Interpreting machine learning functions as physical observables

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with Dimitrios Bachtis and Biagio Lucini

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Part of work with Dimitrios Bachtis & Biagio Lucini

- ✓ **Extending machine learning classification capabilities with histogram reweighting**

  Phys. Rev. E 102 (2020) 033303 [2004.14341 [cond-mat.stat-mech]]

- ✓ **Mapping distinct phase transitions to a neural network**

  Phys. Rev. E 102 (2020) 053306 [2007.00355 [cond-mat.stat-mech]]

- ✓ **Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration**

  Phys. Rev. Res. 3 (2021) 013134 [2010.00054 [hep-lat]]

- ✓ Quantum field-theoretic machine learning

  Phys. Rev. D 103 (2021) 074510 [2102.09449 [hep-lat]] → see earlier talk by Dimitrios in this session

- ✓ Inverse renormalization group in quantum field theory (+ Francesco Di Renzo) → see next year's conference

  [2107.00466 [hep-lat]].

Three take-home messages

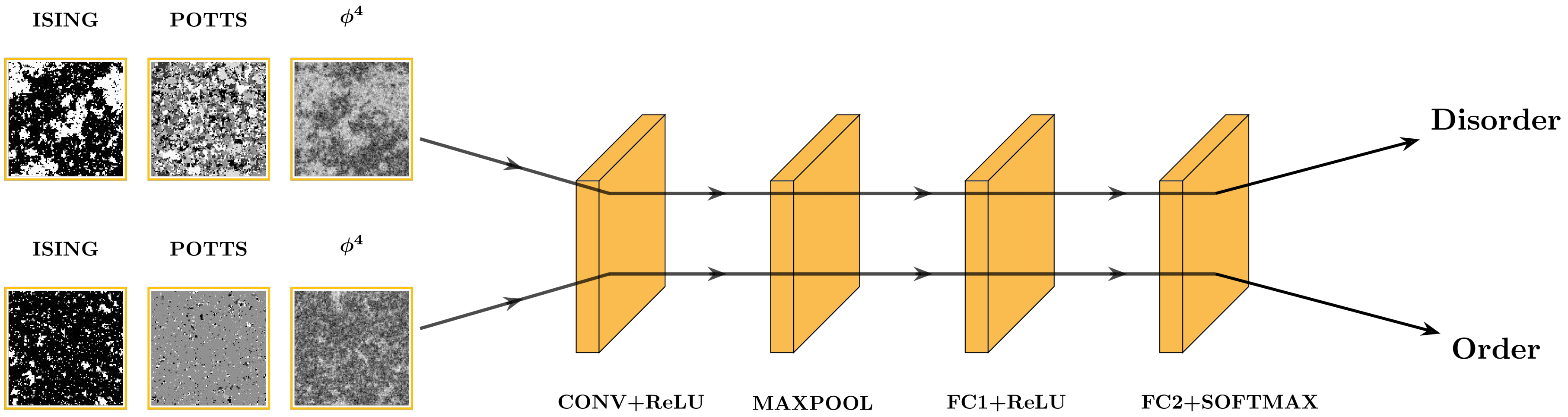
1. ML outputs as physical observables

2. Critical behaviour from NN observables only

