Stochastic Interpolants

Based on "Stochastic Interpolations: A Unifying Framework for Flows and Diffusions" (2025) by Albergo, Boffi, Vanden-Eijnden

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Contents

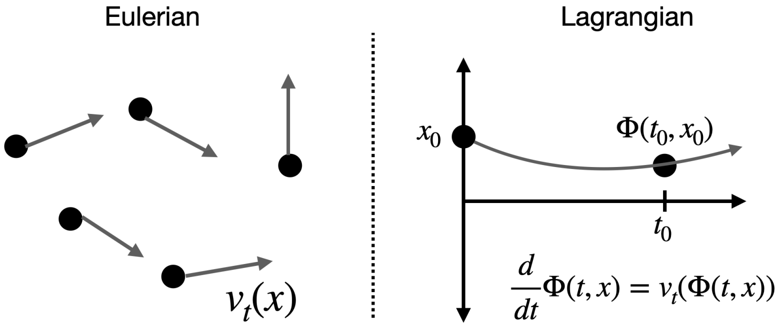
Review from Last Week

Continuity Equation

Continuity Equation

Let $(v_t, t \geq 0)$ be a time dependent velocity field, then

$$\partial_t \rho_t + \nabla \cdot (v_t \rho_t) = 0.$$



Fokker Planck

Fokker Planck PDE

Let $(b_t, t \geq 0)$ be smoothly varying vector valued function, and recall $\Delta = \sum_{j=1}^{d} \partial_{x_j}^2$, then

$$\partial_t \rho_t + \nabla \cdot (b_t \rho_t) = \varepsilon \Delta \rho_t.$$

Observe that this writes as

$$\partial_t \rho_t + \nabla \cdot \left(\left(b_t^{FP} - \varepsilon \nabla \log \rho_t \right) \rho_t \right) = 0.$$

It holds that $X_t \sim \rho_t$, where

$$dX_t = b_t^{FP}(X_t)dt + \sqrt{2\varepsilon} dB_t, \quad X_0 \sim \rho_0$$

Stochastic Interpolation

Stochastic Interpolation [ABVE25]

Let ρ_0, ρ_1 be two probability densities, a stochastic interpolant between ρ_0 and ρ_1 is the stochastic process defined as

$$x_t := I(t, x_0, x_1) + \gamma(t)z, \quad t \in [0, 1],$$

where

- $I(0, x_0, x_1) = x_0$, $I(1, x_0, x_1) = x_1$, $\gamma(0) = \gamma(1) = 0$,
- $(x_0, x_1) \sim \nu$ that is coupling of ρ_0, ρ_1
- $z \sim N(0, \mathrm{Id})$ is independent of (x_0, x_1)

Stochastic Interpolation

Specific choices of $x_t = \alpha(t)x_0 + \beta(t)x_1 + \gamma(t)z$

Stochastic Interpolant		$\alpha(t)$	$\beta(t)$	$\gamma(t)$
Arbitrary ρ_0 (two-sided)	linear	$1-t$	t	$\sqrt{at(1-t)}$
	trig	$\cos\frac{\pi}{2}t$	$\sin\frac{\pi}{2}t$	$\sqrt{at(1-t)}$
	enc-dec	$\cos^2(\pi t)1_{[0,\frac{1}{2})}(t)$	$\cos^2(\pi t)1_{(\frac{1}{2},1]}(t)$	$\sin^2(\pi t)$
Gaussian ρ_0 (one-sided)	linear	$1-t$	t	0
	trig	$\cos\frac{\pi}{2}t$	$\sin\frac{\pi}{2}t$	0
	SBDM (VP)	$\sqrt{1-t^2}$	t	0
Mirror		0	1	$\sqrt{at(1-t)}$

Figure: [ABVE25, Table 1], note “one-sided” setting includes diffusion models

Stochastic Interpolation

Given $x_t = I(t, x_0, x_1) + \gamma(t)z$, let $x_t \sim \rho_t$

Transport Equation

The PDE $\partial_t \rho_t + \nabla \cdot (b_t \rho_t) = 0$ is satisfied with

$$b(t, x) = \mathrm{E}[\dot{x}_t | x_t = x] = \mathrm{E}[\partial_t I(t, x_0, x_1) + \dot{\gamma}(t)z | x_t = x]$$

