From lattice field theory to machine learning and back

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UKRI CENTRE FOR DOCTORAL TRAINING IN ARTIFICIAL INTELLIGENCE, MACHINE LEARNING AND ADVANCED COMPUTING

Swansea University
Prifysgol Abertawe

EuCAIFCon Apr 2024

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UKRI CENTRE FOR DOCTORAL TRAINING IN ARTIFICIAL INTELLIGENCE, MACHINE LEARNING AND ADVANCED COMPUTING

- 5 cohorts of O(11) PhD students each
- first cohort has graduated
- final cohort of 17 students started in Oct 2023

- 60% particle physics/astronomy
- 25% computer science/maths
- 15% health

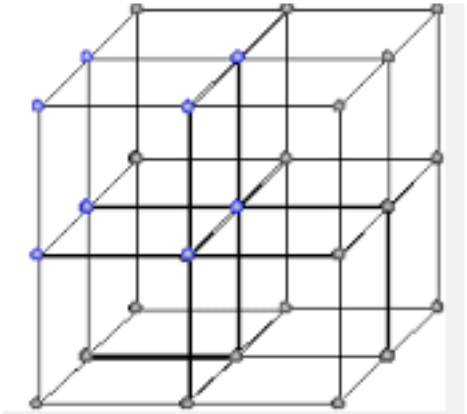
Prifysgol Aberystwyth University · Prifysgol Bangor University · University of Bristol · Cardiff University Prifysgol Caerdydd · Swansea University Prifysgol Abertawe · Supercomputing Wales Uwchgyfrifiadura Cymru

Lattice field theory (LFT) ←→ ML

- many fascinating connections between ML and statistical physics/field theory
- what can we learn that is relevant for → or ← direction

lattice field theory: very loosely speaking

- many fluctuating degrees of freedom on a lattice/graph <-> Markov random fields
- thermalisation and non-equilibrium dynamics <-> learning
- stochastic quantisation and Langevin dynamics <-> diffusion models
- renormalisation group
- …



Conceptual and practical questions

can experience in quantum field theory help in understanding ML and vice versa?

- quantum field-theoretic machine learning

  Dimitrios Bachtis, GA, Biagio Lucini, Phys. Rev. D 103 (2021) 074510 [2102.09449 [hep-lat]]

- scalar field restricted Boltzmann machines as an ultraviolet regulator

  Chanju Park, Biagio Lucini, GA, Phys. Rev. D 109 (2024) 034521 [2309.15002 [hep-lat]]

- stochastic quantisation and diffusion models

  Lingxiao Wang, GA, Kai Zhou, JHEP (to appear) [2309.17082 [hep-lat]]

  NeurIPS 2023 2311.03578 [hep-lat]

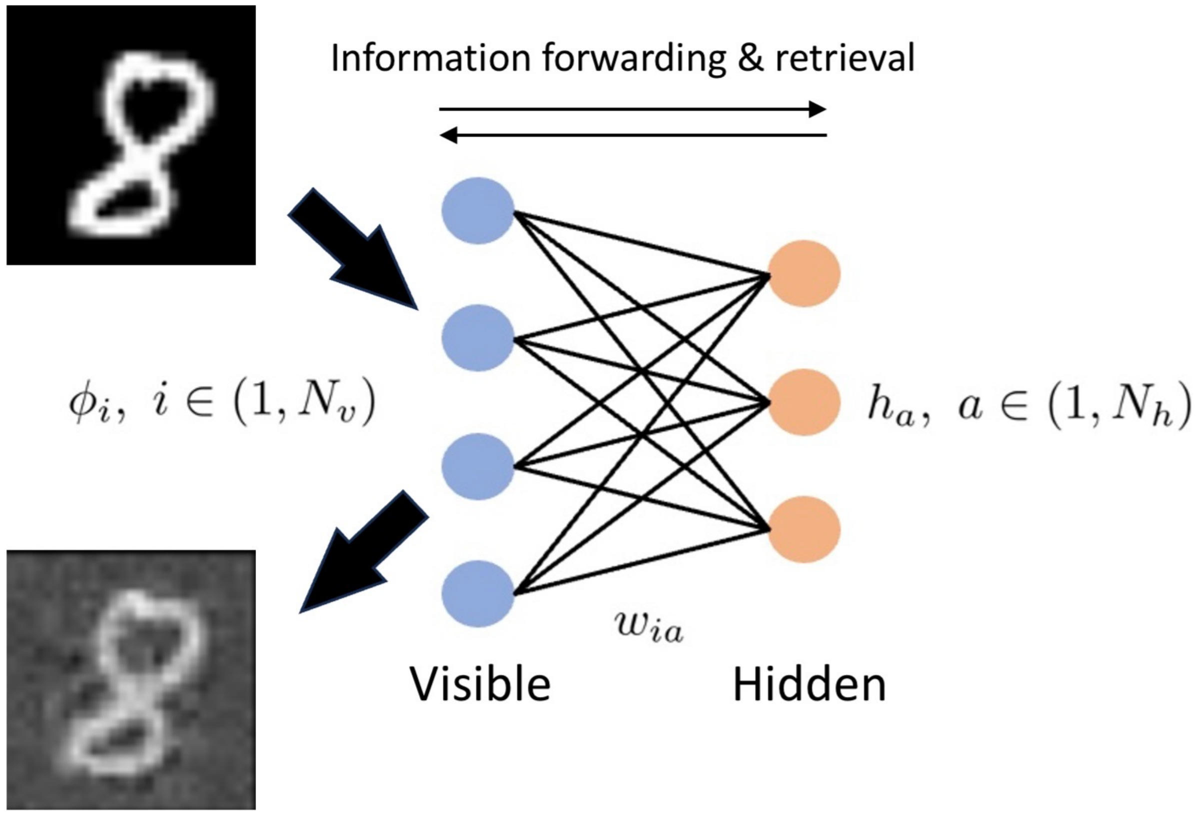
Topic 1

scalar field restricted Boltzmann machines as an ultraviolet regulator

Chanju Park, Biagio Lucini, GA

Phys. Rev. D 109 (2024) 034521 [2309.15002 [hep-lat]]

Restricted Boltzmann Machine: generative network

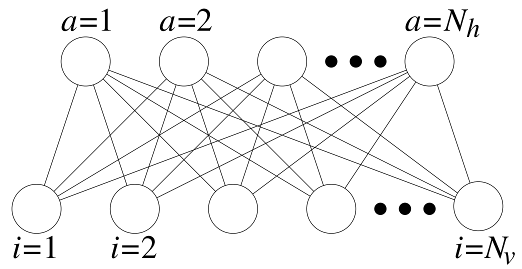


- energy-based method
- probability distribution
- binary or continuous d.o.f.

