Applications of Machine Learning to Lattice Quantum Field Theory

Biagio Lucini

(work in collaboration with G. Aarts and D. Bachtis)

Strong and Electro-Weak Matter 2022, Paris, France, June 2022

Overview

- Augmenting physical knowledge with Machine Learning
- Methods and models
- Quantitative characterization of phase transitions with Machine Learning
- Deriving new observables with Machine Learning
- Inverting the renormalization group flow with Machine Learning
- Summary and perspectives

Machine Learning for Phase Transitions

Recent and current problems investigated include

- Can a Machine Learning algorithm detect a phase transition?
- Which algorithms are "better"?
- Can we find the order parameter?
- Can we reconstruct the symmetry that drives the transition?
- To which precision can we determine the transition temperature?
- With which accuracy can we measure quantities such as critical exponents?
- Can we see the *features* (e.g, topological excitations) that are relevant for the transition?
- Can machine learning invert the Renormalisation Group flow?

The Ising Model in D=2 dimensions

Prifysgol Abertawe Swansea University

- Popular testbed for new numerical approaches, as it has analytic solution at $h = 0$
- Variables: spins $\sigma_i = \pm 1$ distributed on a L^2 grid
- Hamiltonian

$$\mathcal{H} = -\mathcal{J} \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i \ , \qquad \mathcal{J} > 0$$

$\mathbb{Z}_2$ symmetry $\sigma_i \mapsto -\sigma_i$

- Partition function at temperature T

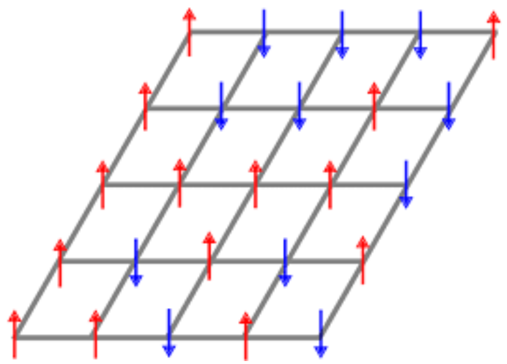
$$Z(\beta, h) = \sum_{\{\sigma_i = \pm 1\}} e^{-\beta \mathcal{H}} = e^{-\beta F} \ , \qquad \beta = (kT)^{-1}$$

For $h = 0$ phase transition at $T_c = \frac{2}{k\left(\log(1+\sqrt{2})\right)} = 2.2691853\ldots$

- Phase transition driven by spontaneous breaking of $\mathbb{Z}_2$ symmetry, with order parameter

$$m = \frac{1}{L^2 Z} \sum_{\{\sigma_i = \pm 1\}} \sigma_i e^{-\beta \mathcal{H}} = \frac{1}{L^2} \langle \sum_i \sigma_i \rangle$$

For $L \to \infty$, $m \neq 0$ for $T < T_c$, while $m = 0$ for $T > T_c$



The Ising critical point

- At $L = \infty$ the magnetic susceptibility has a divergence at T_c:

$$\chi = \frac{1}{L^2}\left(\langle\left(\sum_i \sigma_i\right)^2\rangle - \langle\sum_i \sigma_i\rangle^2\right) \underset{T\to T_c^{\pm}}{\propto} |T - T_c|^{-\gamma}$$

- At finite volume, the latter singularity gets smoothened down into a peak $\chi_{\text{max}}(T_c(L))$ and

$$|T_c(L) - T_c| \propto L^{-\frac{1}{\nu}} \ , \qquad \chi_{\text{max}}(T_c(L)) \propto L^{\frac{\gamma}{\nu}}$$

- Finite size scaling: extract γ and ν from the variation with L of $\chi_{\text{max}}(T_c(L))$

The other critical exponents can be derived from scaling relations

Fisher Law:	$\gamma = \nu(2 - \eta)$,
Widom Law:	$\gamma = \beta(\delta - 1)$,
Rushbrooke Law:	$\alpha + 2\beta + \gamma = 2$,
Josephson Law:	$\nu d = 2 - \alpha$,

The self-interacting scalar field in D=2

Prifysgol Abertawe Swansea University

- Action

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

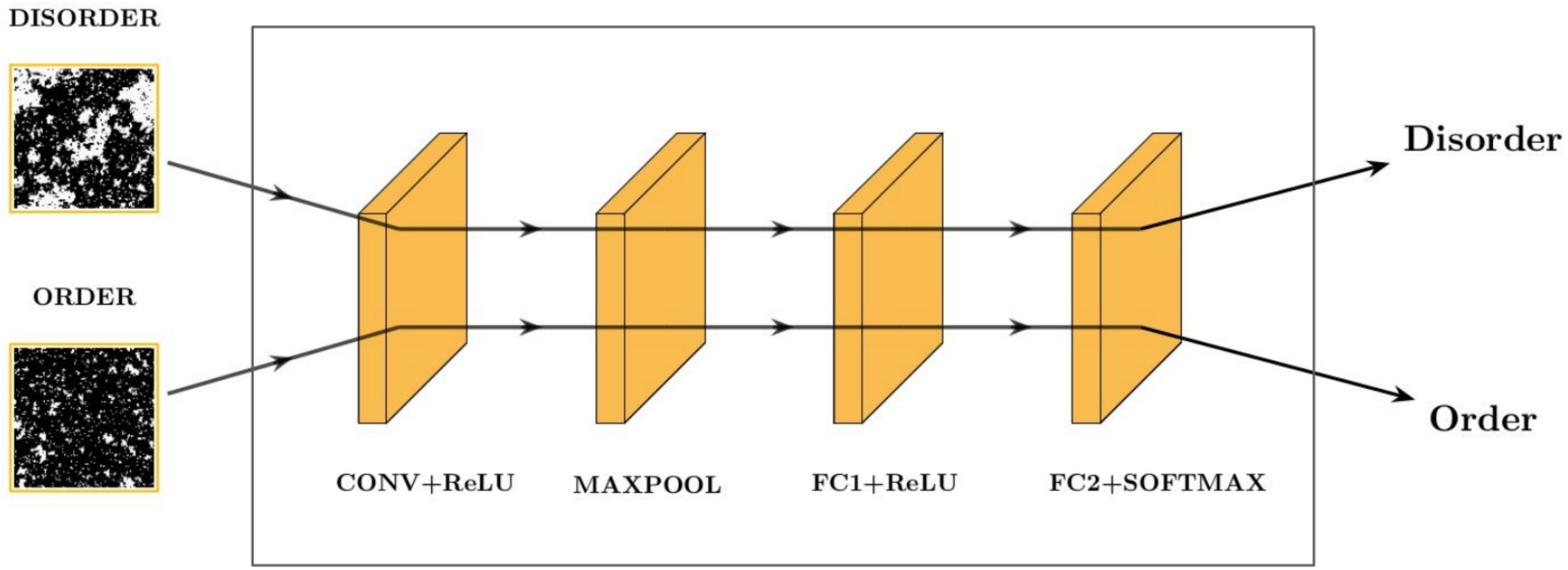
- We fix $\kappa_L = 1$ and find a line of critical points, depending on the ratio λ_L / μ_L^2
- We consider the reference critical values

