Neural Samplers and PDE Solvers Based on Diffusion Processes

Julius Berner

Caltech

May 2, 2024

Overview

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- SDE-based losses for neural PDE solver

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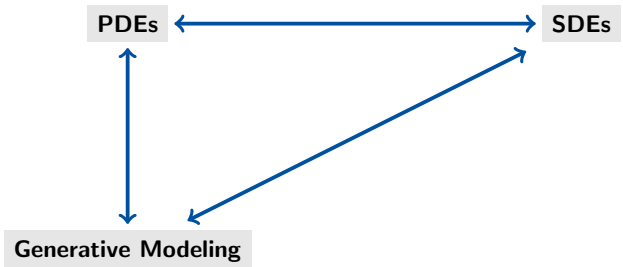
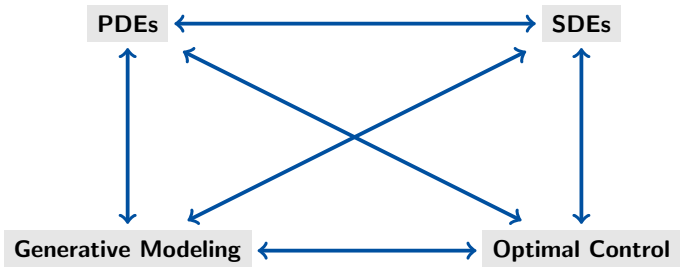
- The role of PDEs in generative modeling and sampling



Overview

- SDE-based losses for neural PDE solver
- The role of PDEs in generative modeling and sampling
- Di usion models, Schrodinger bridges, and optimal control



Neural PDE solver

Partial differential equation (PDEs)

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Fluid dynamics

Pressure

Horizontal velocity

Atmospheric and oceanic modeling

Initial geopotential height

After 1h

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Goal: Approximate the solution $u \ 2 \ V$ of a PDE

$$Lu = 0 \quad \text{on } D;$$

given by a di erential operator L on a domain D with suitable boundary conditions on $@D$.

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Diffusion models

- $D = \mathrm{R}^d \quad [0; T]$
- $Lu = @_t u + \mathrm{div}(u \;) \quad \frac{1}{2} \; ^2 \; u$
- $u(\; ; 0) = p_{\text{target}}$

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Approximate the di erential operator L by di erence quotients on a grid.

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For instance:

$$@_{x_i x_i} u(x) \quad \frac{u(x_i \quad h) \quad 2u(x_i) + u(x_i + h)}{h^2}$$

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Approximate the differential operator L by difference quotients on a grid.

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$$\partial_{x_i x_i} u(x) \approx \frac{u(x_i - h) - 2u(x_i) + u(x_i + h)}{h^2}$$

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For instance (Galerkin approx. for linear u):

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$$\sum_{i=1}^{n} c_i \langle L(v_i), v_j \rangle = \langle f, v_j \rangle$$

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high accuracies, theoretical guarantees
needs to be tailored to the PDE, slow/infeasible for fine grids or high dims.

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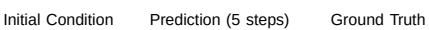
Given data (from classical solvers, simulations, or real-world observations) learn the mapping from parameters/inputs to the PDE solution.



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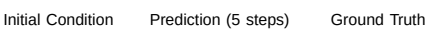

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needs (high-resolution) training data

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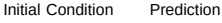

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$$\min \; \|Lu\|_k + \text{BoundaryLoss}(u)$$

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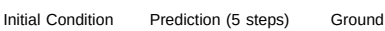

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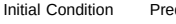

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applicable to most PDEs, unlimited data
sensitive to hyperparameters, (higher-order) derivatives needed

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SDE-based neural PDE solver

Neural PDE solvers based on stochastic representations

Stochastic representations / (un)supervised:
For certain PDEs, solutions can be written as expectations over suitable random variables
and we can regress noisy but cheap simulations.

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without derivatives, include boundary conditions without penalty terms

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Kolmogorov (backward) equations

$$@u = \frac{1}{2}\,\text{trace}\left(\quad {}^{>} r\ {}^{2}u \right)$$

"

di usion coe cient

$$\partial_t u = \tfrac{1}{2}\,\mathrm{trace}\left(\;^{\top} \nabla^2 u \right) \quad \nabla u$$

diffusion coefficient / drift coefficient

Kolmogorov (backward) equations

$$\partial_t u = \tfrac{1}{2}\,\mathrm{trace}\left(\sigma\sigma^{\top}\nabla^2 u\right) + b\cdot\nabla u, \qquad u(x,T) = \varphi(x).$$

σ: diffusion coefficient / b: drift coefficient

φ: terminal condition

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$$@u = \tfrac{1}{2}\,\text{trace}\,(\;^{>} r\;^{2}u) \;-\; r\;u; \qquad u(x;T) = \;'\;(x):$$

" " "

di usion coe cient / drift coe cient terminal condition

Method can be extended to models for drift{di usion processes (e.g., di usion models), optimal control problems (HJB equation), uid dynamics, and option pricing.

