AI applications in QFT
Part III: Selected applications

Gert Aarts

MITP, Mainz, July 2025

Outline

biased selection of examples

- Gaussian restricted Boltzmann machines
- detection of phase transitions
- inverse renormalisation group
- (sign problem and diffusion models)
- outlook

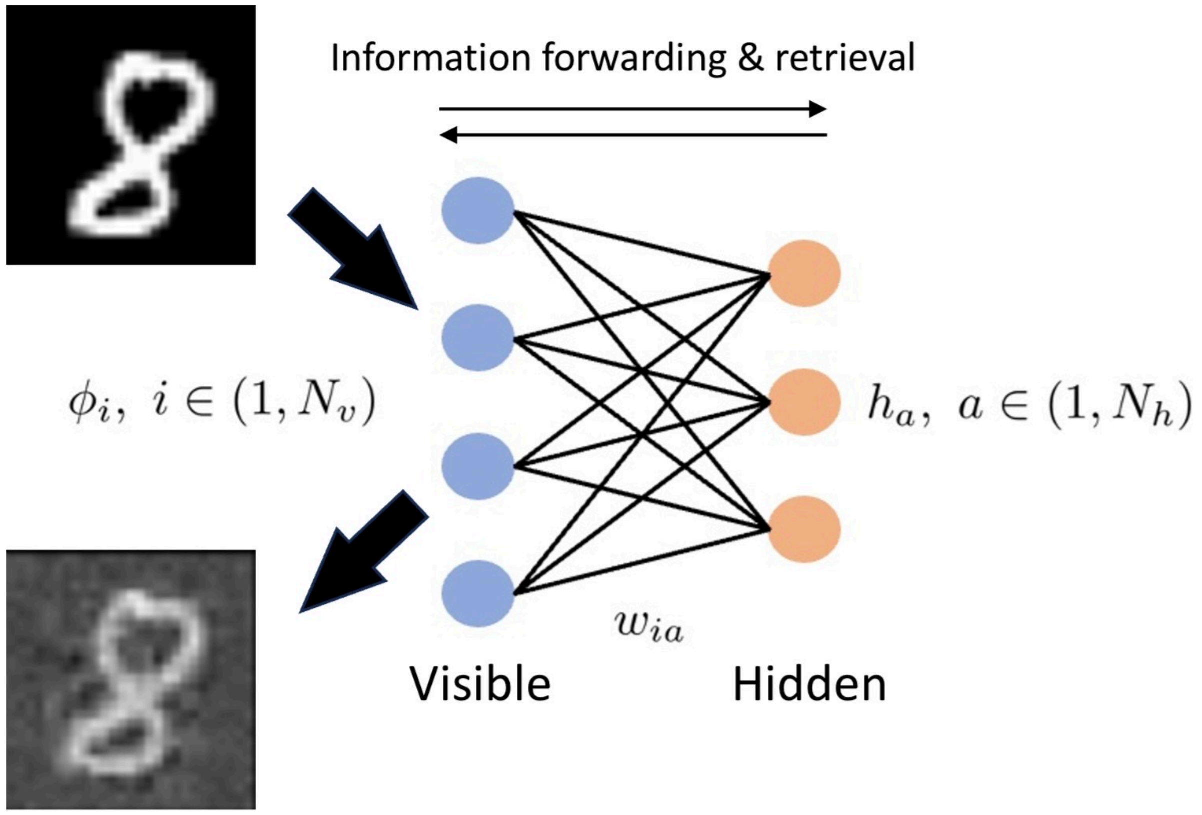
GA, B Lucini, **Chanju Park**, PRD **109** (2024) 034521 [2309.15002 [hep-lat]]

Dimitrios Bachtis, GA, B Lucini, PRE **102** (2020) 033303 [2004.14341 [cond-mat.stat-mech]] and PRE **102** (2020) 053306 [2007.00355 [cond-mat.stat-mech]]

Dimitrios Bachtis, GA, F di Renzo, B Lucini PRL **128** (2022) 081603 [2107.00466 [hep-lat]]

GA, **Diaa Habibi**, L Wang, K Zhou, PoS(Lattice 2024) [2412.01919 [hep-lat]]

Restricted Boltzmann Machine: generative network



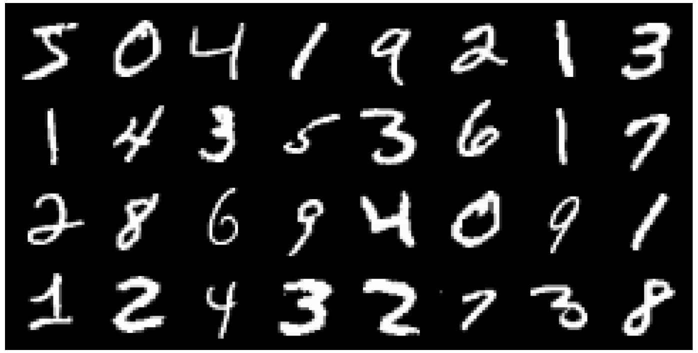
- energy-based method
- probability distribution
- binary or continuous d.o.f.

$$p(\phi, h) = \frac{1}{Z} e^{-S(\phi,h)}$$

$$Z = \int D\phi Dh\, e^{-S(\phi,h)}$$

Scalar field RBM as a generative network

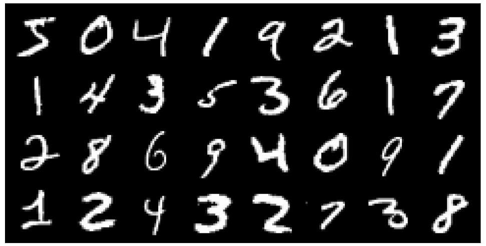
- input data: MNIST → 28 x 28 images → each image is a vector with 784 components
- encoded in the variable ϕ on the visible layer
- train Gaussian RBM to model/learn the probability distribution



$$p(\phi) = \int Dh\, p(\phi, h) = \frac{1}{Z} \exp\left(-\frac{1}{2}\phi^T K \phi + J^T \phi\right)$$

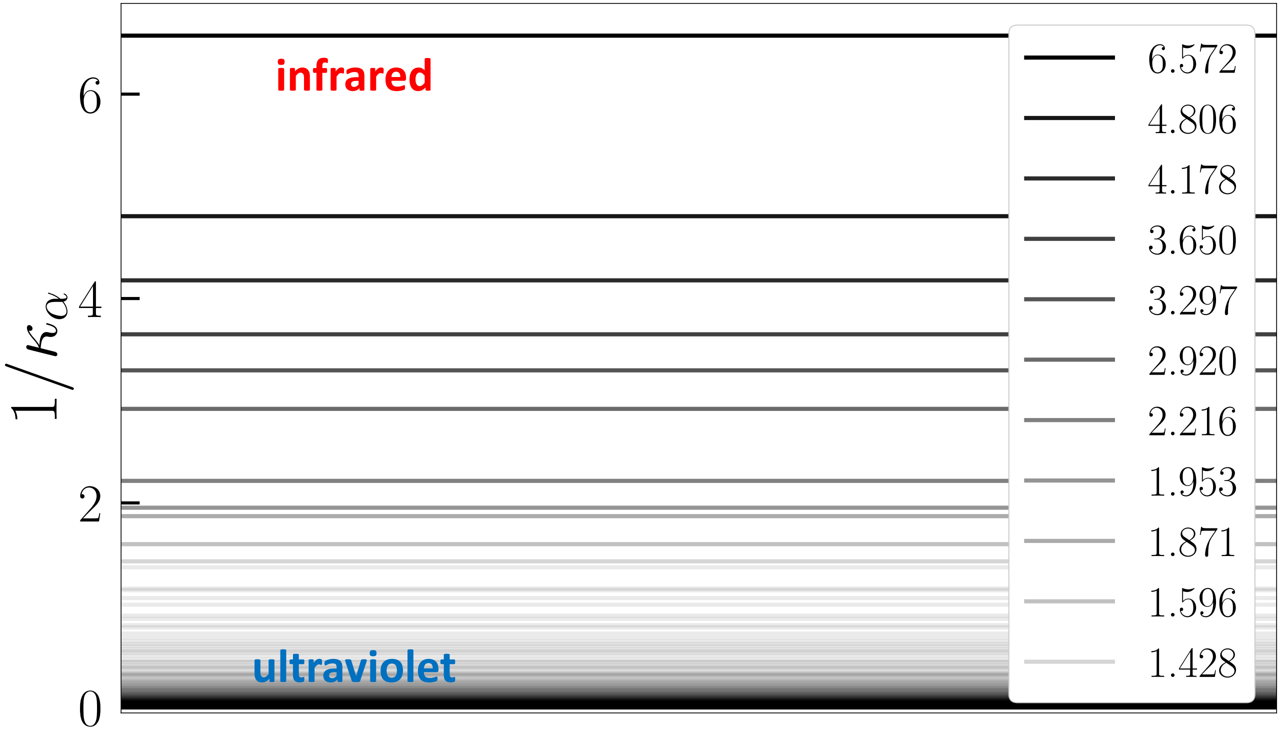
- kernel $K = \mu^2 \mathbb{1} - \sigma_h^2 W W^T$ depends on the weight matrix W : determine optimal W
- generate new images

MNIST kernel: two-point function

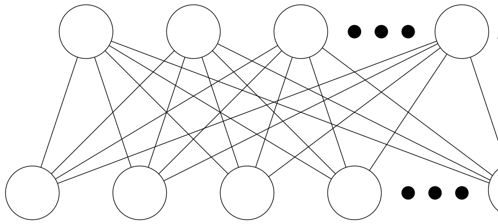


- take MNIST data set (28 x 28 images)
- compute spectrum of two-point correlator $K^{-1}_{ij} = \langle \phi_i \phi_j \rangle_{\text{data}}$
- inverse spectrum $1/\kappa$
- this spectrum should be reproduced by RBM kernel $K = \mu^2 \mathbb{1} - \sigma_h^2 W W^T$

784 eigenvalues



Scalar field RBM



- distribution: $p(\phi,h) = \frac{1}{Z} e^{-S(\phi,h)}$ $\quad S(\phi,h) = \frac{1}{2}\mu^2\phi^T\phi + \frac{1}{2\sigma_h^2}(h-\eta)^T(h-\eta) - \phi^T W h$
- $M \times N = N_v \times N_h$ weight matrix W
- induced distribution on visible layer $p(\phi) = \int Dh\, p(\phi,h) = \frac{1}{Z}\exp\left(-\frac{1}{2}\phi^T K \phi + J^T\phi\right)$
- all information is stored in quadratic operator $K = \mu^2 \mathbb{1} - \sigma_h^2 W W^T$, with spectrum (use SVD)

$$D_K = \mathrm{diag}\big(\underbrace{\mu^2 - \sigma_h^2\xi_1^2, \mu^2 - \sigma_h^2\xi_2^2, \ldots, \mu^2 - \sigma_h^2\xi_N^2}_{N}, \underbrace{\mu^2, \ldots, \mu^2}_{M-N}\big)$$

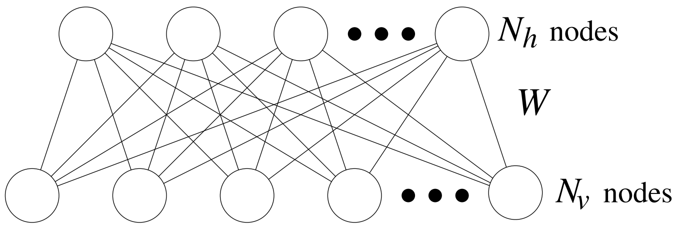
Scalar field RBM as an ultraviolet regulator

