DeepMind

From Denoising Diffusion Models to Dynamic Transport Models

Arnaud Doucet with Yuyang Shi, Valentin De Bortoli & Andrew Campbell https://arxiv.org/abs/2303.16852

> Fondements Mathématiques de l'IA 2 Octobre 2023

Generative Modeling

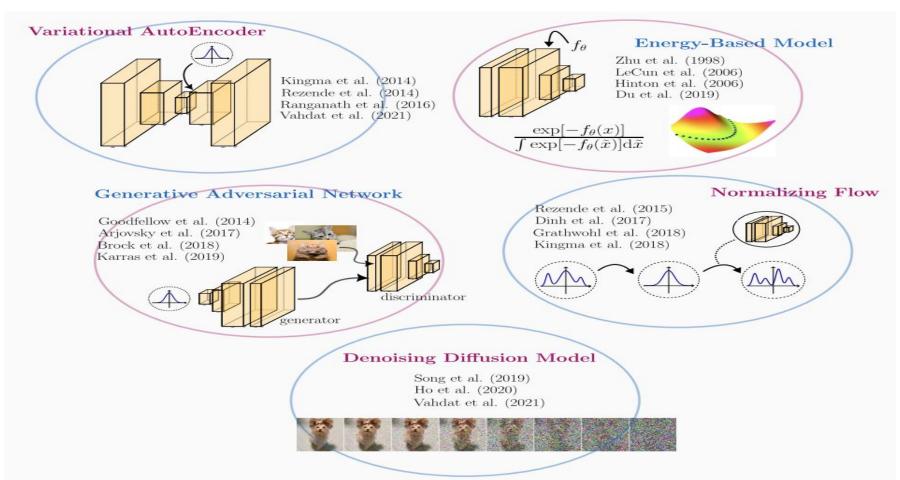
- Formulation: Given samples $(x_i)_{i=1}^N$ from distribution π , generate new samples distributed approximately from π .
- Numerous applications, e.g. data augmentation for downstream tasks (e.g. videos for self-driving cars), high-resolution nowcasting, data-driven priors for inverse problems/Bayesian inference.



From Ho et al., NeurIPS 2020



Generative Models



Denoising Diffusion Models



DALLE-3 OpenAI

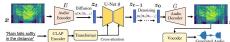




Imagen Google



Riffusion

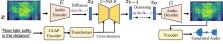


Make-an-audio





Stable Diffusion



Public

Runway

Denoising Diffusions aka Score-Based Generative Models

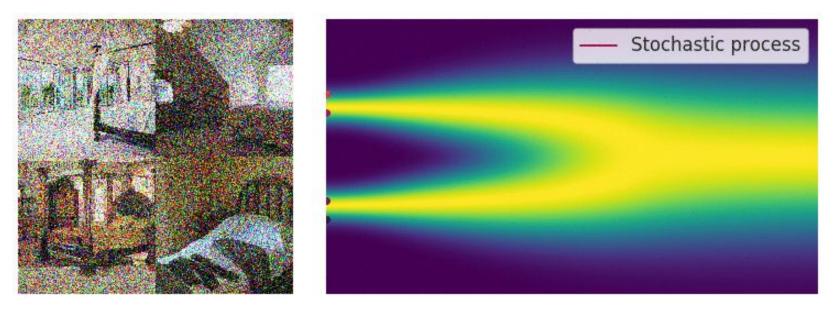
Public

- Having a hard time keeping up with the literature?
 - List of references: https://scorebasedgenerativemodeling.github.io/
- Advantages of the method:
 - State-of-the-art results Dhariwal and Nichol (2021); Karras et al. (2022).
 - High flexibility Poole et al. (2022); Rombach et al. (2022); Balaji et al. (2022); Saharia et al. (2022).
 - Theoretical analysis De Bortoli et al. (2021b); Chen et al. (2022); Pidstrigach (2022); Lee et al. (2022).
- Some drawbacks:
 - **Statistical understanding** is still limited.



Figure 1: DDM results. Image extracted from Dhariwal and Nichol (2021).

