledge of its critical region. We can therefore study it by calculating its critical exponents.



Mapping distinct phase transitions to a neural network, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E 102, 053306 (2020).

Neural Networks as Physical Observables





	μ_c^2	ν	γ/ν
CNN+Reweighting	-0.95225(54)	0.99(34)	1.78(7)

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

Mapping distinct phase transitions to a neural network, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E 102, 053306 (2020).

Neural Networks as Physical Observables

We have answered this question:

➔ How to discover unknown phase transitions with machine learning.

Summary:

1. Using an Ising-trained neural network we were able to predict the phase diagrams for the q-state Potts models and the φ^4 scalar field theory.
2. Having obtained the knowledge of the critical region for the φ^4 theory we then calculated the critical exponents and the critical squared mass for the 2d φ^4 theory.

Mapping distinct phase transitions to a neural network, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E 102, 053306 (2020).

Neural Networks as Physical Observables

How can we explain that the neural network function is a statistical-mechanical observable?

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

Parameters, constraints or fields that interact with a system have conjugate variables which represent the response of the system to the perturbation of the corresponding parameter.

Can we make the same statement about the neural network function f?

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

Parameters, constraints or fields that interact with a system have conjugate variables which represent the response of the system to the perturbation of the corresponding parameter.

Can we make the same statement about the neural network function f?

Conjugate variables are expressed as derivatives of the free energy in terms of the associated field. To be able to make the same statement we should start by expressing the neural network function f in terms of the free energy/partition function.

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

The neural network function f is an intensive property. It is interpreted as a probability and is bound between [0,1]. It therefore doesn't have the proper dependence on the size of the system.

This can be very easily solved by multiplying f with the volume V of the system and recast it as an extensive property:

$$V f$$

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

The (extensive) neural network function Vf can then be included as a term within the Hamiltonian. We consider that Vf couples to an arbitrary external field Y and define a modified Hamiltonian for the Ising model:

$$E_Y = E - VfY.$$

If Y=0, we have the original Hamiltonian of the Ising model.

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

If we take a derivative of the logarithm of the partition function in terms of the external field Y we arrive at the expectation value of the neural network function f:

$$\langle f \rangle = \frac{1}{\beta V} \frac{\partial \log Z_Y}{\partial Y} = \frac{\sum_\sigma f_\sigma \exp[-\beta E_\sigma + \beta V f_\sigma Y]}{\sum_\sigma \exp[-\beta E_\sigma + \beta V f_\sigma Y]}$$

If Y=0, we have the original expression of the expectation value.

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

The derivative of the expectation value of the neural network function gives:

$$\chi_f = \frac{\partial \langle f \rangle}{\partial Y} = \beta V (\langle f^2 \rangle - \langle f \rangle^2)$$

χ is a susceptibility. It measures the response of the neural network function f to changes in the associated external field Y.

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

The derivative of the expectation value of the neural network function gives:

$$\chi_f = \frac{\partial \langle f \rangle}{\partial Y} = \beta V (\langle f^2 \rangle - \langle f \rangle^2)$$

χ is a susceptibility. It measures the response of the neural network function f to changes in the associated external field Y.

What happens if Y ≠0?

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

To investigate what happens when Y ≠0, we could do Monte Carlo sampling on the modified Hamiltonian to obtain configurations:

$$E_Y = E - V f Y$$

An alternative option is to use reweighting to calculate expectation values of the modified system by using configurations of the original.

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

Expectation value of an arbitrary observable <O> during a Monte Carlo simulation in the modified system:

$$\langle O \rangle = \frac{\sum_{i=1}^{N} O_{\sigma_i} \tilde{p}_{\sigma_i}^{-1} \exp[-\beta E_{\sigma_i} + \beta V f_{\sigma_i} Y]}{\sum_{i=1}^{N} \tilde{p}_{\sigma_i}^{-1} \exp[-\beta E_{\sigma_i} + \beta V f_{\sigma_i} Y]}$$

By choosing $\tilde{p}_{\sigma_i}$ equal to the probabilities of the original system:

$$\langle O \rangle = \frac{\sum_{i=1}^{N} O_{\sigma_i} \exp[\beta V f_{\sigma_i} Y]}{\sum_{i=1}^{N} \exp[\beta V f_{\sigma_i} Y]}$$

This form of reweighting is **Hamiltonian-agnostic**.

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

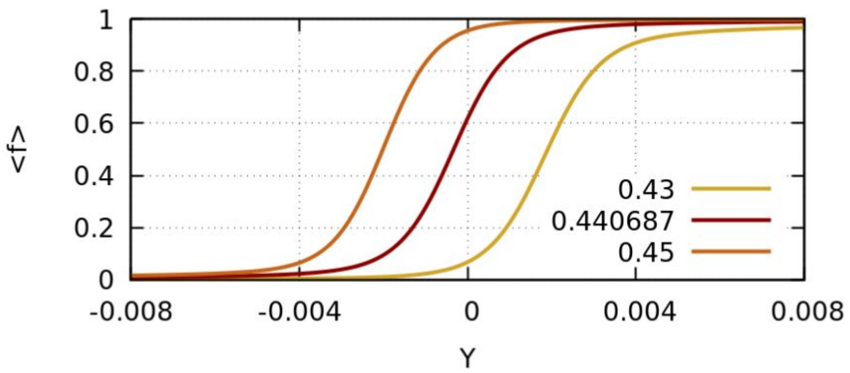


FIG. 2. Mean neural network function $\langle f \rangle$ versus external field Y at inverse temperature $\beta = 0.43, 0, 440687, 0.45$ (right to left). The statistical uncertainty is comparable with the width of the lines.

Recall that:

β=0.43-> symmetric phase

β_c≅0.440687 -> inverse critical temperature

β=0.45-> broken-symmetry phase

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

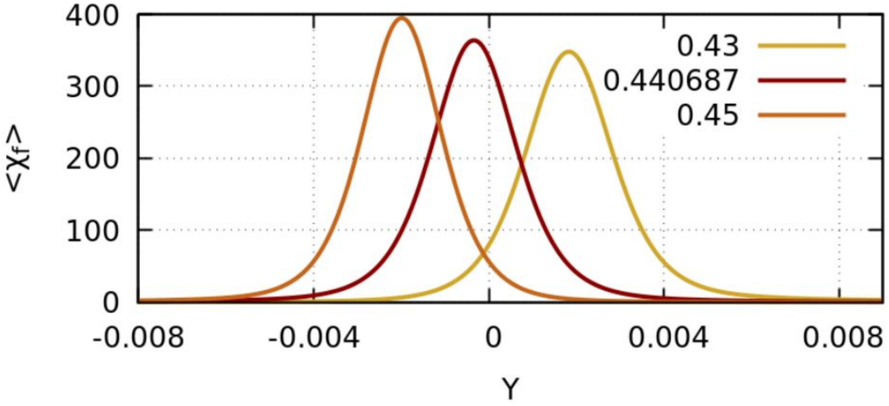


FIG. 3. Mean susceptibility of the neural network function $\langle \chi_f \rangle$ versus external field Y at inverse temperature $\beta = 0.43, 0, 440687, 0.45$ (right to left). The statistical uncertainty is comparable with the width of the lines.

Recall that the inverse critical temperature is $\beta_c \cong 0.440687$.

