Diffusion models and stochastic quantisation

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Physics for AI, Oxford, March 2025

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with Lingxiao Wang and Kai Zhou, JHEP 05 (2024) 060 [2309.17082 [hep-lat]]

NeurIPS workshop 2023 *ML and the Physical Sciences* 2311.03578 [hep-lat]

+ **Diaa Habibi**, NeurIPS workshop 2024, 2410.21212 [hep-lat]

Lattice 2024 2412.01919 [hep-lat]

+ Qianteng Zhu, Wei Wang, NeurIPS workshop 2024, 2410.19602 [hep-lat]

submitted to JHEP, 2502.05504 [hep-lat]

Physics for AI, Oxford, March 2025

ML seems to be everywhere: perspective from a theoretical physicist

- many concepts in ML are familiar to theoretical and computational physicists
- neural networks, say, are systems with many fluctuating degrees of freedom
- training – or learning – is a minimisation process, typically achieved with stochastic gradient descent (SGD)
- linear (matrices) and nonlinear (activation functions) transformations

Machine learning is the new playground!

many concepts in ML are familiar to theoretical and computational physicists

keywords:

- neural networks as statistical systems
- stochastic dynamics
- random matrix theory
- learning: non-equilibrium evolution and "thermalisation"
- phase diagrams of neural networks, spin glasses
- …

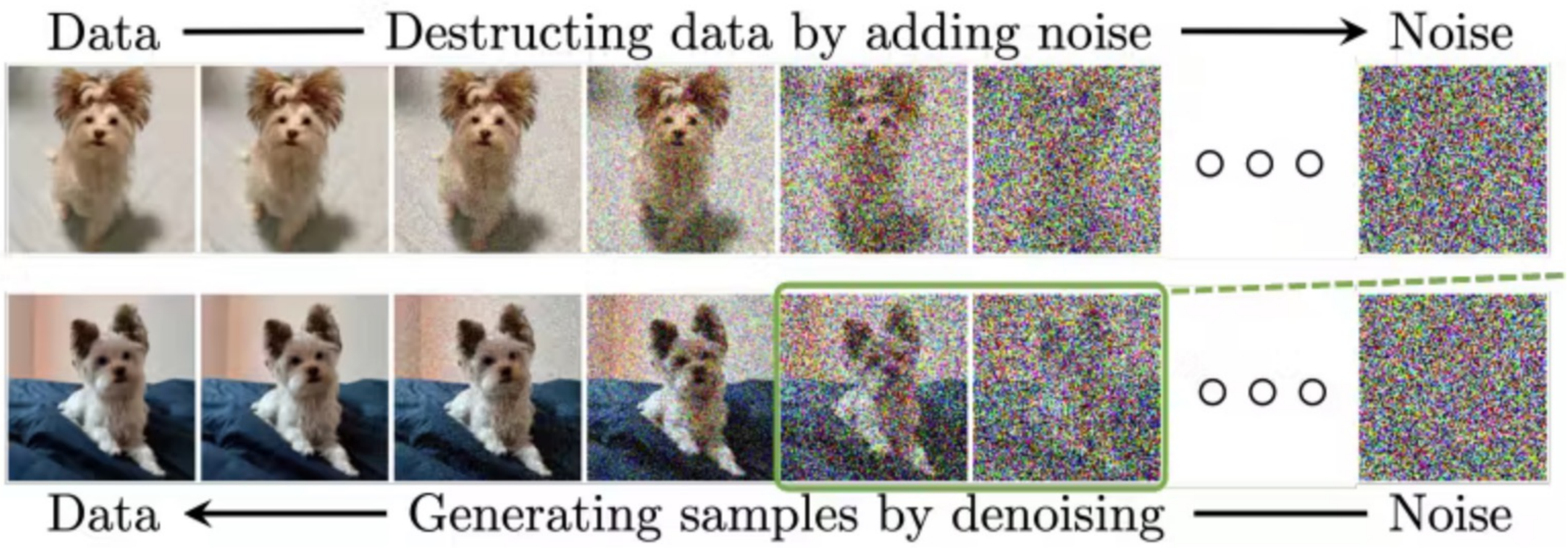
picture of a playground

this talk: diffusion models & lattice field theory & statistical field theory

Outline

- generative AI and diffusion models
- basics: stochastic differential equations (SDEs) and Fokker-Planck equations (FPEs)
- relation between diffusion models and stochastic quantisation in lattice field theory
- detailed study using tools of statistical field theory
- outlook

Generative AI using diffusion models



https://encord.com/blog/diffusion-models/

denoising

Generative Modeling by Estimating Gradients of the Data Distribution
Yang Song, Stefano Ermon
arXiv:1907.05600 [cs.LG]

interpolation

Score-Based Generative Modeling through Stochastic Differential Equations
Yang Song, Jascha Sohl-Dickstein, Diederik P. Kingma, Abhishek Kumar, Stefano Ermon, Ben Poole
arXiv:2011.13456 [cs.LG]

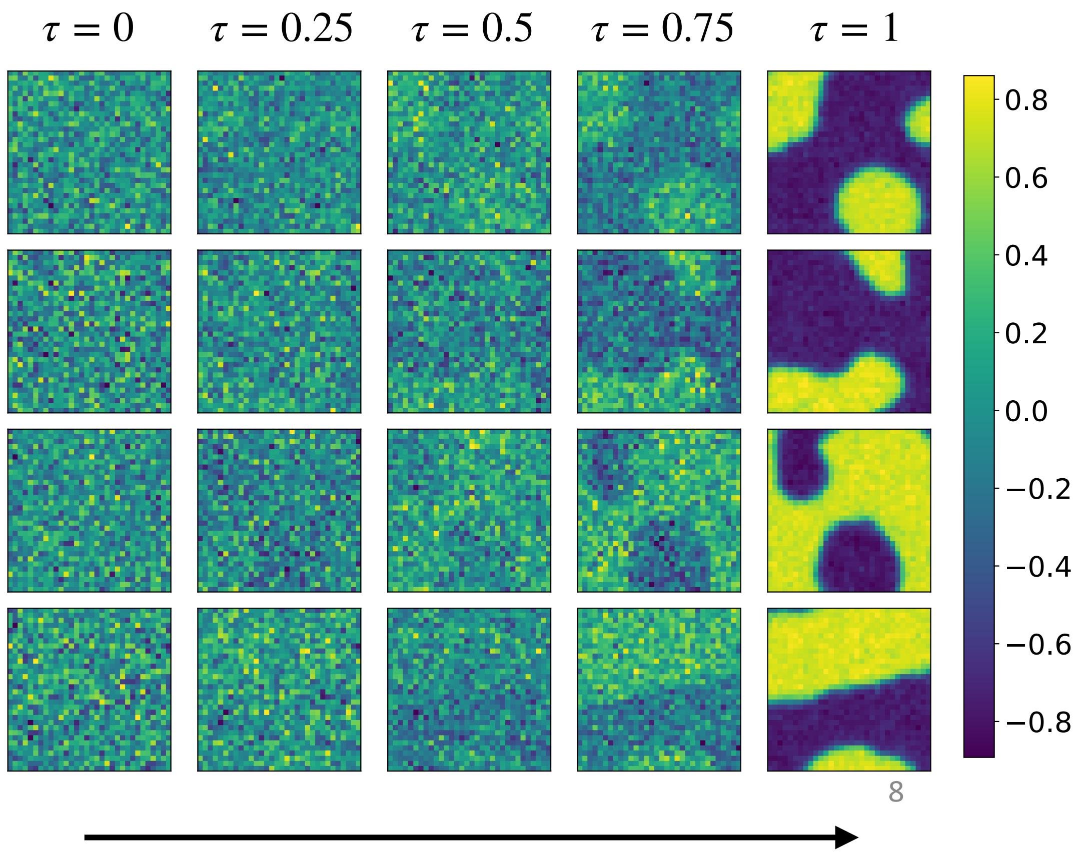
Diffusion model for 2d ϕ^4 lattice scalar theory

- 32^2 lattice, choice of action parameters in symmetric and broken phase
- training data set generated using Hybrid Monte Carlo (HMC)

- first application of diffusion models in lattice field theory

generating configurations:

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



L Wang, GA, K Zhou, JHEP 05 (2024) 060 [2309.17082 [hep-lat]]

Diffusion models: stochastic dynamics

employ stochastic dynamics to generate images or configurations

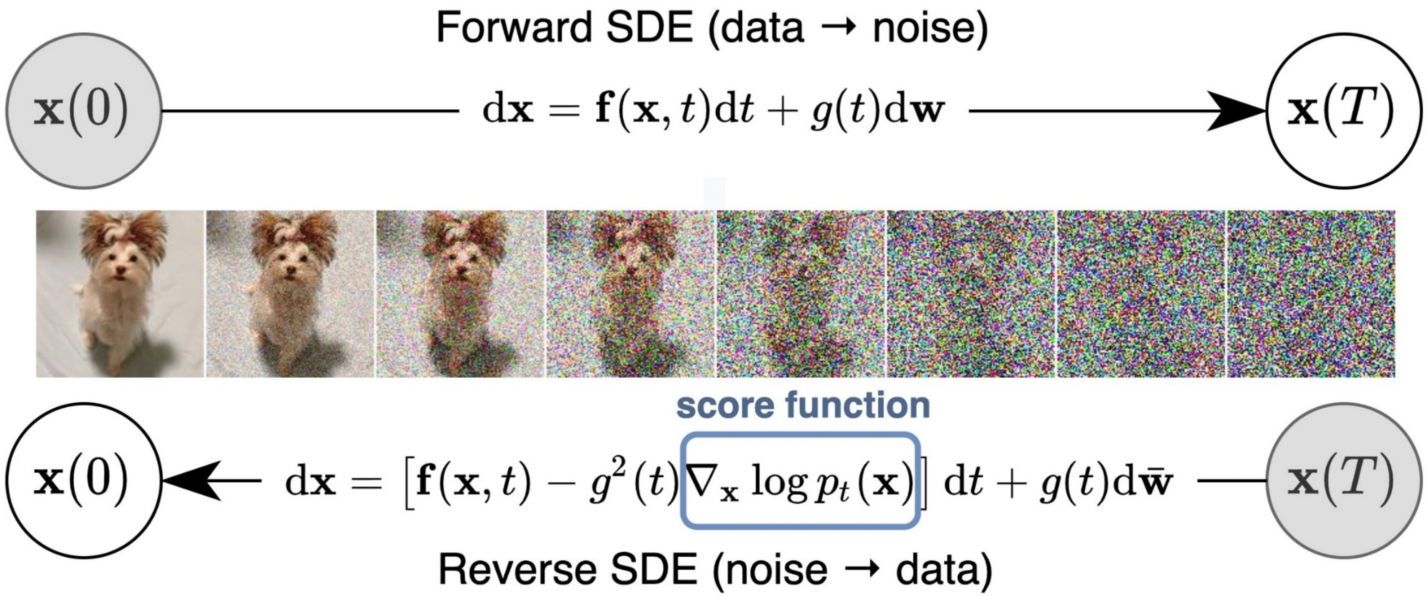
- start with data set of images or configurations

- make the images more blurred by applying noise (forward process)