$$\lambda_L = 0.7 \; , \qquad \mu_L^2 = -0.95153(16)$$

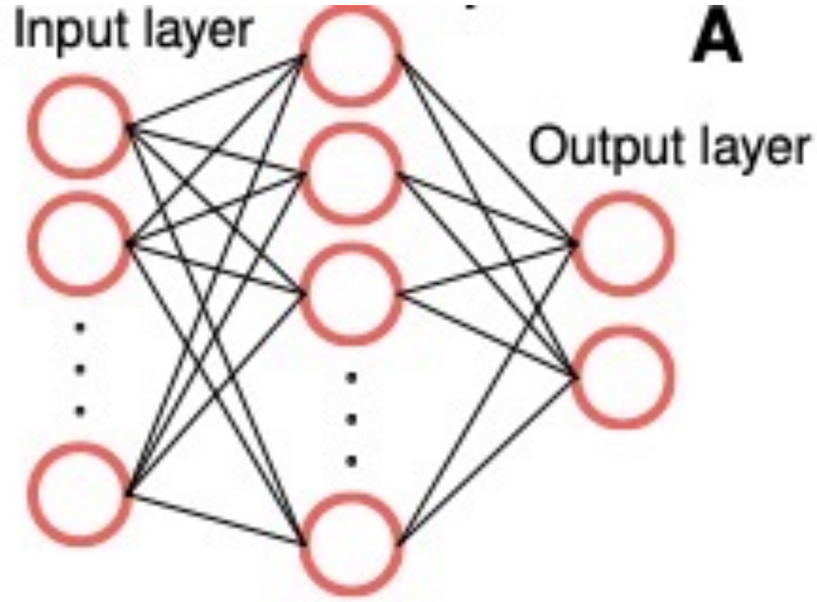
[D. Schaich, W. Loinaz, arXiv:0902.0045]

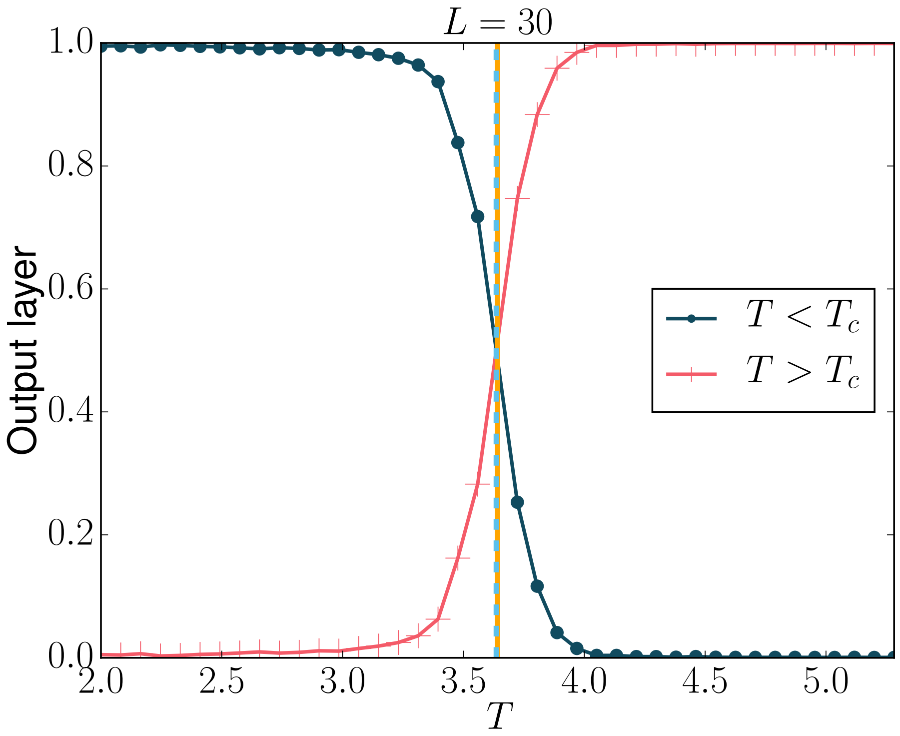
Convolutional Neural Networks

$f(\sigma_i)$



Exposing the phase structure





- Neural Network trained on a square lattice
- Critical temperature on the triangular lattice determined at the permille level (finite size shift?)

[Carrasquilla and Melko, Nature Physics volume 13, pages 431–434 (2017), arXiv:1605.1735]

Summary of other results

[C. Giannetti, B. Lucini and D. Vadacchino, Nucl.Phys.B 944 (2019) 114639, arXiv:1812.06726]

- Critical exponents reproduced with very good accuracy

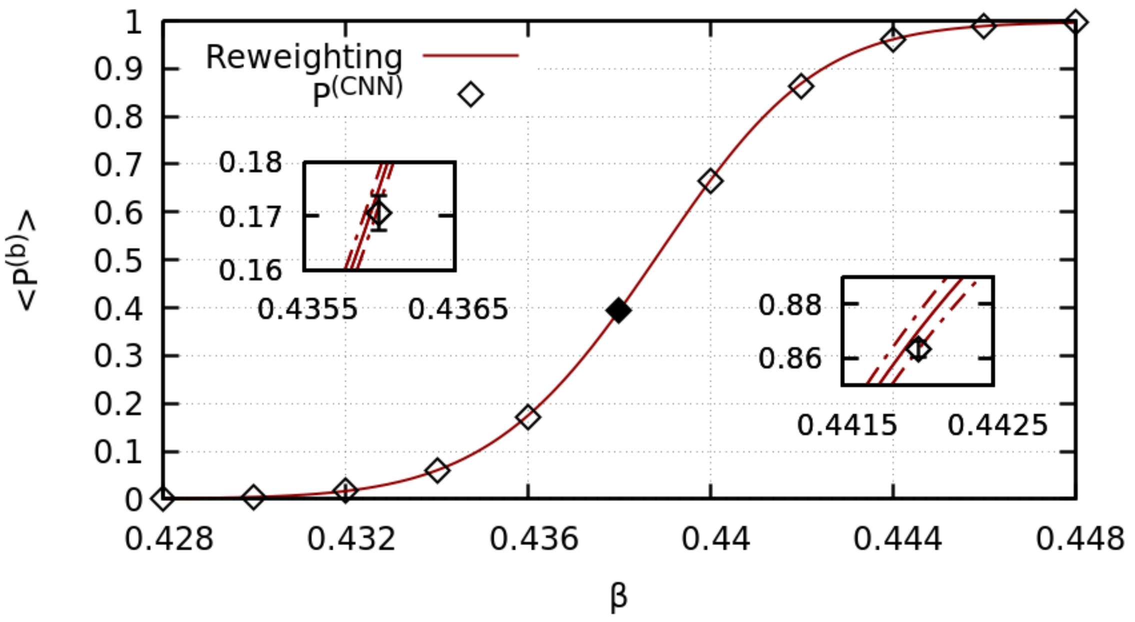
Method	T_c	ν	χ_r^2	γ/ν	χ_r^2
Reweighting	2.26922(33)	1.004(48)	0.36	1.7634(68)	0.46
	2.26925(11)	1 (exact)	0.3	7/4 (exact)	0.66
SVM	2.26968(66)	0.95(18)	0.79	1.733(10)	1.54
	2.26954(25)	1 (exact)	0.65	7/4 (exact)	2.06