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

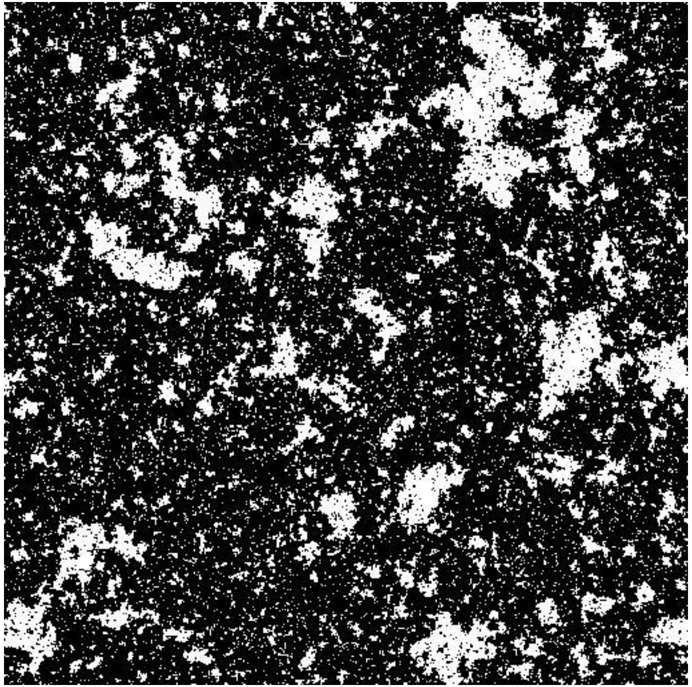
Neural Networks as Physical Observables

Can we study the phase transition induced by the neural network field Y based on a renormalization group approach?

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

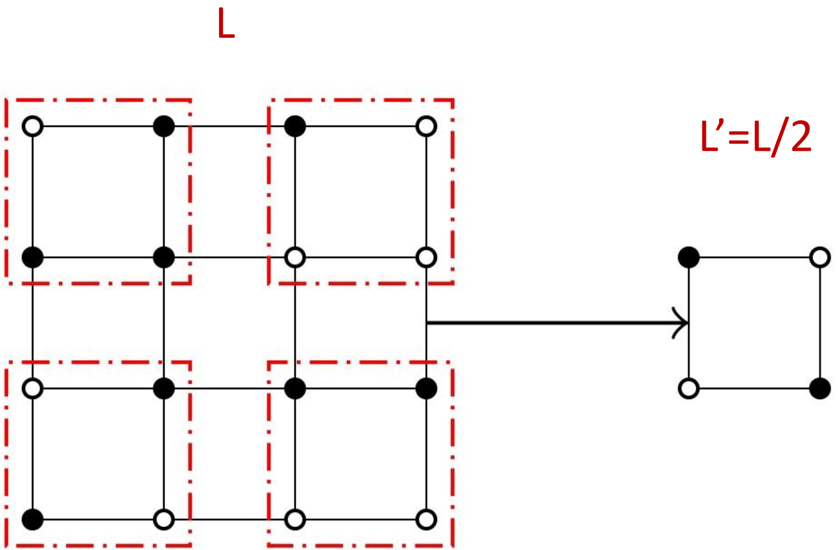
Neural Networks as Physical Observables

L



Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

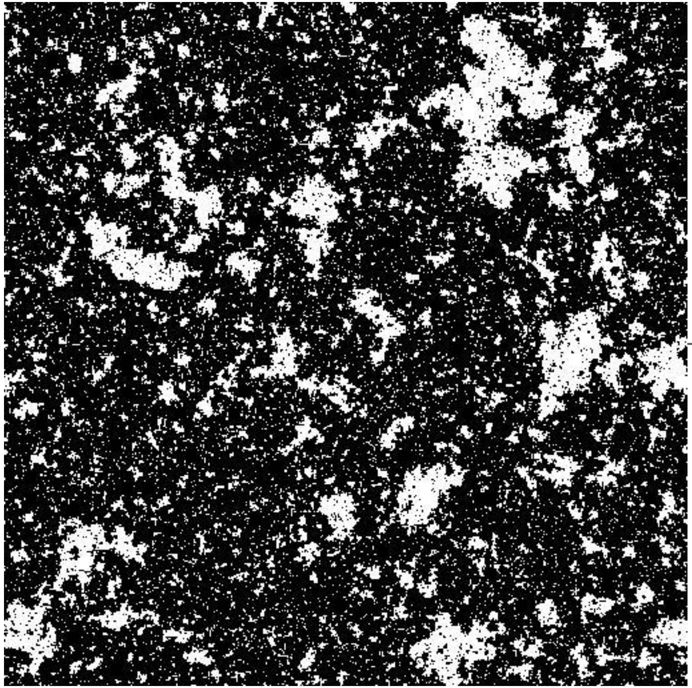


Spin blocking transformation with a rescaling factor of $b=2$ and the majority rule

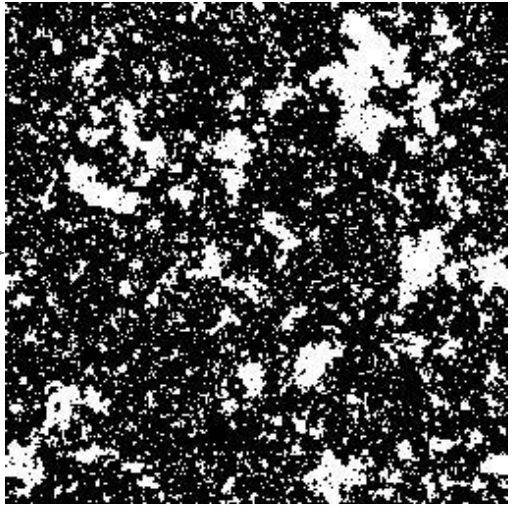
Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

L



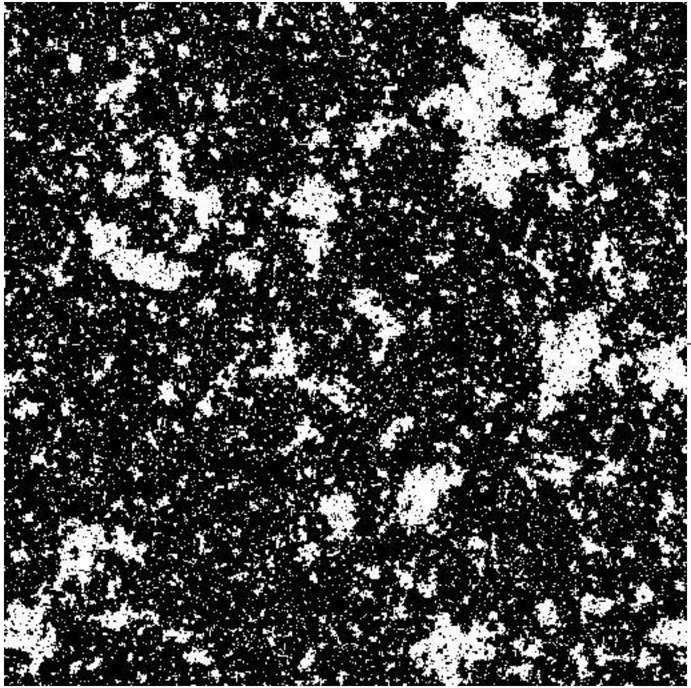
L’=L/2



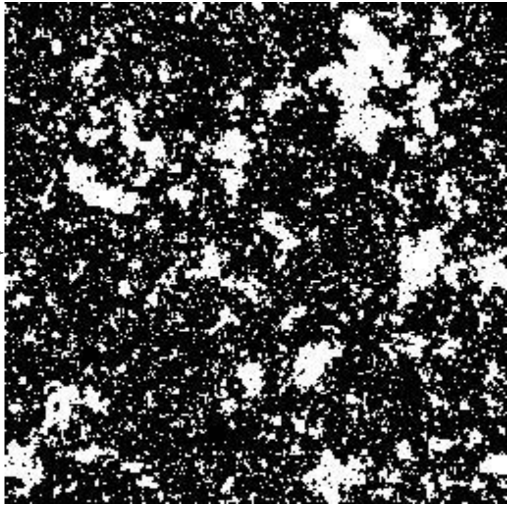
Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