- learn steps in this process

  … and then revert it

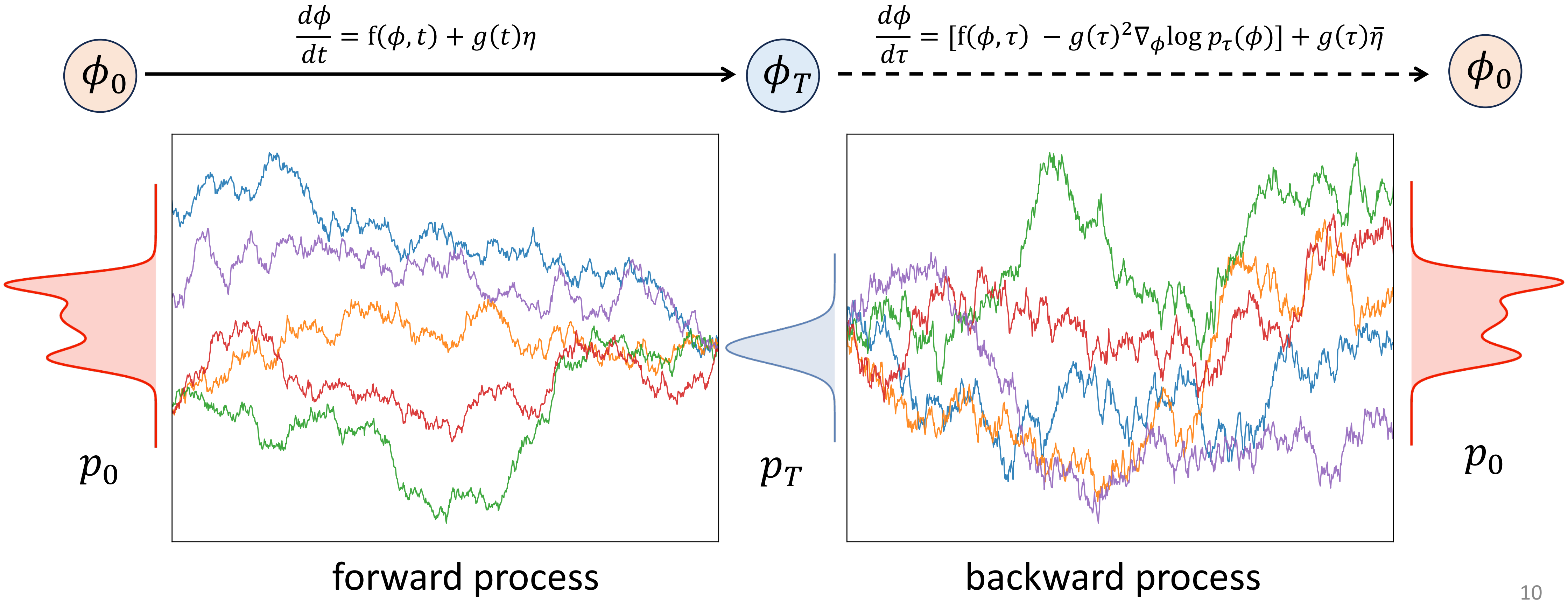
- create new images from noise



https://theaisummer.com/diffusion-models/

Prior and target distributions

- in terms of distributions: p_0 is target (non-trivial), p_T is the prior (easy)



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- **basics: stochastic differential equations (SDEs) and Fokker-Planck equations (FPE)**
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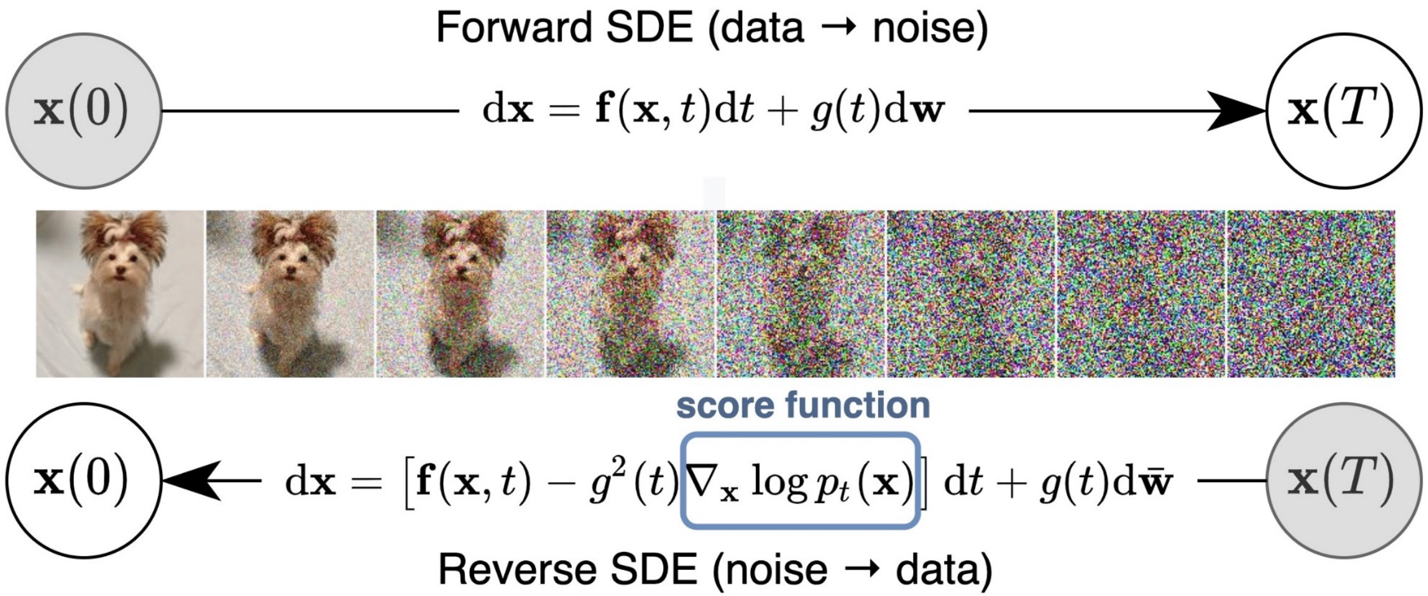
Diffusion models

three ingredients:

- target distribution, consisting of real-world data or from known distribution (in physics)
- forward stochastic process
- backward stochastic process



https://theaisummer.com/diffusion-models/

Stochastic different equations (SDEs)

- two main approaches:

  - denoising diffusion probabilistic models (DDPMs), variance preserving schemes
  - variance expanding schemes

- unified description using SDEs [Yang Song, et al, arXiv:2011.13456 [cs.LG]]

- here: basic intro to set the stage

- notation can differ (Brownian motion, Wiener process, continuous time, …)

➢ I'll be non-rigorous but hopefully (!) correct

Stochastic different equations (SDEs)

- one degree of freedom $\dot{x}(t) = \frac{1}{2}K[x(t)] + \eta(t)$ describe distribution $P(x) \sim e^{-S(x)}$
- force/drift term $K(x) = \nabla \log P(x) = -S'(x)$ stochastic term $\langle \eta(t)\eta(t') \rangle = \delta(t-t')$
- simple discretisation $x_{n+1} = x_n + \frac{\epsilon}{2}K(x_n) + \sqrt{\epsilon}\eta_n$ $\langle \eta_n \eta_{n'} \rangle = \delta_{nn'}$
- express dynamics in terms of probability distribution

$$\langle O[x(t)] \rangle_\eta = \int dx\, P(x,t) O(x) = \langle O(t) \rangle_P$$

- replace noise average by average over distribution: $P(x,t)$ satisfies Fokker-Planck equation

$$x_{n+1} = x_n + \frac{\epsilon}{2} K(x_n) + \sqrt{\epsilon}\eta_n \qquad \langle \eta_n \eta_{n'} \rangle = \delta_{nn'}$$

SDEs and FPEs

$$\langle O[x(t)] \rangle_\eta = \int dx\, P(x,t) O(x) = \langle O(t) \rangle_P$$

- consider $\langle O(x_{n+1}) \rangle_\eta - \langle O(x_n) \rangle_\eta$
- Taylor expand $O(x_{n+1}) = O(x_n) + O'(x_n) \left(\frac{\epsilon}{2} K(x_n) + \sqrt{\epsilon}\eta_n \right) + \frac{\epsilon}{2} O''(x_n) \eta_n \eta_n + \mathcal{O}\left(\epsilon^{3/2}\right)$
- noise average $\langle O(x_{n+1}) \rangle_\eta - \langle O(x_n) \rangle_\eta = \frac{\epsilon}{2} \langle O'(x_n) K(x_n) \rangle_\eta + \frac{\epsilon}{2} \left\langle O''(x_n) \right\rangle_\eta$
- average over distribution $\int dx\, \partial_t P(x,t) O(x) = \frac{1}{2} \int dx\, P(x,t) \left[O'(x) K(x) + O''(x) \right]$
- partial integration, for all $O(x)$: $\partial_t P(x,t) = \frac{1}{2} \partial_x \left(\partial_x - K(x) \right) P(x,t)$ FPE

Fokker-Planck equation, stationary solution

- FPE: $\partial_t P(x,t) = \frac{1}{2}\partial_x \left(\partial_x - K(x)\right) P(x,t)$
- stationary solution: $\partial_t P(x,t) = 0$ $\qquad K(x) = \nabla \log P(x) = -S'(x)$
- if force is derivative of action: $\left(\partial_x - K(x)\right) P(x) = 0 \quad \Leftrightarrow \quad \left(\partial_x + S'(x)\right) P(x) = 0$
- stationary distribution: $P(x) \sim e^{-S(x)}$ expected result

standard result for Brownian motion, add a few more ingredients:

- time dependent noise strength, or diffusion coefficient
- time dependent force

Time-dependent noise, diffusion coefficient

- to cover information at all scales in data set: time dependent noise

$$\dot{x} = \frac{1}{2} g^2(t) K[x(t)] + g(t)\eta(t)$$

- corresponding FPE: $$\partial_t P(x,t) = \frac{1}{2} g^2(t) \partial_x \left[\partial_x - K(x)\right] P(x,t)$$

- can hence also be seen as reparameterisation of ‘time’

- in ML jargon: noise schedulers

Many degrees of freedom, field theory

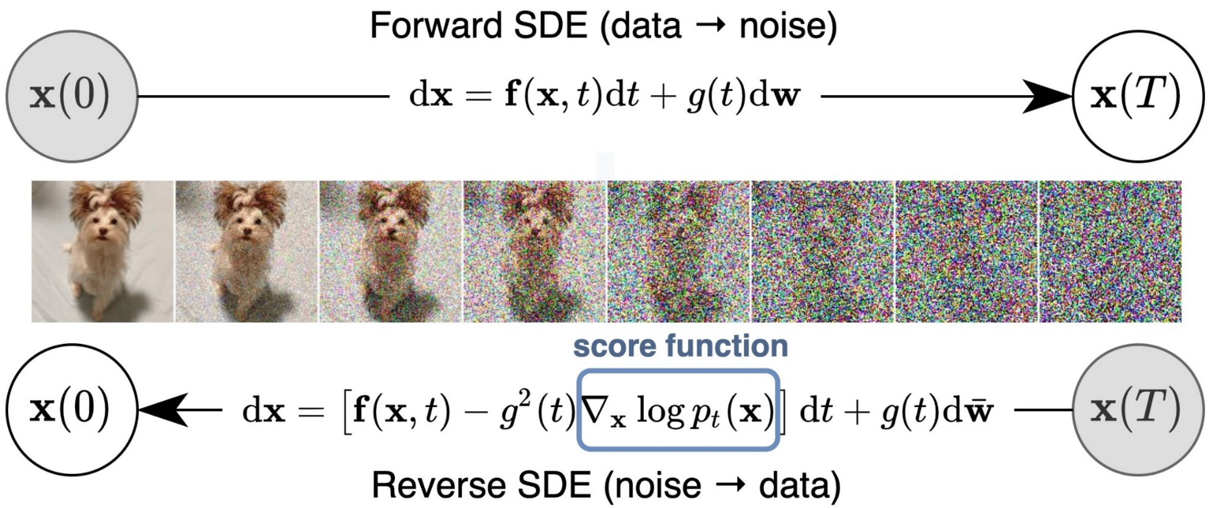
- distributions are functionals (path integrals) $$P[\phi] = \frac{1}{Z} e^{-S[\phi]} \qquad Z = \int D\phi \, e^{-S[\phi]}$$

- SDE $$\frac{\partial \phi(x,t)}{\partial t} = \frac{1}{2} g^2(t) K[\phi(x),t] + g(t)\eta(x,t)$$