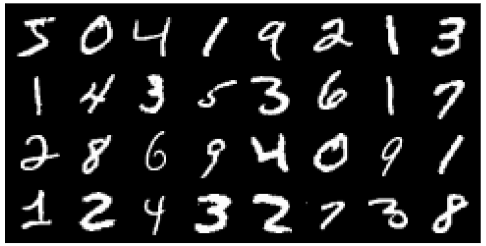
- spectrum $$D_K = \text{diag}(\underbrace{\mu^2 - \sigma_h^2\xi_1^2, \mu^2 - \sigma_h^2\xi_2^2, \ldots, \mu^2 - \sigma_h^2\xi_{N_h}^2}_{N_h}, \underbrace{\mu^2, \ldots, \mu^2}_{N_v - N_h})$$

- what if $N_h < N_v$? not all eigenvalues can be reproduced

- role of hyperparameter μ^2 ? if chosen too low, not all eigenvalues can be reproduced

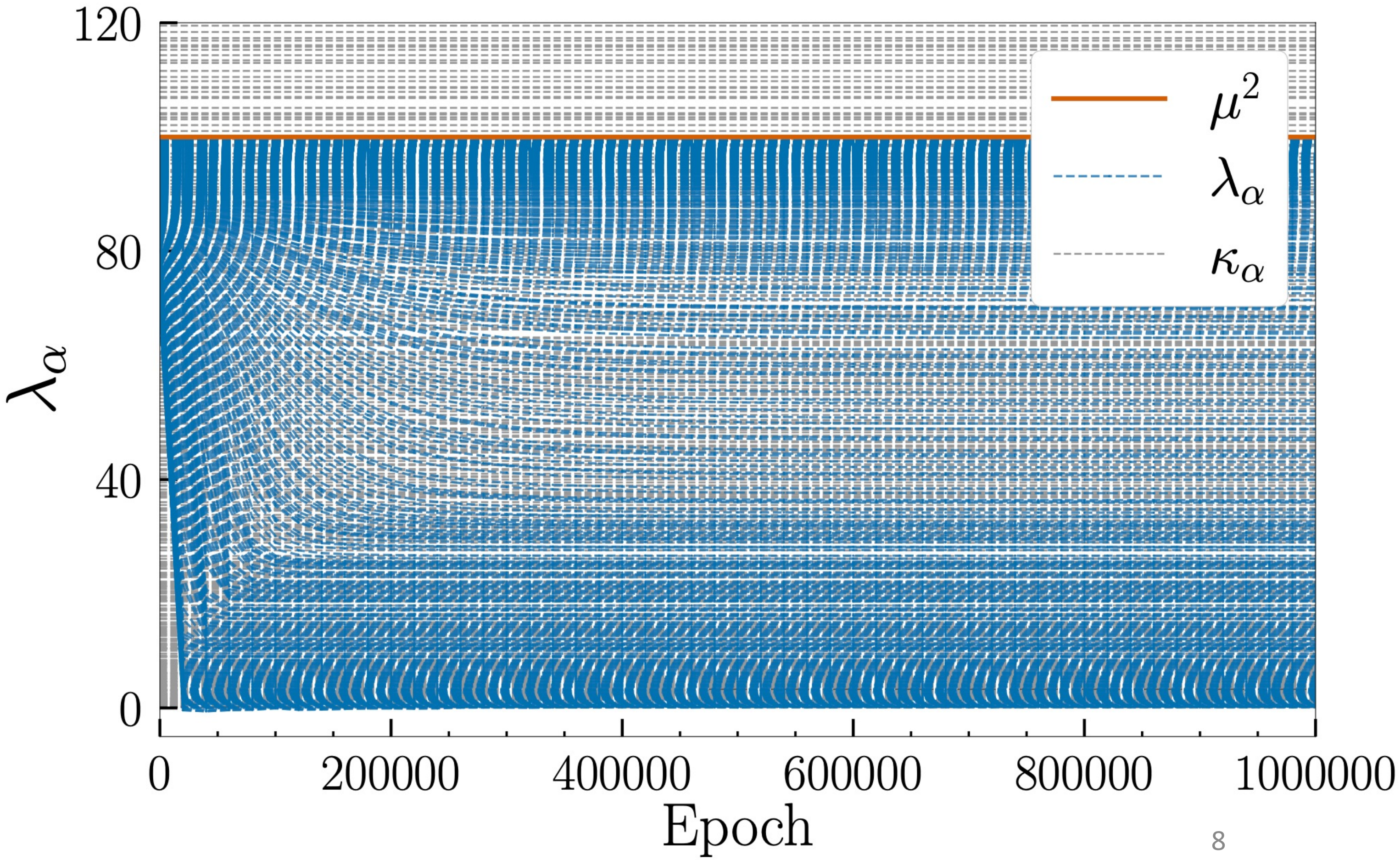
- both N_h and μ^2 act as **ultraviolet regulators**





MNIST with fixed RBM mass

- $N_v = N_h = 784$
- fixed RBM mass $\mu^2 = 100$
- spectrum regulated
- infrared modes learned approximately correctly (see below)



MNIST with $N_h \leq N_v$

what is the effect of including incomplete spectrum?

removal of ultraviolet modes affects generative power

(a) $N_h = 784$

(b) $N_h = 225$

(c) $N_h = 64$

(d) $N_h = 36$

(e) $N_h = 16$

(f) $N_h = 4$

Summary RBM

- simplest case of Gaussian RBM: two scalar fields with bilinear interaction
- when phrased as a LFT: spectrum, IR and UV cutoffs
- role of hyperparameters understood as UV regulators of spectrum
- even this simple case has good generative power

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Classification of phases of matter

Published: 13 February 2017

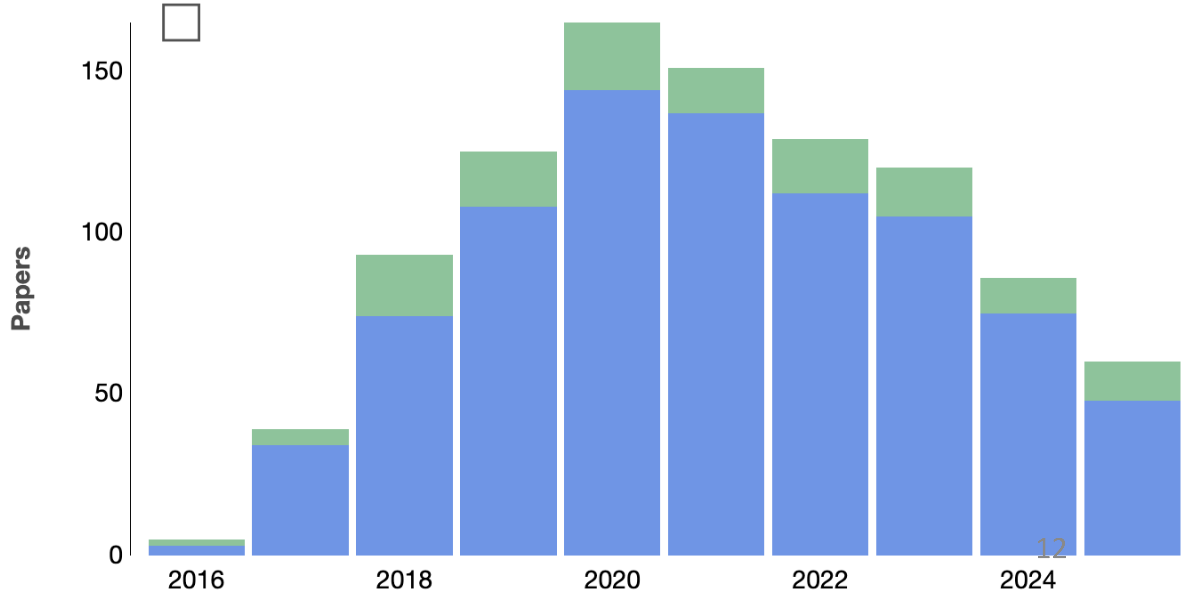
Machine learning phases of matter

Juan Carrasquilla & Roger G. Melko

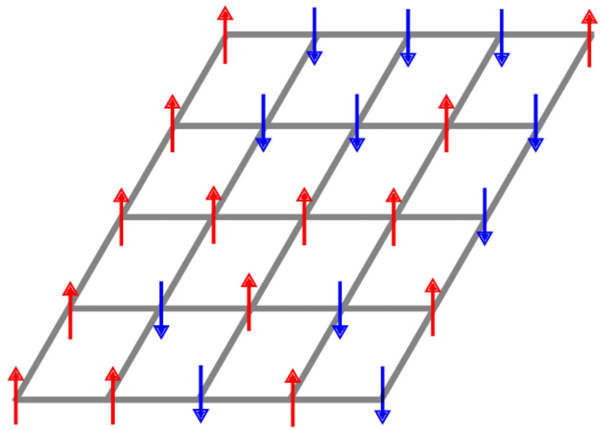
Nature Physics **13**, 431–434(2017) | Cite this article

arXiv:1605.01735v1 [cond-mat.str-el]

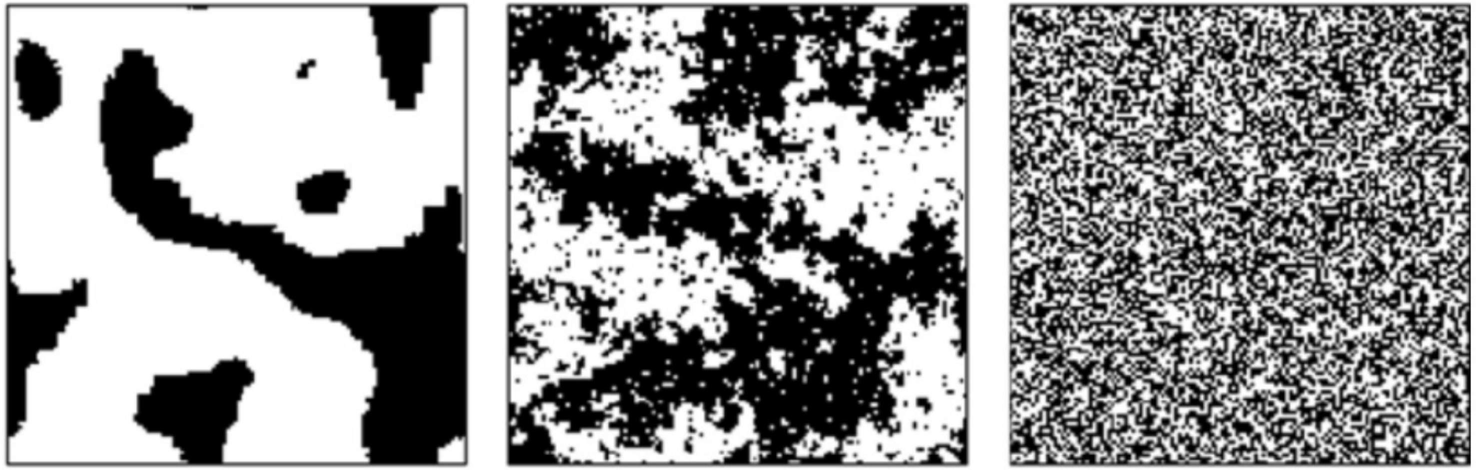
> 1700 citations since 2017 (Google Scholar)



Classification of phases of matter



- matter can exist in different phases
- prototype: 2d Ising model -> ordered/disordered or cold/hot phases
- task: determine phase a configuration is in, determine critical coupling or temperature