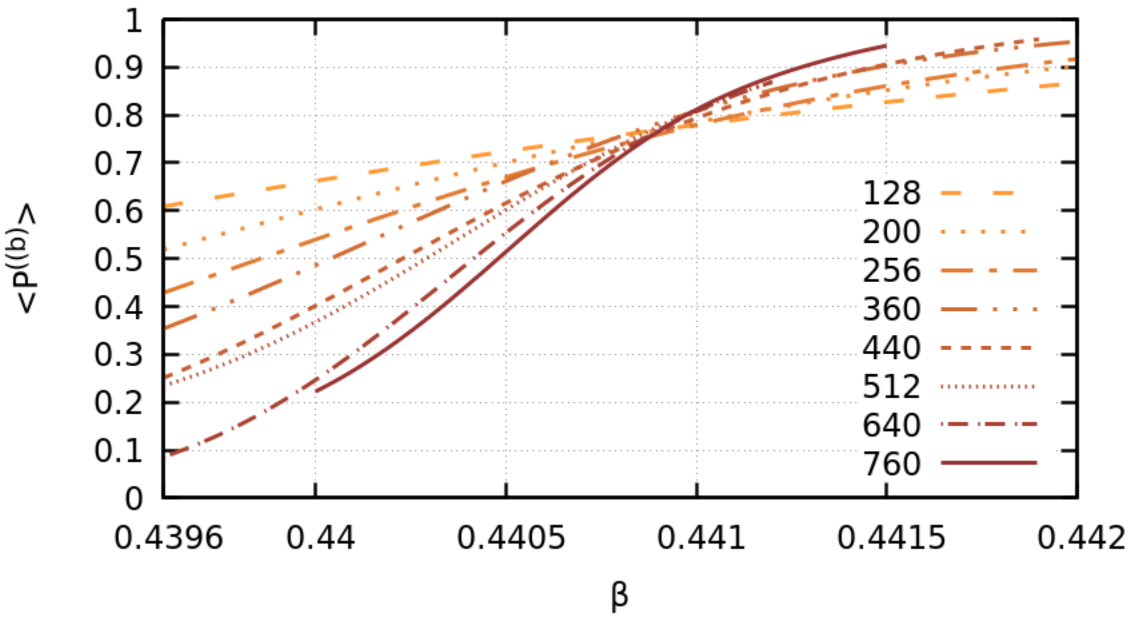
- The machine learning method (SVM) finds the (square of the) magnetization as the decision function
- The symmetry is encoded in the kernel transformation
- Independence of the (sensibly chosen) training temperatures

Probability of classification as an observable

NN trained away from the phase transition: $\beta \leq 0.41$ and $\beta \geq 0.47$

The probability of classification reweighted using a single point agrees with direct measurement
→ this probability is a thermodynamic observable!

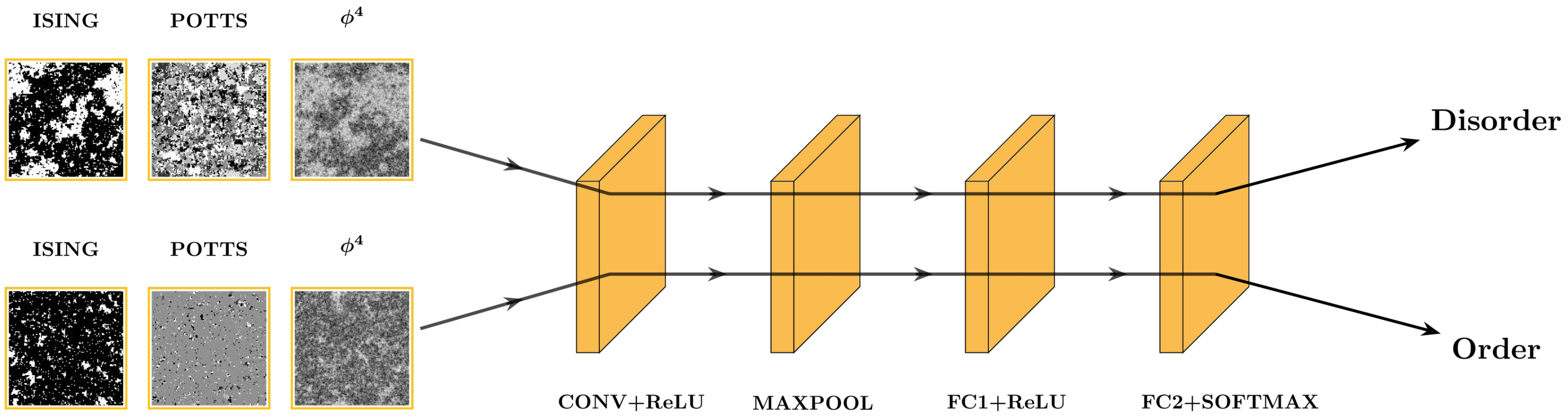


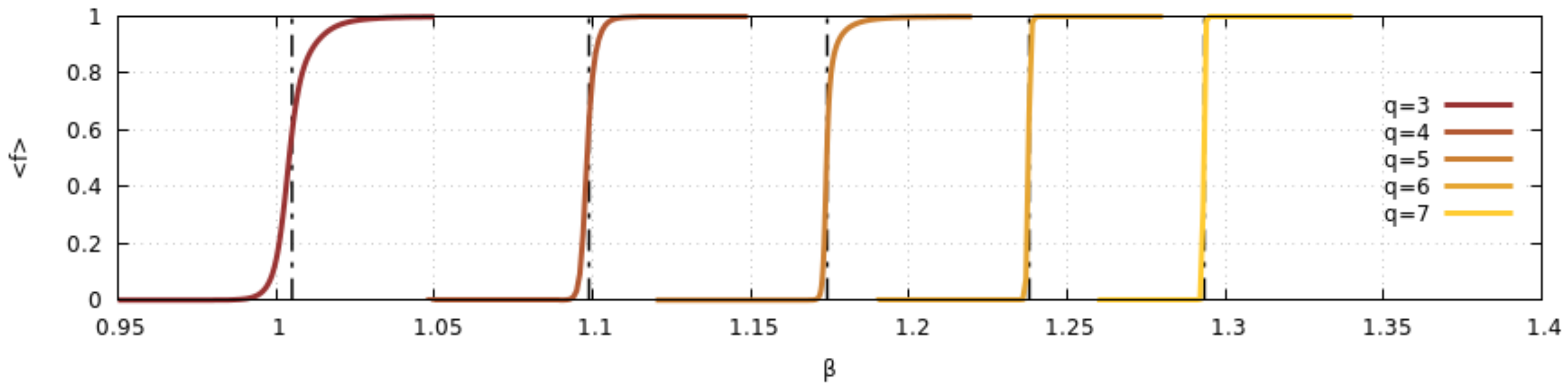


[D. Bachtis, G. Aarts and B. Lucini, Phys. Rev.E 102 (2020) 3, 033303, arXiv:2004.14341]