- FPE $$\partial_t P[\phi,t] = \frac{1}{2} g^2(t) \int d^n x \, \frac{\delta}{\delta\phi(x)} \left(\frac{\delta}{\delta\phi(x)} - K[\phi(x),t] \right) P[\phi,t]$$

Evolving distributions

- apply this framework to evolve distributions forward and backward



SDE/FPE evolves distribution in time

- forward evolution: start from data, erase information but learn along the way
- add increasing levels of noise, simplest case: no drift term $\dot{x}(t) = g(t)\eta(t)$ $\eta \sim \mathcal{N}(0,1)$
- time-dependent noise strength: $g(t) = \sigma^{t/T}$ $0 \leq t \leq T$
- solution: $x(t) = x_0 + \int_0^t ds\, g(s)\eta(s)$ $\Rightarrow$ $x(t) = x_0 + \sigma(t)\eta(t)$
- variance keeps increasing $\langle (x(t) - x_0)^2 \rangle = \sigma^2(t)$ $\sigma^2(t) = \int_0^t ds\, g^2(s)$
- 'erases' the information from the initial data set

FPE: $\partial_t P_t(x) = \frac{1}{2} g^2(t) \partial_x^2 P_t(x)$

Example: forward evolution

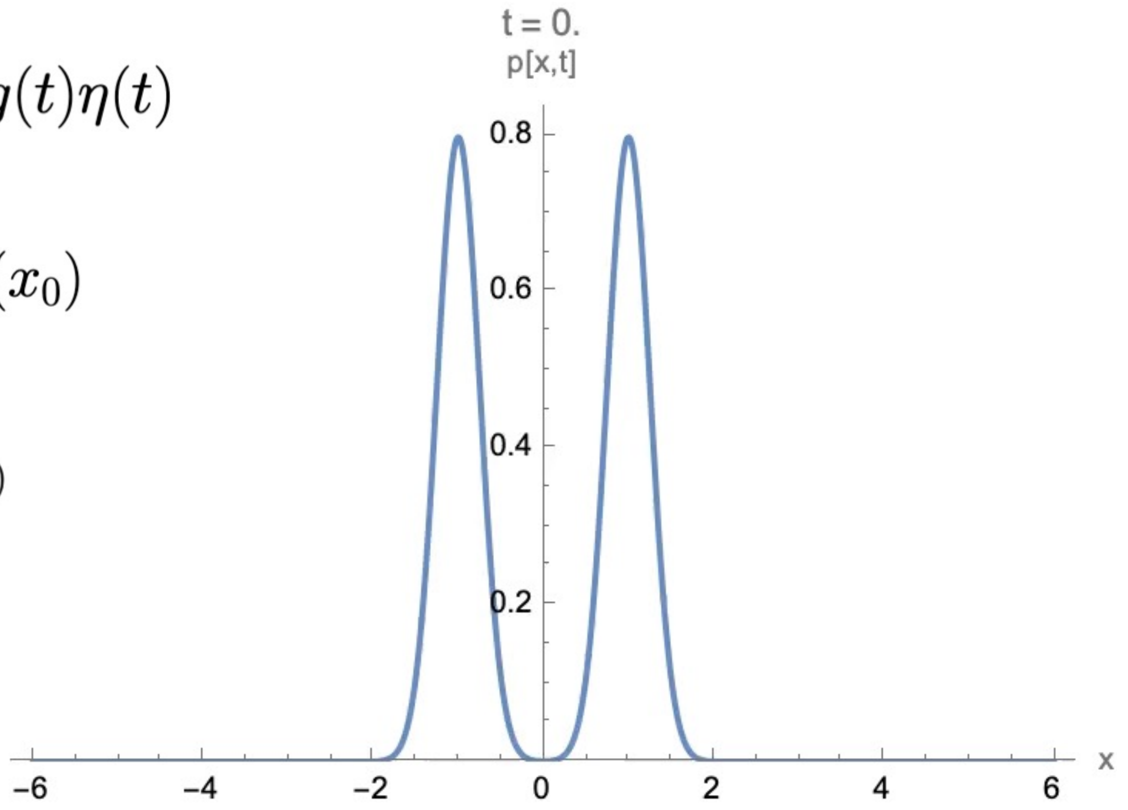
- initial distribution $P_0(x_0)$: two Gaussian peaks

- add noise in variance-expanding scheme $\dot{x}(t) = g(t)\eta(t)$

- analytical description $P_t(x) = \int dx_0 \, P_t(x|x_0) P_0(x_0)$

$$P_t(x|x_0) = \mathcal{N}(x; x_0, \sigma^2(t)) = \frac{1}{\sqrt{2\pi\sigma^2(t)}} e^{-(x-x_0)^2/(2\sigma^2(t))}$$

- peak structure erased



Manifold hypothesis

- logical separation between data (distribution $P_0(x_0)$) and stochastic process

$$P_t(x) = \int dx_0\, P_t(x|x_0) P_0(x_0)$$

$$P_t(x|x_0) = \mathcal{N}(x; x_0, \sigma^2(t)) = \frac{1}{\sqrt{2\pi\sigma^2(t)}} e^{-(x-x_0)^2/(2\sigma^2(t))}$$

- manifold hypothesis: real-world data concentrated on low-dimensional manifolds embedded in a high-dimensional space (the ambient space)

- at the end of the forward process, the entire high-dimensional space should be covered

- adding noise with increasing strength ensures all data structures are captured

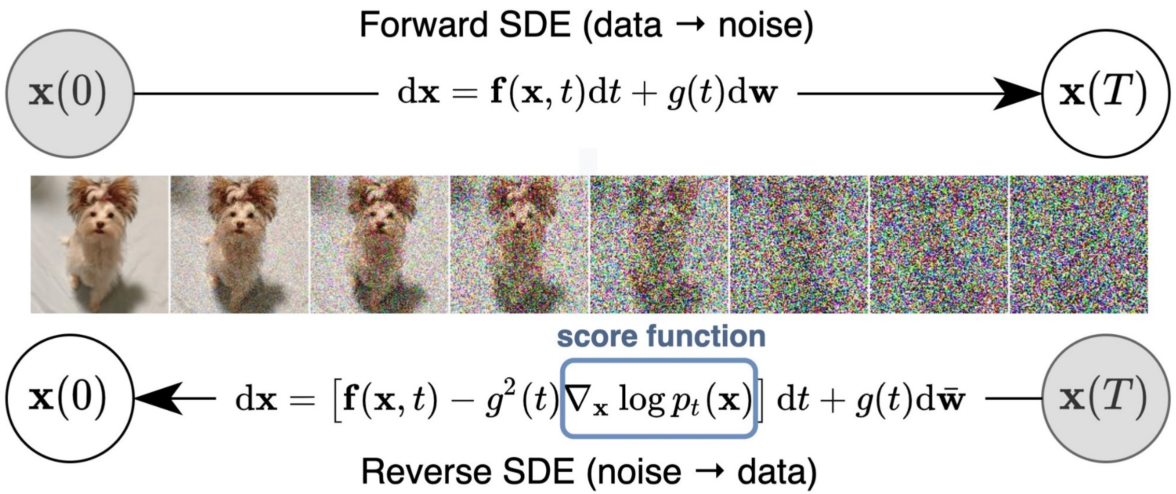
Backward evolution: the score

- structure emerges from noise: add a drift term, the score

- from structure of FPE: drift drives distribution to desired target distribution

- use Anderson equation [B.D.O. Anderson (1982)] $\tau = T - t$

$$x'(\tau) = -K(x(\tau), T-\tau) + g^2(T-\tau)\partial_x \log(P(x, T-\tau)) + g(T-\tau)\eta(\tau)$$



- SDE includes new term: score $\nabla \log P_t(x)$

$0 \leq t \leq T$

noise profile $g(t) = \sigma^{t/T}$

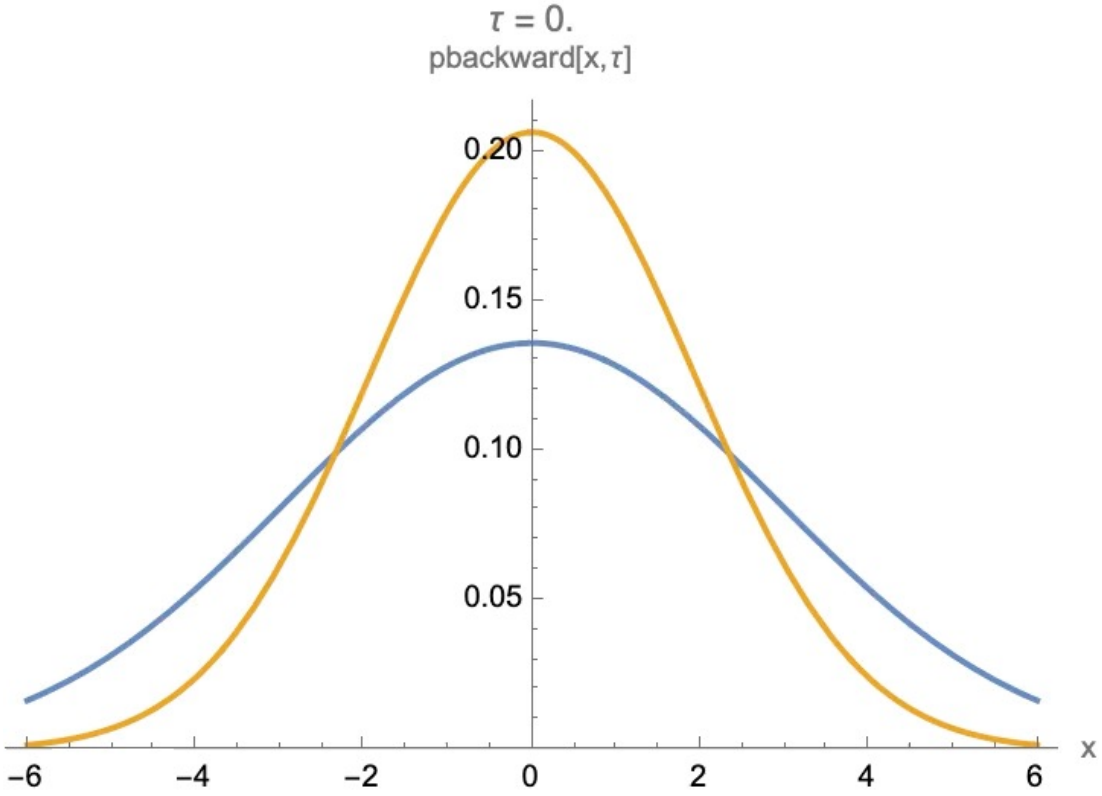
Example: backward evolution

- target distribution: two Gaussian peaks
- forward process $\dot{x}(t) = K(x(t), t) + g(t)\eta(t)$
- corresponding backward process