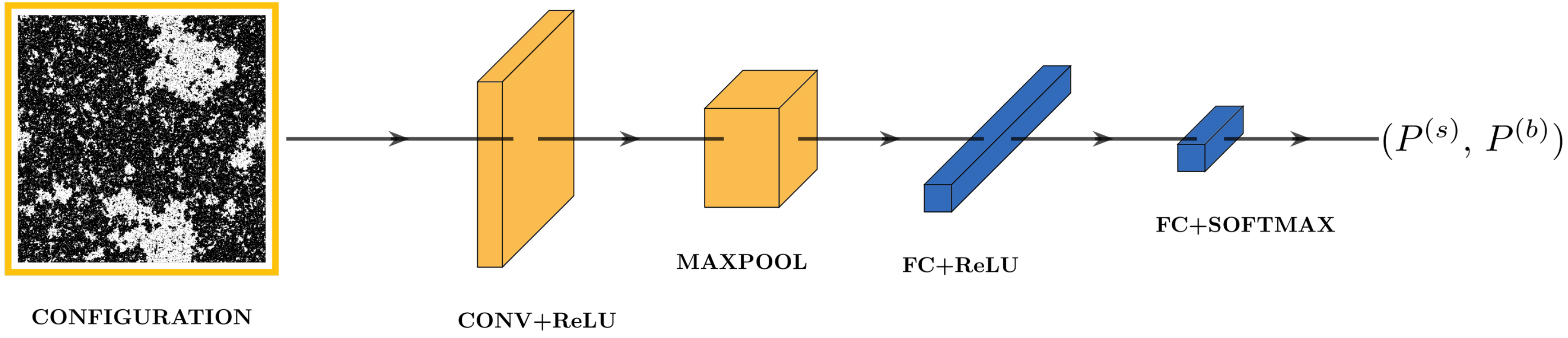


ordered -- ? -- disordered

ML excels in pattern finding

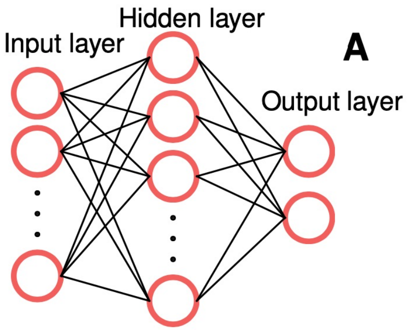
- supervised learning problem:

  use sets of configurations deep in the ordered and in the disordered phase
- 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

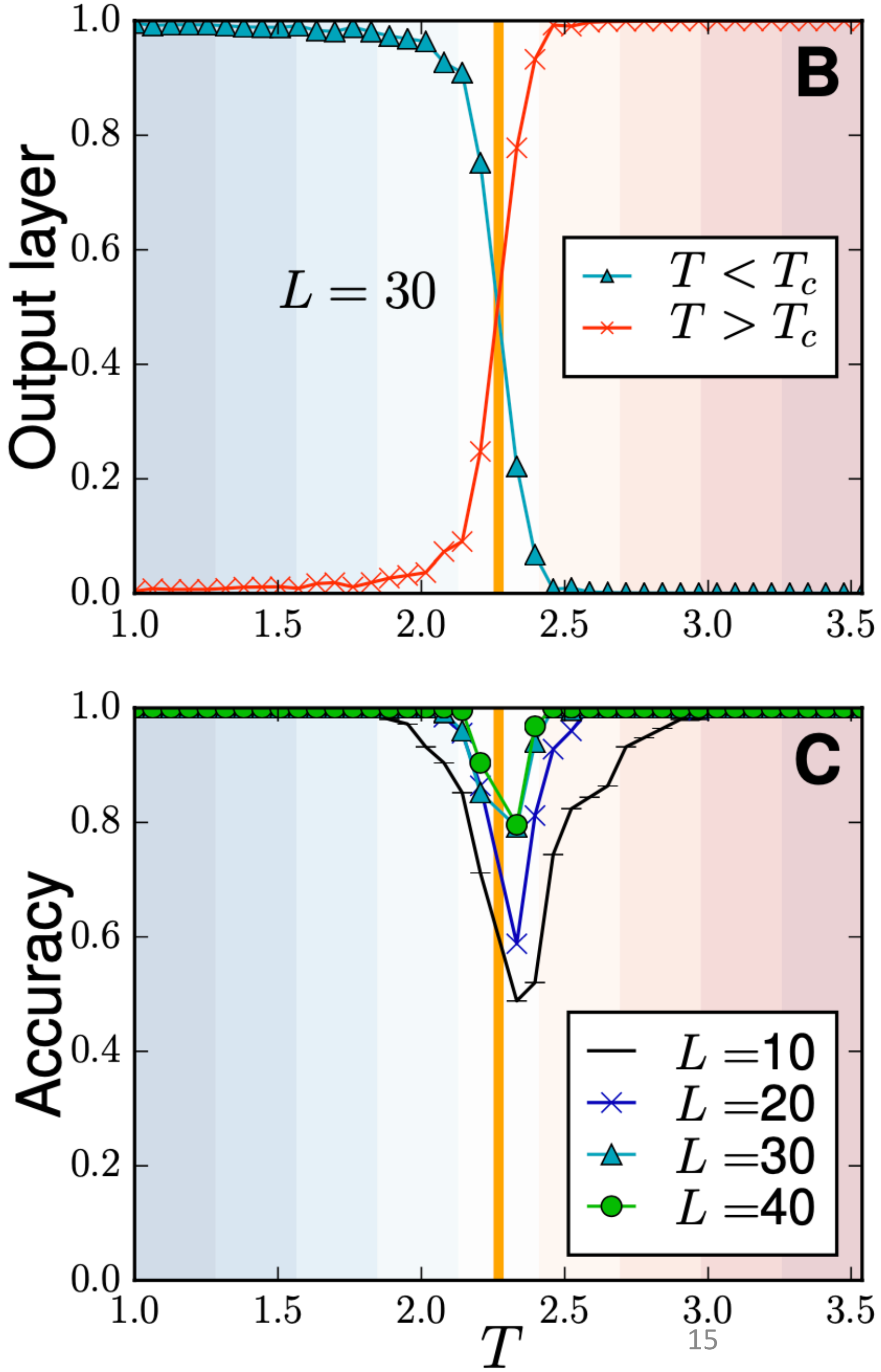


- new, unseen configurations -- > determine **probability** to be (dis)ordered

Carrasquilla-Melko



- two-dimensional Ising model
- feed-forward network with one hidden layer
- output layer: phase 1 or phase 2
- precision improves with increasing volume
- no need to identify order parameter
- extended to square ice and Ising gauge models



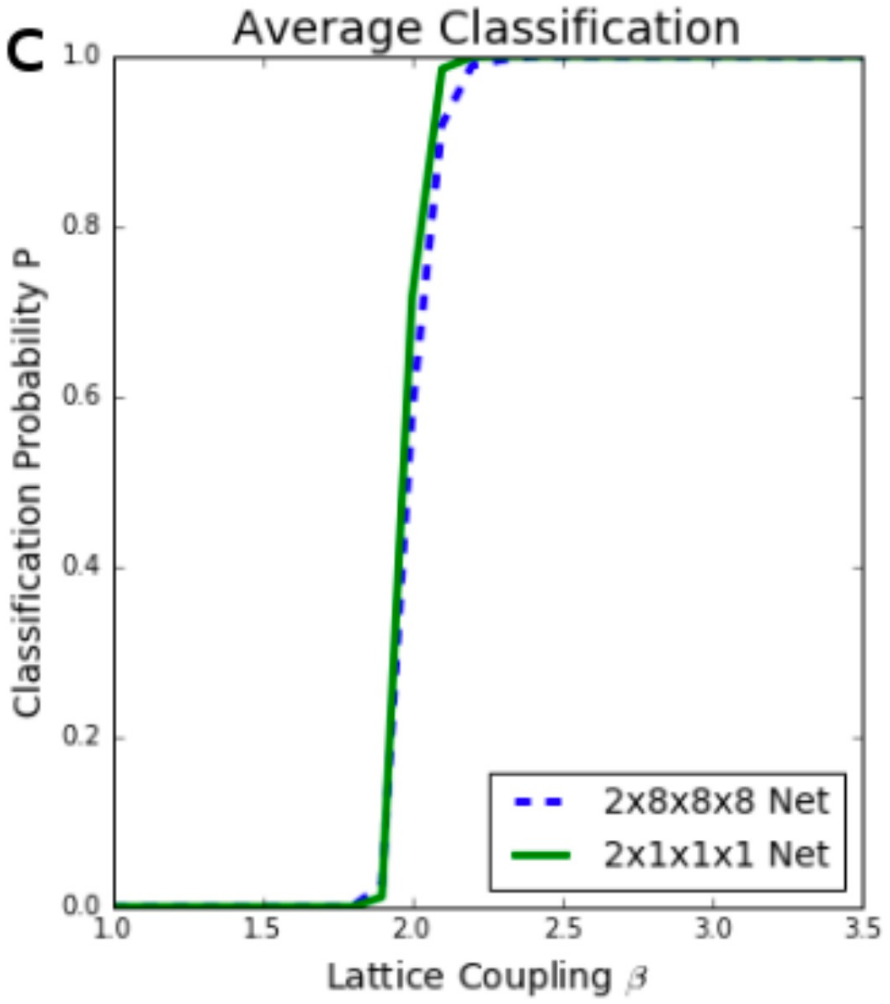
First application in LFT

- *Unsupervised learning of phase transitions: From principal component analysis to variational autoencoders*

  S Wetzel, *PRE* 96 (2017) 2, 022140

- *Machine learning of explicit order parameters: from the Ising model to SU(2) lattice gauge theory*

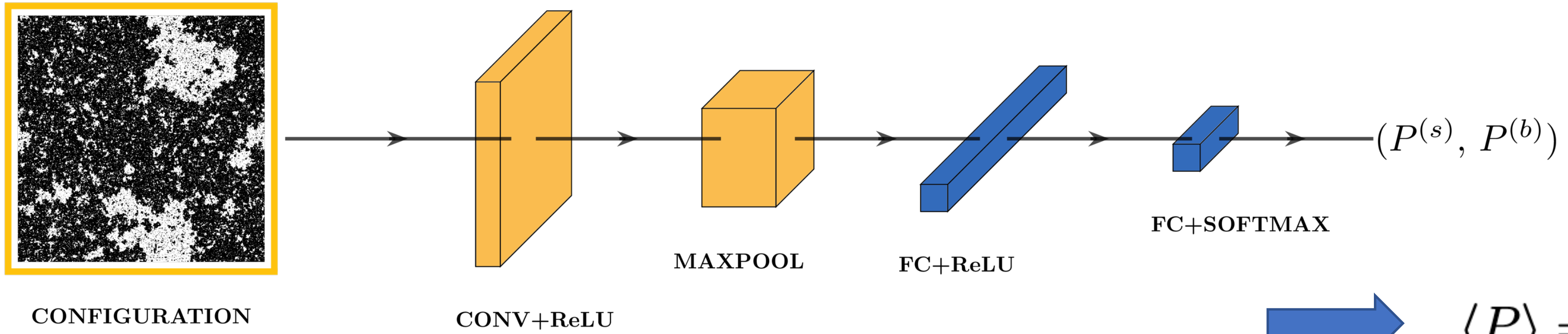
  S Wetzel and M Scherzer
  PRB 96 (2017) 18, 184410
  [1705.05582 [cond-mat.stat-mech]]



thermal transition in SU(2) LGT

Output of NN as a physical observable

- well-established procedure, what can one 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