Transfer learning

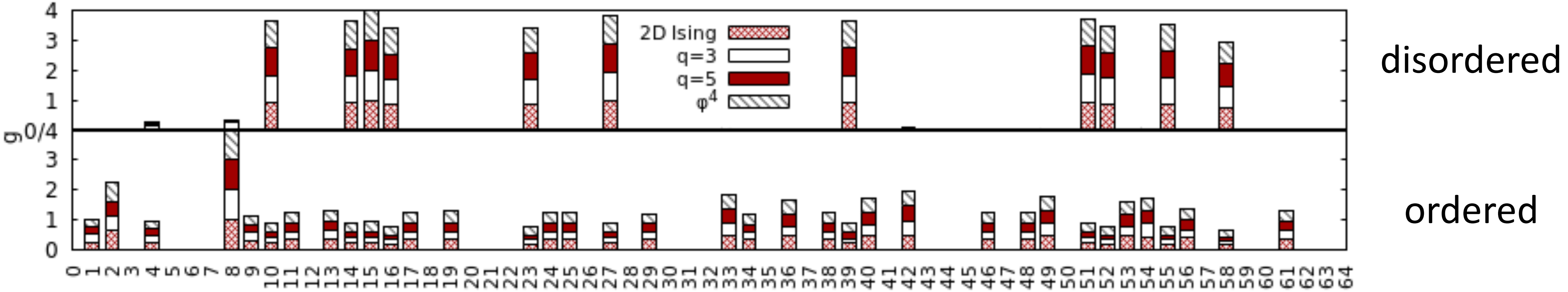
[D. Bachtis, G. Aarts and B. Lucini, Phys.Rev.E 102 (2020) 5, 053306, arXiv:2007.00355]





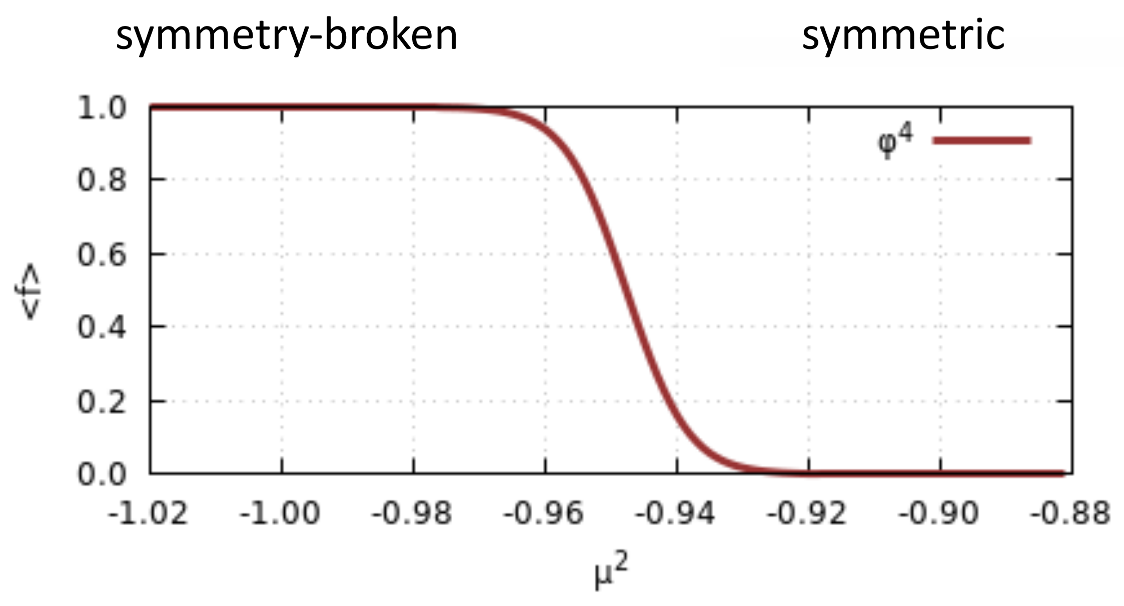
A Convolutional Neural Network trained on Ising 2D can locate the order-disorder transition in other spin models

Towards interpretability: activation functions in NN

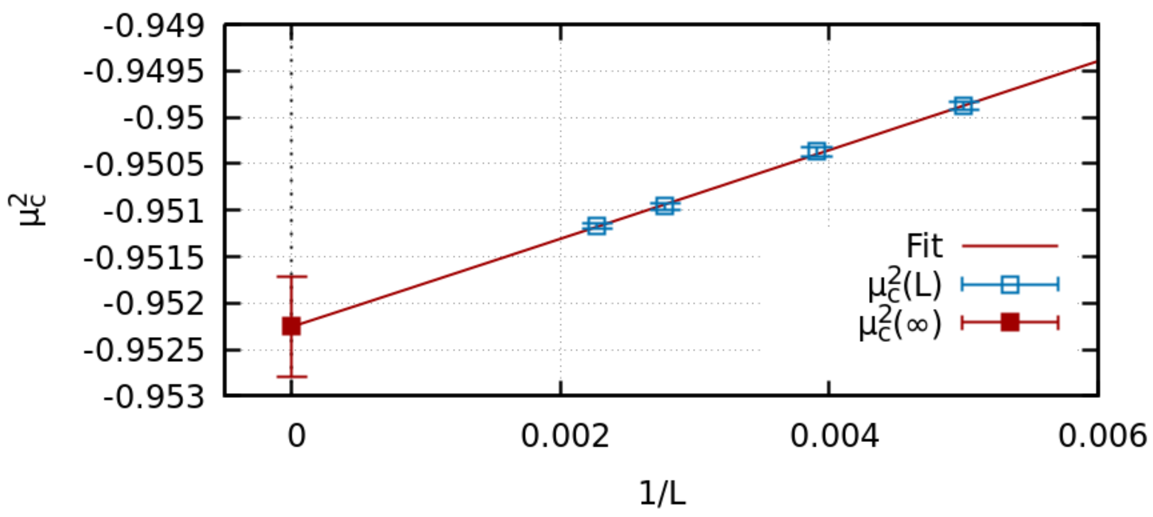


Universal features distinguish ordered and disordered phases, irrespective of e.g. order of transition

ϕ^4 scalar field theory



- reweight in mass parameter, μ^2
- identify regions where phase is clear
- retrain NN using $\mu^2 < -1.0$ and $\mu^2 > -0.9$
- repeat finite-size scaling analysis as in 2d Ising model



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

- same universality class as 2d Ising model
- critical mass in agreement with results obtained with standard methods (Binder cumulant, susceptibility)

Coupling f to the Hamiltonian

Define an observable variable Y conjugated to f and write an extended Hamiltonian