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

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

Scalar field RBM



- treat RBM as a lattice field theory with action

$$S(\phi, h) = \sum_i \frac{1}{2}\mu_i^2\phi_i^2 + \sum_a \frac{1}{2\sigma^2}(h_a - \eta_a)^2 - \sum_{i,a} \phi_i w_{ia} h_a$$

- only quadratic terms, add interactions later, e.g ϕ^4 terms
- learn weight matrix w_{ia} and bias η_a (put to 0 below)
- induced distribution on visible layer

$$p(\phi) = \int Dh\, p(\phi, h) = \frac{1}{Z}\exp\left(-\frac{1}{2}\sum_{i,j}\phi_i K_{ij}\phi_j + \sum_i J_i\phi_i\right)$$

Gaussian scalar field RBM

- induced distribution on visible layer $p(\phi) = \int Dh\, p(\phi, h) = \frac{1}{Z} \exp\left(-\frac{1}{2} \sum_{i,j} \phi_i K_{ij} \phi_j + \sum_i J_i \phi_i \right)$
- scalar field with kinetic (all-to-all) term $K_{ij} = \mu_i^2 \delta_{ij} - \sigma^2 \sum_a w_{ia} w_{aj}^T$
  and source $J_i = \sum_a w_{ia} \eta_a$
- unusual Gaussian LFT: what is the weight matrix W and bias η?
- learn from data or directly from known distribution
- simplest case: target theory = LFT of free scalar field in 1 or 2d, $K^{\phi} \approx p^2 + m^2$

$$WW^T = \frac{1}{\sigma^2}\left(\mu^2 \mathbb{1} - K^\phi\right) \equiv \mathcal{K}$$

Infinite # of solutions ($N_h = N_v$)

infinite # solutions for weight matrix, use that $\mathcal{K}$ is symmetric and positive-definite

1. Cholesky decomposition $\mathcal{K} = LL^T$: $W = L$ triangular

2. diagonalisation $\mathcal{K} = ODO^T = O\sqrt{D}O^T O\sqrt{D}O^T$: $W = W^T = O\sqrt{D}O^T$

3. non-uniqueness: internal symmetry $W \to WO_R$ → $\phi^T W h \to \phi^T W O_R h = \phi^T W h'$

in practice

- realisation depends on initialisation
- non-observable degeneracy due to internal symmetry on hidden layer

$$K_{ij} = \mu_i^2 \delta_{ij} - \sigma^2 \sum_a w_{ia} w_{aj}^T$$

Dependence on N_h and μ^2

- what if $N_h < N_v$? role of hyperparameter μ^2?

- use LFT insights: target distribution is scalar field theory
- method: SVD of weight matrix $W = U\,\Xi\,V^T$

- quadratic kernel $K = \mu^2 \mathbb{1} - \sigma_h^2 U \Xi \Xi^T U^T = U\left[\mu^2 \mathbb{1} - \sigma_h^2 \Xi \Xi^T\right] U^T \equiv U D_K U^T$

- eigenvalues of quadratic kernel

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

- both N_h and μ^2 act as **ultraviolet regulators** train RBM with persistent contrastive divergence

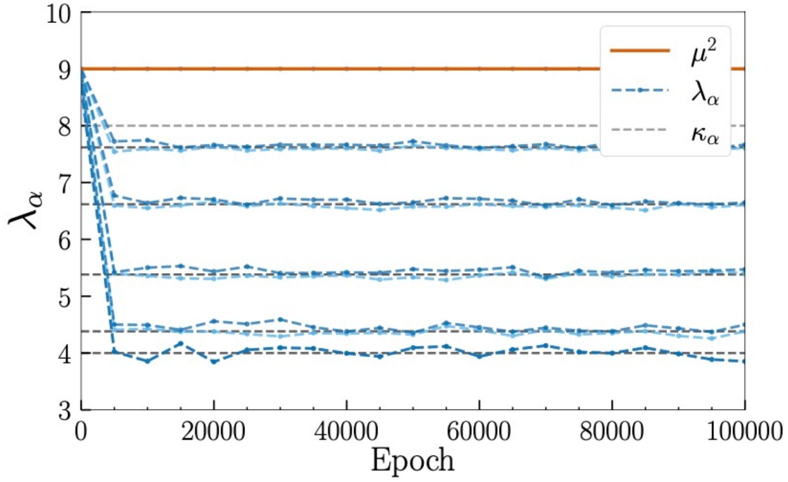
What if $N_h < N_v$?

- example: scalar LFT
  with $N_v = 10$ nodes

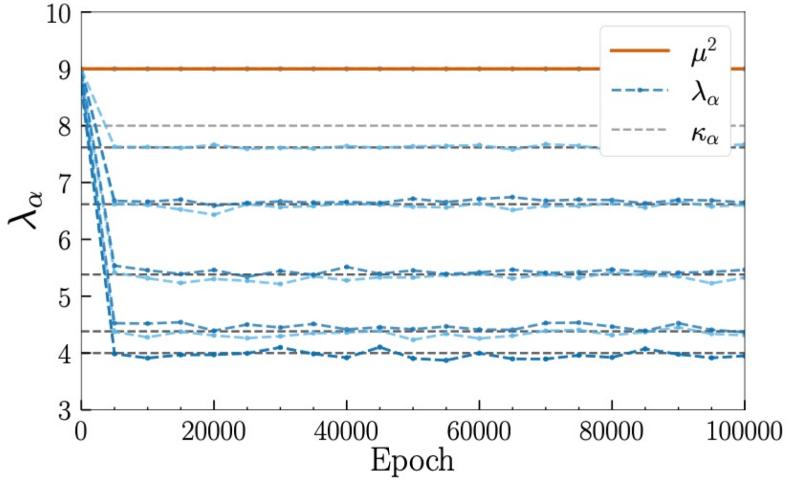
- exact spectrum:
  $$\kappa \sim p^2 + m^2$$