L, ξ



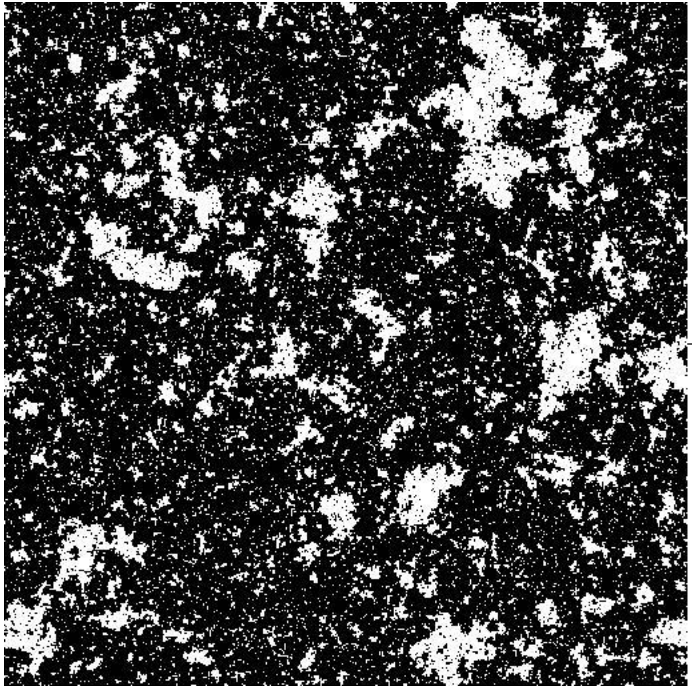
$L'=L/2$, $\xi'=\xi/2$



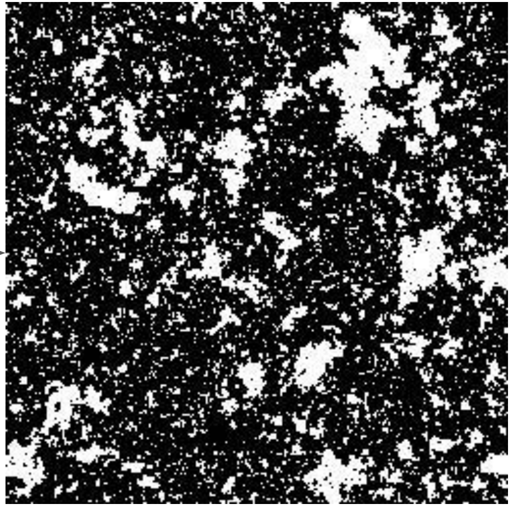
Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

L, ξ, β

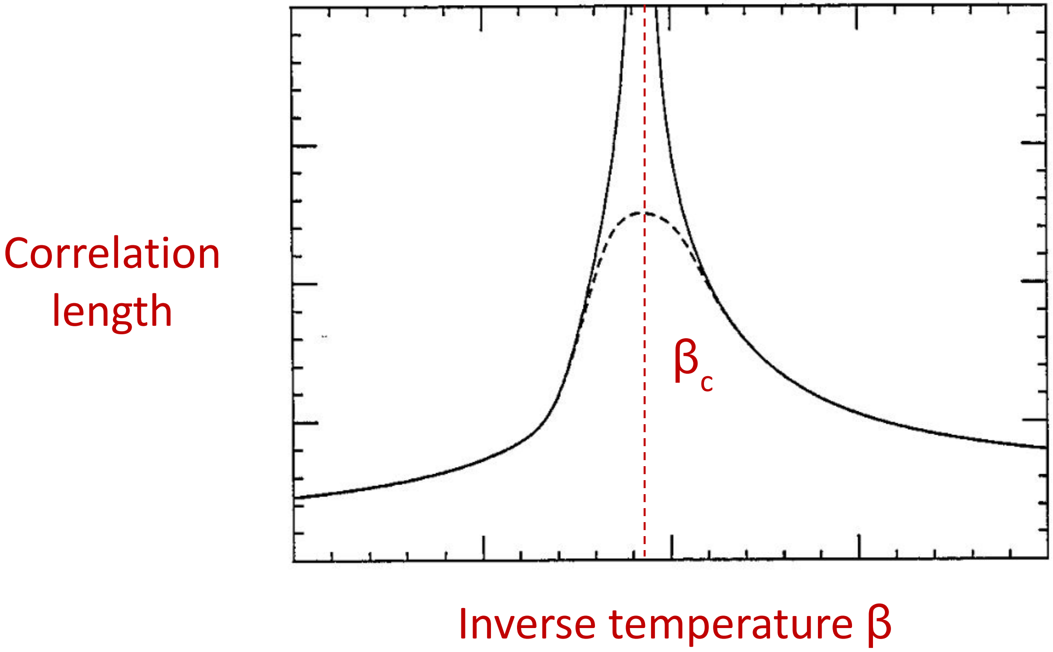


L’=L/2, ξ’=ξ/2, β’



Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

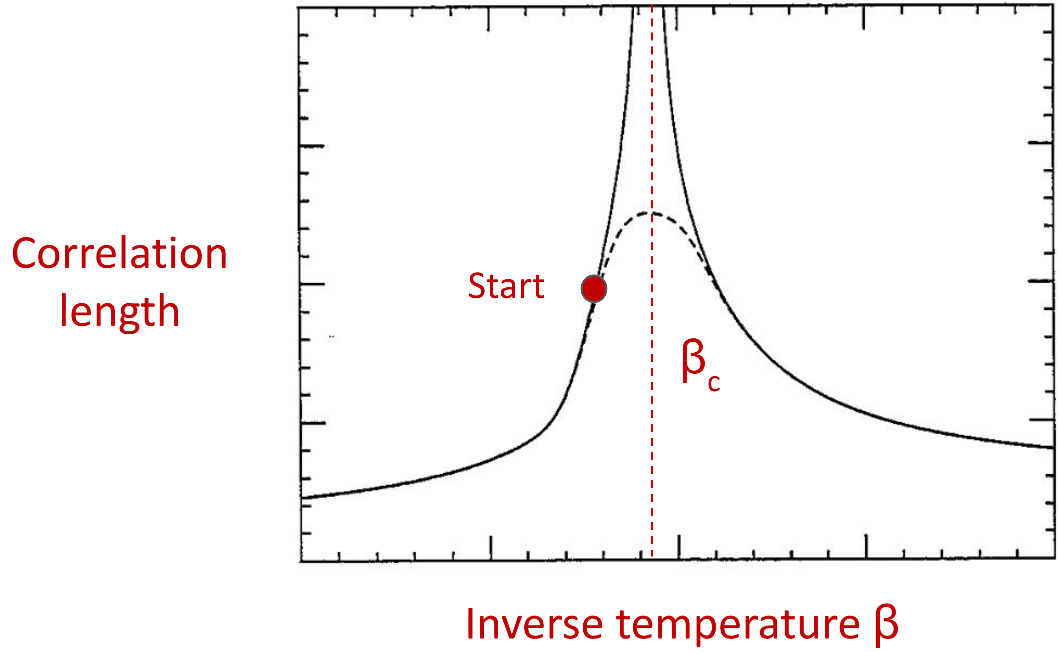
Neural Networks as Physical Observables



Altered figure from (Newman, Barkema) book (Fig 4.1)