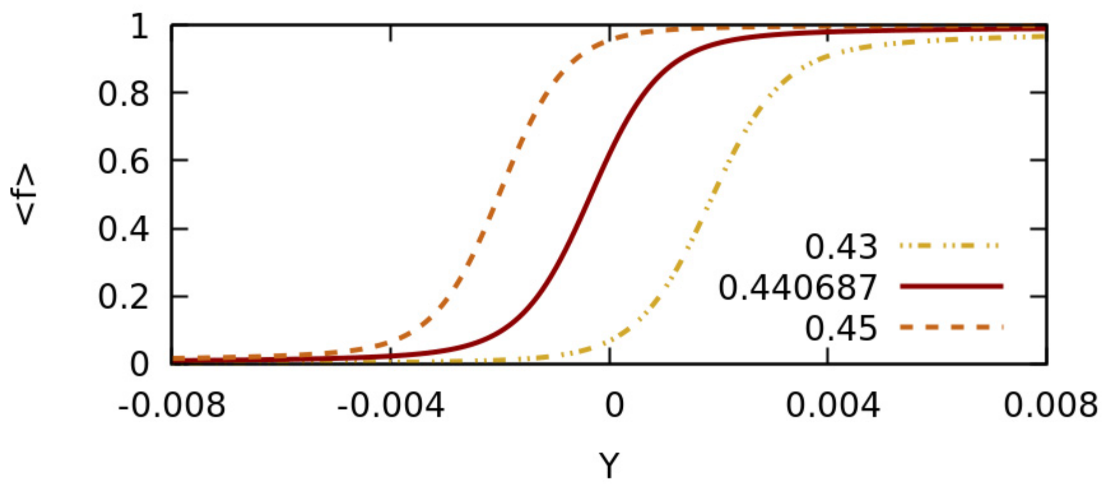
$$E_Y = E - V f Y.$$

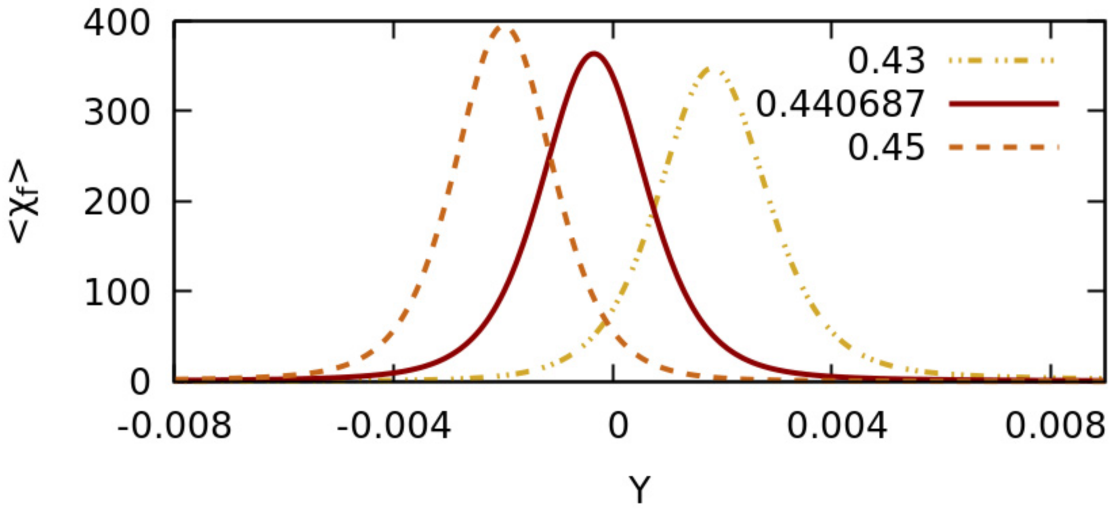
Now f can be computed using path integral methods

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

Note that Y define a new direction for reweighting and that reweighting in this direction does not require the knowledge of E_Y

Induced phase transition





Critical exponents calculated with Renormalisation Group methods

	β_c	ν	θ_Y, θ
RG+NN	0.44063(21)	1.01(2)	$\theta_Y = 0.534(3)$
Exact	$\ln(1+\sqrt{2})/2$	1	$\theta = 8/15$

f allows access to the magnetic critical exponent θ

The Inverse Renormalisation Group

[D. Bachtis, G. Aarts, F. Di Renzo, and B. Lucini, Phys. Rev. Lett., 128:081603 (2022)]

Prifysgol Abertawe
Swansea University

Purpose: generating configurations on larger lattices starting from smaller ones near criticality with negligible computational cost

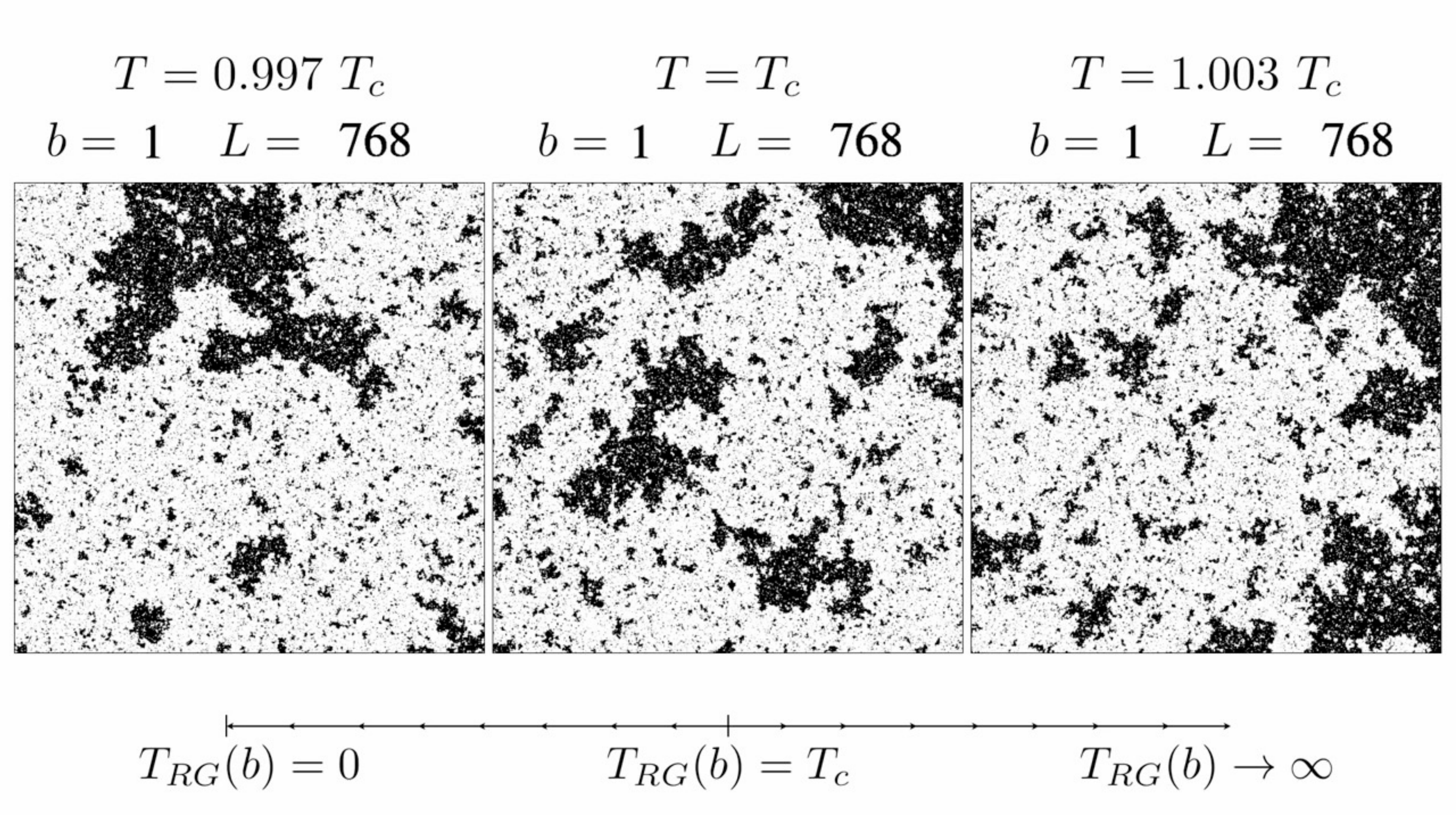
Not a new idea, e.g.