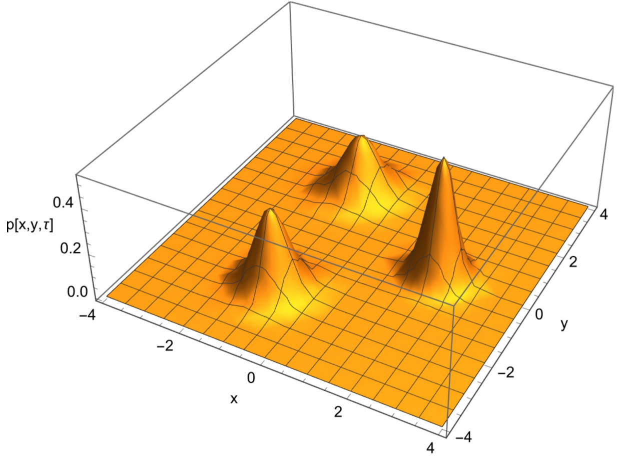
$$
\begin{aligned}
x'(\tau) = & - K(x(\tau), T - \tau) \\
& + g^2(T - \tau)\partial_x \log(P(x, T - \tau) \\
& + g(T - \tau)\eta(\tau)
\end{aligned}
$$

with $\tau = T - t$

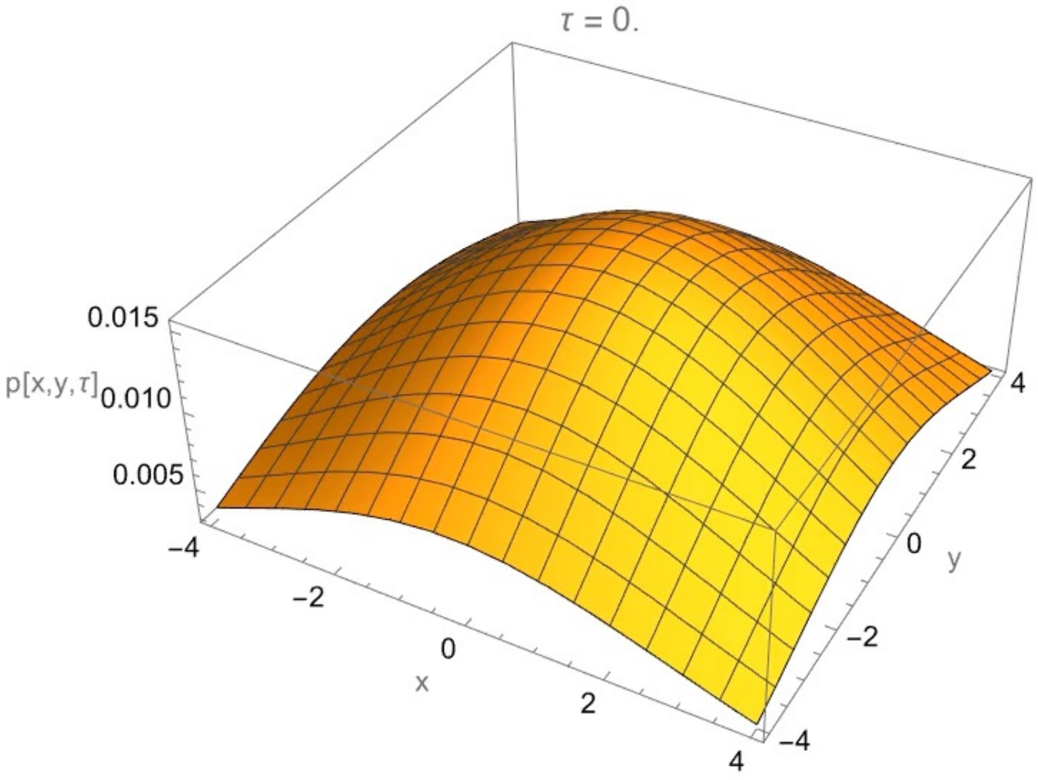
solve FPE for backward process using two initial distributions



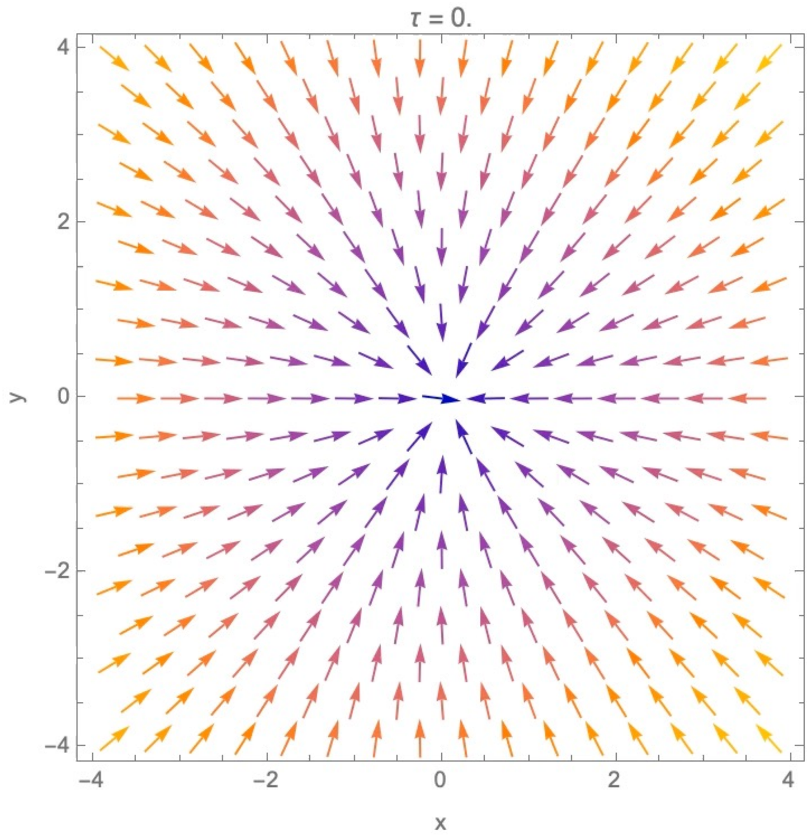
2D example: three Gaussian peaks



backward process, starting from wide normal distribution

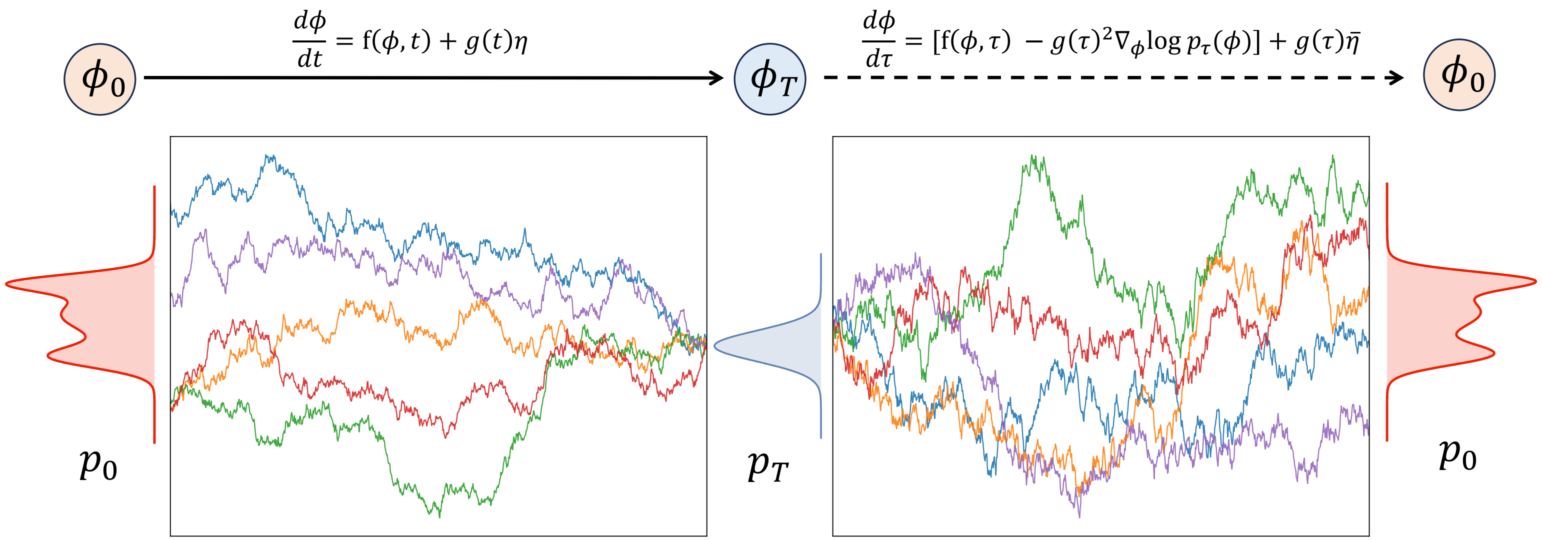


score $\nabla P_t(x, y)$ during backward process



Where does ML come in?

- so far, analysis of SDEs and FPEs
- time-dependent distribution $P(x,t) = P_t(x)$ describes forward and backward process
- in general **score** $\nabla \log P_t(x)$ is not known, needs to be "learnt" during forward process
- score matching
- minimise loss function



Score matching: learn the drift for backward process

- one degree of freedom, variance-expanding scheme: $\dot{x}(t) = g(t)\eta(t) \qquad \eta \sim \mathcal{N}(0,1)$
- time-dependent distribution $P(x,t) = P_t(x)$ describes forward and backward process
- so-called **score** $\nabla \log P_t(x)$ is not known, needs to be "learnt"
- loss function $\mathcal{L}(\theta) = \frac{1}{2}\int_0^T dt\, \mathbb{E}_{P_t(x)} \left[\sigma^2(t)\, \|s_\theta(x,t) - \nabla \log P_t(x)\|^2\right] \qquad \sigma^2(t) = \int_0^t ds\, g^2(s)$
- $s_\theta(x,t)$ approximates score, vector field learnt by some neural network
- introduce conditional distribution $P_t(x) = \int dx_0\, P_t(x|x_0) P_0(x_0)$ initial data $P_0(x_0)$

$$P_t(x) = \int dx_0\, P_t(x|x_0) P_0(x_0)$$

Score matching: learn the drift

- loss function $\mathcal{L}(\theta) = \frac{1}{2}\int_0^T dt\, \mathbb{E}_{P_t(x)}\left[\sigma^2(t)\, \| s_\theta(x,t) - \nabla \log P_t(x) \|^2\right]$
- diffusion process $\dot{x}(t) = g(t)\eta(t)$ easily solved $x(t) = x_0 + \sigma(t)\eta(t)$ $\quad \sigma^2(t) = \int_0^t ds\, g^2(s)$
- conditional distribution $P_t(x|x_0) = \mathcal{N}(x; x_0, \sigma^2(t)) = \frac{1}{\sqrt{2\pi\sigma^2(t)}} e^{-(x-x_0)^2/(2\sigma^2(t))}$
- and hence $\nabla \log P_t(x_t|x_0) = -(x_t - x_0)/\sigma^2(t)$
- loss function $\mathcal{L}(\theta) = \frac{1}{2}\int_0^T dt\, \mathbb{E}_{P_t(x_t)}\left[\left\| \sigma(t) s_\theta(x_t,t) + \frac{x_t - x_0}{\sigma(t)} \right\|^2\right]$

$$= \frac{1}{2}\int_0^T dt\, \mathbb{E}_{P_t(x_t)}\left[\| \sigma(t) s_\theta(x_t,t) + \eta(t) \|^2\right]$$

tractable, computable

ML applications

- two main approaches, depending on choice of drift in forward process:
  - denoising diffusion probabilistic models (DDPMs), variance preserving schemes

    linear drift term $$\dot{x}(t) = -\frac{1}{2}g^2(t)x(t) + g(t)\eta(t)$$

  - variance expanding schemes

    no drift term $$\dot{x}(t) = g(t)\eta(t)$$

- in both cases the transition amplitude $P_t(x|x_0)$ is known analytically and setup works

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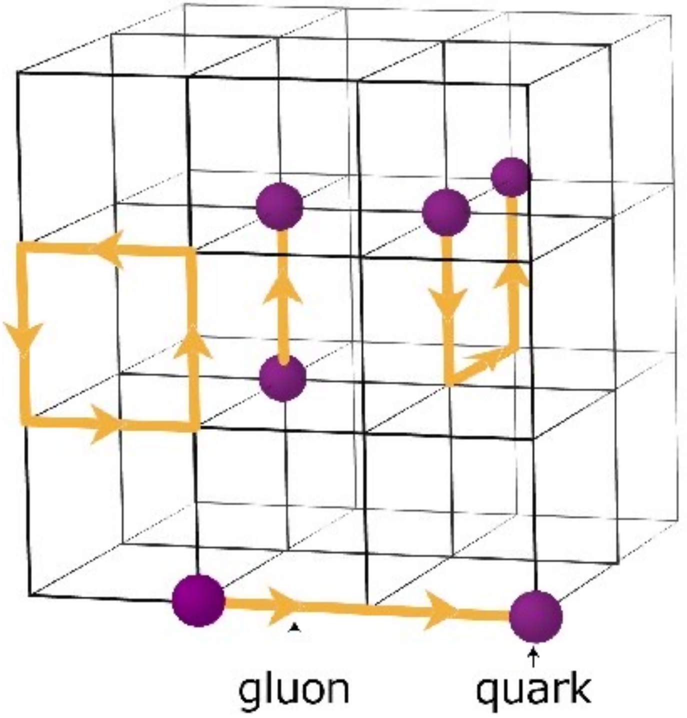
Lattice field theory