- reproduced by RBM (λ) from smallest eigenvalue upwards

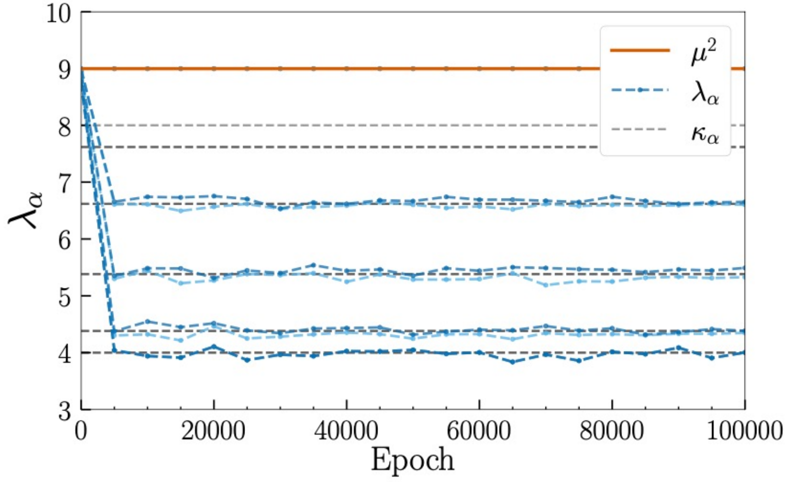
- higher modes are moved to cut-off scale (μ^2)



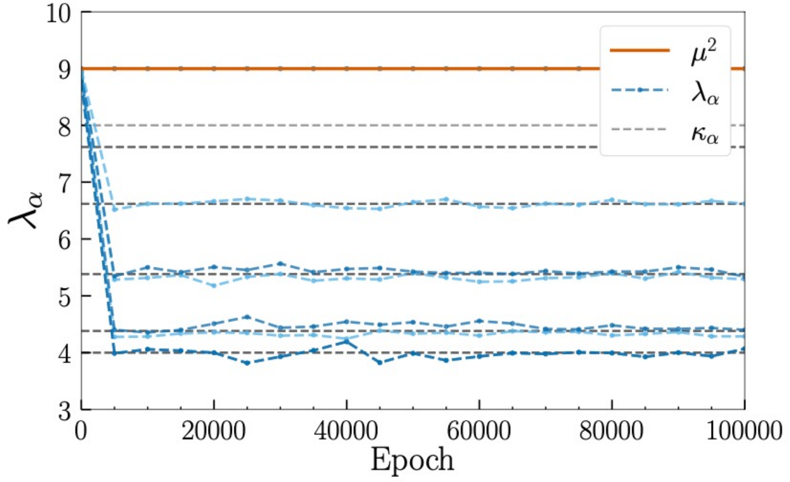
(a) $N_h = 9$



(b) $N_h = 8$



(c) $N_h = 7$



(d) $N_h = 6$

What if RBM mass $\mu^2 < \lambda_{max}$?

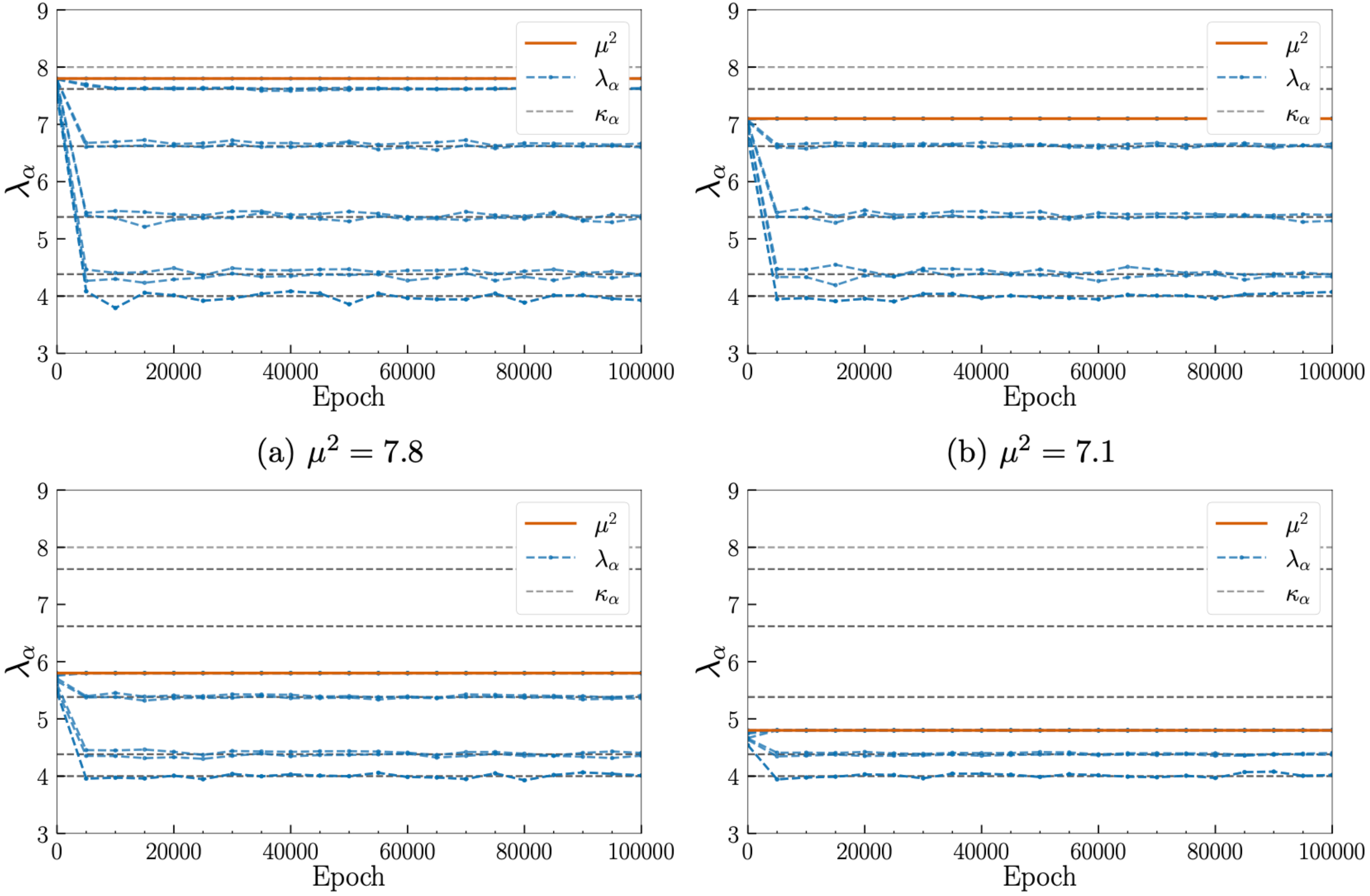
- example: scalar LFT
  with $N_v = 10$ nodes