- R.H. Swendsen, Phys. Rev. Lett., 42:859–861 (1979)
- D. Ron, R.H. Swendsen, and A. Brandt, Phys. Rev. Lett., 89:275701 (2002)
- S. Efthymiou, M.J.S. Beach, and R.G. Melko, Phys. Rev. B, 99:075113, (2019)
- S.-H. Li and L. Wang, Phys. Rev. Lett., 121:260601 (2018)
- K. Shiina, H. Mori, Y. Tomita, H.K. Lee, and Y. Okabe, Scientific Reports, 11(1):9617 (2021)

Our work presents the first IRG calculation for a Quantum Field Theory

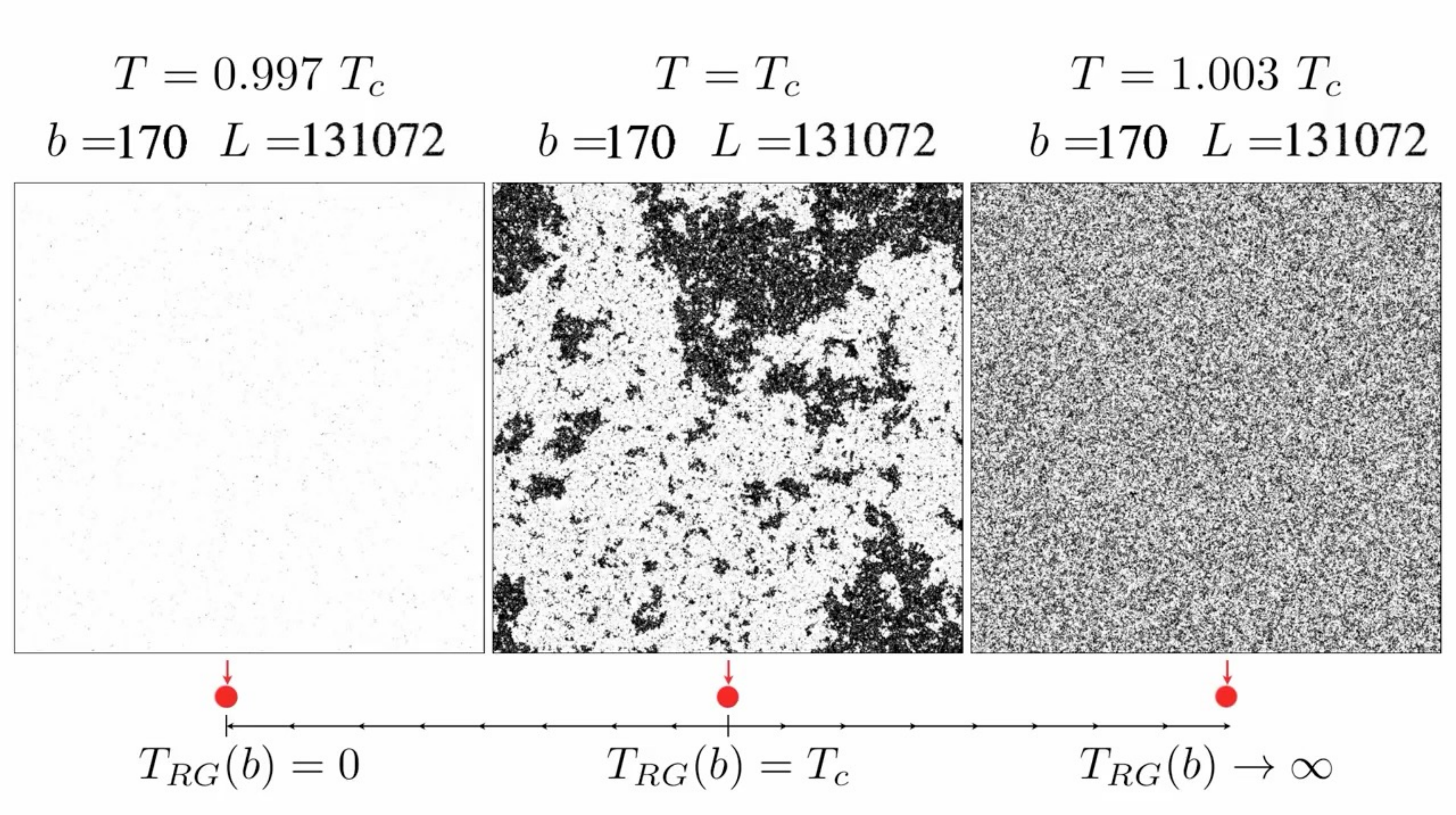
How the Renormalisation Group works

[Adapted from https://blog.dougashton.net/2012/04/the-renormalisation-group/ , video released under CC BY-SA 4.0]



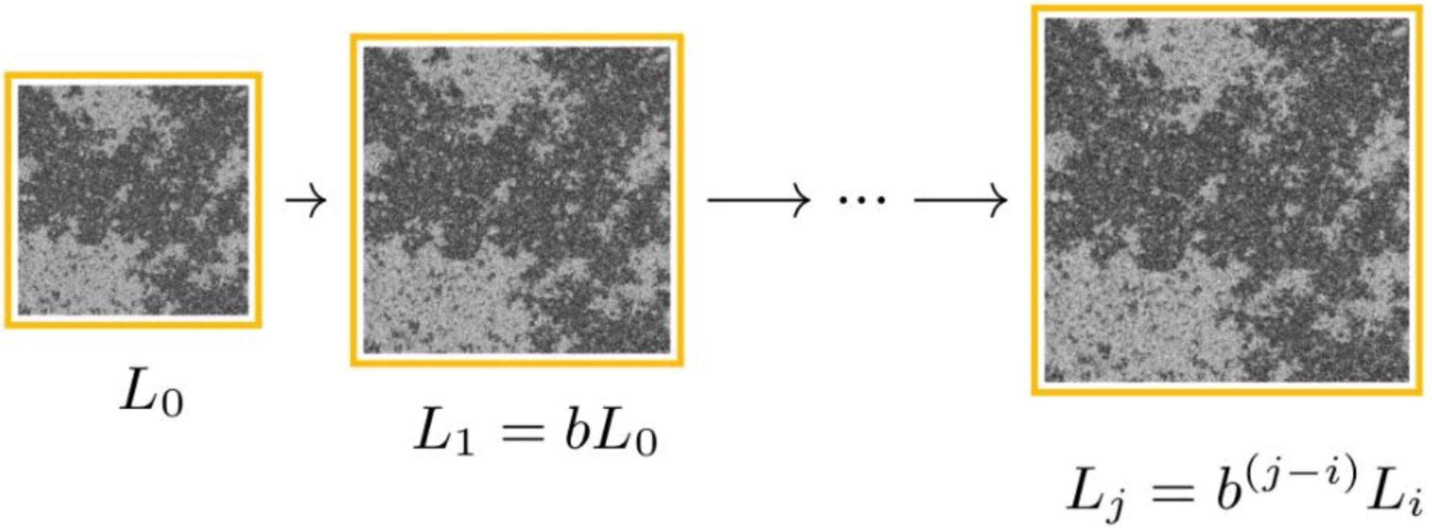
How we expect the IRG to work

[Adapted from https://blog.dougashton.net/2012/04/the-renormalisation-group/ , video released under CC BY-SA 4.0]



Benefits of the IRG

- Overcome critical slowing down $\tau \propto \xi^z$
- More precise calculations of observables at criticality
- Better insights on the infrared dynamics of the model
- Can grow the lattice size indefinitely



Known problem: the RG is not invertible

To invert the RG, we would need to grow the number of degrees of freedom, but the process is not unique

E.g., for a blocked spin equal to +1 possibilities (majority rules) include

+1	+1
+1	-1

-1	+1
+1	+1

-1	+1
+1	-1

-1	+1
+1	-1

…

Even worse for the scalar field, e.g.