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

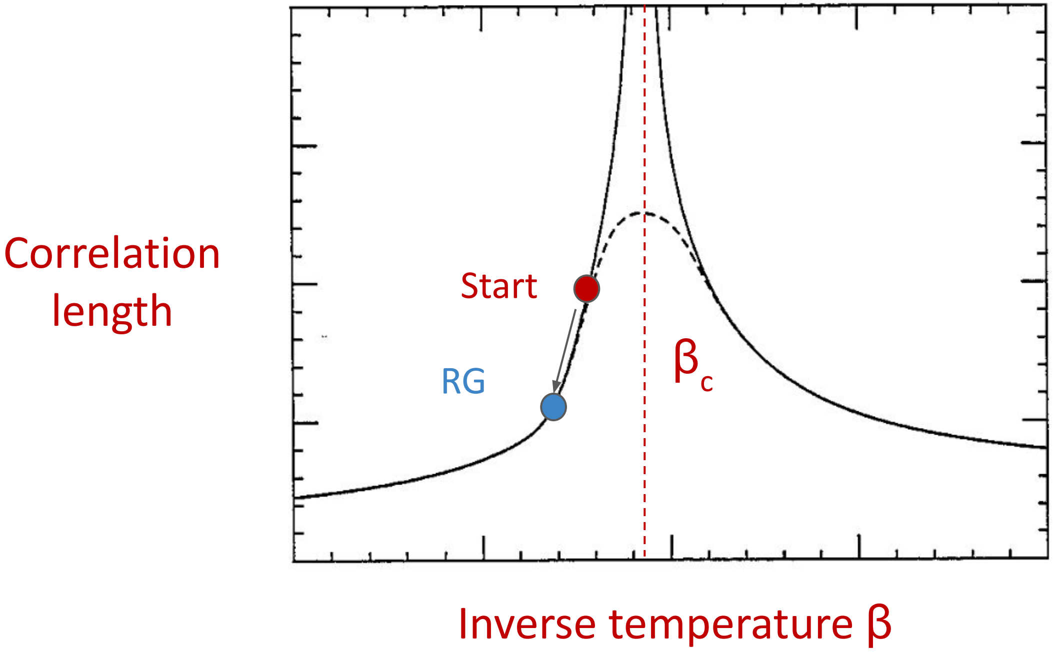
Neural Networks as Physical Observables



Altered figure from (Newman, Barkema) book (Fig 4.1)

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

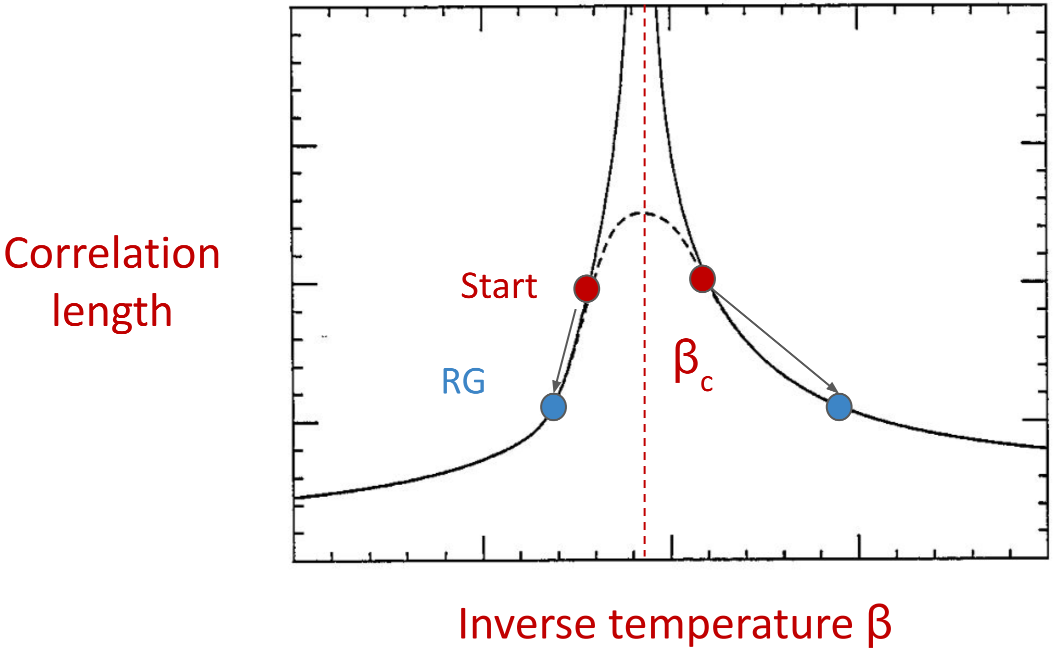
Neural Networks as Physical Observables



Altered figure from (Newman, Barkema) book (Fig 4.1)

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables



Altered figure from (Newman, Barkema) book (Fig 4.1)

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

There is one inverse temperature where the original and the rescaled systems have the same correlation length: the inverse critical temperature β_c=0.440687.

At the inverse critical temperature β_c the correlation length diverges, it becomes infinite, and intensive observable quantities of the two systems will become equal.

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

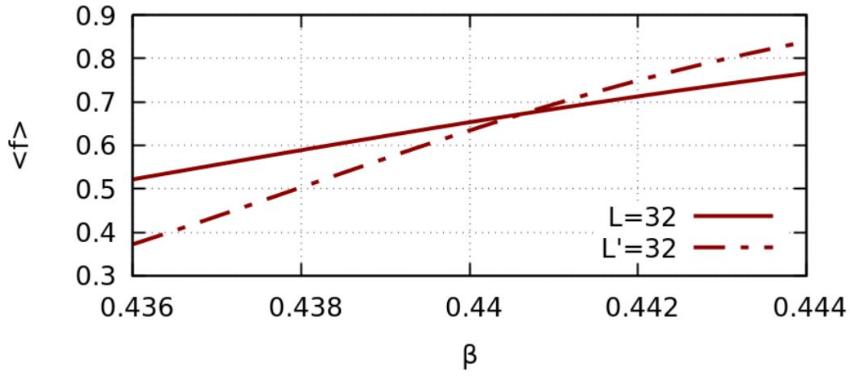
There is one inverse temperature where the original and the rescaled systems have the same correlation length: the inverse critical temperature β_c=0.440687.

At the inverse critical temperature β_c the correlation length diverges, it becomes infinite, and intensive observable quantities of the two systems will become equal.

We can use the neural network function f as an observable to locate the critical point.