$$\langle P \rangle = \frac{1}{Z} \sum_i P_i e^{-\beta E_i}$$

Output of NN as physical observable

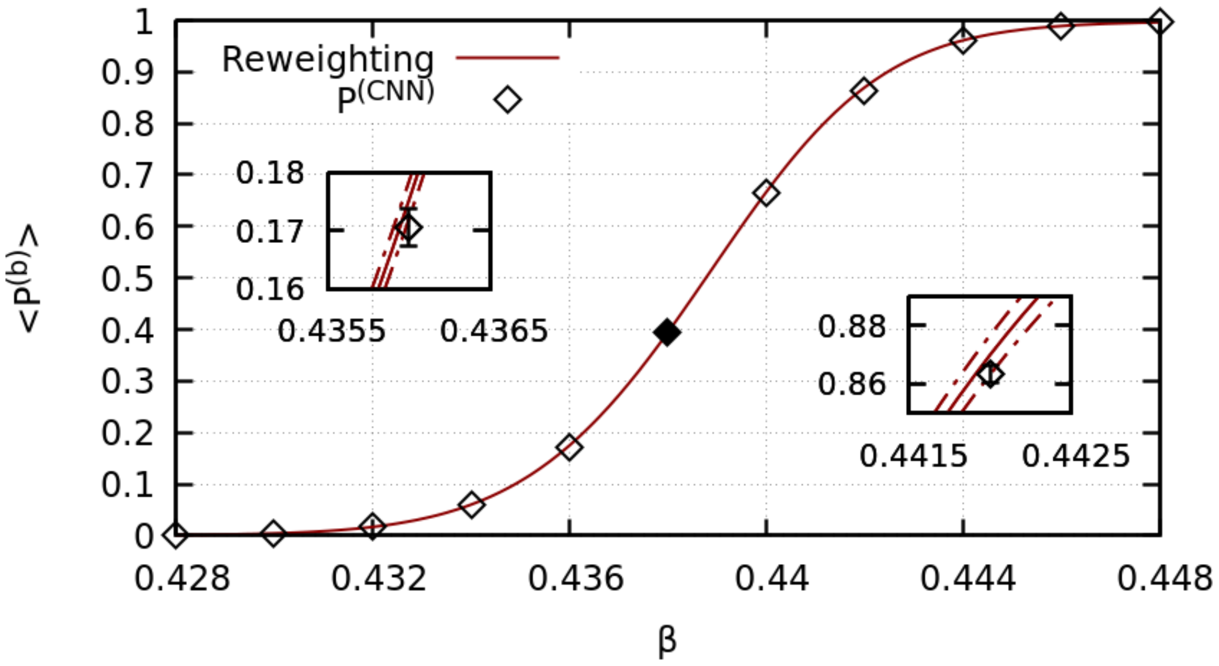
- opens up possibility to use "standard" numerical/statistical methods

  ➡ histogram reweighting: extrapolation to other parameter values

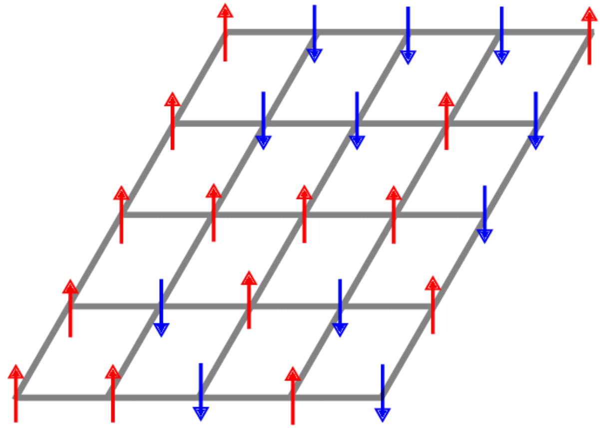
- starting from computation at given β_0: extrapolate to other β values

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

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



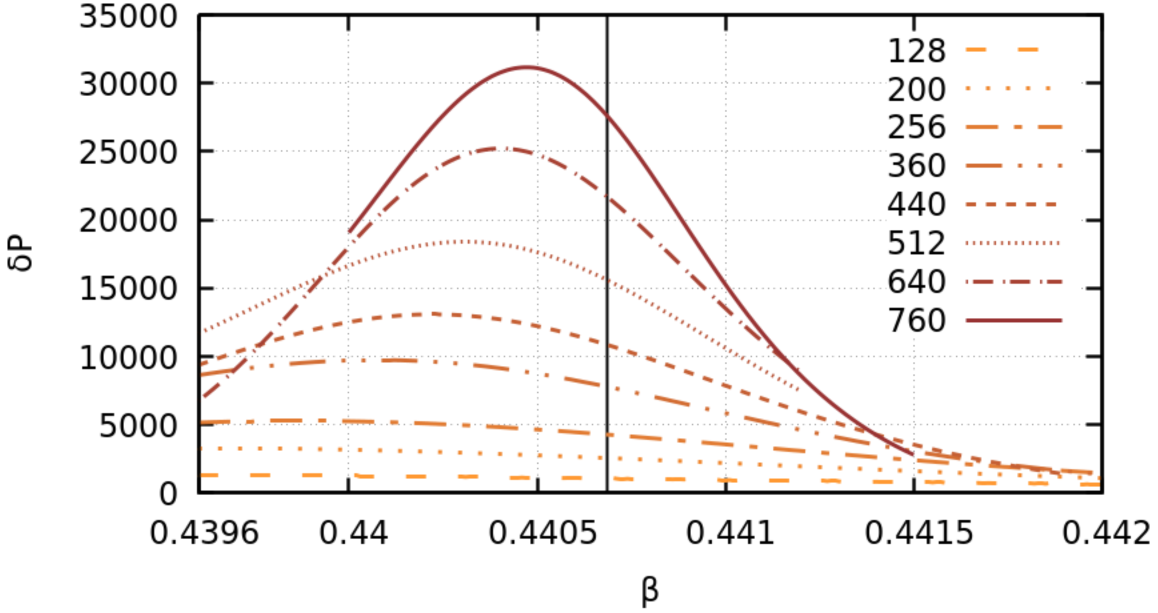
2d Ising model: finite-size scaling

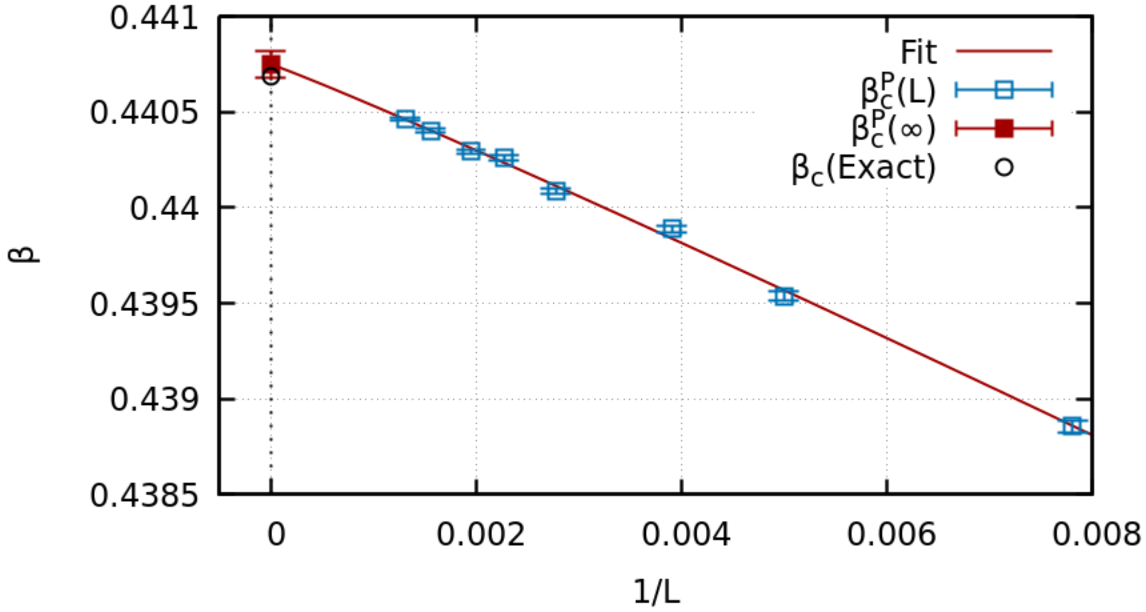


- $Z = \mathrm{Tr}\, e^{-\beta E}$ with $E = -\sum_{<ij>} s_i s_j$ $(s_i = \pm 1)$
- critical coupling or inverse temperature β_c
- correlation length ξ, magnetic susceptibility χ diverge at transition
- critical exponents $\xi \sim |t|^{-\nu}$ $\chi \sim |t|^{-\gamma}$ reduced temperature $t = \dfrac{\beta_c - \beta}{\beta_c}$
- $\nu = 1,$ $\gamma/\nu = 7/4,$ $\beta_c = \frac{1}{2}\ln(1+\sqrt{2}) \approx 0.440687$
- finite-size scaling $|t| = \left|\dfrac{\beta_c - \beta_c(L)}{\beta_c}\right| \sim \xi^{-\frac{1}{\nu}} \sim L^{-\frac{1}{\nu}}$ $\chi \sim L^{\gamma/\nu}$

Critical behaviour from NN observables

determine L dependent susceptibility δP and its maximum at $\beta_c(L)$





extract critical properties from NN observables only

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

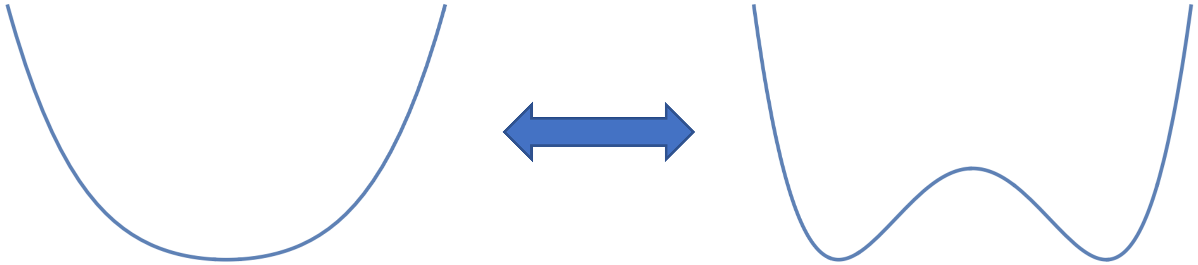
Transfer learning with histogram reweighting

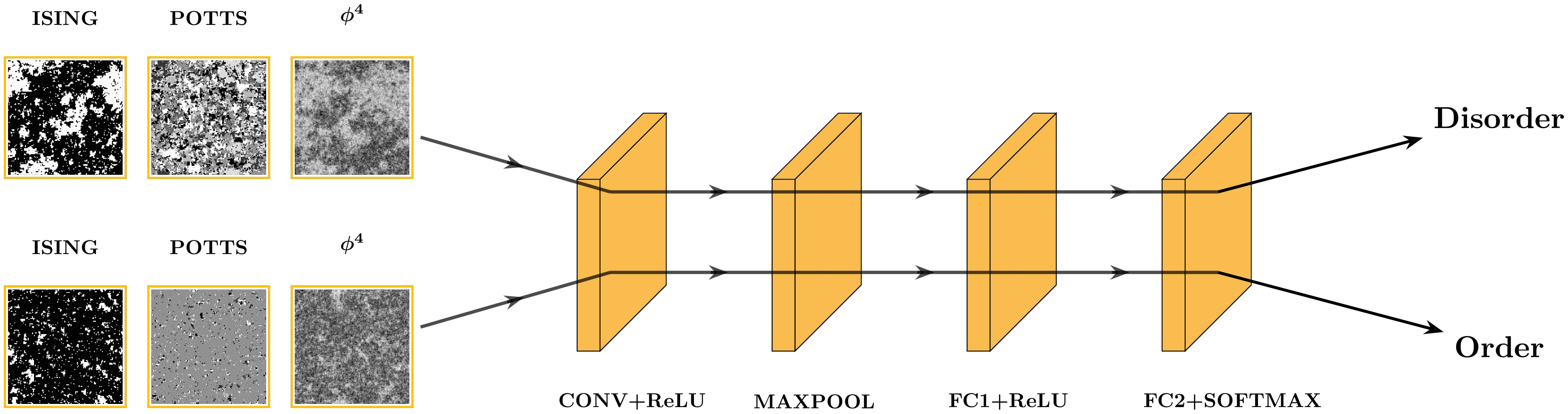
- NN has learned patterns in 2d Ising model
- are these sufficiently universal to predict the structure of phase transitions in other systems?
- what about universality class, order of transition, type of degrees of freedom?