3. Extend Hamiltonians with ML predictive functions

ML excels in pattern finding

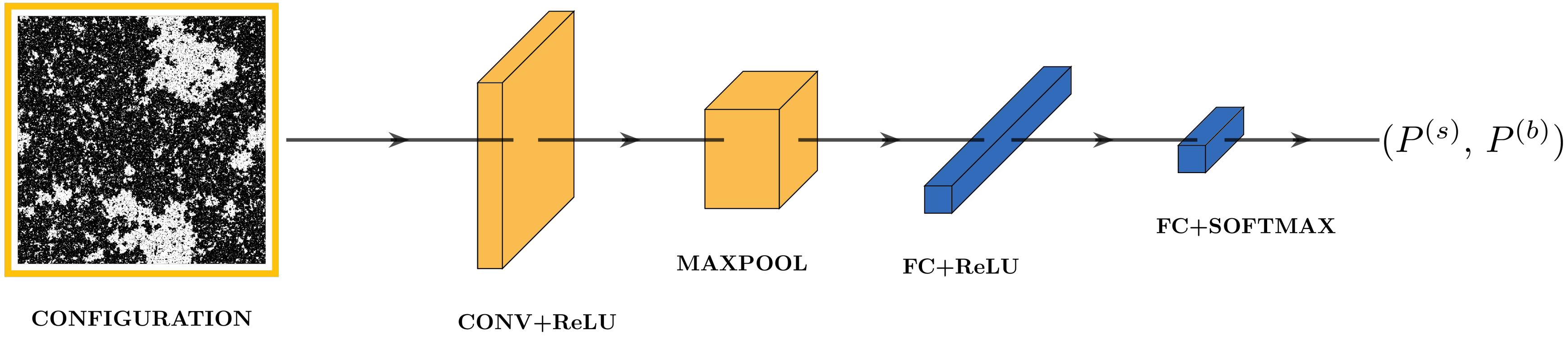
- supervised learning problem: use sets of configurations deep in the ordered and the disordered phase of Ising model, Potts models, φ^4 theory, …
- input: configurations < -- > output: ordered/disordered
- "train the ML algorithm", i.e. adjust parameters in the neural network so that it reproduces the correct classification for the training set



- new, unseen configurations -- > determine probability to be (dis)ordered

1. ML outputs as physical observables

- by now well-established procedure, what can we add?
- interpret output from a NN as an observable in a statistical system
- input: configurations, distributed according to Boltzmann weight
- output: observable, “order parameter” in statistical system



$$\Rightarrow \; < P > = \frac{1}{Z}\sum_i P_i \, e^{-\beta E_i}$$

Output of NN as physical observable

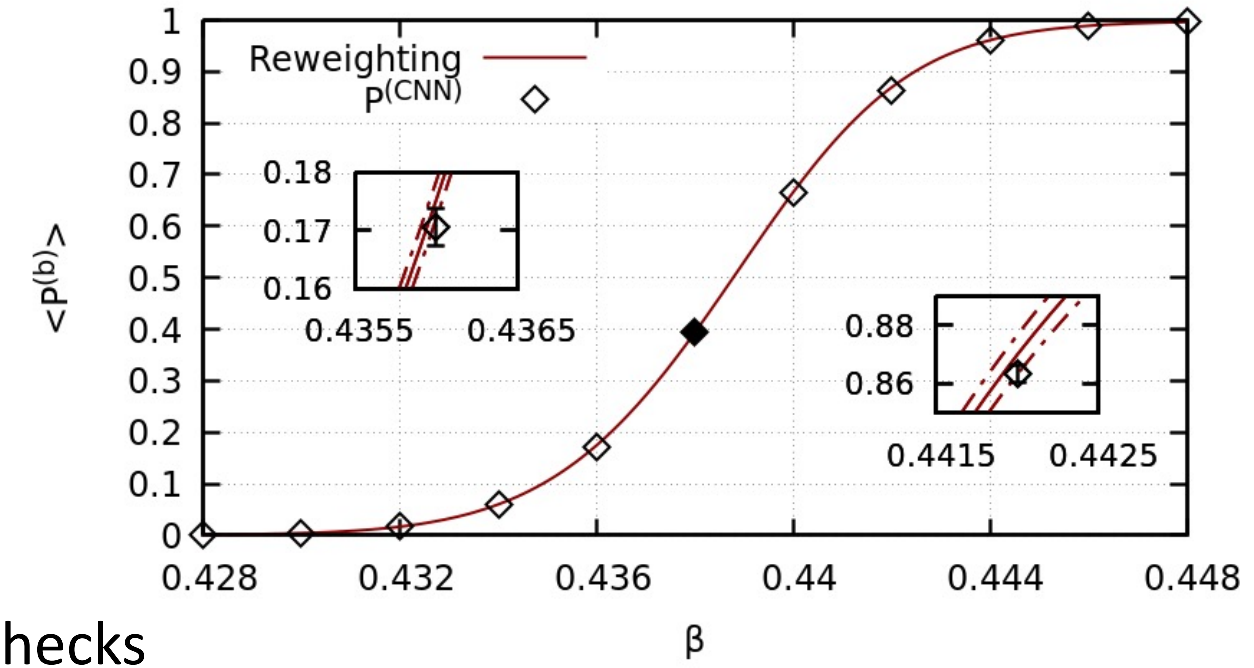
2d Ising model
$\beta_c = \frac{1}{2}\ln(1+\sqrt{2})$
~ 0.440687
train NN at $\beta \leq 0.41$
and $\beta \geq 0.47$