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

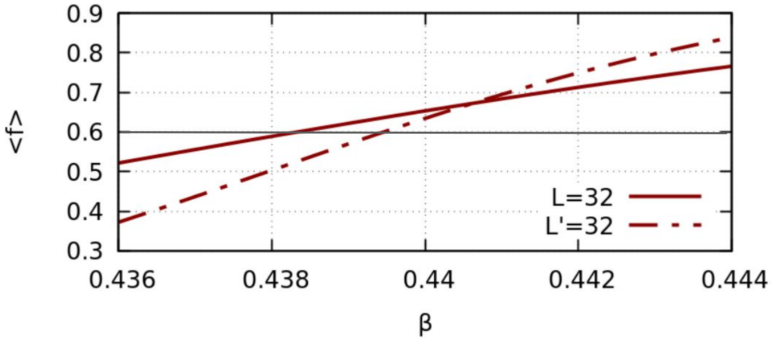


At the intersection point:

$$f(\beta_c) = f'(\beta_c)$$

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables



More generally:

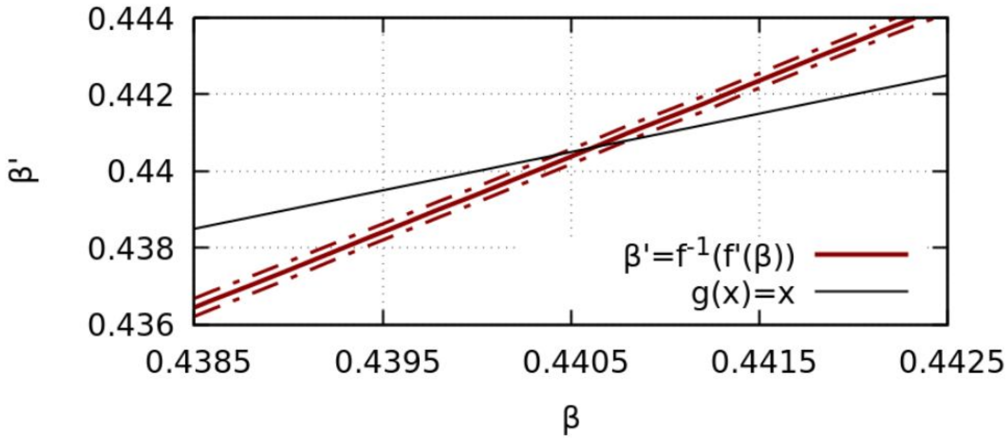
$$f(\beta') = f'(\beta)$$

We can form a mapping between the rescaled and the original inverse temperature:

$$\beta' = f^{-1}(f'(\beta))$$

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables



$$\beta_c = 0.44063(21)$$

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

The original and the rescaled systems have a different distance from the critical point.

This distance can be measured by defining the reduced inverse temperature for the original and the rescaled system:

$$t = \frac{\beta_c - \beta}{\beta_c}$$

Original

$$t' = \frac{\beta_c - \beta'}{\beta_c}$$

Rescaled

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

The original and the rescaled systems have different correlation lengths.

They should therefore diverge to the thermodynamic limit according to different relations:

$$\xi \sim |t|^{-\nu} \qquad\qquad \xi' \sim |t'|^{-\nu}$$

Original | Rescaled

The correlation length exponent is the same because both the original and the rescaled systems are Ising models.

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

By dividing the two relations of the correlation lengths we obtain:

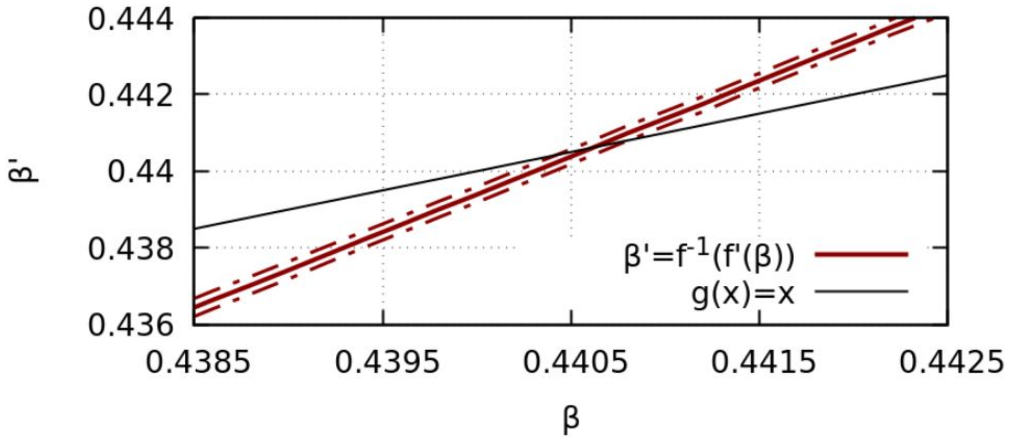
$$\left(\frac{t}{t'}\right)^{-\nu} = b.$$

We then substitute and linearize the renormalization group transformation based on a Taylor expansion to leading order, to obtain:

$$\nu = \frac{\log b}{\log \left.\frac{d\beta'}{d\beta}\right|_{\beta_c}}$$

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables



$$\nu = \frac{\log b}{\log \left. \frac{d\beta'}{d\beta} \right|_{\beta_c}}$$

$$\beta_c = 0.44063(21) \qquad \nu = 1.01(2)$$

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

The neural network field Y induces a phase transition.

Then Y affects the correlation length. Another exponent can be defined that governs the divergence of the correlation length precisely at the critical point:

$$\xi \sim |Y|^{-\theta_Y}$$

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

Similarly to the inverse temperatures a mapping can be formed that relates the original and the rescaled neural network field:

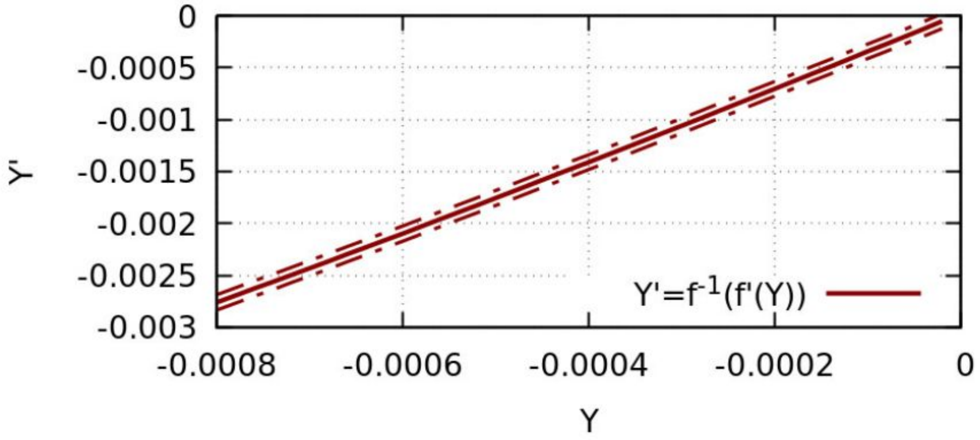
$$Y' = f^{-1}(f'(Y))$$

A new expression can be obtained that allows numerical calculation of the exponent θ_y at the vicinity of the phase transition:

$$\theta_Y = \frac{\log b}{\log \left.\frac{dY'}{dY}\right|_{Y=0}}$$

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables



$$\theta_Y = 0.534(3)$$

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

The Ising model has two relevant operators that govern the divergence of the correlation length, ν and θ.

Exact: $\xi \sim |t|^{-\nu}$ ν=1 $\xi \sim |h|^{-\theta}$ θ=0.5333...