- exact spectrum:

$$\kappa \sim p^2 + m^2$$

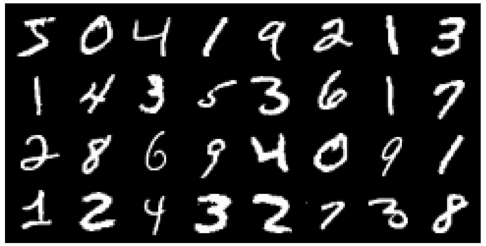
- reproduced by RBM (λ) from smallest eigenvalue upwards

- higher modes are suppressed at cut-off scale (μ^2)

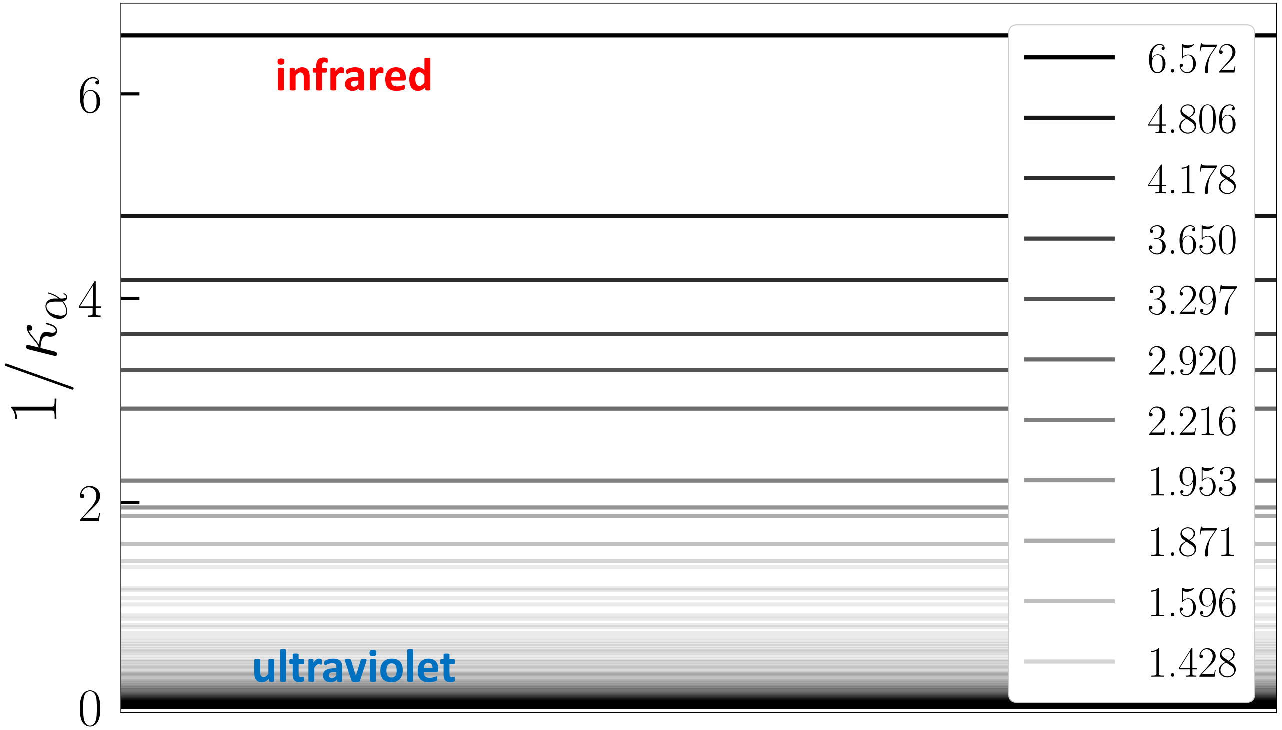


(a) $\mu^2 = 7.8$ (b) $\mu^2 = 7.1$ (c) $\mu^2 = 5.8$ (d) $\mu^2 = 4.8$

RBM as ultraviolet regulator

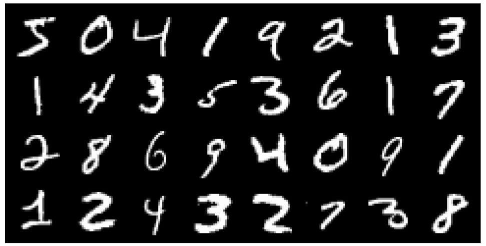


- relevant for “real” data sets? MNIST: 28x28 images of digits
- compute spectrum of two-point correlator $K_{ij}^{-1} = < \phi_i \phi_j >_{data}$
- inverse spectrum $1/\kappa$
- infrared safe
- ultraviolet divergent