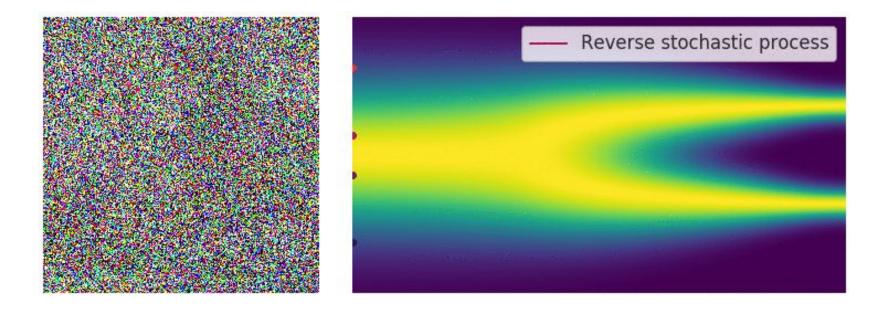
Introduction: Noising Mechanism



Bimodal distribution progressively diffused to Gaussian distribution

Song et al. 'Score-Based Generative Modeling through Stochastic Differential Equations' (2021)

Introduction: Denoising Mechanism



Discrete-Time: Noising Process

Forward diffusion process (fixed)

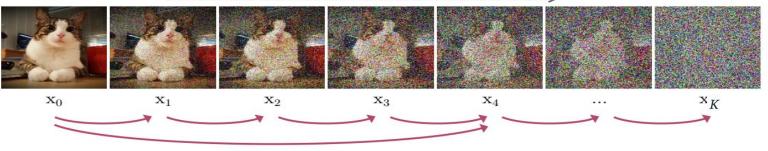


Fig. from Kreis, Gao and Vahdat, tutorial CVPR 2022.

• At sample level: Given data sample X_0 , set for k = 0, ..., K - 1

$$\mathbf{X}_{k+1} = \sqrt{1-eta}\mathbf{X}_k + \sqrt{eta}\epsilon_{k+1}, \quad \epsilon_{k+1} \sim \mathcal{N}(0,I)$$

At distribution level:

Data

$$q(x_{0:K}) = \underbrace{q_0(x_0)}_{ ext{data dist}} \quad \prod_{k=0}^{K-1} \underbrace{q(x_{k+1}|x_k)}_{\mathcal{N}(x_{k+1};\sqrt{1-eta}x_k,eta I)}$$

so $q(x_k|x_0) = \mathcal{N}(x_k; \sqrt{\alpha_k}x_0, (1-\alpha_k)I)$ with $\alpha_k = (1-\beta)^k$ (Ho et al., 2020)

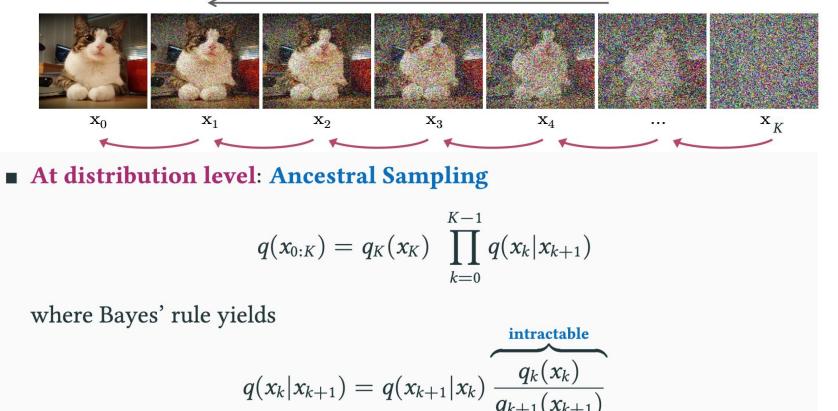


Noise

Discrete-Time: Denoising Process

Data

Reverse denoising process (generative)



• At sample level: Sample $\mathbf{X}_K \sim q_K$ then $\mathbf{X}_k \sim q(\cdot | \mathbf{X}_{k+1})$ for k = K - 1, ..., 0.

Noise

Discrete-Time: Denoising Process First step: Use the fact that

$$q(x_k|x_{k+1}) = rac{q(x_{k+1}|x_k)q_k(x_k)}{q_{k+1}(x_{k+1})} \propto q(x_{k+1}|x_k) \exp(\log q_k(x_k))$$

where $q_k \approx q_{k+1}$ and a Taylor expansion yields

$$\log q_k(x_k) \approx \log q_{k+1}(x_{k+1}) + \nabla \log q_{k+1}(x_{k+1})^{\mathrm{T}}(x_k - x_{k+1}) \quad (*)$$