Estimated: $\xi \sim |t|^{-\nu}$ ν=1.01(2) $\xi \sim |Y|^{-\theta_Y}$ $\theta_Y = 0.534(3)$

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Neural Networks as Physical Observables

We have answered these questions:

- ➔ How to include machine learning functions within Hamiltonians to induce phase transitions.
- ➔ How to utilize the renormalization group to obtain critical exponents using machine learning functions.

Summary:

1. We introduced neural network functions as physical terms within Hamiltonians by coupling them to a fictitious field and expressing them in terms of the system's partition function/free energy.
2. We observed that the neural network field Y induces an order-disorder phase transition, in contrast to the field of the conventional order parameter which always breaks the symmetry explicitly by favoring an ordered state, irrespective of its sign.
3. We utilized the renormalization group to extract the two relevant operators of the 2d Ising model using the neural network function f and its fictitious field Y.

Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (arXiv:2010.00054).

Inverse renormalization group

Can we devise an **inverse renormalization group** approach that can be applied for an arbitrary number of steps to iteratively increase the lattice size of the system?

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

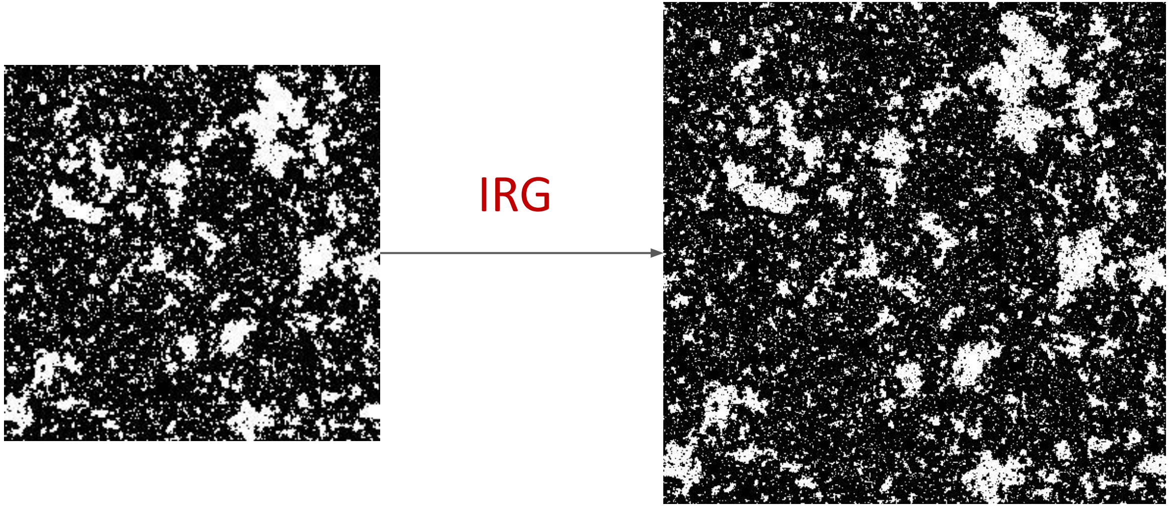
Can we devise an **inverse renormalization group** approach that can be applied for an arbitrary number of steps to iteratively increase the lattice size of the system?

If yes, then we can obtain configurations of systems with larger lattice size without simulating them, hence evading the critical slowing down effect.

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

In the inverse renormalization group new degrees of freedom will be introduced within the system.



Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

Inversion of a majority rule in the **Ising** model

Original degree of freedom

+1

Possible rescaled degrees of freedom

+1	+1
+1	-1

-1	+1
+1	+1

-1	+1
+1	-1

-1	+1
+1	-1

…

For the inverse renormalization group in the Ising model, see:

Inverse Monte Carlo Renormalization Group Transformations for Critical Phenomena, D. Ron, R. Swendsen, A. Brandt, Phys. Rev. Lett. 89, 275701 (2002)

Inverse renormalization group

Inversion of a summation in the φ^4 model

Original degree of freedom

0.40

Possible rescaled degrees of freedom

0.01	0.36
0.02	0.01

-421.1	90.1
0.5	330.9

…

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

Inversion of a summation in the $\boldsymbol{\varphi^4}$ model

Original degree of freedom

0.40

Possible rescaled degrees of freedom

0.01	0.36
0.02	0.01

-421.1	90.1
0.5	330.9

…

Too complicated!

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

We can learn a set of transformations that can mimic the inversion of a standard renormalization group transformation.

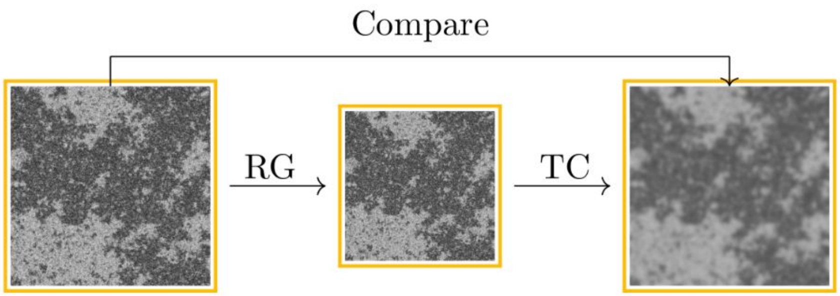


FIG. 3. Illustration of the optimization approach. Transposed convolutions (TC) are applied on configurations produced with the renormalization group (RG) to construct a set of configuration which is compared with the original.

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

$$\begin{array}{|c|c|}\hline 3 & 1 \\ \hline 2 & 0 \\ \hline \end{array} \; * \; \begin{array}{|c|c|}\hline w_{11} & w_{12} \\ \hline w_{21} & w_{22} \\ \hline \end{array}$$

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

$$\begin{array}{|c|c|}\hline 3 & 1 \\ \hline 2 & 0 \\ \hline\end{array} \; * \; \begin{array}{|c|c|}\hline w_{11} & w_{12} \\ \hline w_{21} & w_{22} \\ \hline\end{array}$$

Example

$$\begin{array}{|c|c|}\hline 3 & 1 \\ \hline 2 & 0 \\ \hline\end{array} \; * \; \begin{array}{|c|c|}\hline 2 & 3 \\ \hline 0 & 1 \\ \hline\end{array} \; =$$

$$\begin{array}{|c|c|c|}\hline 6 & 3 & \\ \hline 0 & 3 & \\ \hline & & \\ \hline\end{array} + \begin{array}{|c|c|c|}\hline & 2 & 3 \\ \hline & 0 & 1 \\ \hline & & \\ \hline\end{array} + \begin{array}{|c|c|c|}\hline & & \\ \hline 4 & 6 & \\ \hline 0 & 1 & \\ \hline\end{array} + \begin{array}{|c|c|c|}\hline & & \\ \hline & 0 & 0 \\ \hline & 0 & 0 \\ \hline\end{array} =$$

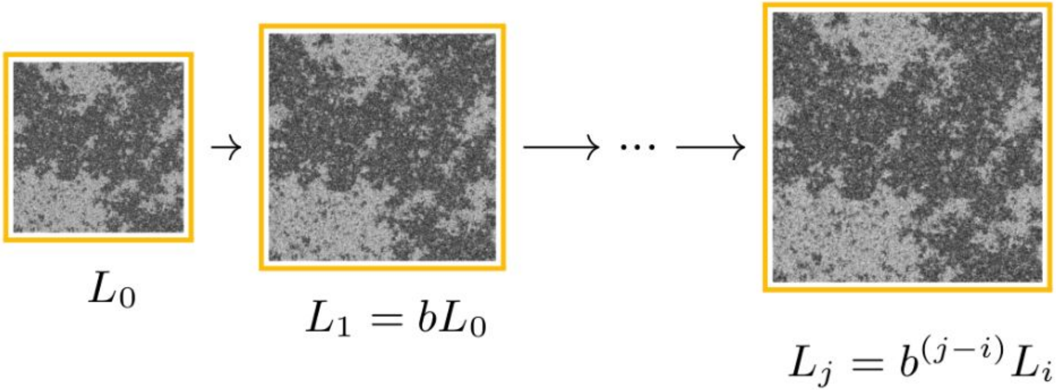
$$\begin{array}{|c|c|c|}\hline 6 & 5 & 3 \\ \hline 4 & 9 & 0 \\ \hline 0 & 1 & 0 \\ \hline\end{array}$$

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

The benefit:

Once learned, we can apply this set of inverse transformations iteratively to arbitrarily increase the size of the system.



Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

The set of transformations can be applied iteratively to arbitrarily increase the lattice size:

$$L_j = b^{(j-i)} L_i \qquad\qquad j > i \geq 0, \text{ and } L_0 = L$$

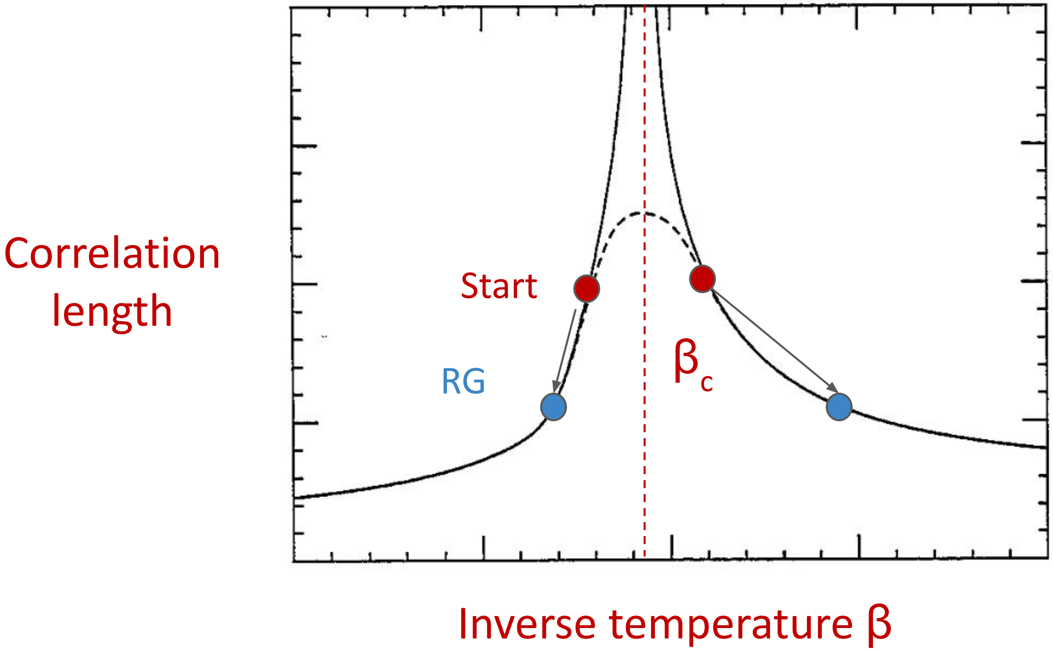
However the increase in the lattice size will induce an analogous increase in the correlation length of the system:

$$\xi_j = b^{(j-i)} \xi_i$$

What are the implications?

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

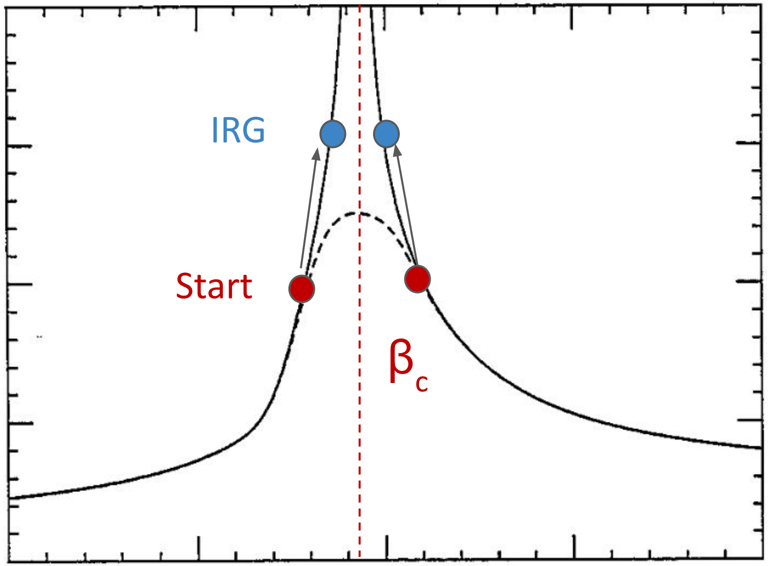
Inverse renormalization group



Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

Correlation length

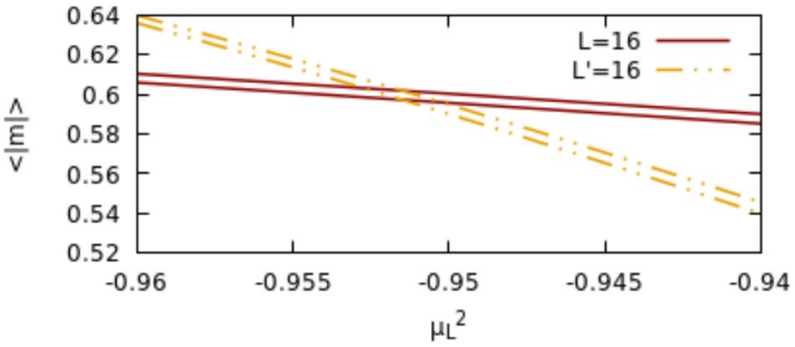


Inverse temperature β

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

First, we verify that the **standard MC** renormalization group method works in the φ^4 theory:

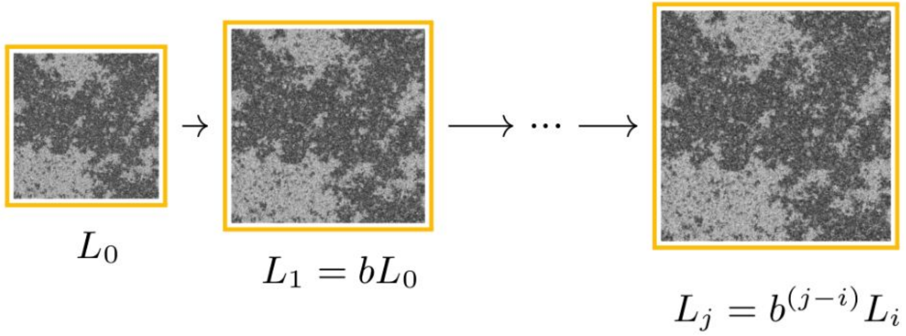


Then we invert the standard transformation that we verified as being successful.