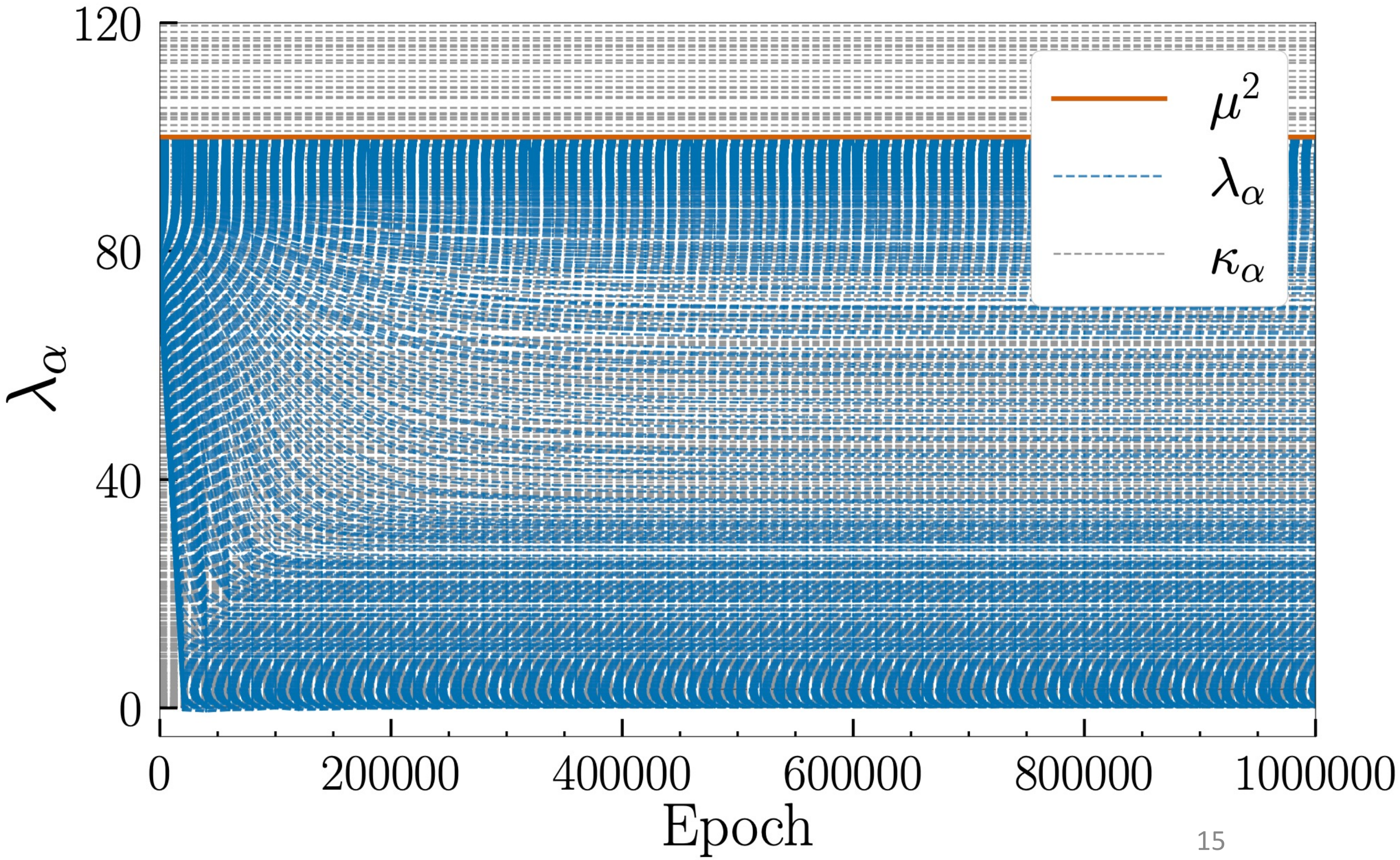


784 eigenvalues

MNIST with fixed RBM mass



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



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) $N_h = 4$

Topic 2

stochastic quantisation and diffusion models

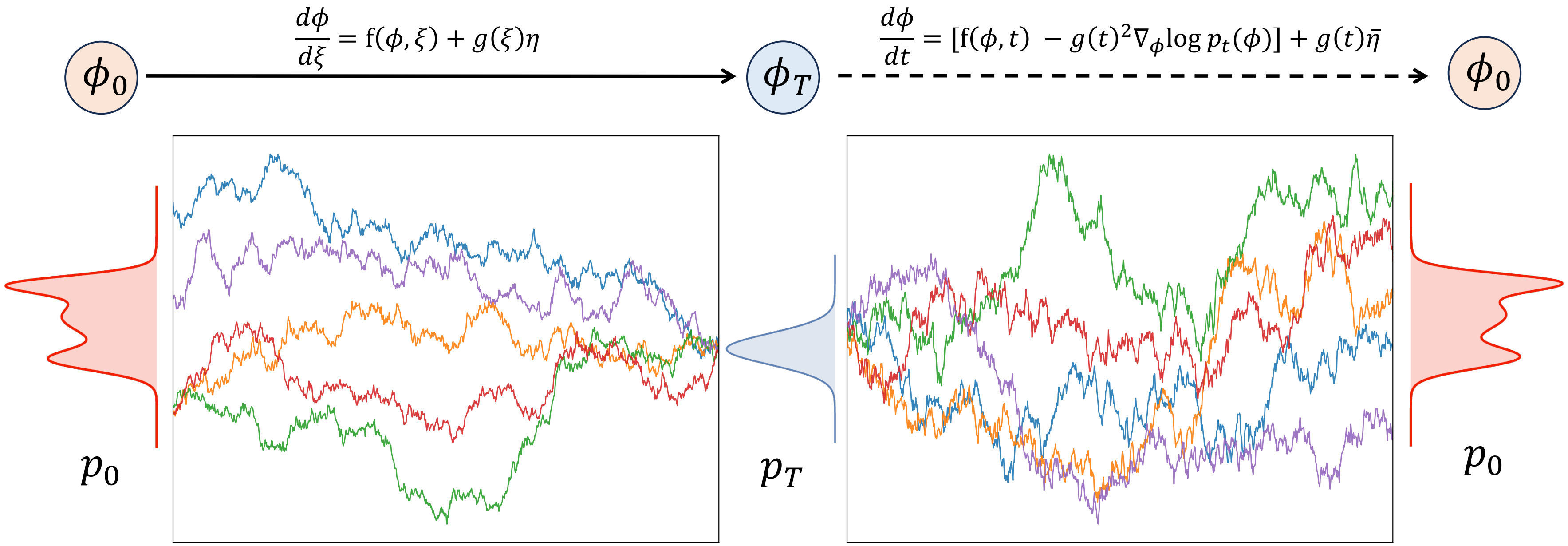
Lingxiao Wang, GA, Kai Zhou

JHEP (to appear) [2309.17082 [hep-lat]]