Fokker Planck Equation

The PDE $\partial_t \rho_t + \nabla \cdot (b_t^{FP} \rho_t) = \varepsilon \Delta \rho_t$ is satisfied with

$$s(t, x) = \nabla \log \rho(t, x) = -\gamma^{-1}(t)\mathrm{E}[z | x_t = x]$$
$$b^{FP} = b + \varepsilon s$$

Choice of Coupling

What's the point of choosing $(X_0, X_1) \sim \nu$? Another **design choice**

- Diffusion models [SSDK+20], one marginal is noise and assume independent
- [AGB+24] analyzes theoretical and practical advantages of ν selection
- Another meaningful coupling is Schrödinger bridge [SDBCD23, DBKMD24]

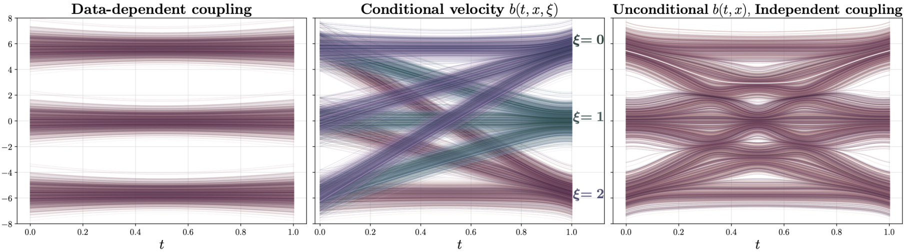


Figure: [AGB+24, Figure 3], Gaussian mixture with 3 modes, different couplings of endpoints

Deterministic vs Stochastic Trajectories

Two Approaches to Generative Modeling

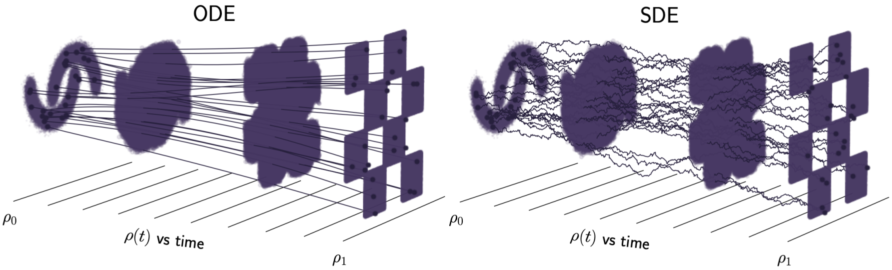


Figure: ODE vs SDE Generative Modeling [ABVE25, Figure 1]

An Algorithmic Question: Which one is "better"?

Generative Modeling (ODE)

Deterministic transport (ODE), estimate $b(t,x)$ such that

$$\partial_t \rho_t + \nabla \cdot (b_t \rho_t) = 0 \tag{1}$$

[ABVE25, Lemma 21], Endpoint Error

Consider $\rho(t,x), \hat{\rho}(t,x)$ satisfying (1) with $b(t,x), \hat{b}(t,x)$, respectively. Then

$$\mathrm{KL}(\rho(1)|\hat{\rho}(1)) = \int_0^1 \int_{\mathbb{R}^d} \left\langle \nabla \log \hat{\rho}(t,x) - \nabla \log \rho(t,x), \hat{b}(t,x) - b(t,x) \right\rangle \rho(t,x) dx dt$$

- Key ideas in proof are: (1) interpolation in time, (2) integration by parts :)
- **Problem:** error not controlled entirely by $(\hat{b} - b)$

Generative Modeling (ODE)

As $\rho(0,\cdot) = \hat{\rho}(0,\cdot)$,

$$\mathrm{KL}(\rho(1)|\hat{\rho(1)}) = \mathrm{KL}(\rho(1)|\hat{\rho(1)}) - \mathrm{KL}(\rho(0)|\hat{\rho(0)}) = \int_0^1 \frac{d}{dt}\mathrm{KL}(\rho(t)|\hat{\rho}(t))dt.$$