- simulate a quantum field theory on a Euclidean spacetime lattice

- generate ensembles of configurations, using importance sampling, e.g. Hybrid Monte Carlo (HMC)

- Quantum Chromodynamics (QCD) remains an outstanding challenge:
  - need four-dimensional lattices, with many degrees of freedom
  - light quarks are numerically expensive, due to inversion of Dirac operator
  - chiral symmetry is nontrivial to implement
  - need to take the continuum and infinite volume limit
  - HMC and other algorithms suffer from critical slowing down

- Lattice QCD simulations run on national HPC facilities

Lattice field theory simulations

- create sequence of configurations to estimate observables
- statistically independent, satisfy detailed balance, ergodic
- based on Boltzmann weight $P(\phi) \sim e^{-S(\phi)}$ importance sampling
- hybrid Monte Carlo (HMC) widely used
- some issues: critical slowing down near phase transitions, topological freezing in the presence of topological sectors, …
- stochastic quantisation, early proposal for LFT simulations (Parisi & Wu 1980)

Diffusion models and stochastic quantisation

- images/configurations are generated during backward process

- stochastic process with time-dependent drift and noise strength

$$\frac{\partial \phi(x,\tau)}{\partial \tau} = g^2(\tau)\nabla_\phi \log P(\phi;\tau) + g(\tau)\eta(x,\tau)$$

- write $P(\phi;\tau) = \frac{e^{-S(\phi,\tau)}}{Z}$ such that $\nabla_\phi \log P(\phi,\tau) = -\nabla_\phi S(\phi,\tau)$

- then $$\frac{\partial \phi(x,\tau)}{\partial \tau} = -g^2(\tau)\nabla_\phi S(\phi,\tau) + g(\tau)\eta(x,\tau)$$

Diffusion models and stochastic quantisation

- then $$\frac{\partial \phi(x,\tau)}{\partial \tau} = -g^2(\tau)\nabla_\phi S(\phi,\tau) + g(\tau)\eta(x,\tau)$$
- very familiar to (lattice) field theorists
- stochastic quantisation (Parisi & Wu 1980)
- path integral quantisation via a stochastic process in fictitious time $$\frac{\partial \phi(x,\tau)}{\partial \tau} = -\nabla_\phi S(\phi) + \sqrt{2}\eta(x,\tau)$$
- stationary solution of associated Fokker-Planck equation $P(\phi) \sim e^{-S(\phi)}$

Diffusion models and stochastic quantisation

$$\frac{\partial\phi(x,\tau)}{\partial\tau} = g^2(\tau)\nabla_\phi \log P(\phi;\tau) + g(\tau)\eta(x,\tau)$$

$$\frac{\partial\phi(x,\tau)}{\partial\tau} = -\nabla_\phi S(\phi) + \sqrt{2}\eta(x,\tau)$$

similarities and differences:

✓ SQ: fixed drift, determined from known action
constant noise variance (but can be generalised using kernels)
thermalisation followed by long-term evolution in equilibrium

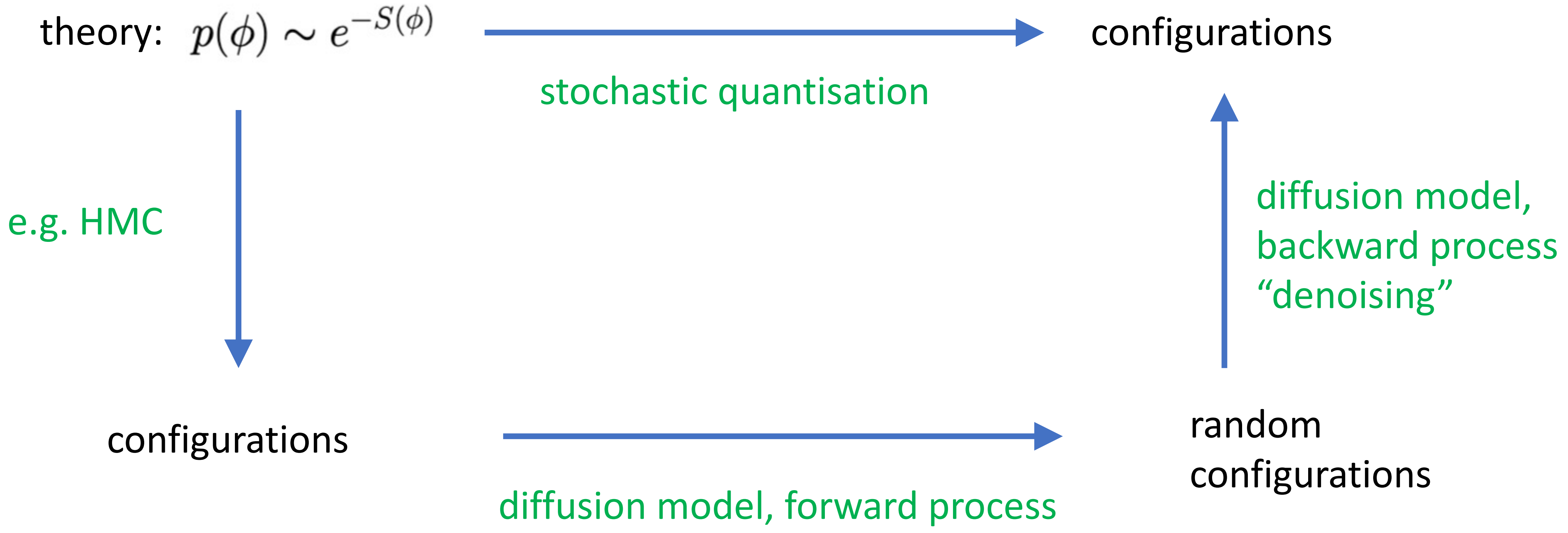
✓ DM: drift and noise variance time-dependent, learn from data
evolution between $0 \leq \tau \leq T = 1$, many short runs

side remark:
I worked on stochastic quantisation in QCD and theories with a sign problem during 2008-2015

GA and IO Stamatescu, Stochastic quantisation at finite chemical potential, JHEP 09 (2008) 018 [0807.1597 [hep-lat]]

Diffusion models and stochastic quantisation

- diffusion models as an alternative approach to stochastic quantisation



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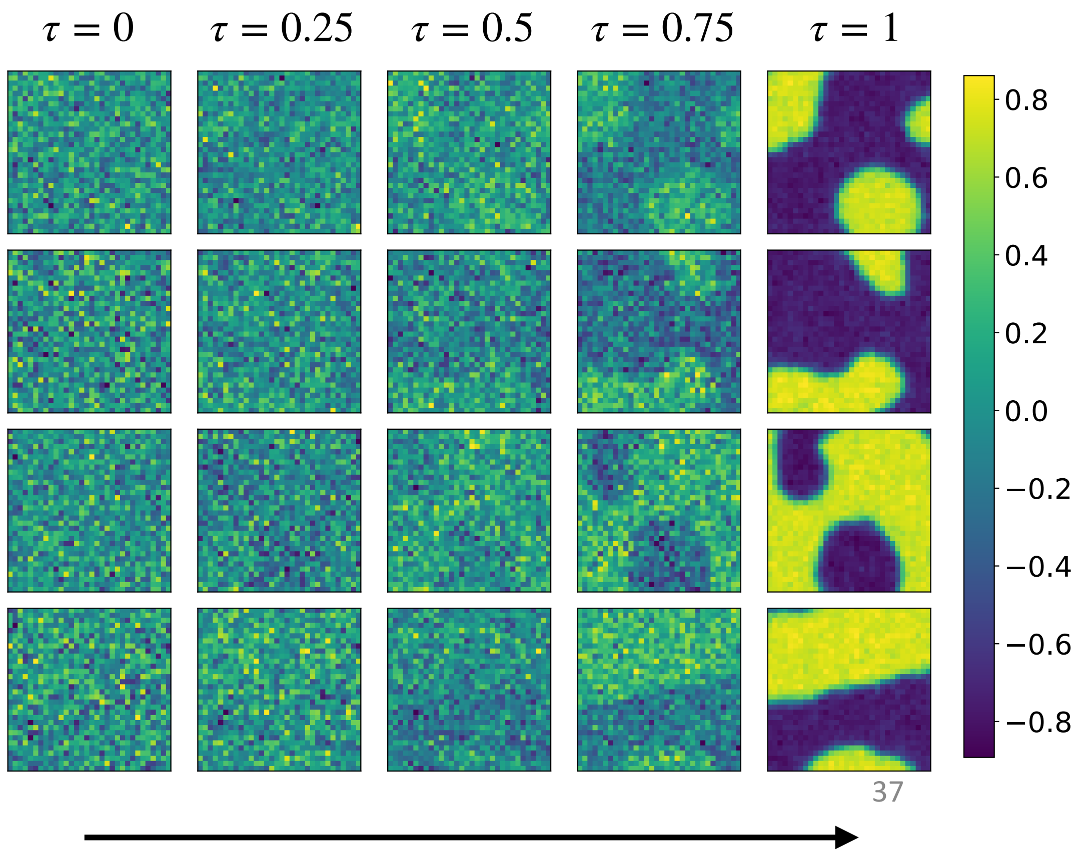

generating configurations:

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

L Wang, GA, K Zhou, JHEP 05 (2024) 060 [2309.17082 [hep-lat]]

Diffusion models for LFT

- in “real-world” applications the target or data distribution is not known analytically
- only samples are available for learning or training
- in physics applications, we usually know the theory and and hence the distribution
- this allows for use of physical intuition in designing diffusion models
- physics-conditioned DMs for lattice gauge theory [2502.05504 [hep-lat]]
- inclusion of accept/reject step to make algorithm exact [2502.05504 [hep-lat]]

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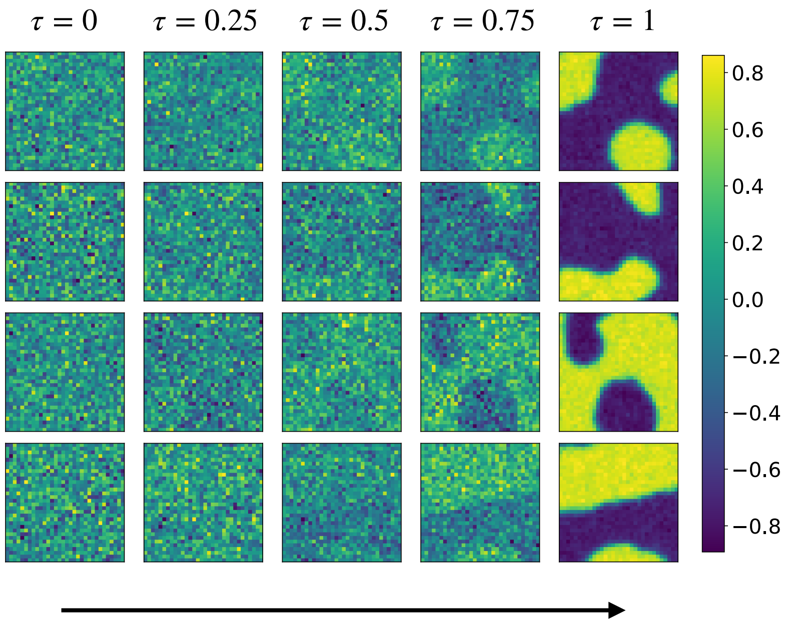
Diffusion models



ok, so it seems to work: many questions

- correlations: how are they destroyed and rebuilt?
- usually attention is on two-point function or variance
- but higher n-point functions contain interactions in field theory
- essential for applications in field theory, correlations = interactions
- focus on moments and cumulants

discuss forward and backward process in more detail

GA, **Diaa Habibi**, L Wang, K Zhou [2410.21212 [hep-lat]]