Second step: Combining $q(x_{k+1}|x_k)$ and (*)

$$q(x_k|x_{k+1}) \approx q(x_{k+1}|x_k) \exp[\nabla \log q_{k+1}(x_{k+1})^{\mathrm{T}}(x_k - x_{k+1})]$$
$$\approx \mathcal{N}\left(x_k; \frac{1}{\sqrt{1-\beta}} \left(x_{k+1} + \beta \underbrace{\nabla \log q_{k+1}(x_{k+1})}_{\text{intractable}}\right), \beta I\right) \quad (\mathbf{C})$$

From Discrete-Time to Continuous-Time

• Noising diffusion: consider the diffusion $(\mathbf{X}_t)_{t \in [0,T]}$

$$\mathrm{d}\mathbf{X}_t = -\gamma \mathbf{X}_t \mathrm{d}t + \sqrt{2\gamma} \mathrm{d}\mathbf{B}_t, \quad \mathbf{X}_0 \sim q_0.$$

where $(\mathbf{B}_t)_{t \in [0,T]}$ is a Brownian motion and let $q_t = \text{Law}(\mathbf{X}_t)$. \rightsquigarrow transports **data to noise**, i.e. q_0 to $q_T \approx \mathcal{N}(0, I)$.

• **Denoising diffusion** (Anderson, 1982) : the time-reversal $(\mathbf{Y}_t)_{t \in [0,T]}$ with $\mathbf{Y}_t = \mathbf{X}_{T-t}$ verifies

$$\mathrm{d}\mathbf{Y}_t = \gamma(\mathbf{Y}_t + 2
abla \log q_{T-t}(\mathbf{Y}_t))\mathrm{d}t + \sqrt{2\gamma}\mathrm{d}\mathbf{W}_t, \quad \mathbf{Y}_0 \sim q_T,$$

where $(\mathbf{W}_t)_{t \in [0,T]}$ is a Brownian motion. \rightsquigarrow transports **noise to data**, i.e. $q_T \approx \mathcal{N}(0, I)$ to q_0 .

Problem: Score $\nabla \log q_t$ is **intractable**.

Score Approximation

"Ideal" denoising diffusion:

$$\mathrm{d}\mathbf{Y}_t = \gamma(\mathbf{Y}_t + 2
abla \log q_{T-t}(\mathbf{Y}_t))\mathrm{d}t + \sqrt{2\gamma}\mathrm{d}\mathbf{W}_t, \quad \mathbf{Y}_0 \sim q_T,$$

induces path measure \mathbb{P} .

Approximate denoising diffusion:

$$\mathrm{d}\mathbf{Y}_t = \gamma(\mathbf{Y}_t + 2s_{ heta}(T-t,\mathbf{Y}_t))\mathrm{d}t + \sqrt{2\gamma}\mathrm{d}\mathbf{W}_t, \quad \mathbf{Y}_0 \sim \mathcal{N}(0,I),$$

induces path measure \mathbb{Q}_{θ} .

• Learning the score: Minimizing $KL(\mathbb{P}||\mathbb{Q}_{\theta})$ w.r.t. θ is equivalent to minimizing

$$egin{aligned} \mathcal{L}(heta) &= \int_0^T \mathbb{E}[||s_ heta(t,\mathbf{X}_t) -
abla \log q_t(\mathbf{X}_t)||^2] \mathrm{d}t \ &= \int_0^T \mathbb{E}[||s_ heta(t,\mathbf{X}_t) -
abla \log q_{t|0}(\mathbf{X}_t|\mathbf{X}_0)||^2] \mathrm{d}t + C. \end{aligned}$$



What's the score?

Tweedie's formula

$$abla \log q_t(\mathbf{X}_t) = \mathbb{E}[
abla \log q_{t|0}(\mathbf{X}_t|\mathbf{X}_0)].$$

Explicit expression: Ornstein–Uhlenbeck transition

$$q_{t|0}(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\alpha_t}\mathbf{x}_0, (1-\alpha_t)I)$$

SO

$$abla \log q_t(\mathbf{X}_t) = rac{\sqrt{lpha_t} \quad \overbrace{\mathbb{E}[\mathbf{X}_0 | \mathbf{X}_t]}^{\text{denoiser}} - \mathbf{X}_t}{1 - lpha_t}.$$

Learning the score \iff Learning a denoiser



Benefits of Continuous-Time

- **Sophisticated numerical integrators**, predictor-corrector schemes.
- Probability flow ODE (Song et al., 2021):

$$\mathrm{d}\mathbf{X}_t = -\gamma(\mathbf{X}_t + \nabla \log q_t(\mathbf{X}_t))\mathrm{d}t, \quad \mathbf{X}_0 \sim q_0$$

admits same marginals as noising diffusion; i.e. Law(\mathbf{X}_t) = q_t \rightsquigarrow transports **data to noise**, i.e. q_0 to $q_T \approx \mathcal{N}(0, I)$.