Recall that $\mathrm{KL}(p|q) = \mathrm{E}_p[\log(dp/dq)]$, so

$$\begin{aligned}\frac{d}{dt}\mathrm{KL}(\rho(t)|\hat{\rho}(t)) &= \frac{d}{dt}\int_{\mathbb{R}^d} \log\left(\frac{\rho(t,x)}{\hat{\rho}(t,x)}\right)\rho(t,x)dx \\ &= \int_{\mathbb{R}^d} \partial_t\left(\log\left(\frac{\rho(t,x)}{\hat{\rho}(t,x)}\right)\right)\rho(t,x) + \left(\log\left(\frac{\rho(t,x)}{\hat{\rho}(t,x)}\right)\right)\partial_t\rho(t,x)dx\end{aligned}$$

Recall that $\partial_t\rho(t) = -\nabla\cdot(\rho(t)b(t))$, so integration by parts gives

$$\int_{\mathbb{R}^d}\left(\log\left(\frac{\rho(t,x)}{\hat{\rho}(t,x)}\right)\right)\partial_t\rho(t,x)dx = \int_{\mathbb{R}^d}\langle\nabla\log\rho(t) - \nabla\log\hat{\rho}(t), b(t)\rangle\rho(t,x)dx$$

Generative Modeling (ODE)

For the other term,

$$
\begin{aligned}
&\int_0^1 \int_{\mathbb{R}^d} \big(\partial_t \log \rho(t) - \partial_t \log \hat{\rho}(t)\big)\, \rho(t,x) dx dt \\
&= \int_0^1 \int_{\mathbb{R}^d} \left(\frac{\partial_t \rho(t)}{\rho(t)} - \frac{\partial_t \hat{\rho}(t)}{\hat{\rho}(t)} \right) \rho(t,x) dx dt \\
&= \int_0^1 \int_{\mathbb{R}^d} \left(-\frac{\nabla \cdot (\rho(t) b(t))}{\rho(t)} + \frac{\nabla \cdot (\hat{\rho}(t)\hat{b}(t))}{\hat{\rho}(t)} \right) \rho(t,x) dx dt \\
&= \int_0^1 \left(-\int_{\mathbb{R}^d} \left(\nabla \cdot (b(t) - \hat{b}(t)) \right) \rho(t,x) dx \right) dt \\
&+ \int_0^1 \int_{\mathbb{R}^d} \left(-\langle \nabla \log \rho(t), b(t) \rangle + \langle \nabla \log \hat{\rho}(t), \hat{b}(t) \rangle \right) \rho(t,x) dx dt.
\end{aligned}
$$

Generative Modeling (ODE)

Using integration by parts,

$$-\int_{\mathbb{R}^d} \left(\nabla \cdot (b(t) - \hat{b}(t))\right) \rho(t,x)dx = \int_{\mathbb{R}^d} \langle b(t) - \hat{b}(t), \nabla \log \rho(t) \rangle \rho(t,x)dx,$$

so previous slide becomes

$$\begin{aligned}
&\int_0^1 \int_{\mathbb{R}^d} \left(\partial_t \log \rho(t) - \partial_t \log \hat{\rho}(t)\right) \rho(t,x)dxdt \\
&= \int_0^1 \int_{\mathbb{R}^d} \langle b(t) - \hat{b}(t), \nabla \log \rho(t) \rangle \rho(t,x)dxdt \\
&+ \int_0^1 \int_{\mathbb{R}^d} \left(-\langle \nabla \log \rho(t), b(t) \rangle + \langle \nabla \log \hat{\rho}(t), \hat{b}(t) \rangle\right) \rho(t,x)dxdt \\
&= \int_0^1 \langle \hat{b}(t), \nabla \log \hat{\rho}(t) - \nabla \log \rho(t) \rangle \rho(t,x)dxdt.
\end{aligned}$$

Combing terms gives final solution!

Generative Modeling (SDE)

Fokker-Planck, estimate $b(t, x)$ such that

$$\partial_t \rho_t + \nabla \cdot (b_t^{FP} \rho_t) = \varepsilon \Delta \rho_t \tag{2}$$

[ABVE25, Lemma 22], Endpoint Error

Consider $\rho(t, x), \hat{\rho}(t, x)$ satisfying (2) with $b^{FP}(t, x), \hat{b}^{FP}(t, x)$, respectively. Then

$$\mathrm{KL}(\rho(1)|\hat{\rho}(1)) \leq \frac{1}{4\varepsilon} \int_0^1 \int_{\mathbb{R}^d} \left| b^{FP}(t, x) - \hat{b}^{FP}(t, x) \right|^2 \rho(t, x) dx dt$$