Diffusion models in more detail

- forward process $\dot{x}(t) = K(x(t), t) + g(t)\eta(t)$ $0 \leq t \leq T$

noise profile $g(t) = \sigma^{t/T}$

- backward process

$$x'(\tau) = -K(x(\tau), T - \tau) + g^2(T - \tau)\partial_x \log P(x, T - \tau) + g(T - \tau)\eta(\tau)$$

score

$\tau = T - t$

two main schemes

- variance-expanding (VE): no drift $K(x, t) = 0$
- variance-preserving (VP) or denoising diffusion probabilistic models (DDPMs):

linear drift $K(x(t), t) = -\frac{1}{2}k(t)x(t)$

assume first moment vanishes

$$x_0 \to x_0 - \mathbb{E}_{P_0}[x_0]$$

Solve forward process

- forward process $\dot{x}(t) = K(x(t),t) + g(t)\eta(t)$ $\quad K(x(t),t) = -\frac{1}{2}k(t)x(t)$
- initial data from target ensemble $x_0 \sim P_0(x_0)$
- solution $x(t) = x_0 f(t,0) + \int_0^t ds\, f(t,s)g(s)\eta(s)$ $\quad f(t,s) = e^{-\frac{1}{2}\int_s^t ds'\, k(s')}$
- second moment/cumulant/variance $\kappa_2(t) = \mu_2(t) = \mu_2(0)f^2(t,0) + \Xi(t)$

$$\Xi(t) = \int_0^t ds \int_0^t ds'\, f(t,s)f(t,s')g(s)g(s')\mathbb{E}_\eta[\eta(s)\eta(s')] = \int_0^t ds\, f^2(t,s)g^2(s)$$

$$f(t,s) = e^{-\frac{1}{2}\int_s^t ds'\, k(s')}$$

Higher-order moments and cumulants

- moments $\mu_n(t) = \mathbb{E}[x^n(t)]$ and cumulants $\kappa_n(t)$: straightforward algebra

$$\kappa_3(t) = \mu_3(t) = \kappa_3(0) f^3(t,0)$$

$$\mu_4(t) = \mu_4(0) f^4(t,0) + 6\mu_2(0) f^2(t,0)\Xi(t) + 3\Xi^2(t)$$

$$\kappa_4(t) = \mu_4(t) - 3\mu_2^2(t) = \left[\mu_4(0) - 3\mu_2^2(0)\right] f^4(t,0) = \kappa_4(0) f^4(t,0)$$

$$\kappa_5(t) = [\mu_5(0) - 10\mu_3(0)\mu_2(0)]\, f^5(t,0) = \kappa_5(0) f^5(t,0)$$

→ $$\kappa_{n>2}(t) = \kappa_n(0) f^n(t,0)$$

variance-expanding scheme: no drift

$$f(t,0) = 1$$

higher cumulants conserved!

$$\Xi(t) = \int_0^T ds\, f^2(t,s) g^2(s)$$

Proof to all orders

- generating functionals: average over both noise and target distributions

moments $Z[J] = \mathbb{E}[e^{J(t)x(t)}]$ cumulants $W[J] = \log Z[J]$

- noise average $$Z_\eta[J] = \mathbb{E}_\eta[e^{J(t)x(t)}] = \frac{\int D\eta\, e^{-\frac{1}{2}\int_0^t ds\,\eta^2(s) + J(t)\left[x_0 f(t,0) + \int_0^t ds\, f(t,s) g(s) \eta(s)\right]}}{\int D\eta\, e^{-\frac{1}{2}\int_0^t ds\,\eta^2(s)}}$$

- full average $$Z[J] = \mathbb{E}[e^{J(t)x(t)}] = e^{\frac{1}{2}J^2(t)\Xi(t)} \int dx_0\, P_0(x_0) e^{J(t)x_0 f(t,0)}$$

- cumulant generator $$W[J] = \log Z[J] = \frac{1}{2}J^2(t)\Xi(t) + \log \int dx_0\, P_0(x_0) e^{J(t)x_0 f(t,0)}$$

$$f(t,s) = e^{-\frac{1}{2}\int_s^t ds'\, k(s')}$$

$$\Xi(t) = \int_0^T ds\, f^2(t,s) g^2(s)$$

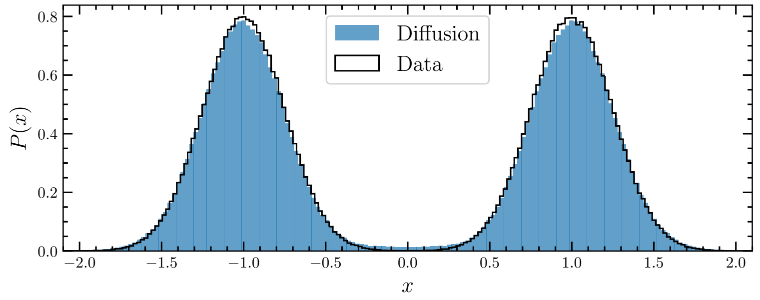
Proof to all orders: cumulants

- cumulant generator $$W[J] = \log Z[J] = \frac{1}{2} J^2(t)\Xi(t) + \log \int dx_0\, P_0(x_0) e^{J(t) x_0 f(t,0)}$$

- 2nd cumulant $$\kappa_2(t) = \frac{d^2 W[J]}{dJ(t)^2}\Big|_{J=0} = \Xi(t) + \mathbb{E}_{P_0}[x_0^2] f^2(t,0)$$ ✓

- higher-order cumulants $$\kappa_{n>2}(t) = \frac{d^n W[J]}{dJ(t)^n}\Big|_{J=0} = \frac{d^n}{dJ(t)^n} \log \mathbb{E}_{P_0}[e^{J(t) x_0 f(t,0)}]\Big|_{J=0} = \kappa_n(0) f^n(t,0)$$ ✓

Toy model: two-peak distribution

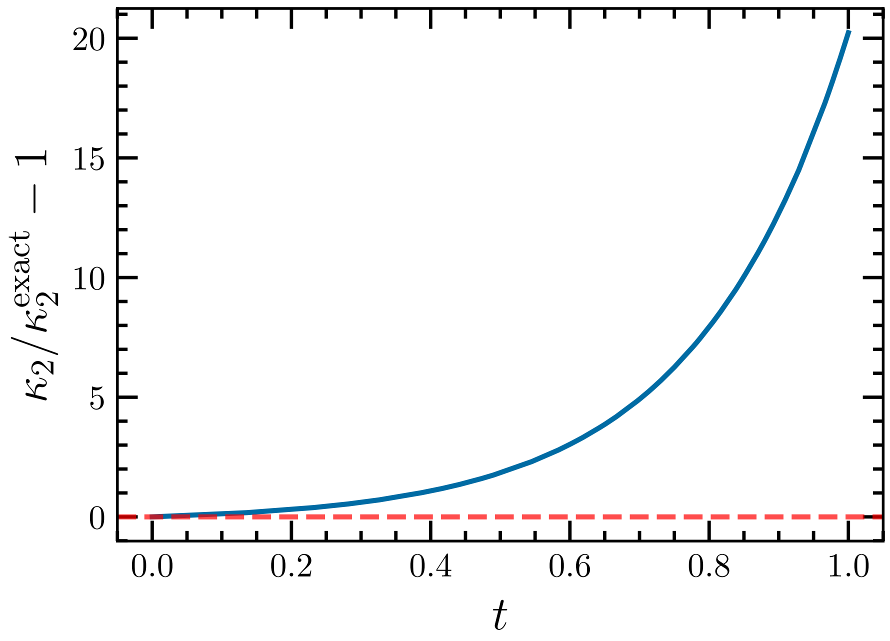


- test the predictions in simple zero-dimensional model
- sum of two Gaussians $$P_0(x) = \frac{1}{2}\left[\mathcal{N}(x;\mu_0,\sigma_0^2) + \mathcal{N}(x;-\mu_0,\sigma_0^2)\right]$$
- exactly solvable, all even cumulants non-zero, time-dependent score is known analytically
- present second moment and higher-order cumulants

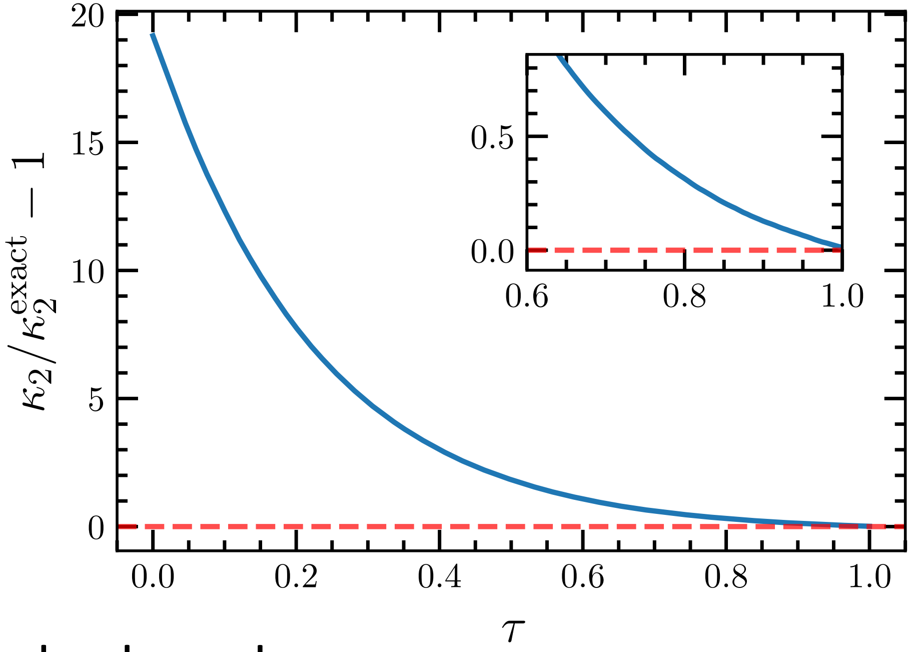
$f(t,s) = 1$

2nd cumulant without drift

- variance-expanding scheme $\kappa_2(t) = \kappa_2(0) + \Xi(t)$ $\Xi(t) = \int_0^t ds\, g^2(s) \sim \sigma^{2t/T}$



forward



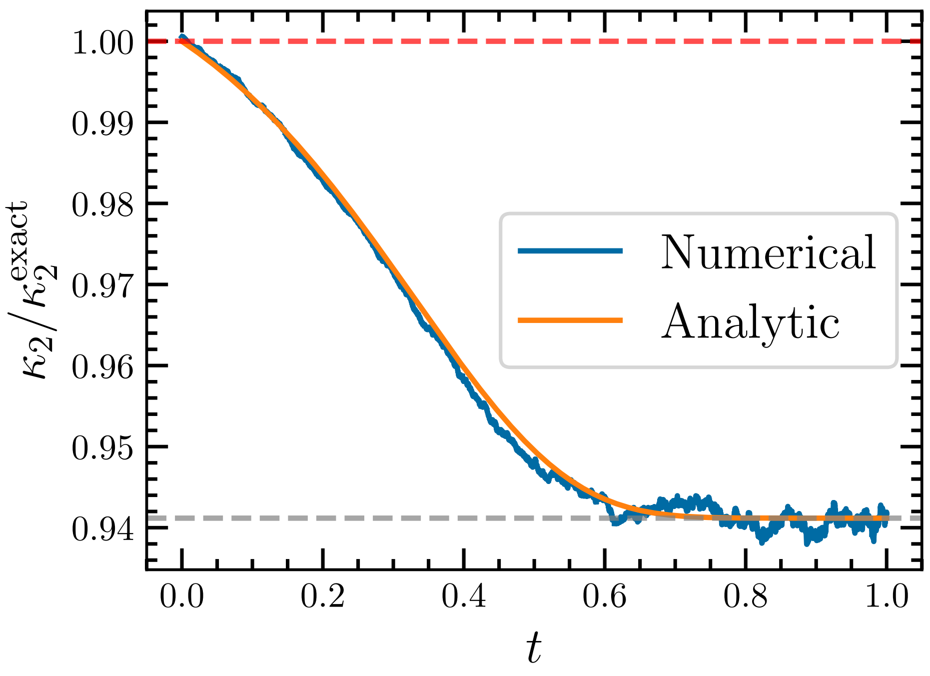
backward

2^{nd} cumulant with drift (DDPM)