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

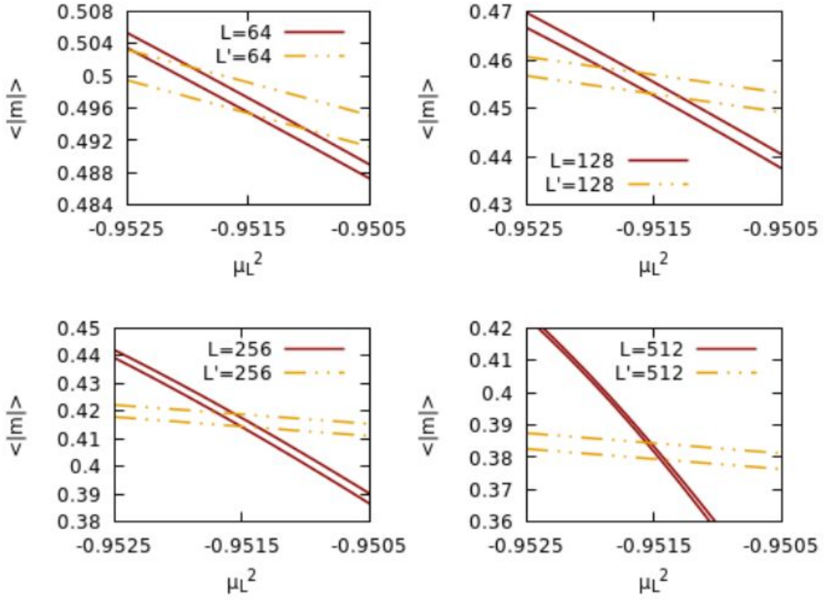
Inverse renormalization group

Now, we start from a lattice size L_0=32 in each dimension and apply the inverse transformations to obtain systems of lattice sizes L_1=64, L_2=128, L_3=256, L_4=512.



Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group



Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

Can we now use the inverse renormalization group approach to calculate critical exponents?

The relations that govern the divergence of the magnetization for an original (i) and a rescaled (j) system are

$$m_i \sim |t_i|^\beta \qquad\qquad m_j \sim |t_j|^\beta$$

They can be equivalently expressed in terms of the correlation length as

$$m_i \sim \xi_i^{-\beta/\nu} \qquad\qquad m_j \sim \xi_j^{-\beta/\nu}$$

where v is the correlation length exponent

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

By dividing the magnetizations (or magnetic susceptibilities), taking the natural logarithm, and applying L'Hôpital's rule, we obtain

$$\frac{\beta}{\nu} = -\frac{\ln \frac{dm_j}{dm_i}\Big|_{K_c}}{\ln \frac{\xi_j}{\xi_i}} = -\frac{\ln \frac{dm_j}{dm_i}\Big|_{K_c}}{(j-i)\ln b}. \qquad \frac{\gamma}{\nu} = \frac{\ln \frac{d\chi_j}{d\chi_i}\Big|_{K_c}}{\ln \frac{\xi_j}{\xi_i}} = \frac{\ln \frac{d\chi_j}{d\chi_i}\Big|_{K_c}}{(j-i)\ln b}.$$

We can use the expressions above to calculate the critical exponents without ever experiencing a critical slowing down effect.

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

TABLE I. Values of the critical exponents γ/ν and β/ν. The original system has lattice size $L = 32$ in each dimension and its action has coupling constants $\mu_L^2 = -0.9515$, $\lambda_L = 0.7$, $\kappa_L = 1$. The rescaled systems are obtained through inverse renormalization group transformations.

L_i/L_j	32/64	32/128	32/256	32/512	64/128	64/256	64/512	128/256	128/512	256/512
γ/ν	1.735(5)	1.738(5)	1.741(5)	1.742(5)	1.742(5)	1.744(5)	1.744(5)	1.745(5)	1.745(5)	1.746(5)
β/ν	0.132(2)	0.130(2)	0.128(2)	0.128(2)	0.128(2)	0.127(2)	0.127(2)	0.126(2)	0.126(2)	0.126(2)

TABLE II. Values of the critical exponents γ/ν and β/ν. The original system has lattice size $L = 8$ in each dimension and its action has coupling constants $\mu_L^2 = -1.2723$, $\lambda_L = 1$, $\kappa_L = 1$. The rescaled systems are obtained through inverse renormalization group transformations.

L_i/L_j	8/16	8/32	8/64	8/128	8/256	8/512	16/32	16/64	16/128	16/256	16/512
γ/ν	1.694(6)	1.708(6)	1.717(6)	1.723(6)	1.727(6)	1.730(6)	1.721(6)	1.728(6)	1.732(6)	1.735(6)	1.737(6)
β/ν	0.154(2)	0.147(2)	0.142(2)	0.139(2)	0.137(2)	0.135(2)	0.140(2)	0.136(2)	0.134(2)	0.132(2)	0.131(2)

L_i/L_j	32/64	32/128	32/256	32/512	64/128	64/256	64/512	128/256	128/512	256/512
γ/ν	1.735(6)	1.738(6)	1.740(6)	1.740(6)	1.741(6)	1.742(6)	1.742(7)	1.743(6)	1.743(7)	1.743(7)
β/ν	0.133(2)	0.131(2)	0.130(2)	0.129(2)	0.129(2)	0.129(2)	0.128(2)	0.128(2)	0.127(2)	0.127(2)

Ising universality class: $\gamma/\nu=1.75$, $\beta/\nu=0.125$.

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Inverse renormalization group

We have answered these questions:

- ➔ How to generate configurations of systems with larger lattice size without having to simulate these systems and without critical slowing down effect.
- ➔ How do inverse renormalization group flows emerge.
- ➔ How to calculate multiple critical exponents with the inverse renormalization group.

Summary:

1. We demonstrated that inverse renormalization group transformations can iteratively increase the lattice size of a system, hence obtaining configurations of larger lattice size, without critical slowing down.
2. We demonstrated that inverse renormalization group flows emerge that drive the system towards its critical point.
3. We demonstrated that multiple critical exponents can be calculated for the φ^4 theory with the inverse renormalization group.

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)

Summary

1) **Interpretation of machine learning functions as physical observables:**
   a) How to construct effective order parameters with machine learning.
   b) How to reweight machine learning functions in parameter space.
   c) How to discover unknown phase transitions with machine learning.
   d) How to include machine learning functions within Hamiltonians to induce phase transitions.
   e) How to utilize the renormalization group to obtain critical exponents using machine learning functions.
2) **Inverse renormalization group with machine learning**:
   a) How to generate configurations of systems with larger lattice size without having to simulate these systems and without critical slowing down effect.
   b) How do inverse renormalization group flows emerge.
   c) How to calculate multiple critical exponents with the inverse renormalization group.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 813942

Thank you for your attention!

Inverse renormalization group

2d φ^4 theory

$$S = -\kappa_L \sum_{\langle ij \rangle} \phi_i \phi_j + \frac{(\mu_L^2 + 4\kappa_L)}{2} \sum_i \phi_i^2 + \frac{\lambda_L}{4} \sum_i \phi_i^4 .$$

The system undergoes a second-order phase transition for a critical value of the mass when

$$\mu_L^2 < 0 \qquad \lambda_L > 0 \qquad \kappa_L > 0$$

We will apply a standard renormalization group transformation, in the vicinity of the phase transition of the φ^4 theory, and calculate the original and renormalized magnetization of the system.

Inverse Renormalization Group in Quantum Field Theory, D. Bachtis, G. Aarts, F. Di Renzo, B. Lucini, Phys. Rev. Lett. 128, 081603 (2022)