Deterministic generation: Let $\mathbf{Y}_t = \mathbf{X}_{T-t}$ then

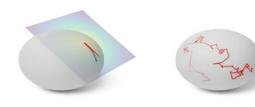
$$d\mathbf{Y}_t = \gamma(\mathbf{Y}_t + \nabla \log q_{T-t}(\mathbf{Y}_t))dt, \quad \mathbf{Y}_0 \sim q_T$$

 \rightsquigarrow transports **noise to data**, i.e. q_0 to $q_T \approx \mathcal{N}(0, I)$.



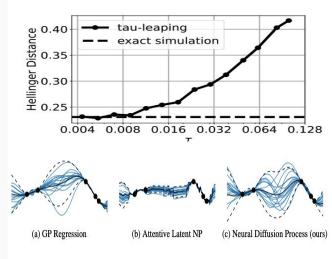
Extensions Beyond \mathbb{R}^d

- **Riemmanian manifolds** (De Bortoli et al., 2022; Huang et al., 2022): applications to protein backbone generation (Watson et al., 2022) and joint grasp and motion optimization (Urain et al., 2022).
- **Discrete state-space** (Campbell et al., 2022): allows to exploit fast samplers from chemical physics.
- **Simplex** (Benton et al., 2022; Richemond et al., 2022): application to compositional data.
- **Function spaces** (Dutordoir et al., 2022; Kerrigan et al., 2022)



(a) A single step of a (b) Many steps yield an ap-Geodesic Random Walk.

proximate trajectory.



Dutortoir et al., "Neural Diffusion Processes"



Public

Trans-dimensional generative modeling via jump diffusions

- Data of varying dimension: molecules with varying number of atoms, videos with varying number of frames; i.e. π lives on $\bigcup_{n=1}^{n_{\max}} \mathbb{R}^n$.
- **Difficulties**: Training *n*_{max} models expensive and conditional generation would require predicting *n* given observations.
- **Jump Diffusion**: We diffuse and kill components until one remains and is Gaussian, time-reversal adds components.

Algorithm 1: Sampling the Generative Process

$$\begin{split} t \leftarrow T \\ \mathbf{X} \sim p_{\text{ref}}(\mathbf{X}) &= \mathbb{I}\{n = 1\} \mathcal{N}(\mathbf{x}; 0, I_d) \\ \text{while } t > 0 \text{ do} \\ \text{if } u < \overleftarrow{\lambda}_t^{\theta}(\mathbf{X}) \delta t \text{ with } u \sim \mathcal{U}(0, 1) \text{ then} \\ \text{Sample } \mathbf{x}^{\text{add}}, i \sim A_t^{\theta}(\mathbf{x}^{\text{add}}, i | \mathbf{X}) \\ \mathbf{X} \leftarrow \text{ins}(\mathbf{X}, \mathbf{x}^{\text{add}}, i) \\ \text{end} \\ \mathbf{x} \leftarrow \mathbf{x} - \overleftarrow{\mathbf{b}}_t^{\theta}(\mathbf{X}) \delta t + g_t \sqrt{\delta t} \epsilon \text{ with } \epsilon \sim \mathcal{N}(0, I_{nd}) \\ \mathbf{X} \leftarrow (n, \mathbf{x}), t \leftarrow t - \delta t \\ \text{end} \\ \end{split}$$

Visualization of the jump-diffusion backward generative process on molecules.

Campbell et al., arXiv:2305.16261, NeurIPS 2023



Public

Beyond Diffusion Models: Transport using ODEs

Diffusion models: noising "transports" π_0 to $\pi_T \approx \mathcal{N}(0, I)$, denoising does the reverse.

Limitations: What if *T* is not large enough? What if you want π_T be non-normal? Do we need diffusions at all?

ODE Transport Models: stochastic interpolants (Albergo and Vanden-Eijnden, 2023), flow matching (Lipman et al., 2023), rectified flow (Liu et al., 2023): Let X₀ ~ π₀ then X₁ = Φ(X₀) ~ π₁ where Φ is built using an ODE whose drift is learned using samples of π₀, π₁.

Connections to **Optimal Transport** unclear.