Kolmogorov (backward) equations

$$\partial_t u = \tfrac{1}{2}\,\mathrm{trace}\big(\sigma^2 \nabla^2 u\big) + \mu \cdot \nabla u, \quad u(x,T) = \psi(x).$$

diffusion coefficient / drift coefficient — terminal condition

Method can be extended to models for drift–diffusion processes (e.g., diffusion models), optimal control problems (HJB equation), fluid dynamics, and option pricing.

Stochastic representation (Itô's lemma):

$$u(x,0) = \mathbb{E}\big[\psi(X_T^x)\big], \qquad \mathbb{E}[Z] = 0;$$

noise with zero expectation

where X^x solves the stochastic differential equation (SDE)

$$dX_t^x = \mu(X_t^x)\,dt + \sigma(X_t^x)\,dB_t; \quad X_0^x = x.$$

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Euler-Maruyama scheme and Monte Carlo sampling

Discretize the SDE

$$dX_t^x = \quad (X_t^x)\,dt + \quad (X_t^x)\,dB_t\,; \quad X_0^x = x;$$

using the Euler-Maruyama scheme with step size t:

$$\hat{X}^x_{t+\ t} = \hat{X}^x_t + \quad (\hat{X}^x_t)\ \ t + \quad (\hat{X}^x_t)\,(B_{t+\ t} \quad B_t) : \qquad \underbrace{\qquad\qquad}_{N\ (0;\ t)}$$

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using the Euler-Maruyama scheme with step size Δt:

$$\hat{X}^x_{t+\Delta t} = \hat{X}^x_t + (\hat{X}^x_t)\,\Delta t + (\hat{X}^x_t)\,(B_{t+\Delta t} - B_t); \quad \underbrace{Z}_{N(0,\Delta t)}$$

- Use Monte Carlo (MC) sampling to approximate the soluti $u(x;0) = E'(X_T^x)$ with MSE $O(m^{-1} + \Delta t)$:

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- Extensions: Combining SDE-based losses with neural operators for the Navier-Stokes eq.

R. Zhang, Q. Meng, R. Zhu, Y. Wang, W. Shi, S. Zhang, Z.-M. Ma, and T.-Y. Liu. Monte Carlo neural operator for learning PDEs via probabilistic representation. arXiv:2302.05104, 2023

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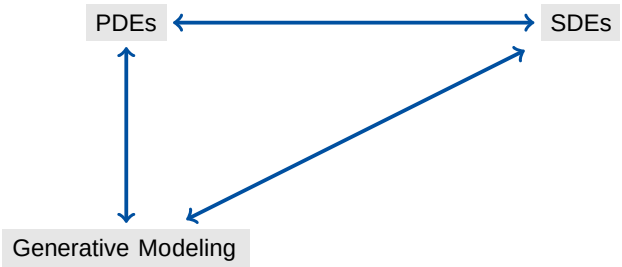
H. C. Nam, J. Berner, and A. Anandkumar. Solving Poisson equations using neural walk-on-spheres. In ICLR 2024 Workshop on AI4Di erentialEquations In Science, 2024

SDE-based generative modeling and sampling



Motivation: Selected applications of di usion models

Image & Video Generation

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Biology and Chemistry

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Sampling from high-dimensional distributions

Task: Sample from a high-dimensional distribution p_{target}.

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p_{target} can be given in the form of:

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Overview of generative models

Fig.: https://lilianweng.github.io/posts/2021-07-11-diffusion-models/

Overview of generative models

Connections: Di usion models give rise to continuous-time normalizing ows and can be viewed as hierarchical VAEs with xed encoder.

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Overview of generative models

Connections: Di usion models give rise to continuous-time normalizing ows and can be viewed as hierarchical VAEs with xed encoder.
Tasks: Flow-based models have been used for Tasks 1 & 2. We show that this is also possible for di usion models.

Fig.: https://lilianweng.github.io/posts/2021-07-11-diffusion-models/

Problems

- We cannot use denoising score matching (or other adaptations of likelihood training / forward-KL divergence):

$$E_{x \sim p_{target},\, n \sim N(0;\, \sigma^2 I)} \left[\left\| u(x + n;\, \sigma) - x \right\|^2 \right]$$

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  - Cannot use the probability flow ODE (score $\nabla \log p_X$ not available during training).