→ transfer learning

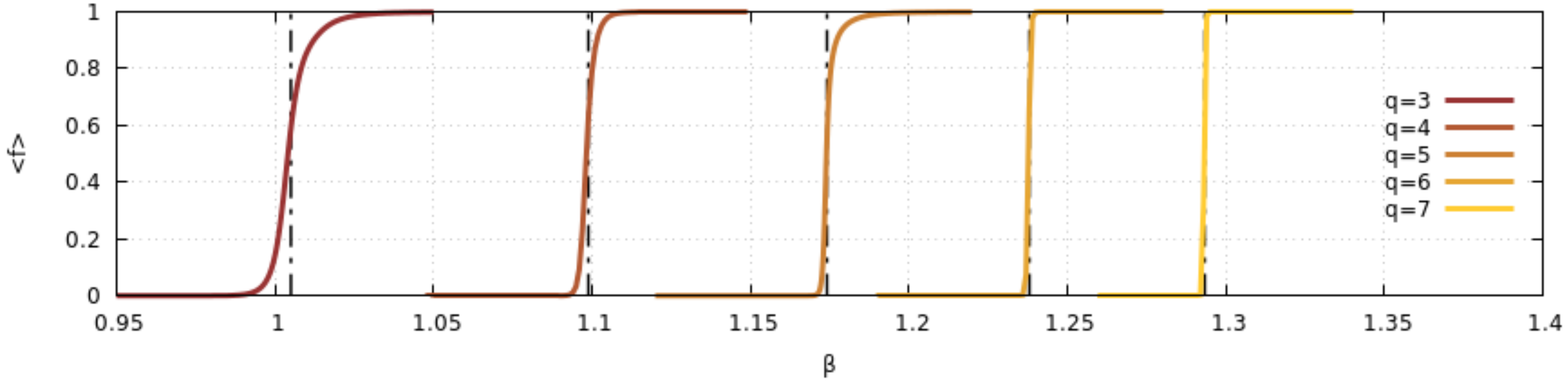
- apply to q-state Potts model (with $q = 3, \dots, 7$) and φ^4 scalar field theory

Transfer learning



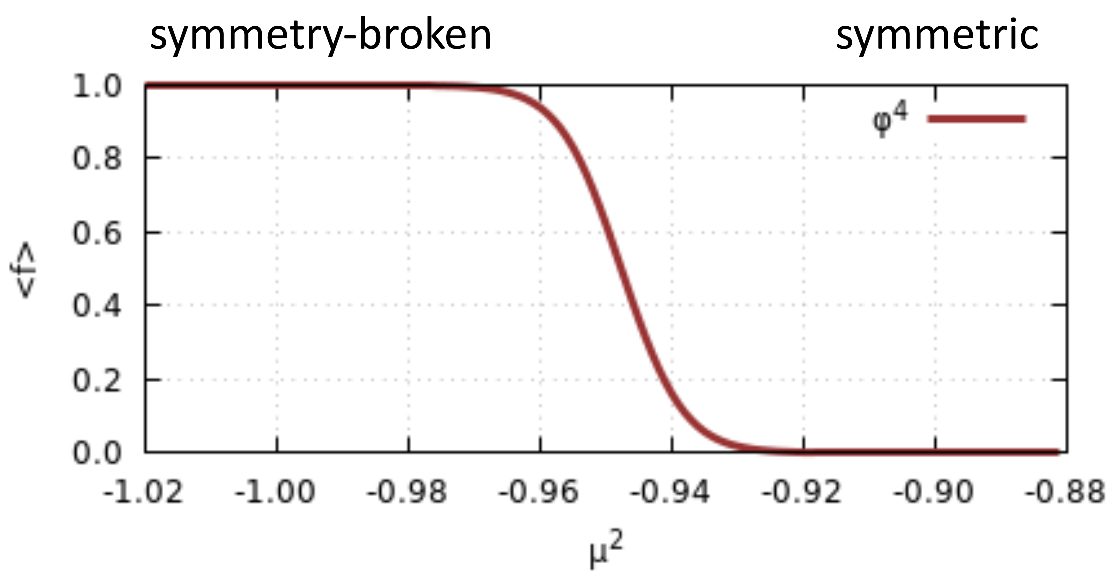


Transfer learning: q-state Potts model

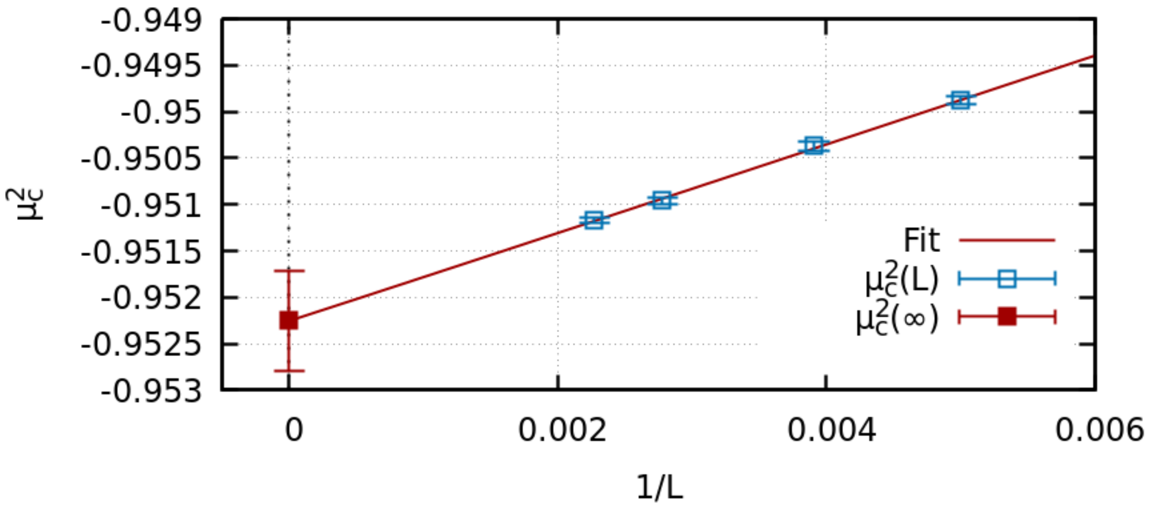


- training on Ising model, not Potts model
- continuous lines using histogram reweighting
- vertical dashed lines indicate expected transition at $\beta_c = \ln(1 + \sqrt{q})$
- $q = 3, 4$: 2nd order transition, $q = 5, 6, 7$: 1st order transition

φ^4 scalar field theory



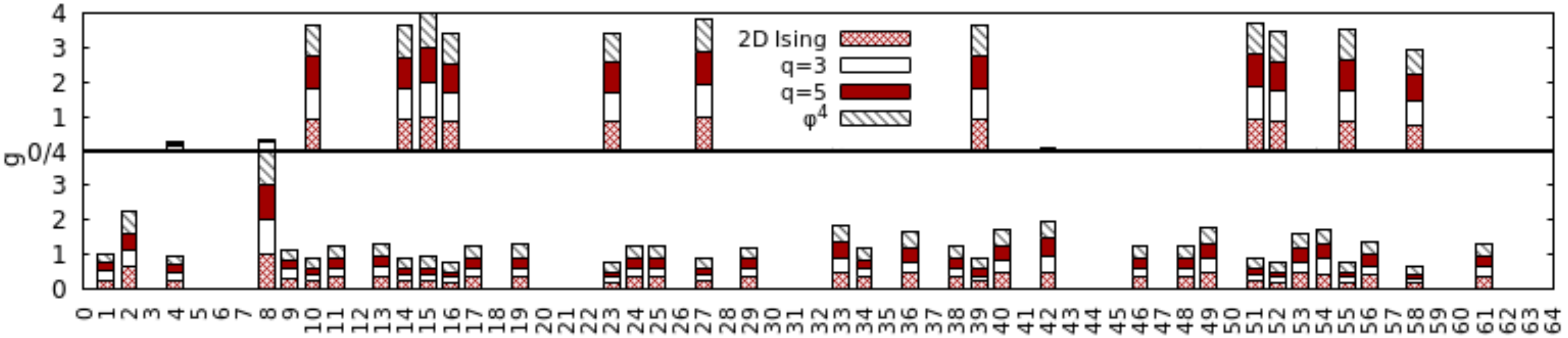
- reweight in mass parameter, μ^2
- identify regions where phase is clear
- retrain NN using $\mu^2 < -1.0$ and $\mu^2 > -0.9$
- repeat finite-size scaling analysis as in 2d Ising model



	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)

Under the hood: activation functions in NN



mean activation functions in the 64 neurons in the fully connected (FC1) layer of 2d Ising-trained neural network, for:

- 2d Ising model
- $q = 3$ and $q = 5$ Potts model
- φ^4 scalar field theory

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

Summary: detection of phase transitions

- train on simplistic systems to study more complicated models
- combine with reweighting to scan parameter space
- reconstruct effective order parameters and locate (unknown) phase transitions
- study infinite-volume limit to make accurate predictions

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- **inverse renormalisation group**
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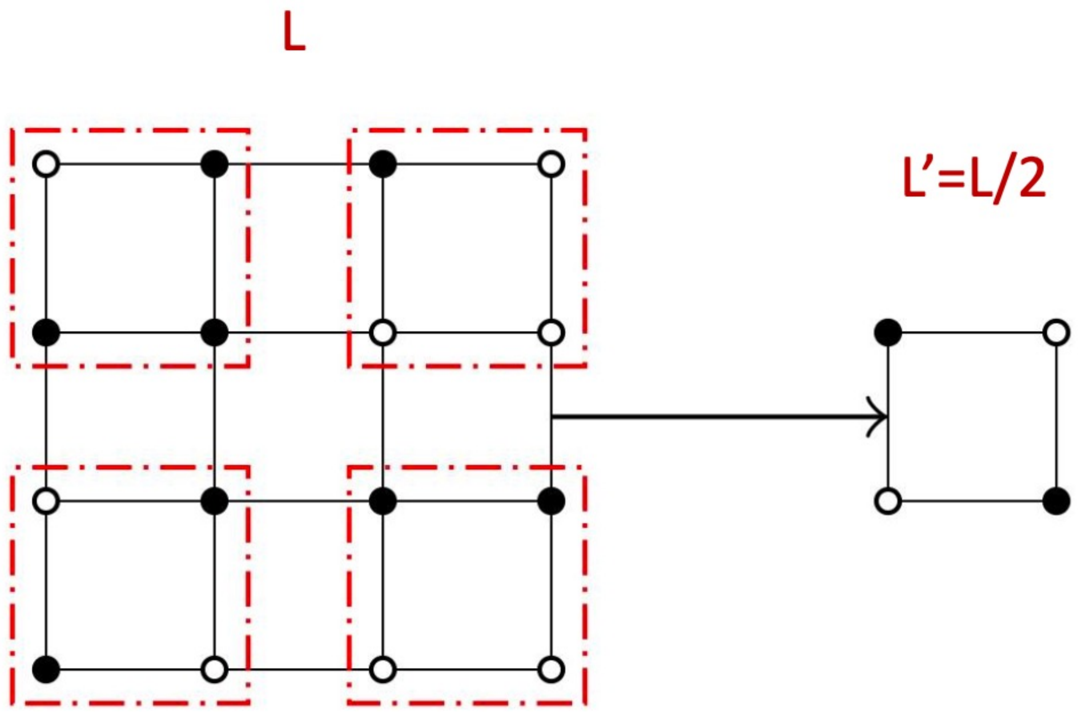
Renormalisation Group (RG)