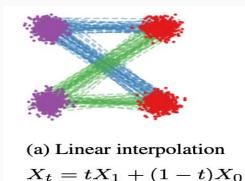


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Transport using ODEs: Flow Matching

Path Measure: Let $\mathbf{X}_0 \sim \pi_0$, $\mathbf{X}_1 \sim \pi_1$ and

$$\mathbf{X}_t = (1-t)\mathbf{X}_0 + t\mathbf{X}_1 \sim \pi_t$$

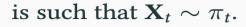




Liu et al.., "Flow Straight and Fast", ICLR 2023

• Useless Transport ODE: As $X_t = X_0 + t(X_1 - X_0)$ then the ODE

$$rac{\mathrm{d} \mathbf{X}_t}{\mathrm{d} t} = \mathbf{X}_1 - \mathbf{X}_0 = rac{\mathbf{X}_1 - \mathbf{X}_t}{1-t}, \qquad \mathbf{X}_0 \sim \pi_0, \ \mathbf{X}_1 \sim \pi_1,$$



Transport using ODEs: Flow Matching

Useful Transport ODE: The ODE with drift

$$v(t, \mathbf{x}) = \mathbb{E}[\mathbf{X}_1 - \mathbf{X}_0 | \mathbf{X}_t = \mathbf{x}] = \frac{\mathbb{E}[\mathbf{X}_1 | \mathbf{X}_t = \mathbf{x}] - \mathbf{x}}{1 - t}$$

is such that $\mathbf{X}_t \sim \pi_t!$

• Learning the Drift: $v_{\theta^{\star}}(t, \mathbf{x}) = (\mathbf{x}_{\theta}^{*}(t, \mathbf{x}) - \mathbf{x})/(1 - t) \approx v(t, \mathbf{x})$ by minimizing

$$\mathcal{L}(heta) = \mathbb{E}[||\mathbf{x}_{ heta}(t,\mathbf{X}_t) - \mathbf{X}_1||^2]$$



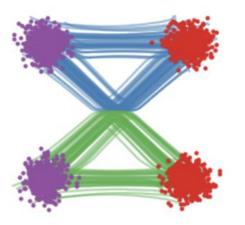
Liu et al.., "Flow Straight and Fast", ICLR 2023

> (a) Linear interpolation $X_t = tX_1 + (1-t)X_0$

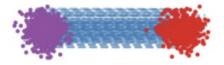
(b) Rectified flow Z_t induced by (X_0, X_1)

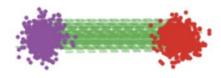


Transport using ODEs: Flow Matching



Non-optimal transport





Optimal transport

Liu et al.., "Flow Straight and Fast", ICLR 2023



Optimal Transport

The unpaired problem:

- Learn a **coupling** Π between π_0 and π_1 .
- Learn to **sample** from this coupling Π .

Optimal transport (Monge-Kantorovich formulation)

Find a **coupling** Π^* such that

$$\Pi^{\star} = \operatorname{argmin} \{ \int_{\mathbb{R}^d imes \mathbb{R}^d} ||x - y||^2 \mathrm{d} \Pi(x, y) \;, \; \Pi_0 = \pi_0, \; \Pi_1 = \pi_1 \}.$$

• Sample from π_0 and then $\Pi_{1|0}^*$ to get a sample from π_1 .

Limitations of the formulation:

- Can be unstable.
- Even for discrete data, very costly.

- Solution? Entropic regularization!
 - H is the entropy.
 σ² > 0 a regularization parameter.

Schrödinger Bridge: From Static to Dynamic

Static formulation

$$\Pi^{\star} = \operatorname{argmin} \{ \int_{\mathbb{R}^{d} \times \mathbb{R}^{d}} \frac{1}{2} \| x - y \|^{2} d\Pi(x, y) - \sigma^{2} \mathbf{H}(\Pi) , \Pi_{0} = \pi_{0}, \ \Pi_{1} = \pi_{1} \}.$$

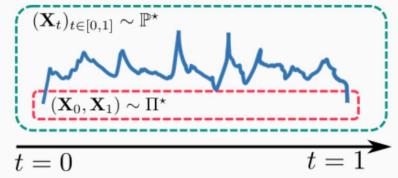
Dynamic formulation

Find \mathbb{P}^* a **path measure** such that

$$\mathbb{P}^{\star} = \operatorname{argmin}\{\operatorname{KL}(\mathbb{P}|\mathbb{Q}) \ , \mathbb{P}_0 = \pi_0, \ \mathbb{P}_1 = \pi_1 \}.$$

▶ \mathbb{Q} is associated with $(\sigma \mathbf{B}_t)_{t \in [0,1]}$, with $(\mathbf{B}_t)_{t \in [0,1]}$ a **Brownian motion**.