Spoiler: Take the divergence on the path space $C([0, T]; \mathbb{R}^d)$ rather than the target space $\mathbb{R}^d$, i.e., $D_{KL}(P_{X^u} \,|\, P_{\text{target}})$.

SDE-based generative modeling and sampling

Goal: Learn the drift of a SDE X such that X_T approximates a given distribution.

Connections to PDEs

Goal: $X_T \quad p_{\text{target}}$ with generative SDE

$dX_s = \quad (X_s; s)\, ds + \quad dB_s; \quad X_0 \quad p_{\text{prior}}$:

$= 0$: continuous-timenormalizing ow .

Connections to PDEs

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Fokker-Planck equation for density p_X :

$@p_X = \quad \text{div}(p_X \quad) + \frac{1}{2} \quad ^2 \quad p_X$:

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Connections to PDEs

Goal: $X_T \sim p_{\text{target}}$ with generative SDE

$$dX_s = (X_s; s)\,ds + dB_s; \quad X_0 \sim p_{\text{prior}}:$$

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Fokker-Planck equation for density p_X:

$$\partial p_X = \operatorname{div}(p_X \ ) + \tfrac{1}{2}\ ^2 p_X:$$

$= 0$: continuity equation.

Regularization: minimize energy

$$\inf \int_0^T E\ k\ (X_s; s)k^2\ ds:$$

> 0: Dynamic Schrödinger bridge.

$= 0$: Optimal W_2-transport.

J.-D. Benamou and Y. Brenier. A computational uid mechanics solution to the Monge-Kantorovich mass transfer problem. Numerische Mathematik, 84(3):375{393, 2000

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$$dX_s = v(X_s, s)\,ds + \sigma\, dB_s, \quad X_0 \sim p_{\text{prior}}:$$

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$$\partial_t \Phi = \frac{1}{2}\|\nabla\Phi\|^2 - \frac{\sigma^2}{2}\Delta\Phi:$$

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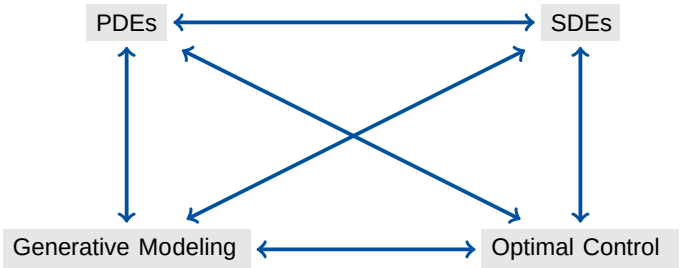
Di usion models, Schrodinger bridges, and optimal control



Framework: Time-reversals

General setting: Forward & backward transitions between prior p_{prior} and target p_{target}.

p_{prior}

p_{target}

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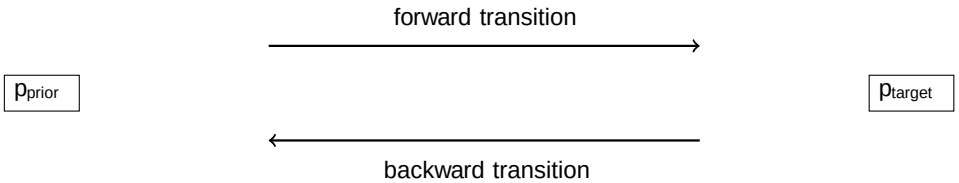

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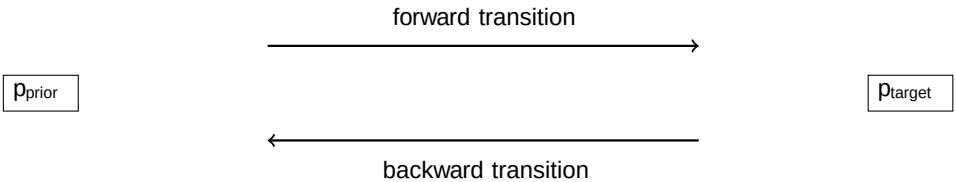

Examples: VI in latent variable models (VAEs), (optimal) transport, (Schrödinger) bridges.

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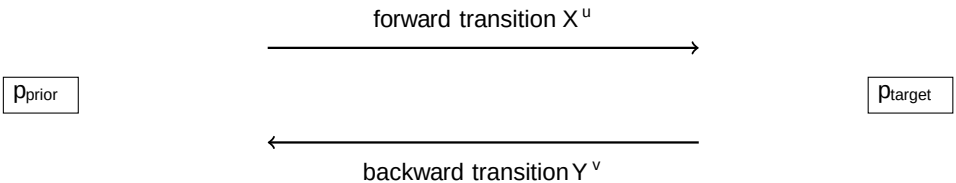

Examples: VI in latent variable models (VAEs), (optimal) transport, (Schrödinger) bridges.