- standard renormalisation group: coarse-graining,
  blocking transformation, integrating out degrees of freedom, …

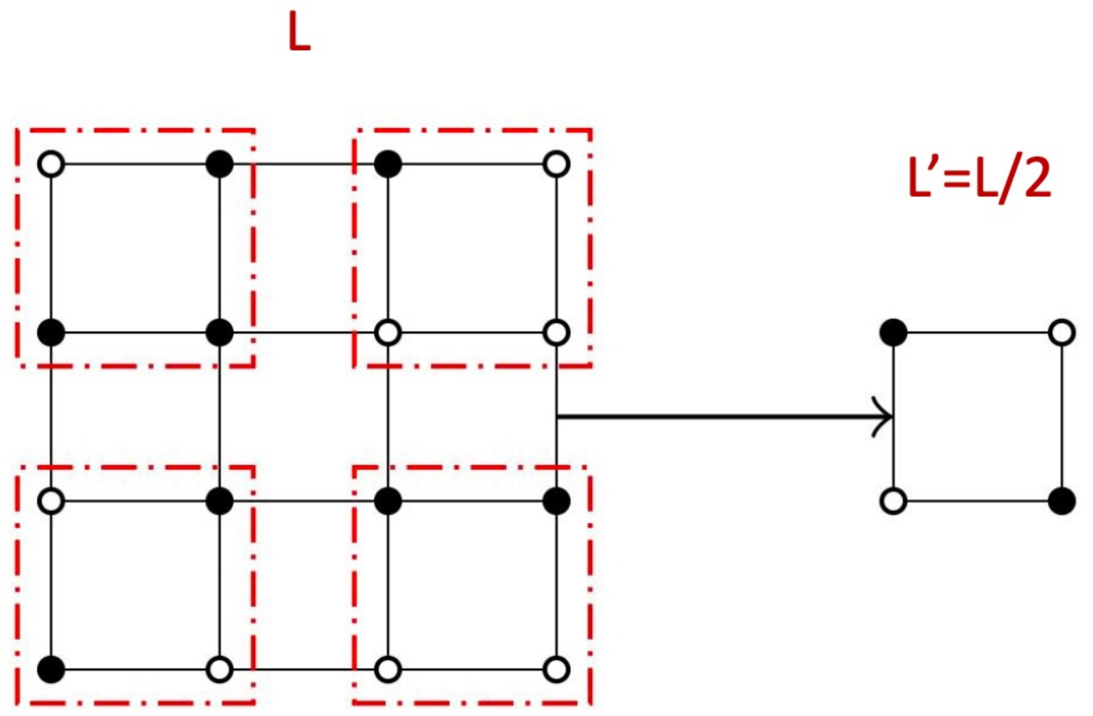
- Ising model: Kadanoff block spin
- majority rule
- reduction of degrees of freedom
- study critical scaling

- not invertible: semi-group



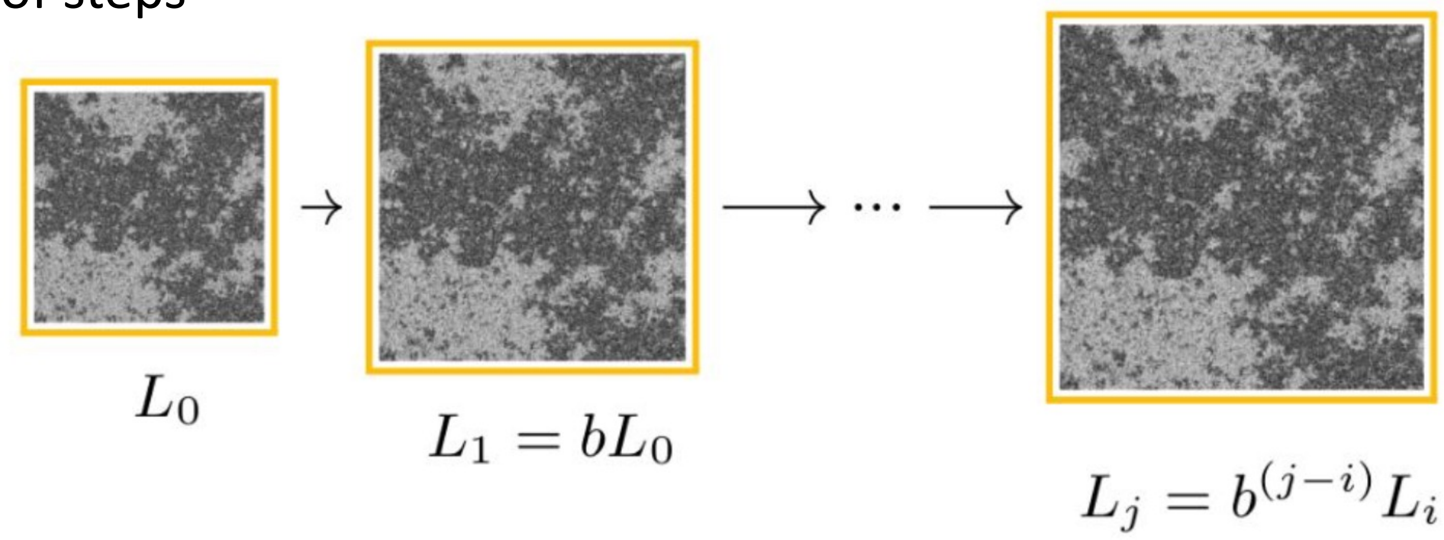
Renormalisation group

- generates flow in parameter space
- due to repeated blocking: run out of degrees of freedom
- need to start with large system to
  apply RG step multiple times
- large systems, close to a transition,
  suffer from critical slowing down



Inverse renormalisation group

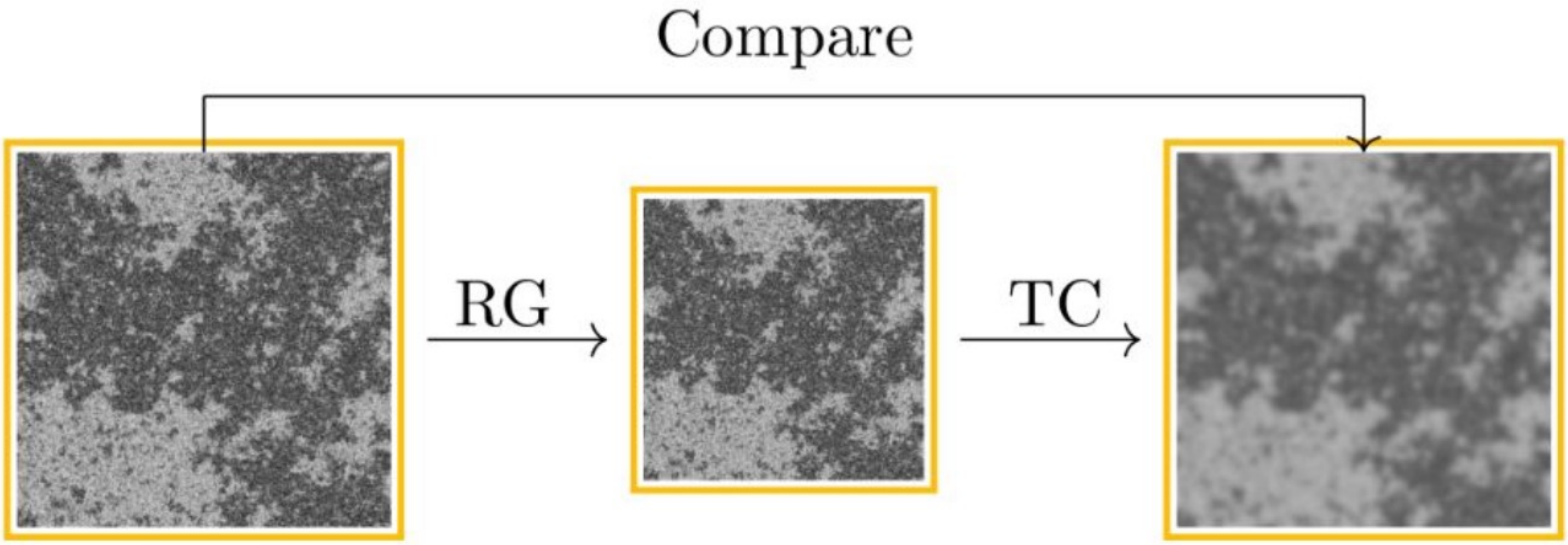
- what if we could invert the RG?
- add degrees of freedom, fill in the 'details'
- inverse flow in parameter space
- can be applied arbitrary number of steps
- evade critical slowing down



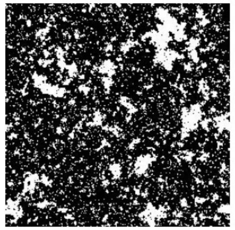
for Ising model: Inverse Monte Carlo Renormalization Group Transformations for Critical Phenomena,
D. Ron, R. Swendsen, A. Brandt, Phys. Rev. Lett. 89, 275701 (2002)

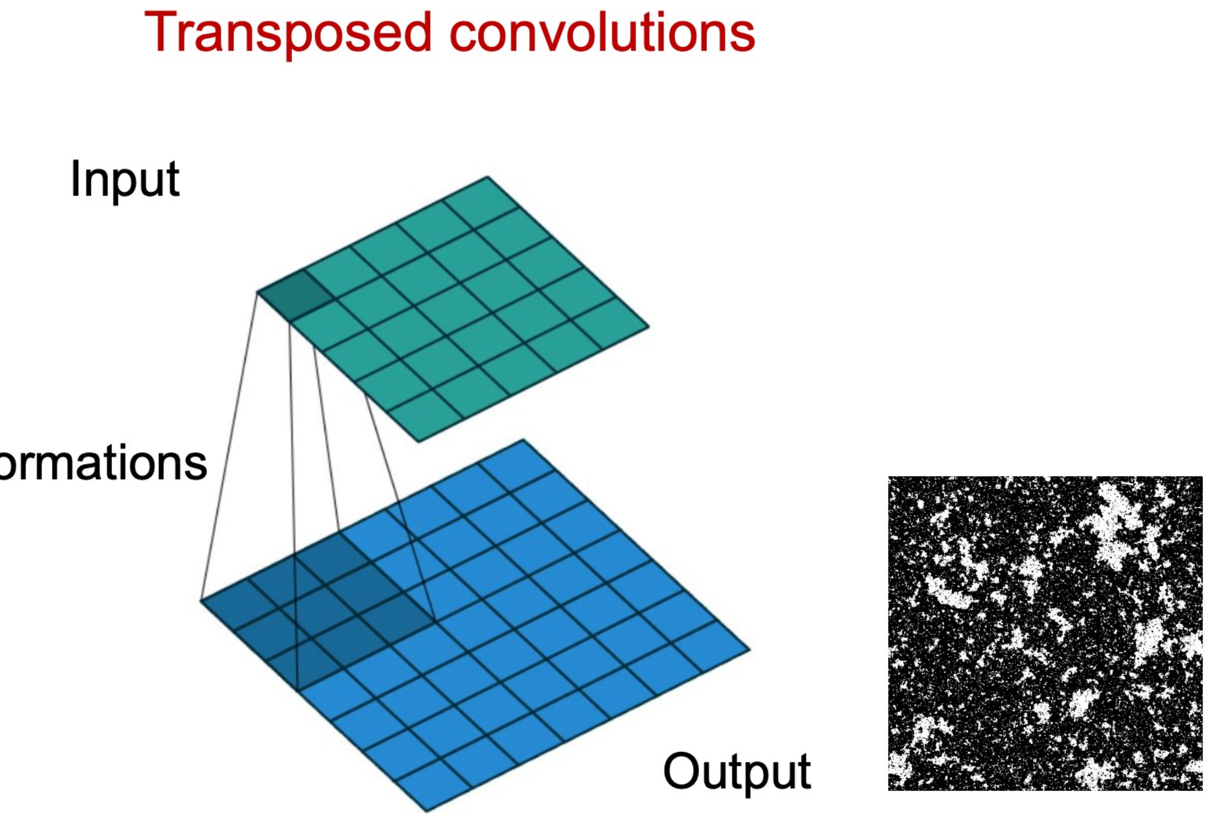
How to devise an inverse transformation?