• From dynamic to static: $\mathbb{P}_{0,1}^{\star} = \Pi^{\star}$.





Schrödinger Bridge Problem

Dynamic formulation (Schrödinger Bridge)

Find \mathbb{P}^* a **path measure** such that

$$\mathbb{P}^{\star} = \operatorname{argmin}\{\operatorname{KL}(\mathbb{P}|\mathbb{Q}) , \mathbb{P}_0 = \pi_0, \ \mathbb{P}_1 = \pi_1 \}.$$

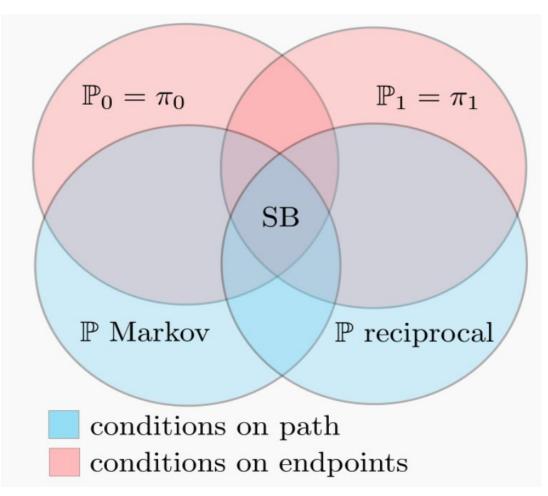
▶ \mathbb{Q} is associated with $(\sigma \mathbf{B}_t)_{t \in [0,1]}$, with $(\mathbf{B}_t)_{t \in [0,1]}$ a **Brownian motion**.

• \mathbb{P}^* is called the **Schrödinger Bridge**.

- Can be thought of:
 - Closest path measure to Q such that,
 - the marginal constraints are respected.
- Given Π^* , how to sample from \mathbb{P}^* ?
 - Sample $(\mathbf{X}_0, \mathbf{X}_1) \sim \Pi^{\star}$.
 - ► Sample $\mathbf{X}_t = (1 t)\mathbf{X}_0 + t\mathbf{X}_1 + \sigma\sqrt{t(1 t)}\mathbf{Z}, \mathbf{Z} \sim N(0, \text{Id}).$
 - " \mathbb{P}^* is in the **reciprocal class** of \mathbb{Q} " (see Thieullen (1993)).

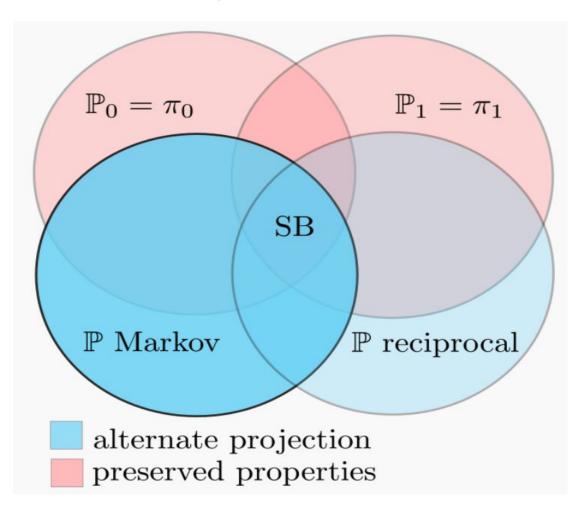


Schrödinger Bridge



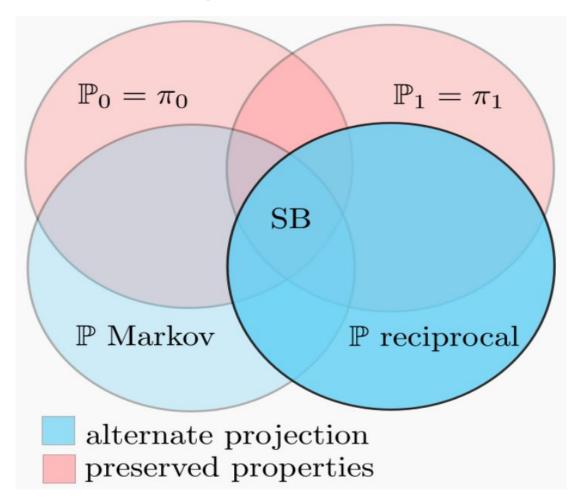


Iterative Markovian Fitting



6

Iterative Markovian Fitting





Markovian Projection

Start with \mathbb{P} non-Markov, $(\mathbf{X}_t)_{t \in [0,1]} \sim \mathbb{P}$,

$$d\mathbf{X}_t = b(t, \mathbf{X}_t, \mathbf{X}_1) dt + \sigma d\mathbf{B}_t$$

future dependency

with $b(t, \mathbf{X}_t, \mathbf{X}_1)$ linear in \mathbf{X}_1 .