0.01	0.36
0.02	0.01

-421.1	90.1
0.5	330.9

…

compatible with a blocked spin value 0.4

What we mean by inverting the RG then?

Prifysgol Abertawe Swansea University

- We start from a set of configuration generated via a Monte Carlo on a lattice of size L
- Using a Machine Learning algorithm, from those we derive a set of configurations on a lattice L' = b L (typically, b=2)
- We assume that the ensemble at L' as distributed according to the Boltzmann measure at L
- This enables us to compute (and to reweight!) observables at L'
- Using crossing of curves, we compute critical quantities

Advantage: numerical effort done on small lattices, hence relatively cheap

Critical to the process: blocking method, ML algorithm and assumption of Boltzmann distribution

The blocking method

Prifysgol Abertawe Swansea University

- Given a block B with generic point i, consider

$$\phi_B^+ = \frac{\sum_{i \in B} \phi(i)\theta(\phi(i))}{\sum_{i \in B} \theta(\phi(i))} \quad \text{and} \quad \phi_B^- = \frac{\sum_{i \in B} \phi(i)\theta(-\phi(i))}{\sum_{i \in B} \theta(-\phi(i))}$$

- Now, set

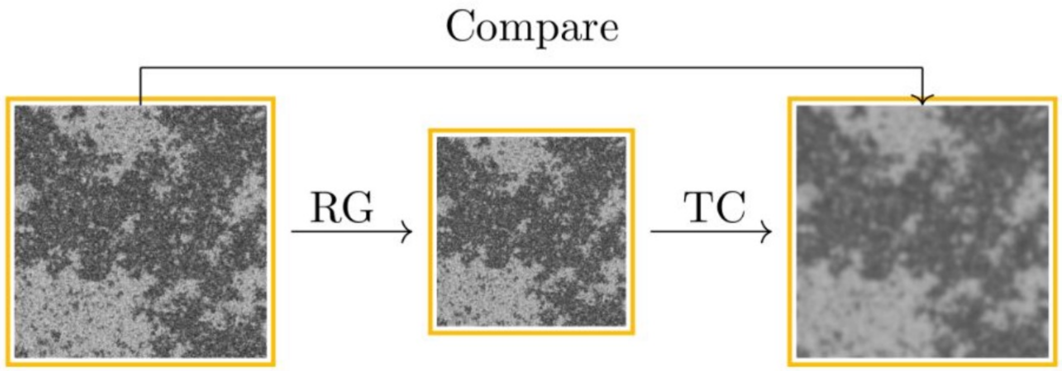
$$\phi_B = \phi_B^+ \theta(\phi_B^+ + \phi_B^-) + \phi_B^- \theta(-\phi_B^+ - \phi_B^-)$$

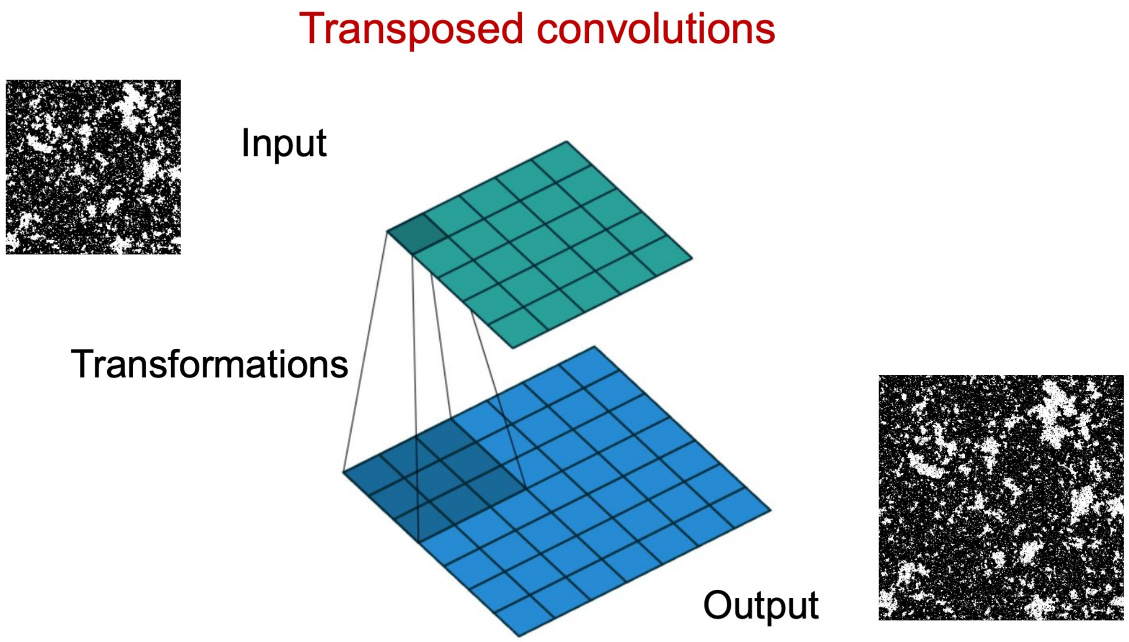
- This is equivalent to the majority rule in the Ising model