Our setting: Controlled SDEs (notation: $\overleftarrow{\beta}(t) := \beta(T - t)$)

$$dX_s^u = \beta(s)u(X_s^u, s)\,ds + \sqrt{\beta(s)}\,dW_s, \quad X_0 \sim p_{\text{prior}},$$
$$dY_s^v = -\overleftarrow{\beta}(s)v(Y_s^v, s)\,ds + \sqrt{\overleftarrow{\beta}(s)}\,dW_s, \quad Y_0 \sim p_{\text{target}}.$$

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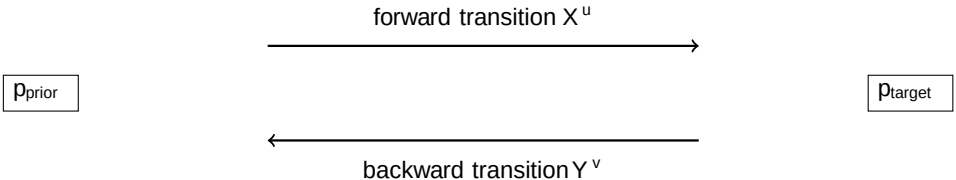

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New objective: Find u, v, such that X^u is the time-reversal $\overleftarrow{Y}^v$ of Y^v, i.e., consider the path measures P_{X^u} and $P_{\overleftarrow{Y}^v}$, a divergence D, and optimize $\min_{u,v} D(P_{X^u} \| P_{\overleftarrow{Y}^v})$.

Unifying objective

How to calculate the divergence $D(P_{X^u} \| P_{Y^v})$?

Unifying objective

How to calculate the divergence $D_{KL}(P_{X^u} \,|\, P_{Y^v})$?

- We combine the PDE perspective with tools from optimal control to derive the Log-likelihood for path measures:

$$\log \frac{dP_{X^u}}{dP_{Y^v}}(X^w) = \int_0^T (u+v)\left(w + \frac{v-u}{2}\right) + \operatorname{div}(v)\,(X_s^w; s)\,ds + \int_0^T (u+v)(X_s^w; s)\,dW_s + \log \frac{p_{\text{prior}}(X_0^w)}{p_{\text{target}}(X_T^w)}$$

zero expectation

L. Richter and J. Berner. Improved sampling via learned di usions. In International Conference on Learning Representations, 2024

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- "Likelihood Schrödinger bridge" (non-unique)

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Mode collapse: Reverse-KL divergence suffers from mode collapse.

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Log-variance divergence

- Our framework allows for other divergences: We proposed the log-variance divergence

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Gaussian mixture

Better mode coverage: Improved performance with D_{LV} (compared against D_{KL}) for PIS, DIS, DDS, and the general bridge sampler.

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Metrics: Log-norm. const., Sinkhorn distance to ground truth, normalized e ective sample size, and average stddev.

Method	Divergence	logZ (rw) #	W^2 #	ESS"	std #
CRAFT		0.012	0.020	-	0.019
PIS	KL	0.249	0.467	0.0051	1.937
	LV	0.001	0.020	0.9093	0.023
DIS	KL	0.015	0.064	0.0226	2.522
	LV	0.017	0.020	0.8660	0.004
DDS	KL	0.005	0.042	0.0737	2.161
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Bridge	KL	0.560	0.393	0.0180	0.698
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Image density and funnel distribution

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Funnel distribution (challenging benchmark for sampling methods):

$$p_{\text{target}}(x) = N(x_1; 0; 9) \prod_{i=2}^{10} N(x_i; 0; e^{x_1})$$

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DIS	KL	0.032	5.120	0.1383	5.254
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Our improved samplers based on di usion processes are competitive with state-of-the-art methods based on SMC & normalizing ows (CRAFT).

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Many-Well problem

Many-Well: typical problem in molecular dynamics with

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Problem	Method	$\log Z$ #	W^2 #	ESS "	std #
Many-Well	PIS-KL	3.567	1.699	0.0004	1.409
($d = 5; w = 5;$ $= 4$)	**PIS-LV**	**0.214**	**0.121**	**0.6744**	**0.001**
	DIS-KL	1.462	1.175	0.0012	0.431
	DIS-LV	**0.375**	**0.120**	**0.4519**	**0.001**
Many-Well	PIS-KL	0.101	**6.821**	0.8172	0.001
($d = 50; w = 5;$ $= 2$)	**PIS-LV**	**0.087**	6.823	**0.8453**	**0.000**
	DIS-KL	1.785	**6.854**	0.0225	0.009
	DIS-LV	**1.783**	6.855	**0.0227**	0.009

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Thank you for your attention!

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Github: `https://github.com/juliusberner`

Mail: `mail@jberner.info`