Markovian projection = remove the dependency on the future.

Preserve marginals for free!

In practice:

- Loss function $||x_{\theta}(t, \mathbf{X}_t) \mathbf{X}_1||^2$.
- At equilibrium: $x_{\theta}(t, x_t) = \mathbb{E}[\mathbf{X}_1 | \mathbf{X}_t].$
- $\blacktriangleright d\mathbf{X}_t = b(t, \mathbf{X}_t, x_{\theta}(t, \mathbf{X}_t))dt + \sigma d\mathbf{B}_t.$
- The special case of flow matching (Lipman et al., 2022):

$$\blacktriangleright (\mathbf{X}_0, \mathbf{X}_1) \sim \pi_0 \otimes \pi_1, \mathbf{X}_t = t\mathbf{X}_1 + (1-t)\mathbf{X}_0.$$

 $\blacktriangleright d\mathbf{X}_t = (\mathbf{X}_1 - \mathbf{X}_t)/(1-t)dt.$

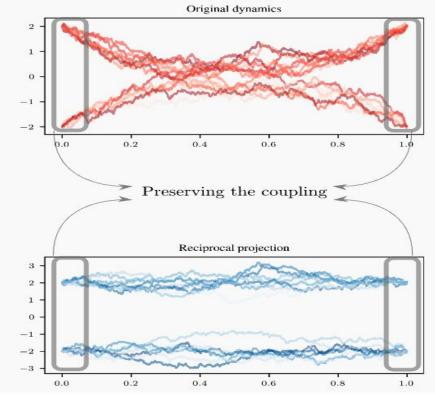


Reciprocal Projection

• \mathbb{P} in the **reciprocal class** if for $(\mathbf{X}_t)_{t \in [0,1]} \sim \mathbb{P}$:

$$\blacktriangleright \mathbf{X}_t = (1-t)\mathbf{X}_0 + t\mathbf{X}_1 + \sigma\sqrt{t(1-t)}\mathbf{Z}, \mathbf{Z} \sim \mathbf{N}(0, \mathrm{Id}).$$

- Same bridge as the Brownian bridge".
- Projection on the reciprocal class (no neural network involved).

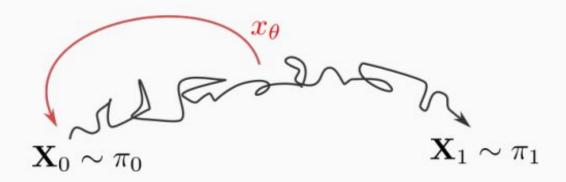




Diffusion Schrödinger Bridge Matching

- Diffusion Schrödinger Bridge matching:
 - Alternating projections on Markov measures and reciprocal class.
 - two networks: x_{θ} (backward), x_{ϕ} (forward).
- DSBM iteration 1: training of the backward
 - Sample from $(\mathbf{X}_0, \mathbf{X}_1) \sim \pi_0 \otimes \pi_1$.
 - ► Sample $\mathbf{X}_t = (1 t)\mathbf{X}_0 + t\mathbf{X}_1 + \sigma\sqrt{t(1 t)}\mathbf{Z}, \mathbf{Z} \sim N(0, \text{Id}).$

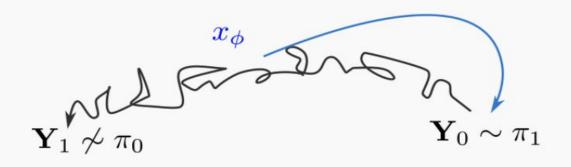
$$\blacktriangleright \text{ Loss } \|x_{\theta}(1-t,\mathbf{X}_t)-\mathbf{X}_0\|^2.$$