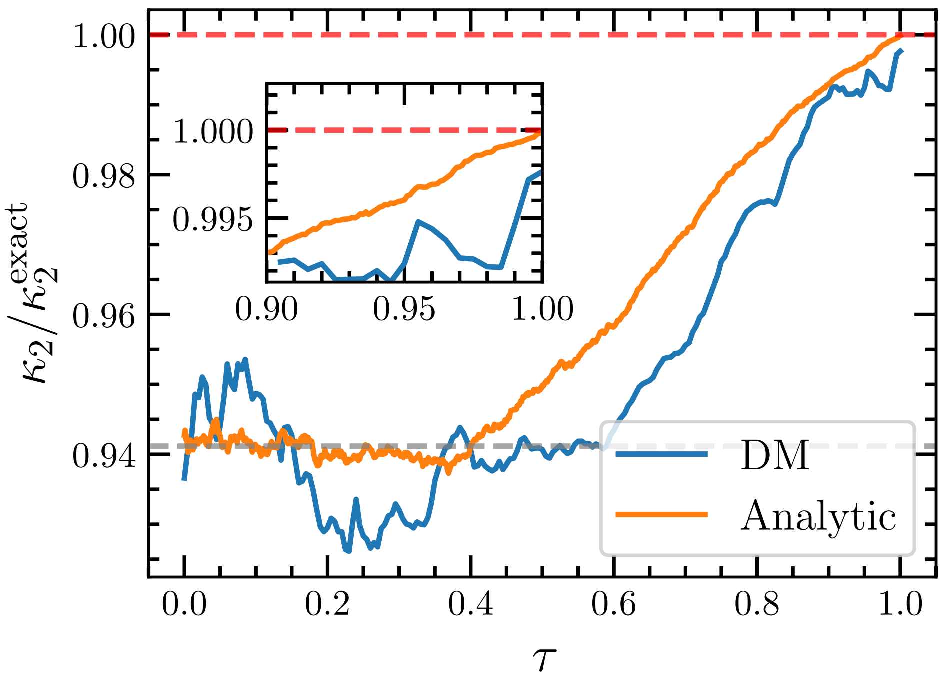
$$f(t,s) = e^{-\frac{1}{2}u(t)+\frac{1}{2}u(s)}$$

$$u(t) = \int_0^t ds\, g^2(s)$$

- variance-preserving scheme $\quad \kappa_2(t) = \mu^2(t) + \sigma^2(t) = \left(\mu_0^2 + \sigma_0^2 - 1\right) f^2(t,0) + 1$



forward



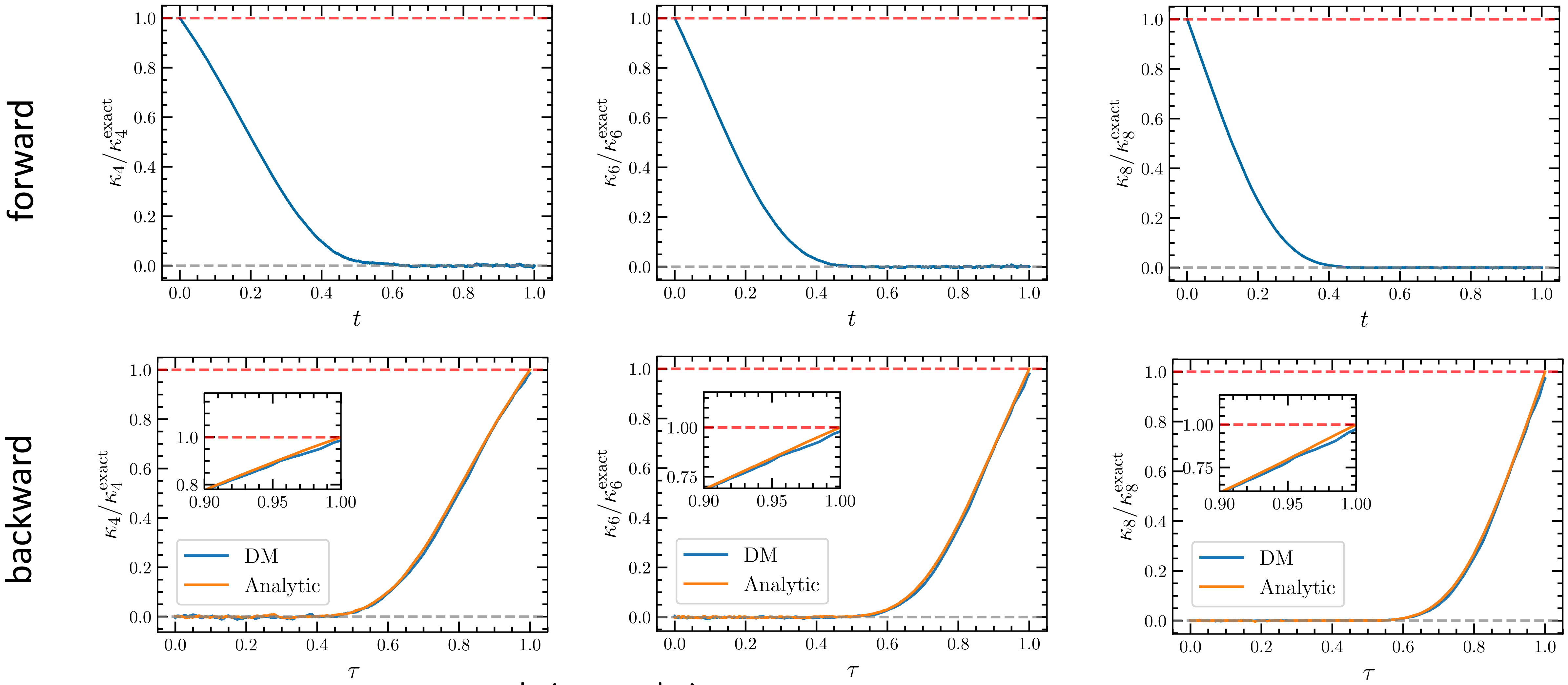
backward

analytic = analytic score

$$\kappa_{n>2}(t) = \kappa_n(0) f^n(t,0)$$

$$f(t,0) \to 0$$

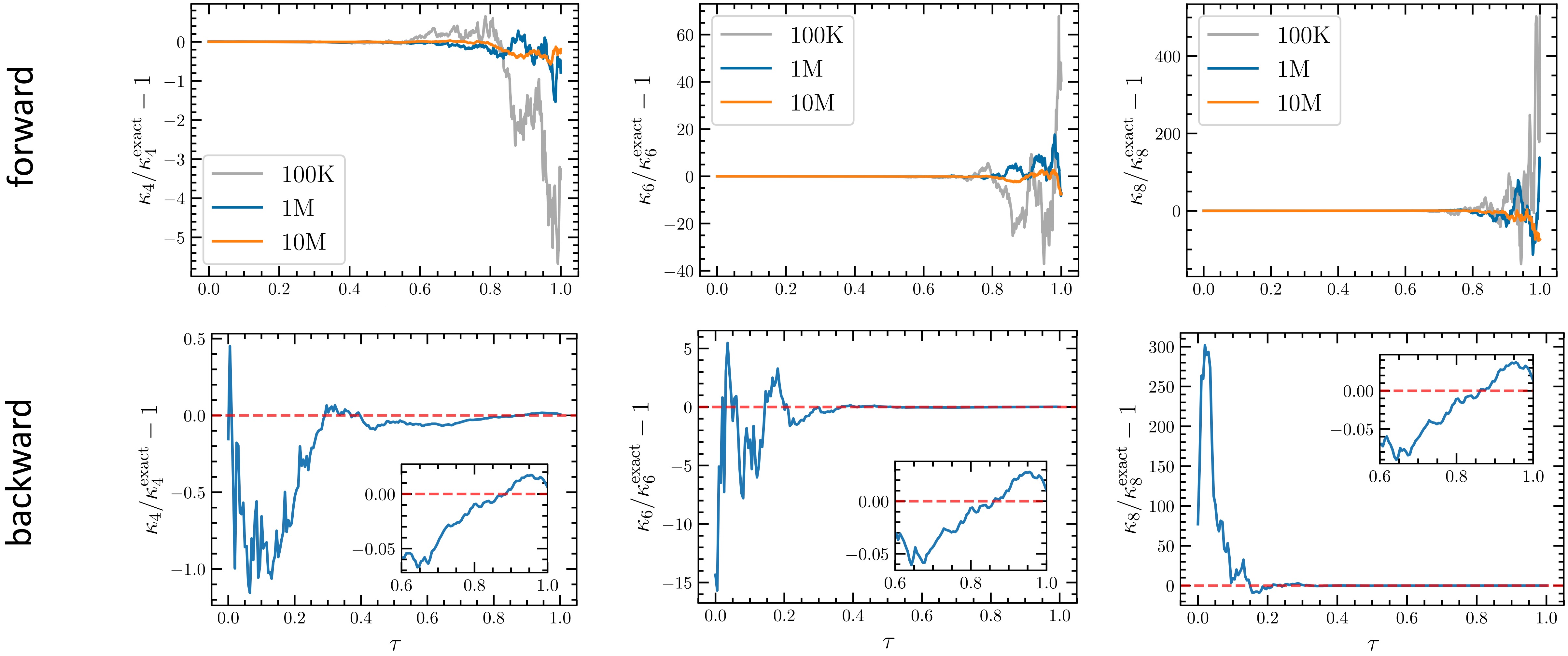
4th, 6th, 8th cumulant with drift (DDPM)



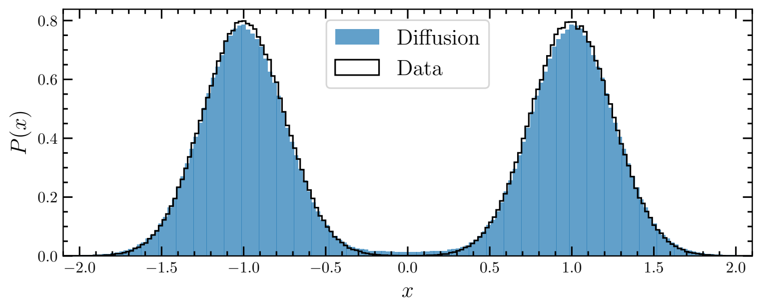
analytic = analytic score

$$\kappa_{n>2}(t) = \kappa_n(0)$$

4^{th}, 6^{th}, 8^{th} cumulant without drift



Comparison between schemes



	κ_2	κ_4	κ_6	κ_8
Exact	1.0625	−2	16	−272
Data	1.0624(5)	−2.000(2)	16.00(2)	−272.0(6)
Variance expanding	1.0692(6)	−2.001(2)	16.03(3)	−272.7(6)
Variance preserving (DDPM)	1.0609(5)	−1.976(2)	15.72(2)	−265.6(6)

expectation values at the end of the backward process

✓ variance-expanding scheme slightly outperforms variance-preserving scheme

Higher-order cumulants

- with drift (DDPM): cumulants go to zero, distribution becomes normal
- without drift (variance-expanding): higher-order cumulants are conserved,
  up to numerical cancellations, required between moments which increase in time
- initial conditions for backward process taken from normal distribution
- score has higher-order cumulants encoded: cumulants are reconstructed