- new degrees of freedom should be introduced
- learn a set of transformations (*transposed convolutions*) to invert a standard RG step
- minimise difference between original and constructed configuration



Inverse renormalisation group





- local transformation
- apply inverse transformations iteratively
- evade critical slowing down
- generate flow in parameter space
- invariance at critical point

Application to φ^4 scalar field theory

- repeated steps
- locking in on critical point

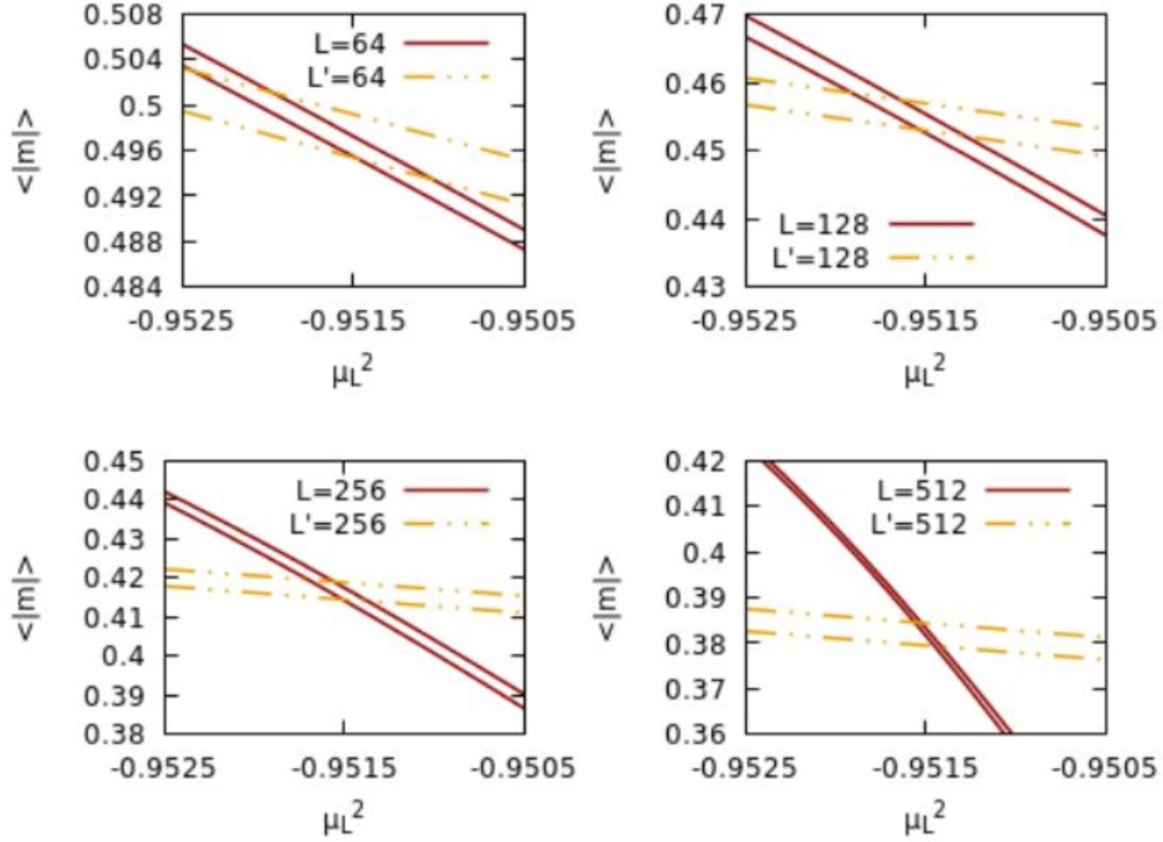


TABLE I. Values of the critical exponents γ/ν and β/ν. The original system has lattice size $L = 32$ in each dimension and its action has coupling constants $\mu_L^2 = -0.9515$, $\lambda_L = 0.7$, and $\kappa_L = 1$. The rescaled systems are obtained through inverse renormalization group transformations.

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)

Application to φ^4 scalar field theory

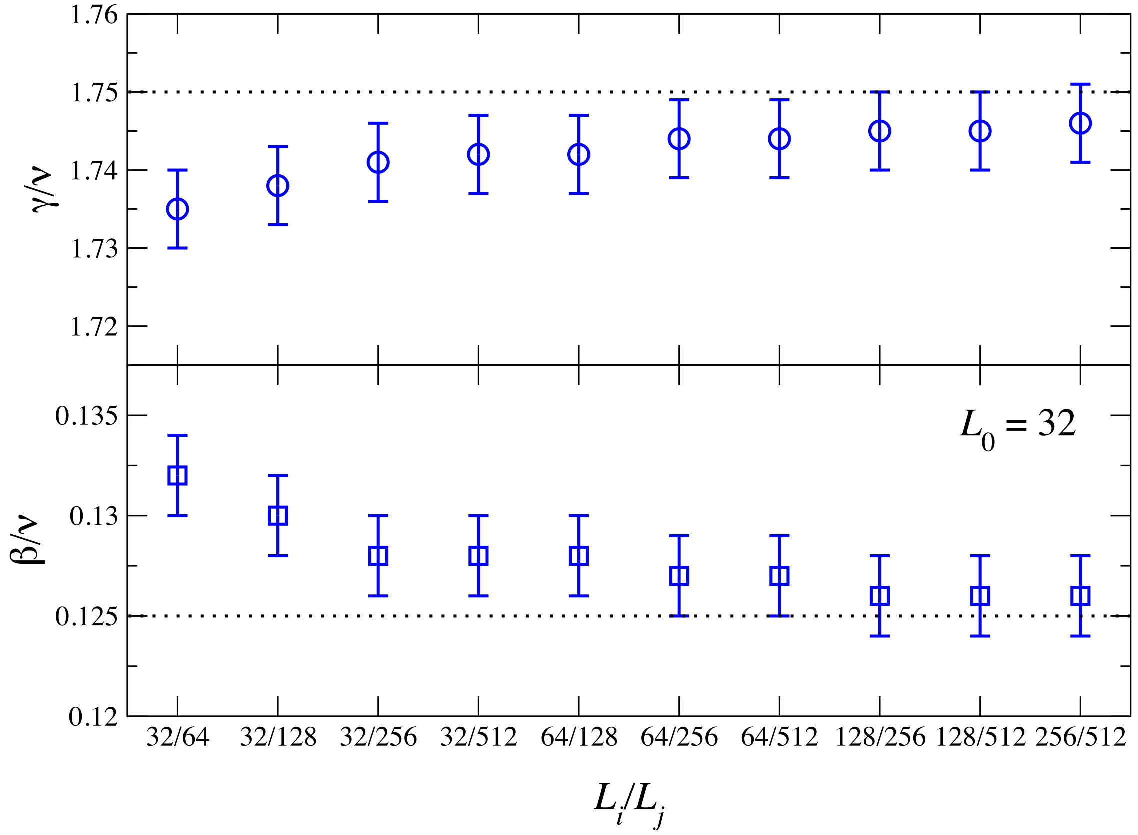
- start with lattice of size 32^2 and apply IRG steps repeatedly
- $32^2 \rightarrow 64^2 \rightarrow 128^2 \rightarrow 256^2 \rightarrow 512^2$
- IRG flow towards critical point
- extract critical exponents

  γ/υ and β/υ from comparison

  between two volumes
- constructed a large (512^2) lattice

  very close to criticality

  without critical slowing down



Summary: inverse RG

- flow to critical point without critical slowing down
- reach large lattices from easy-to-simulate lattice sizes

Dimitrios Bachtis, GA, F di Renzo, B Lucini
PRL **128** (2022) 081603 [2107.00466 [hep-lat]]

some related recent work:

- Super-resolving normalising flows for lattice field theories

  M Bauer, R Kapust, J Pawlowski, F Temmen, 2412.12842 [hep-lat]

- Multilevel generative samplers for investigating critical phenomena

  A Singha, E Cellini, K Nicoli, K Jansen, S Kühn, S Nakajima, 2503.08918 [cs.LG]

- Dreaming up scale invariance via inverse renormalization group

  A Rançon, U Rançon, T Ivek, I Balog, 2506.04016 [cond-mat.stat-mech]

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Stochastic quantisation: complex actions

- stochastic quantisation not limited to real-valued distributions/actions
- extend Langevin process to complex manifold: complex Langevin dynamics (Parisi 1981)

- complexify degrees of freedom $z \to x + iy$

- consider dynamics in complex plane or complexified manifold

$$z \sim \rho(z) \in \mathbb{C} \quad \Rightarrow \quad x, y \sim P(x, y) \in \mathbb{R}$$

- convergence not guaranteed, no general solution of Fokker-Planck equation

(Complex) Langevin dynamics

- observables $\langle O(x)\rangle = \int dx\, \rho(x) O(x)$ $\rho(x) = \frac{1}{Z}\exp[-S(x)]$ $Z = \int dx\, \rho(x)$
- Langevin equation and drift $\dot{x}(t) = K[x(t)] + \eta(t)$ $K(x) = \frac{d}{dx}\log\rho(x) = -\frac{dS(x)}{dx}$
- Fokker-Planck equation (FPE) $\partial_t \rho(x;t) = \partial_x \left[\partial_x - K(x)\right]\rho(x;t)$
- what if weight is complex? drift is complex, FPE only formal
- complexify degrees of freedom $z \to x + iy$
- consider dynamics in complex plane or complexified manifold

Complex Langevin dynamics

- complexify degrees of freedom
- Langevin equation and drift in analytically continued variables

$$\dot{x}(t) = K_x + \eta_x(t), \qquad K_x = \mathrm{Re}\frac{d}{dz}\log\rho(z), \qquad \langle \eta_x(t)\eta_x(t')\rangle = 2N_x\delta(t-t')$$
$$\dot{y}(t) = K_y + \eta_y(t), \qquad K_y = \mathrm{Im}\frac{d}{dz}\log\rho(z), \qquad \langle \eta_y(t)\eta_y(t')\rangle = 2N_y\delta(t-t')$$

- observables

$$N_x - N_y = 1$$

$$\langle O[x(t)+iy(t)]\rangle_\eta = \int dxdy\, P(x,y;t)O(x+iy)$$

introductory lectures on QCD and the sign problem: GA, 1512.05145 [hep-lat]