- opens up possibility to use “standard” numerical/statistical methods

→ histogram reweighting: extrapolation to other parameter values

- starting from computation at given β_0: extrapolate to other β values

$$< P > (\beta) = \frac{\sum P_i e^{-(\beta-\beta_0)E_i}}{\sum e^{-(\beta-\beta_0)E_i}}$$



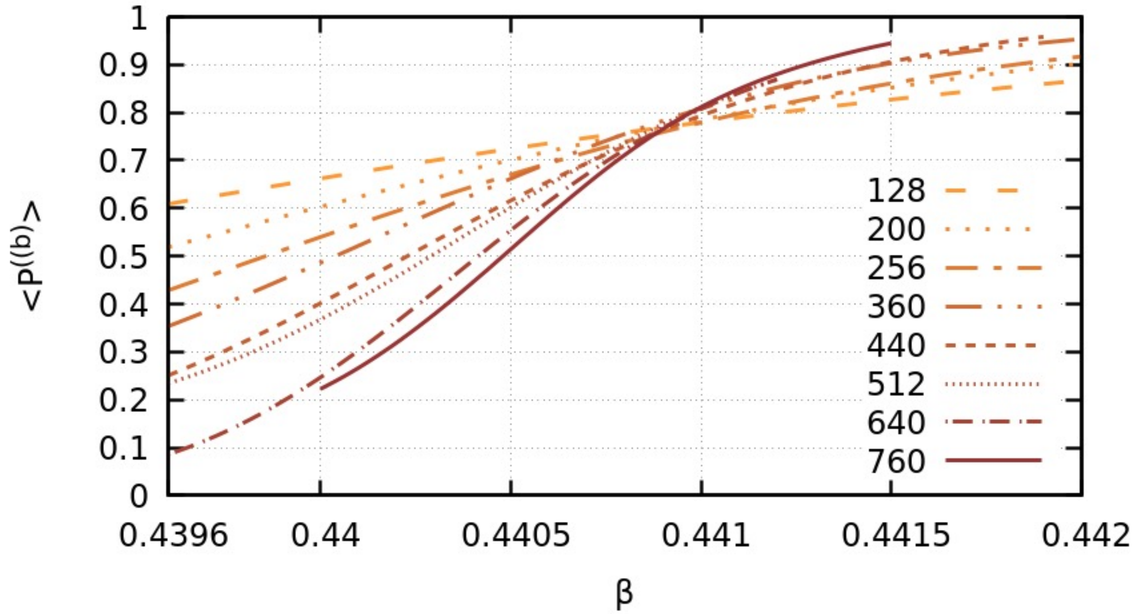
$L = 128$

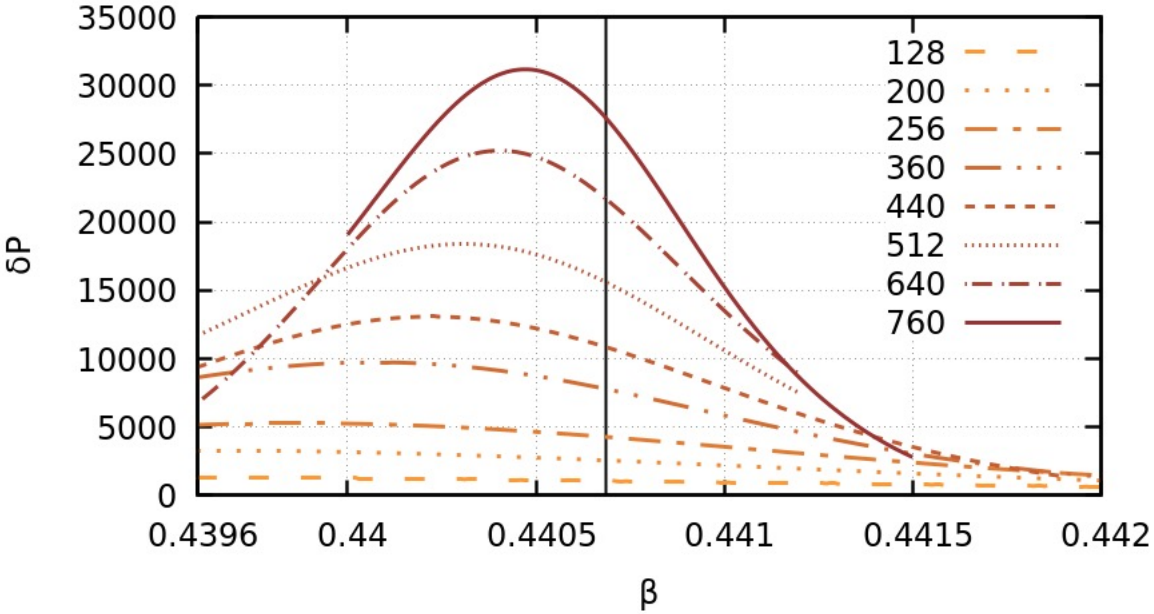
✓ filled diamond at β_0