Diffusion Schrödinger Bridge Matching

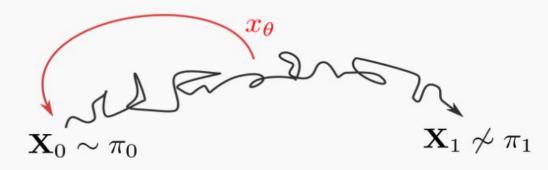
- Diffusion Schrödinger Bridge matching:
 - Alternating projections on Markov measures and reciprocal class.
 - two networks: x_{θ} (backward), x_{ϕ} (forward).
- DSBM iteration 2: training of the forward
 - Sample from $\mathbf{Y}_0 \sim \pi_1$, $d\mathbf{Y}_t = (x_\theta(t, \mathbf{Y}_t) \mathbf{Y}_t)/(1-t)dt + \sigma d\mathbf{B}_t$.
 - Keep $(\mathbf{Y}_0, \mathbf{Y}_1)$.
 - ► Sample $\mathbf{Y}_t = (1 t)\mathbf{Y}_0 + t\mathbf{Y}_1 + \sigma\sqrt{t(1 t)}\mathbf{Z}, \mathbf{Z} \sim N(0, \text{Id}).$
 - Loss $||x_{\phi}(1-t, \mathbf{Y}_t) \mathbf{Y}_0||^2$.





Diffusion Schrödinger Bridge Matching

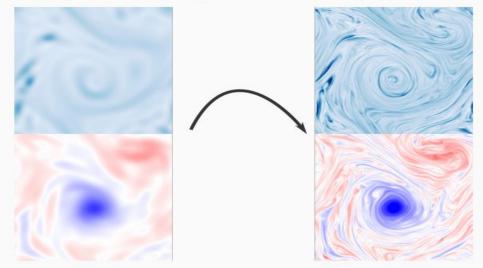
- Diffusion Schrödinger Bridge matching:
 - Alternating projections on Markov measures and reciprocal class.
 - two networks: x_{θ} (backward), x_{ϕ} (forward).
- DSBM iteration 3: training of the backward
 - Sample from $\mathbf{X}_0 \sim \pi_0$, $d\mathbf{X}_t = (x_{\phi}(t, \mathbf{X}_t) \mathbf{X}_t)/(1-t)dt + \sigma d\mathbf{B}_t$.
 - Keep $(\mathbf{X}_0, \mathbf{X}_1)$.
 - ► Sample $\mathbf{X}_t = (1 t)\mathbf{X}_0 + t\mathbf{X}_1 + \sigma\sqrt{t(1 t)}\mathbf{Z}, \mathbf{Z} \sim N(0, \text{Id}).$
 - $larget Loss ||x_{\theta}(1-t,\mathbf{X}_t)-\mathbf{X}_0||^2.$





Climate Science Experiment

- Dataset Bischoff and Deck (2023):
 - Supersaturation and vorticity field.
 - Low resolution $(64 \times 64 \times 2)$ to high resolution $(512 \times 512 \times 2)$.
- **Goal**: superresolution (downscaling)



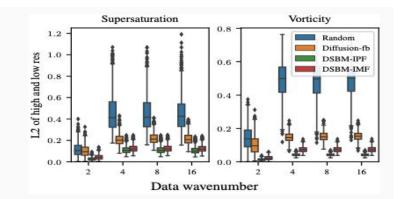
Unpaired problem

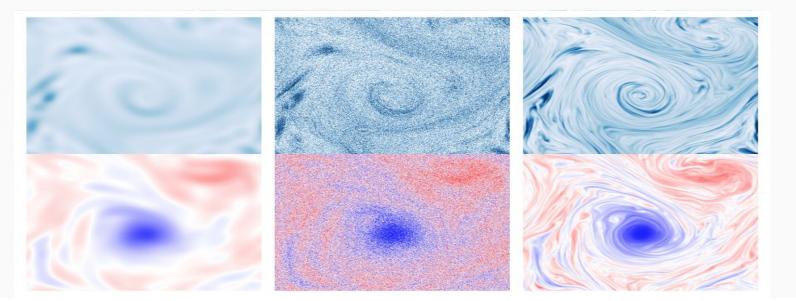
 for downscaling tasks, paired datasets of high and low resolution climate *simulations* do not truly exist, due to deterministic chaos and the feedback of small scale motion to large scales;



Climate Science Experiment

- Same setting as Bischoff and Deck (2023).
- Super resolution task.
- Quality measure (frequency histogram).
- Similarity measure (ℓ_2 with upscaling).





Discussion

 Denoising Diffusion Models provide state-of-the-art performance in numerous domains: image, audio, proteins etc.

Dynamic transport alternatives are now also available.

 A lot of open problems at the interface of control, generative modeling, transport and sampling.