Lattice augmentation with Machine Learning

Prifysgol Abertawe Swansea University

Central concept: transposed convolution

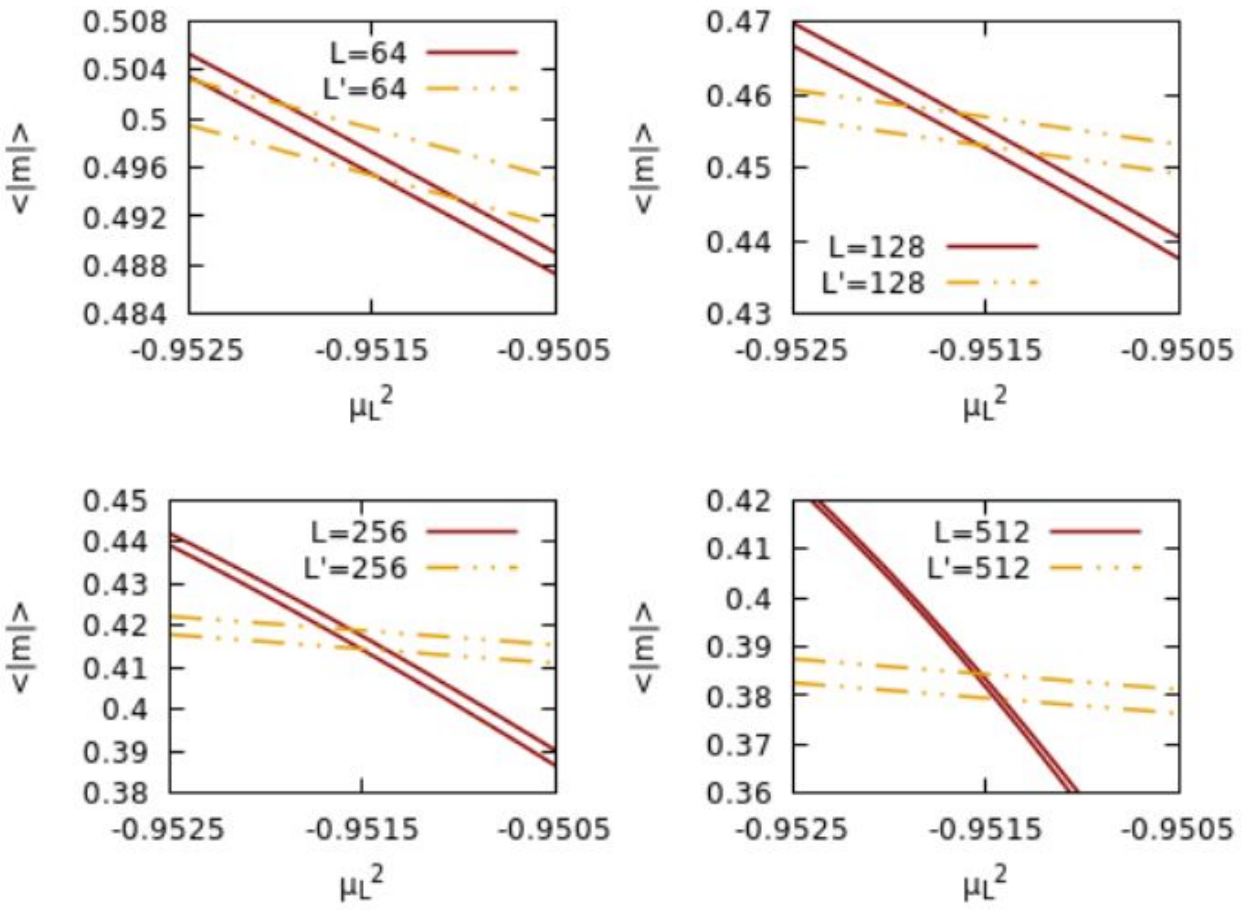




Determining the direction of the RG flow

Prifysgol Abertawe
Swansea University

- Comparison with directly simulated lattices show that in the augmented system **the coupling flows towards the critical point**
- Plotting two different lattice sizes (no need for direct simulation!) the crossing identifies an estimate for the critical coupling



Determining critical quantities

We can rewrite the scaling relationships for the magnetisation

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

in terms of the correlation length

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

to obtain the operational definition of the critical exponent ratio

$$\frac{\beta}{\nu} = -\frac{\ln \frac{dm_j}{dm_i}\Big|_{K_c}}{\ln \frac{\xi_j}{\xi_i}} = -\frac{\ln \frac{dm_j}{dm_i}\Big|_{K_c}}{(j-i)\ln b}$$

Similarly, from χ we get γ/ν

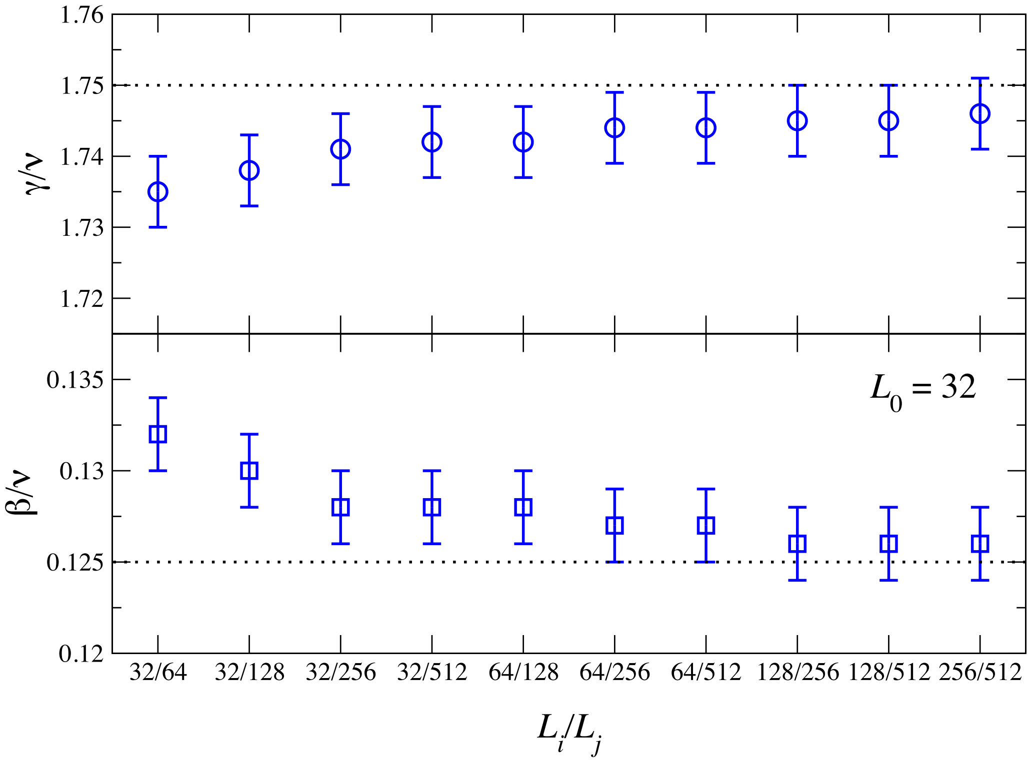
Critical exponents

Method: configurations obtained with a simulation for L=32 and IRG augmentation up to L=512

Ratios of critical exponents extracted for pairs of lattices

Expected asymptotic approach to Ising values clearly observed

All with no critical slowing down!



Conclusions and Outlook

Prifysgol Abertawe Swansea University

- Machine Learning offers a novel angle to look at phase transitions
- It enables precise calculations of critical properties with no assumed knowledge on the underlying symmetry
- Machine Learning exposes novel observables, whose behaviour can offer insights on the dynamics of the phase transition
- A powerful demonstrator of the potential of Machine Learning is the Inverse Renormalisation Group
- Future work focusing on interpretability
- Related work ongoing to derive more efficient and interpretable Machine Learning methods from Quantum Field Theories

  [e.g., D. Bachtis, G. Aarts and B. Lucini, Phys.Rev.D 103 (2021) 7, 074510, arXiv:2107.00466]

License notice

Prifysgol Abertawe
Swansea University

The video on the RG in slide 17 is adapted from https://blog.dougashton.net/2012/04/the-renormalisation-group/ removing the explanatory first part.

The video on the IRG in slide 18 is obtained playing backward the video in slide 17.