✓ line obtained by reweighting in β
✓ open diamonds are independent cross checks

$\beta_c \sim 0.440687$

Finite size scaling with histogram reweighting

Determine L dependent probability P and its susceptibility $\chi = \delta P$





critical exponents

$\xi \sim |t|^{-\nu}$

$|t| \sim \xi^{-1/\nu} \sim L^{-1/\nu}$

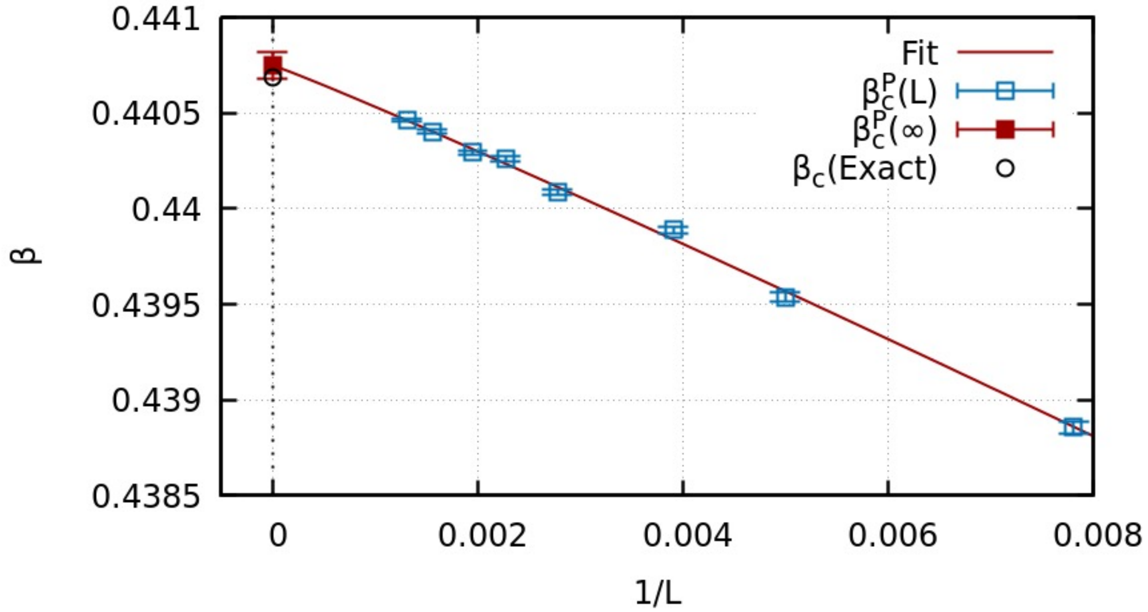
$\chi \sim |t|^{-\gamma} \sim L^{\gamma/\nu}$