NeurIPS 2023 2311.03578 [hep-lat]

Diffusion models

- solve stochastic process with a particular drift/force/score
- drift is learnt during forward diffusion process, starting from data
- new configurations are generated via backward process using learnt drift



Stochastic quantisation

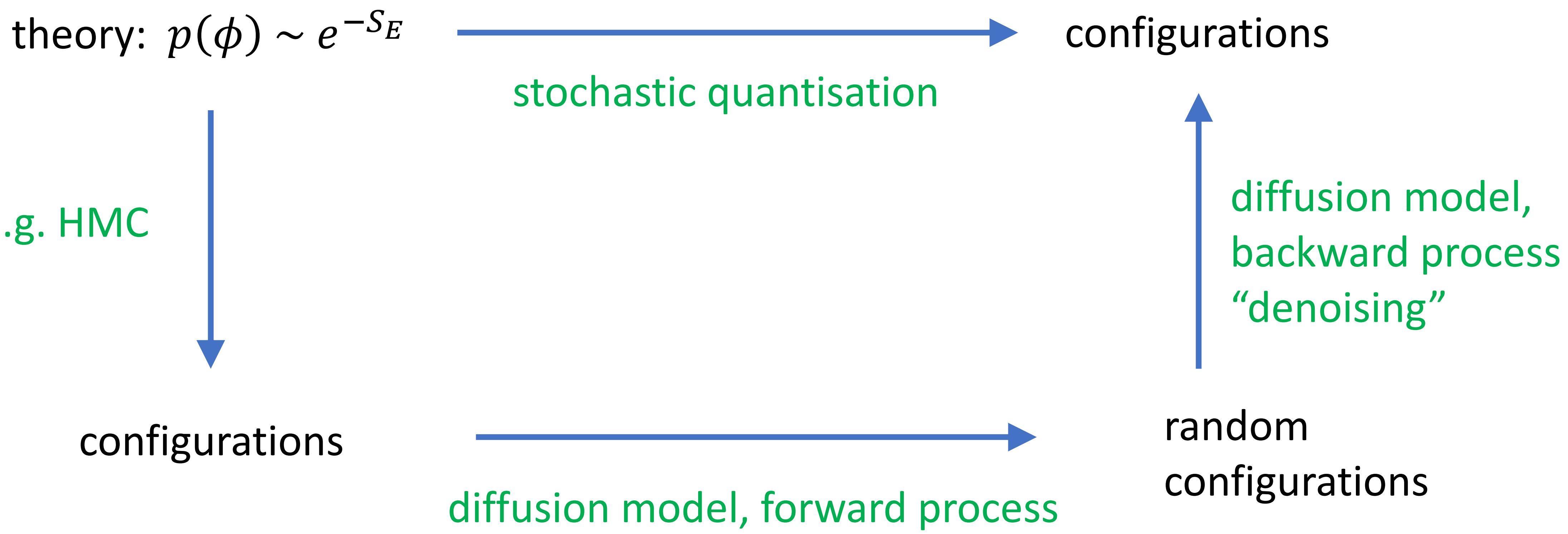
- ideas well-known in quantum field theory: stochastic quantisation (Parisi & Wu 1980)
- path integral quantisation via a stochastic process in fictitious time

$$\frac{\partial\phi(x,\tau)}{\partial\tau} = -\frac{\delta S_E[\phi]}{\delta\phi(x,\tau)} + \eta(x,\tau) \qquad \langle\eta(x,\tau)\eta(x',\tau')\rangle = 2\alpha\delta(x-x')\delta(\tau-\tau')$$

- equilibrium solution ($\tau \to \infty$): distribution $p(\phi) \sim e^{-S_E}$
- convergence guaranteed for real actions due to properties of Fokker-Planck equation
- create samples from Euclidean path integral
- applied to non-abelian gauge theories and QCD in 1980s, but superseded by other methods such as Hybrid Monte Carlo (HMC) [stepsize dependence, efficiency]

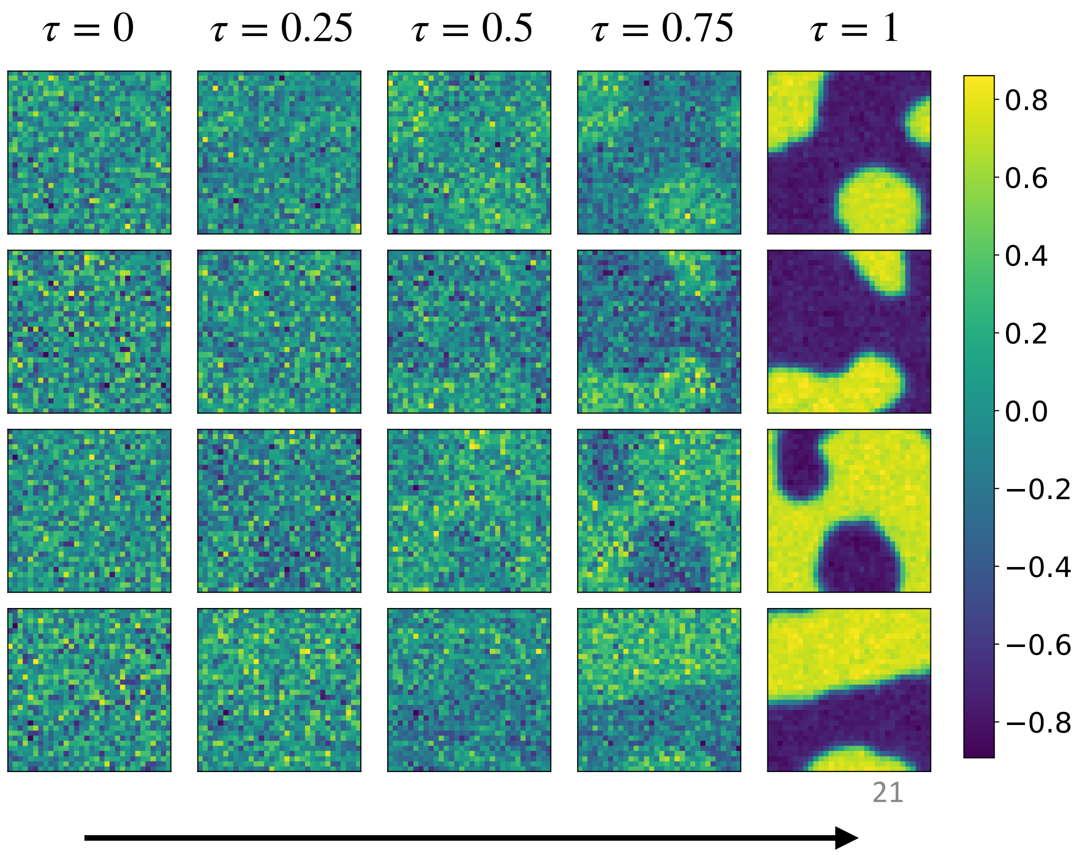
Stochastic quantisation and diffusion models