Generative Modeling (SDE)

Recall that

$$\partial_t \rho_t + \nabla \cdot (b_t^{FP} \rho_t) = \varepsilon \Delta \rho_t \Leftrightarrow \partial_t \rho_t + \nabla \cdot \left(\left(b_t^{FP} - \varepsilon \nabla \log \rho_t \right) \rho_t \right) = 0$$

From previous calculation,

$$\begin{aligned}
&\mathrm{KL}(\rho(1)|\hat{\rho}(1)) \\
&= \int_0^1 \int_{\mathbb{R}^d} \left\langle \nabla \log \hat{\rho}_t - \nabla \log \rho_t, \hat{b}_t^{FP} - \varepsilon \nabla \log \hat{\rho}_t - b_t^{FP} + \varepsilon \nabla \log \rho_t \right\rangle \rho_t(x) dx dt \\
&= \int_0^1 \int_{\mathbb{R}^d} \left(\langle \nabla \log \hat{\rho}_t - \nabla \log \rho_t, \hat{b}_t^{FP} - b_t^{FP} \rangle - \varepsilon \|\nabla \log \hat{\rho}_t - \nabla \log \rho_t\|^2 \right) \rho_t(x) dx dt \\
&\leq \frac{1}{2\eta^2} \int_0^1 \left\| \hat{b}_t^{FP} - b_t^{FP} \right\|^2 \rho_t(x) dx dt + \left(\frac{\eta^2}{2} - \varepsilon \right) \int_0^1 \|\nabla \log \hat{\rho}_t - \nabla \log \rho_t\|^2 \rho_t(x) dx dt,
\end{aligned}$$

using Young's inequality. Then set $\eta = \sqrt{2\varepsilon}$.

Generating Modeling, [ABVE25, Remark 25]

[ABVE25, Theorem 23], Endpoint Error

In the setting as above, let $\hat{b}$ be estimate for b, then

$$\mathrm{KL}(\rho(1)|\hat{\rho}(1)) \leq \frac{1}{2\varepsilon}\left(\text{Error in } \hat{b}\right) + \frac{\varepsilon}{2}\left(\text{Error in } \hat{s}\right)$$

Suppose we have estimates $\hat{b}, \hat{s}$

- Deterministic generative model

$$\frac{d}{dt}\hat{X}_t = \hat{b}(t, \hat{X}_t)$$

- Stochastic generative model

$$d\hat{X}_t = \left(\hat{b}(t, \hat{X}_t) + \varepsilon\hat{s}(t, \hat{X}_t)\right)dt + \sqrt{2\varepsilon}dW_t$$

- The optimal value of ε is

$$\varepsilon^* = \left(\frac{(\text{Error in } \hat{b})}{(\text{Error in } \hat{s})}\right)^{1/2}$$

Generative Modeling

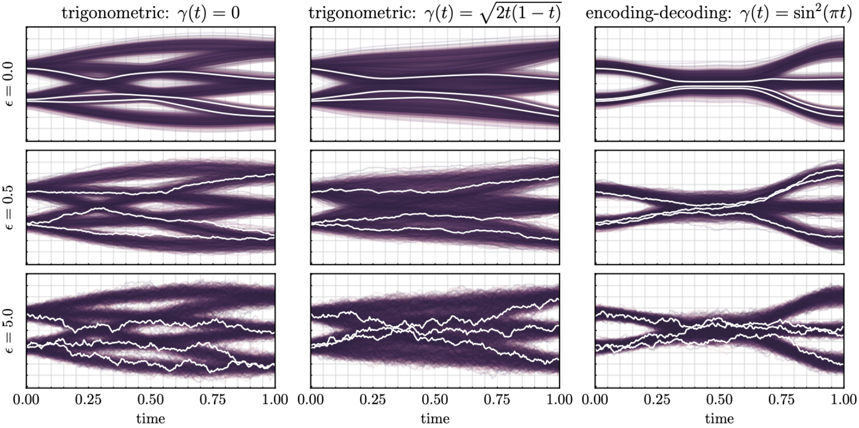


Figure: [ABVE25, Figure 5], Role of ε on sample trajectories

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