determine maximum at $\beta_c(L)$

$\xi \sim |t|^{-\nu}$
$\chi \sim |t|^{-\gamma} \sim L^{\gamma/\nu}$

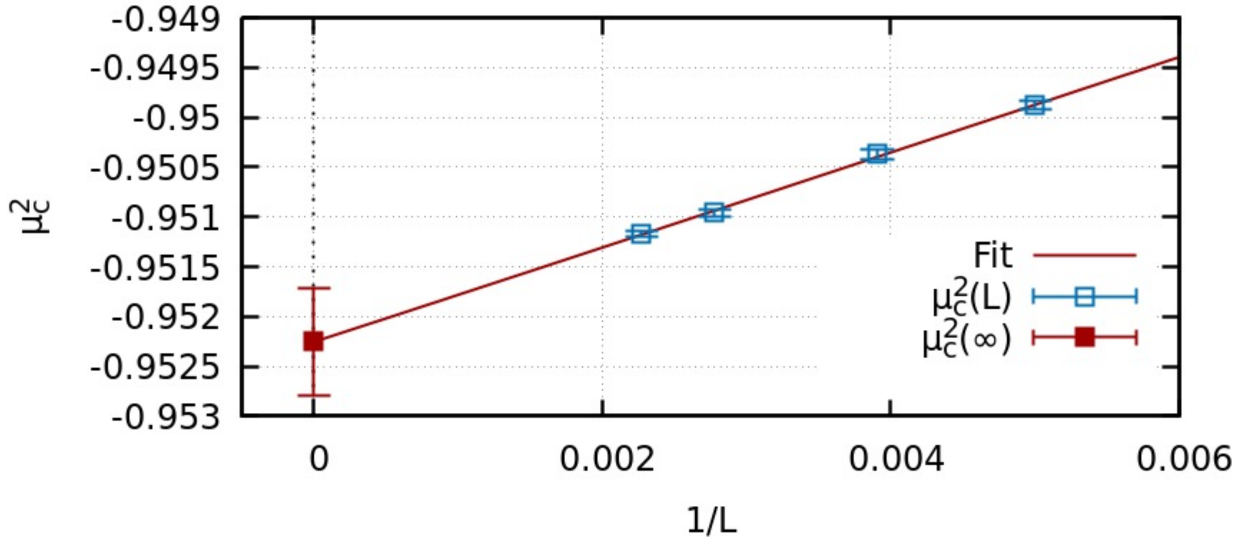
2. Critical behaviour from NN observables only