- diffusion models as an alternative approach to stochastic quantisation



Diffusion model for 2d ϕ^4 scalar theory

- 32^2 lattice, choice of action parameters in symmetric and broken phase
- training data set generated using Hybrid Monte Carlo (HMC)
- variance expanding DM trained using U-Net architecture



generating configurations:

- broken phase
- “denoising” (backward process)
- large-scale clusters emerge, as expected

Diffusion model for 2d ϕ^4 scalar theory

generating configurations in symmetric phase

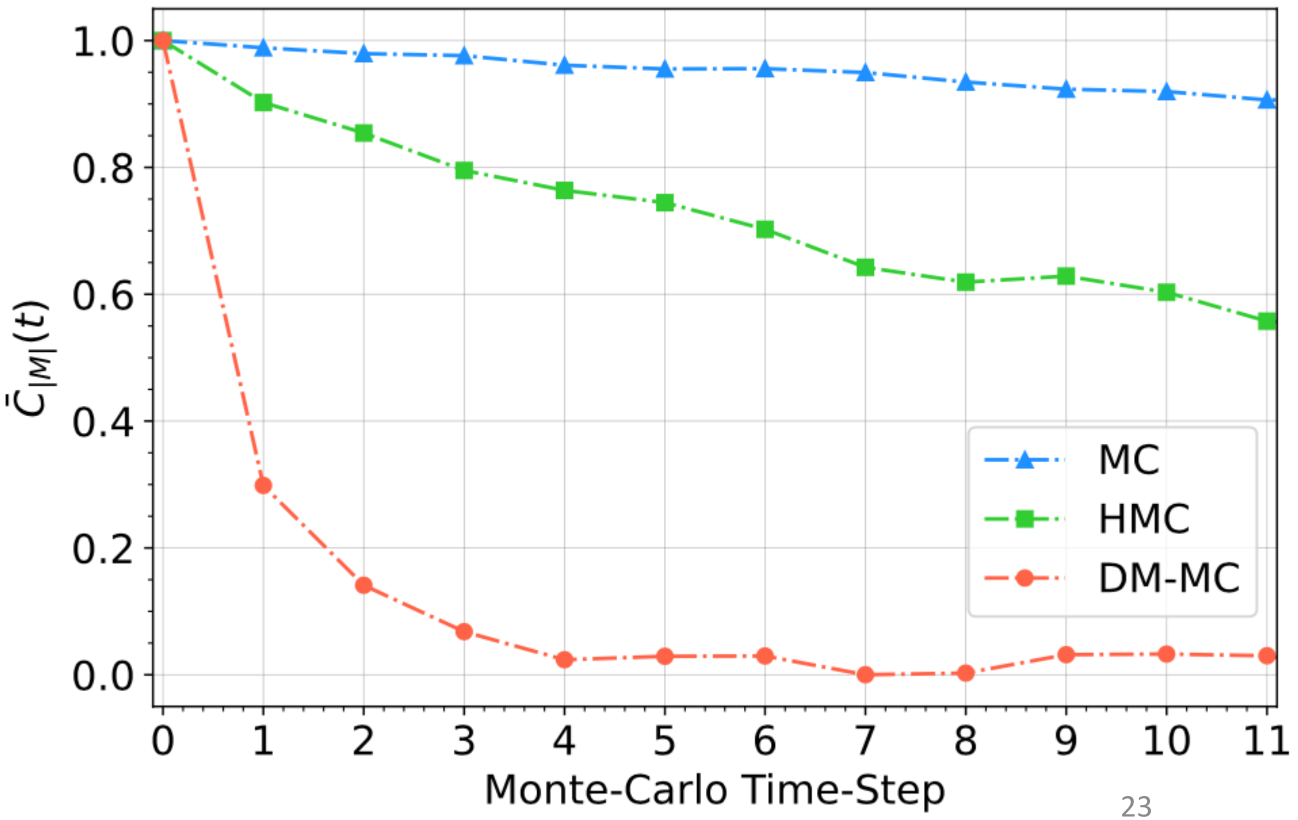
- compute magnetisation $< M >$, susceptibility χ_2, Binder cumulant U_L
- compare with test HMC data set (with same statistics)

data-set	$\langle M \rangle$	χ_2	U_L
Training (HMC)	0.0012± 0.0007	2.5160 ± 0.0457	0.1042 ± 0.0367
Testing (HMC)	0.0018 ± 0.0015	2.4463 ± 0.1099	-0.0198 ± 0.1035
Generated (DM)	0.0017± 0.0015	2.4227 ± 0.1035	0.0484 ± 0.0959

- good agreement is observed

Diffusion model for 2d ϕ^4 scalar theory

- auto-correlation time (first comparison)
- normalised auto-correlation function



overall:

- proof of principle
- expected results obtained
- need to do detailed comparison of precision, speed and scalability

Summary and outlook

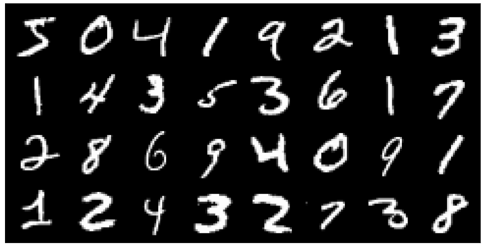
- can experience in quantum field theory help in understanding ML and vice versa?