Two-dimensional scalar fields

extension to scalar fields trivial: each lattice point is treated separately

- forward $\partial_t \phi(x,t) = K[\phi(x,t),t] + g(t)\eta(x,t)$
- backward $\partial_\tau \phi(x,\tau) = -K[\phi(x,\tau),T-\tau] + g^2(T-\tau)\nabla_\phi \log P(\phi,T-\tau) + g(T-\tau)\eta(x,\tau)$
- two-point function $G(x,y;t) \equiv \mathbb{E}[\phi(x,t)\phi(y,t)] = \mathbb{E}_{P_0}[\phi_0(x)\phi_0(y)]f^2(t,0) + \Xi(t)\delta(x-y)$
- moments $\mu_n(x,t) = \mathbb{E}[\phi^n(x,t)]$ independent of x

$$\Xi(t) = \int_0^T ds\, f^2(t,s) g^2(s)$$

Generating functionals

full path integral with sources

- moment generating

$$Z[J] = \mathbb{E}[e^{J(x,t)\phi(x,t)}] = e^{\frac{1}{2}J^2(x,t)\Xi(t)} \int D\phi_0\, P_0[\phi_0] e^{J(x,t)\phi_0(x) f(t,0)}$$

- cumulant generating

$$W[J] = \log Z[J] = \frac{1}{2} J^2(x,t)\Xi(t) + \log \int D\phi_0\, P_0[\phi_0] e^{J(x,t)\phi_0(x) f(t,0)}$$

- higher-order cumulants

$$\kappa_{n>2}(t) = \frac{\delta^n W[J]}{\delta J(x,t)^n}\Big|_{J=0} = \frac{\delta^n}{\delta J(x,t)^n} \log \mathbb{E}_{P_0}[e^{J(x,t)\phi_0(x) f(t,0)}]\Big|_{J=0}$$

variance preserving

$f(t,0) \rightarrow 0$

variance expanding

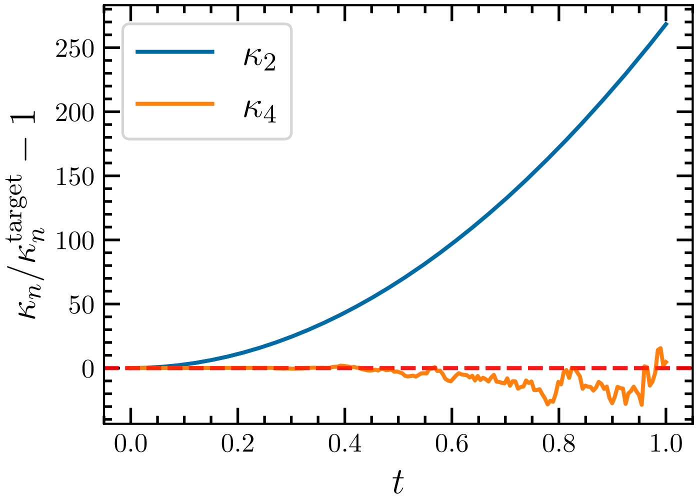
$f(t,0)) = 1$

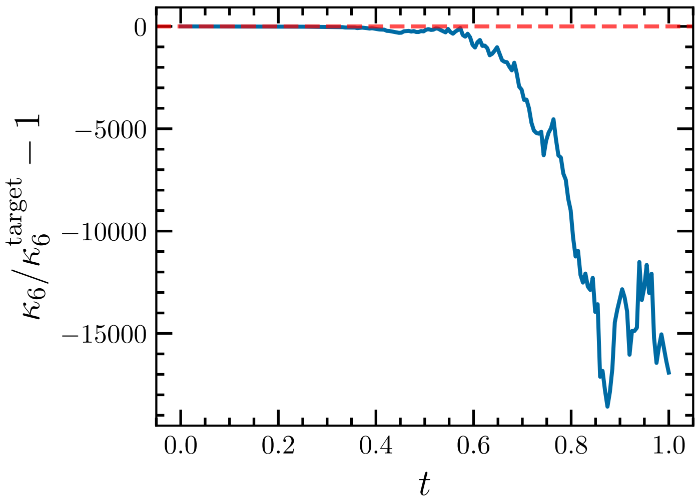
2^{nd}, 4^{th}, 6^{th} cumulant without drift

κ_2, κ_4

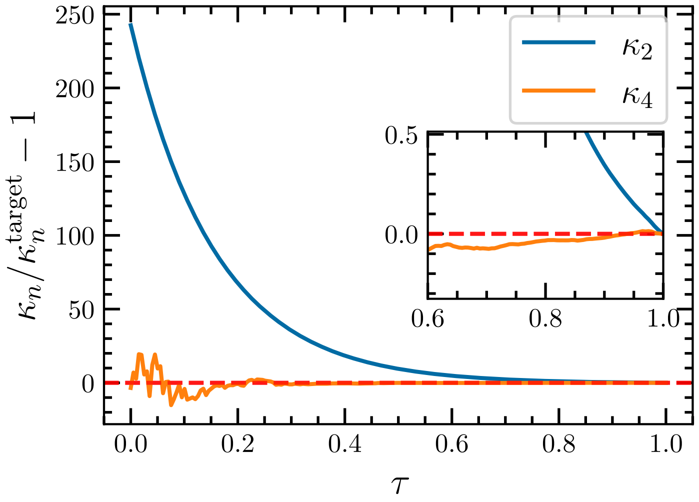
κ_6

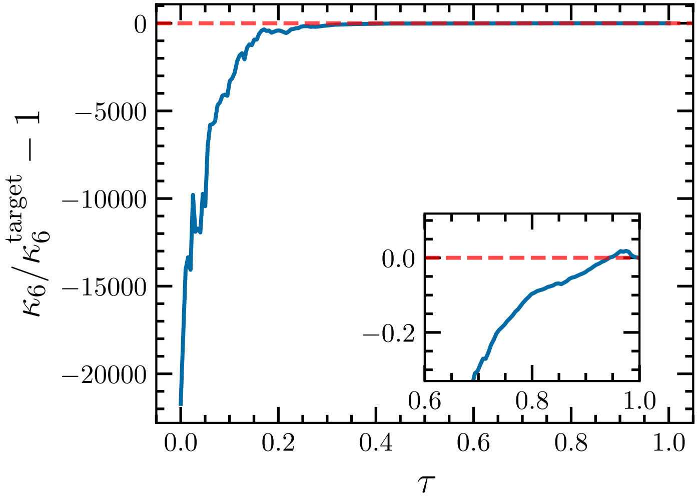
forward





backward





Comparison: trained diffusion model

	κ_2	κ_4	κ_6	κ_8
HMC (normalised)	0.39597(4)	−0.29453(6)	0.90108(28)	−5.8689(25)
Diffusion model	0.39598(4)	−0.29454(7)	0.90113(32)	−5.8694(28)

ϕ^4 theory: $32^2, \kappa = 0.4, \lambda = 0.022, 10^5$ configurations

expectation values at the end of the backward process

excellent agreement

Extensions

- U(1) gauge theory in two dimensions, exactness of algorithm, include accept/reject step
  2502.05504 [hep-lat]

- complex actions → first results at *Lattice* conference, in progress, 2412.01919 [hep-lat]

- fermionic models (Gross-Neveu model, Schwinger model) → in progress

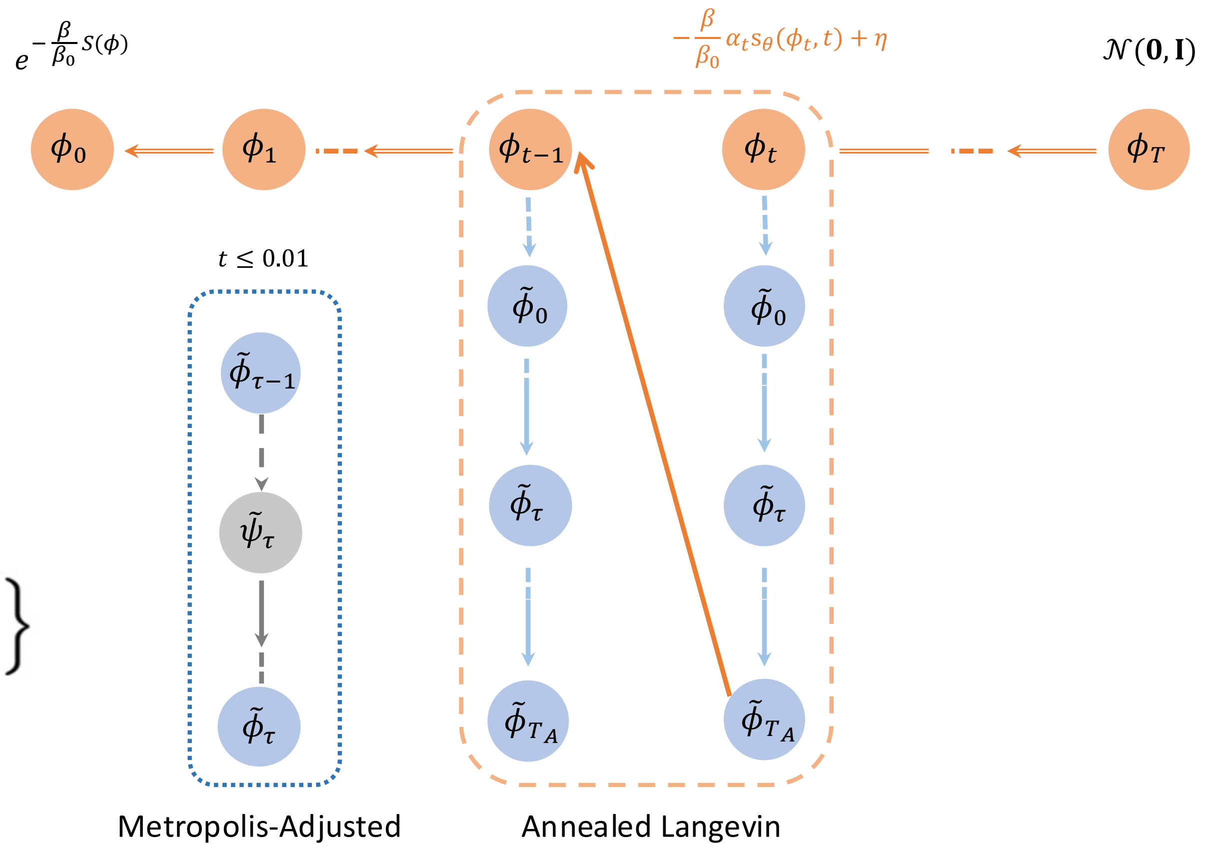
Exactness: include accept/reject step

- since physical probability distribution $p(\phi)$ is known: add corrective factor

- Metropolis-Adjusted Langevin algorithm (MALA)

- accept proposed new configuration $\tilde{\psi}_\tau$ with Metropolis-Hastings step

$$\tilde{\phi}_\tau = \begin{cases} \tilde{\psi}_\tau & \text{with probability} \min\left\{1, \frac{p(\tilde{\psi}_\tau)q(\tilde{\phi}_{\tau-1}|\tilde{\psi}_\tau)}{p(\tilde{\phi}_{\tau-1})q(\tilde{\psi}_\tau|\tilde{\phi}_{\tau-1})}\right\} \\ \tilde{\phi}_{\tau-1} & \text{otherwise} \end{cases}$$



Qianteng Zhu, GA, Wei Wang, Kai Zhou, Lingxiao Wang, 2502.05504 [hep-lat]

Summary and outlook

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

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

- diffusion models offer a new approach for ensemble generation to explore in LFT
- learn from data: requires high-quality ensembles
- closely related to stochastic quantisation
- moment- and cumulant-generating functionals

  higher n-point functions important in LFT applications
- in progress: application to theories with fermions, gauge theories, complex actions, …