2d Ising model



	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

2d φ^4 scalar field theory at fixed λ

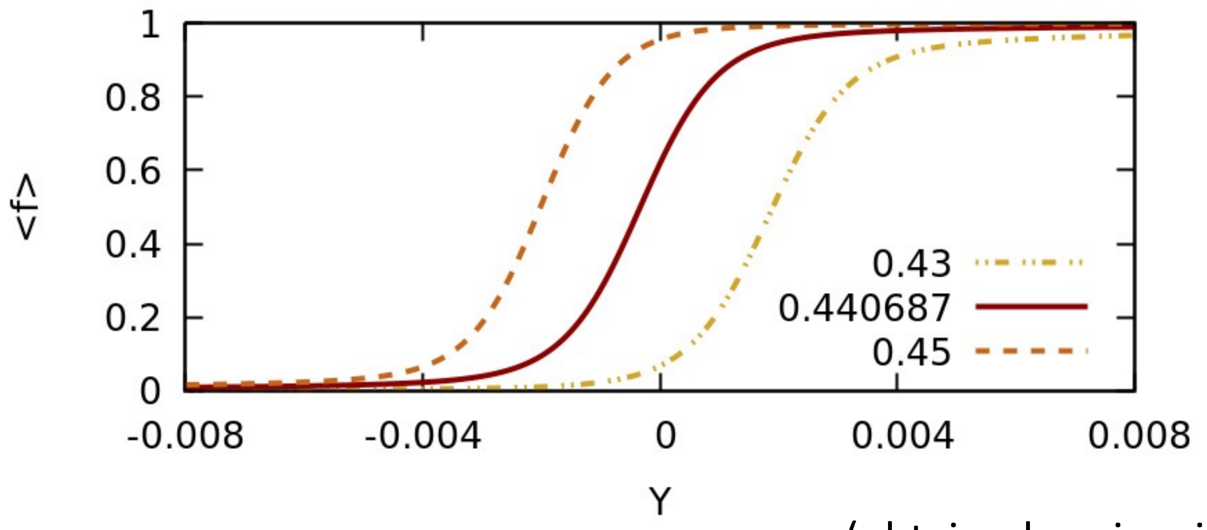


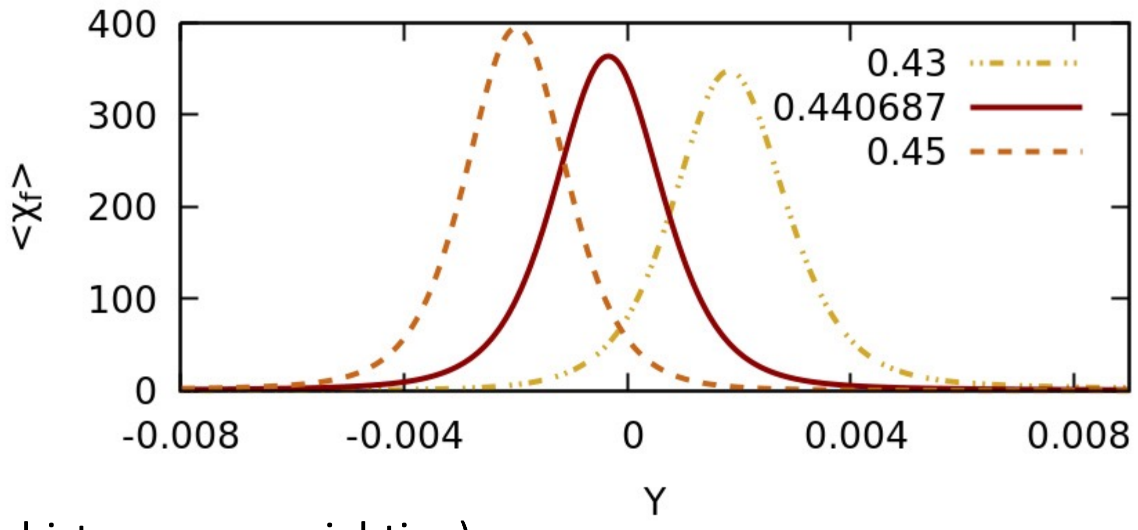
	μ_c^2	ν	γ/ν
CNN+Reweighting	-0.95225(54)	0.99(34)	1.78(7)

same universality class as 2d Ising model

3. Extend Hamiltonians with ML predictive functions

- denote ML predictive function (probability) with f, with $0 \leq f \leq 1$, intensive quantity
- add to system H, coupled to conjugate source, $H_Y = H - VfY$
- generating function: $< f > = \frac{1}{\beta V}\frac{\partial \ln Z_Y}{\partial Y}$, etc
- more importantly: induce symmetry breaking without explicit symmetry breaking





(obtained again with histogram reweighting)

Critical exponent ϑ and external field Y

- access to new critical exponent ϑ_Y : $\xi \sim |Y|^{-\vartheta_Y}$
- similar to external magnetic field $\xi \sim |h_{magnetic}|^{-\vartheta}$
  but without explicit symmetry breaking (!)
- use blocking and RG analysis:

	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	$\theta = 8/15$
	~ 0.440687		~ 0.5333

only used NN quantities, no need for knowledge of order parameter, physical meaning of external field, explicit symmetry breaking

Summary and outlook

- ✓ proposed to identify NN outputs as observables in statistical physics
- ✓ introduced histogram reweighting to employ in supervised machine learning
- ✓ critical properties obtained from a finite-size scaling analysis using quantities derived from NN alone (no need for explicit order parameter, knowledge of symmetries)
- ✓ precision results obtained for critical parameters and exponents
- ✓ quantitative studies of phase transitions based on a synergistic relation between machine learning and statistical mechanics: explore new systems