Complex Langevin dynamics

- FPE $$\partial_t P(x,y;t) = \left[\partial_x\left(N_x\partial_x - K_x\right) + \partial_y\left(N_y\partial_y - K_y\right)\right] P(x,y;t)$$
- cannot be solved, non-integrable $\partial_x K_y \neq \partial_y K_x$
- formal justification $$\int dxdy\, P(x,y) O(x+iy) = \int dx\, \rho(x) O(x)$$
- relation (cannot be verified in practice) $$\rho(x) = \int dy\, P(x-iy, y)$$
- instead, a posteriori criteria for correctness

GA, E Seiler, IO Stamatescu, *Phys. Rev. D* **81** (2010) 054508 [0912.3360]
GA, F James, E Seiler, IO Stamatescu, *Eur. Phys. J. C* **71** (2011) 1756 [1101.3270]

Complex Langevin distributions

- FPE $$\partial_t P(x,y;t) = \left[\partial_x\left(N_x\partial_x - K_x\right) + \partial_y\left(N_y\partial_y - K_y\right)\right] P(x,y;t)$$

real noise:

$$N_x = 1, N_y = 0$$

- want to describe/understand this distribution
  - further sampling
  - criteria for correctness
  - (modify process)

$$P(x,y;t) \geq 0$$

- use diffusion model, learn from CL generated data
- diffusion model does not care what the origin of the data is
- note: no solution to the sign problem if CL fails

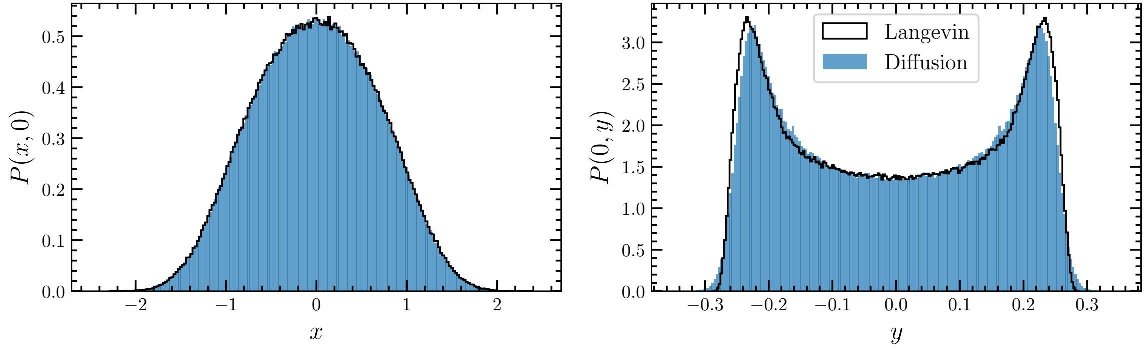
Quartic model

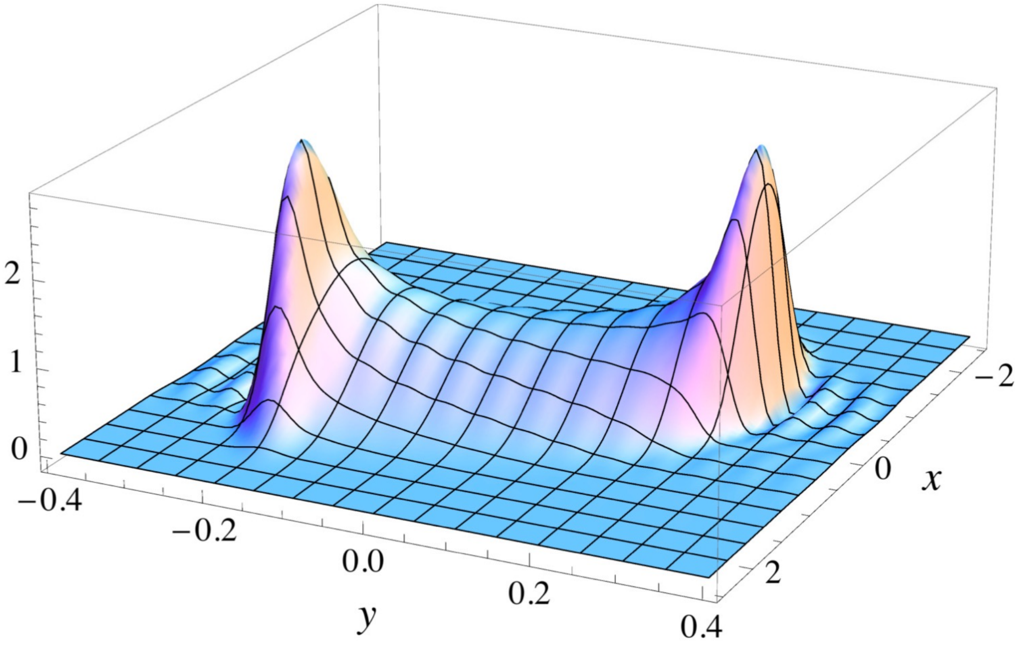
- simple model with quartic coupling $S = \frac{1}{2}\sigma_0 x^2 + \frac{1}{4}\lambda x^4$ $\sigma_0 = A + iB$
- detailed analysis in GA, Giudice, Seiler, *Annals Phys.* **337** (2013) 238 [1306.3075]
- CL converges, provided $3A^2 - B^2 > 0$, dynamics is contained inside a strip, $-y_- < y < y_-$
- this follows from CL drift $$y_-^2 = \frac{A}{2\lambda}\left(1 - \sqrt{1 - \frac{B^2}{3A^2}}\right)$$
- FPE can be solved (approximately) using double expansion in Hermite polynomials
- train diffusion model on CL generated data

Quartic model

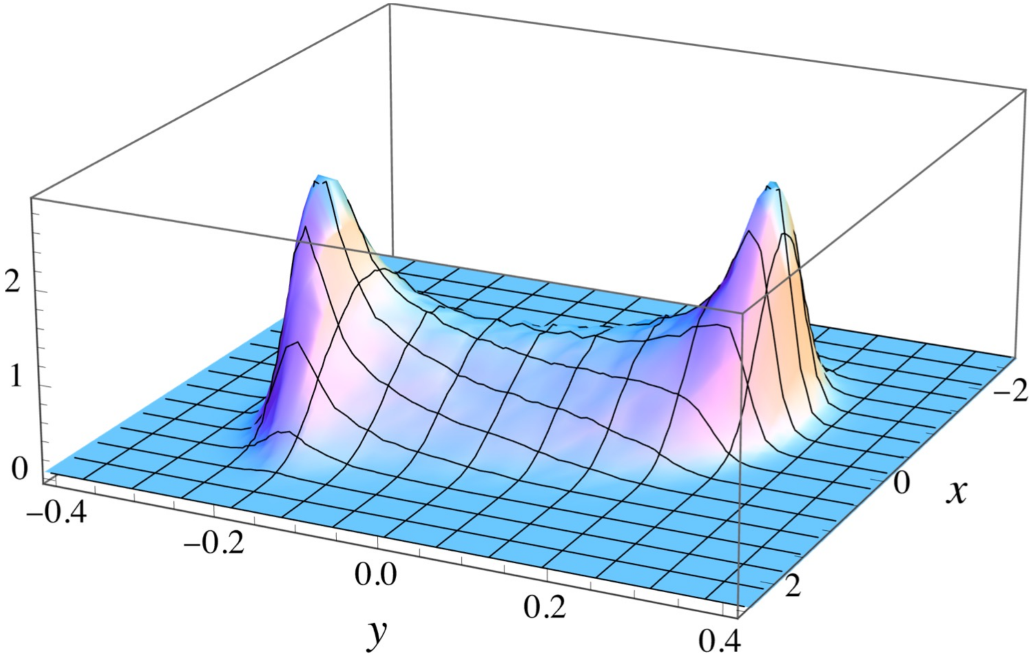
$$A = B = \lambda = 1$$

$$y_- \approx 0.3029$$





solution of FPE using double expansion in Hermite polynomials



solution obtained by sampling from trained diffusion model

GA, Giudice, Seiler, *Annals Phys.* **337** (2013) 238 [1306.3075]

Comparison

cumulants in the quartic model

n	2		4		6		8	
	re	−im	re	−im	re	−im	re	−im
Exact	0.428142	0.148010	−0.060347	−0.100083	−0.00934	0.19222	0.41578	−0.5923
CL	0.4277(5)	0.1478(2)	−0.0597(6)	−0.0991(6)	−0.010(1)	0.188(2)	0.406(4)	−0.57(1)
DM	0.4267(6)	0.1459(2)	−0.0582(6)	−0.0981(5)	−0.008(1)	0.188(2)	0.400(5)	−0.58(1)

expectation values at the end of the backward process

note: diffusion model learns from CL data, not the "exact" value

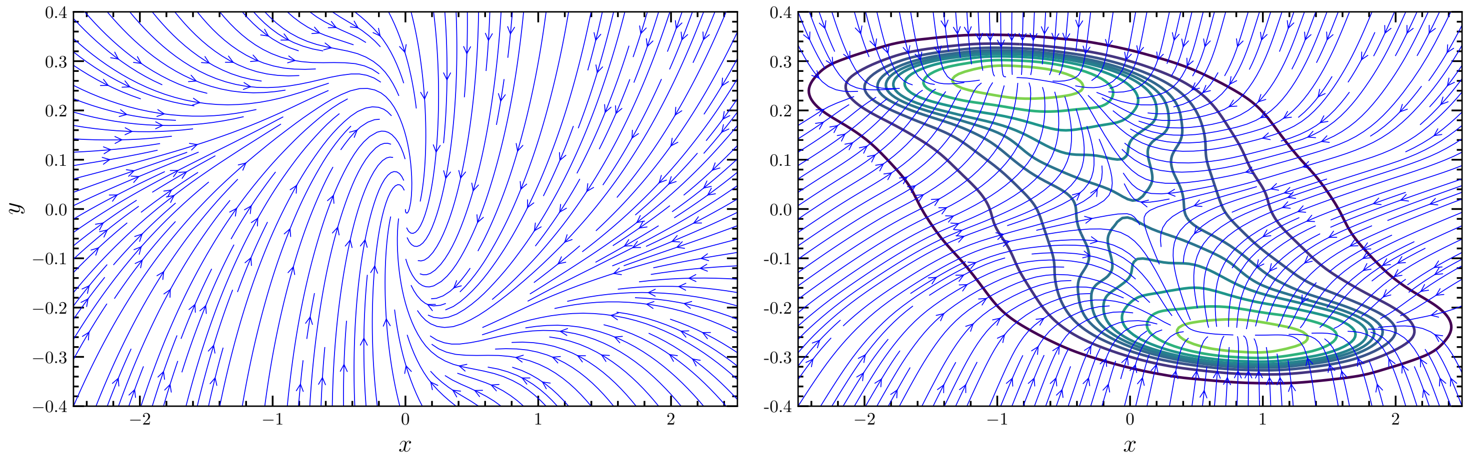
Trained diffusion model: quartic model

two very different processes

complex Langevin:
- non-integrable drift
- noise in real direction
- attractor at origin

diffusion model:
- integrable score
- noise in both directions
- saddle at origin

to explore further



complex Langevin drift diffusion model score

different Fokker-Planck equations

yet same distributions are created for data generation

have obtained access to $\nabla \log P(x, y)$

Summary and outlook

- machine learning offers a fascinating playground for (theoretical) physicists
- applicable to address research questions, including in lattice field theory
- scope to apply theoretical physics knowledge to gain insight into ML algorithms

- many directions to explore
- after learning the basics, first steps are relatively easy

next challenge:

- impose the rigour we are used to from LFT
- improve upon well-established approaches