- two examples of interplay between lattice field theory and ML
  - scalar field RBM as ultraviolet regulator
  - stochastic quantisation and diffusion models

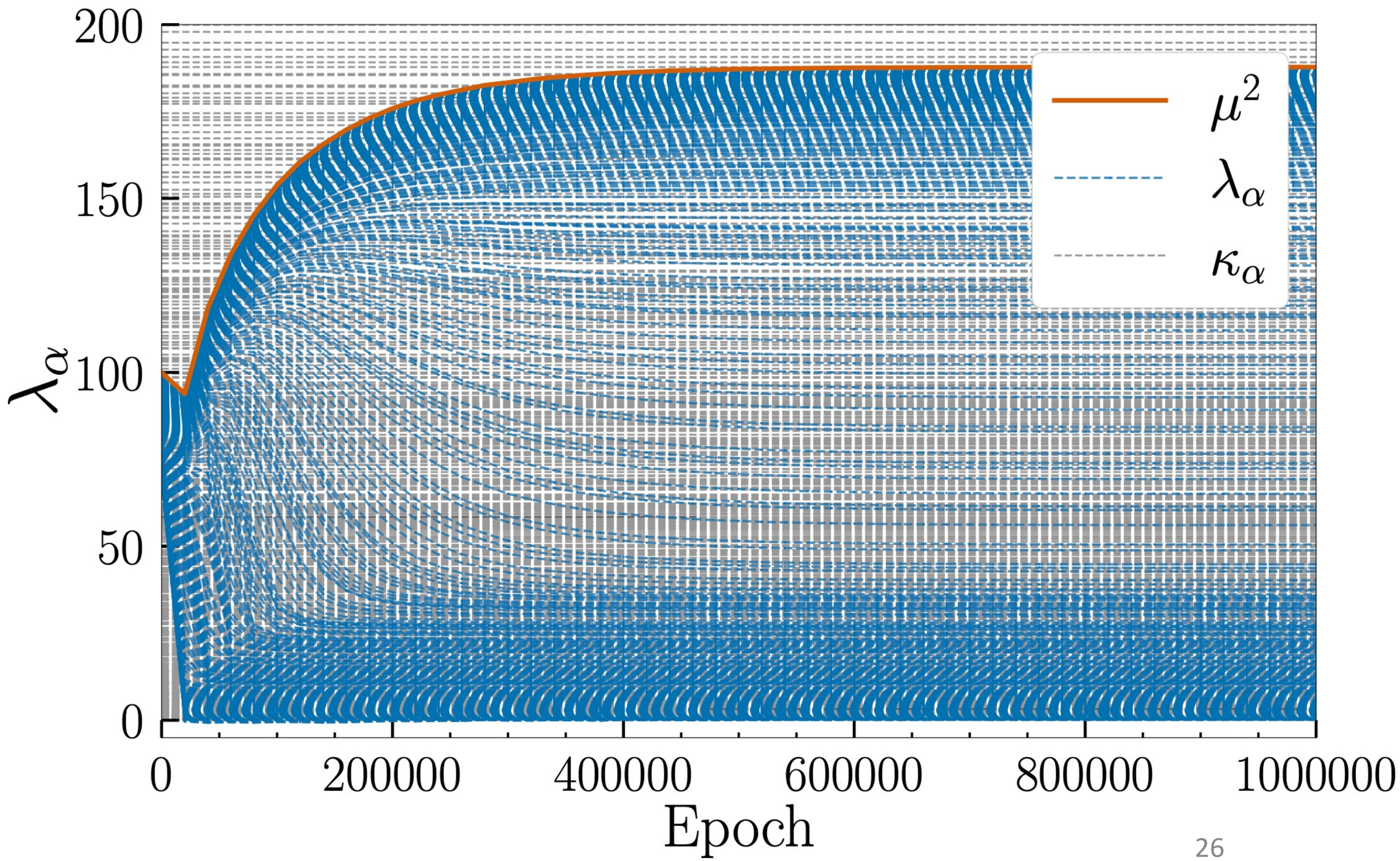
- interplay between statistical/lattice field theory and ML
- many directions to explore

Back-up

MNIST with dynamic RBM mass



- $N_v = N_h = 784$
- dynamical RBM mass μ^2 is learned as well
- spectrum regulated
- ultraviolet cut-off μ^2 increases to include more modes



Interacting scalar field RBM

- Gaussian RBMs can learn Gaussian distributions
- in LFT language: need to include interactions
- various ways to do so, depending on properties of target distribution

- QFT-ML approach: add local potential terms on nodes, e.g. ϕ^4 terms

Quantum field-theoretic machine learning, Bachtis, Aarts, Lucini
Phys. Rev. D 103 (2021) 074510 [2102.09449 [hep-lat]]

- standard RBM approach: use binary hidden layer $h_a = \pm 1$

Scalar-Bernoulli RBM: hidden binary nodes

- induced distribution $p(\phi) = \frac{1}{Z} \exp\left(-S_\phi(\phi) + \sum_a \sum_{n=1}^{\infty} c_n \psi_a^{2n}\right)$ with $\psi_a = \sum_i \phi_i w_{ia} - \eta_a$
- generates all-to-all interactions of all powers of ϕ
- at leading order in W same kinetic term as in Gaussian case
- example of quartic term
  (taking $\eta_a = 0$ for simplicity)
  $$\sum_a \sum_{i,j,k,l} (\phi_i w_{ia})(\phi_j w_{ja})(\phi_k w_{ka})(\phi_l w_{la})$$
- highly non-local, very different from standard field theories, analysis in preparation

Stochastic quantisation: complex actions

- approach not limited to real-valued distributions/actions
- extend Langevin process to complex manifold: complex Langevin dynamics (Parisi 1981)
- complexify d.o.f.: real scalar → complex scalar, $U \in SU(N) \to U \in SL(N, \mathbb{C})$

- convergence not guaranteed, no general solution of Fokker-Planck equation
- a posteriori justification (GA, Seiler, Stamatescu 2009, Nagata, Nishimura, Shimasaki 2016)

- applied to problems at finite (baryon) chemical potential (GA & Stamatescu 2008, Aarts 2009)
- success in some theories, QCD remains difficult (e.g. Sexty 2019)
- introductory lectures: GA, J.Phys.Conf.Ser. 706 (2016) 2, 022004 [1512.05145 [hep-lat]]