Rectified Flow and Stochastic Interpolation

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Transport Mapping Problem

- Generative modelling and data transfer problems can be formulated as **learning transport mapping:**
  Given empirical observations of two distributions π_0, π_1 on $\mathbb{R}^d$, find a transport map $T : \mathbb{R}^d \to \mathbb{R}^d$, which, in the infinite data limit, gives $Z_1 := T(Z_0) \sim \pi_1$ when $Z_0 \sim \pi_0$.
- Examples:
  - Latent variable $\xrightarrow{\text{implicit map}}$ samples: GAN, VAE.
  - Prior distribution $\xrightarrow{\text{explicit flow}}$ samples: Flow and diffusion models.
  - We will focus on the **explicit flow-based** approach.

Simplest Path: Straight Path

- Suppose we have some $X_0 \sim \pi_0$ (prior), $X_1 \sim \pi_1$ (samples) and seek to transform X_0 to X_1.
- A key issue with neural-ODEs is their complex trajectories.
- However, since the paths can be **arbitrary**, a natural idea is to simply connect randomly sampled pairs (X_0, X_1) with **straight lines**, as demonstrated in the Figure 1 and 2.

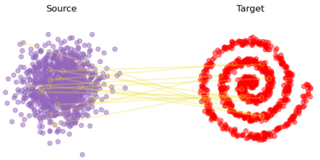

Figure 1: 2D View.

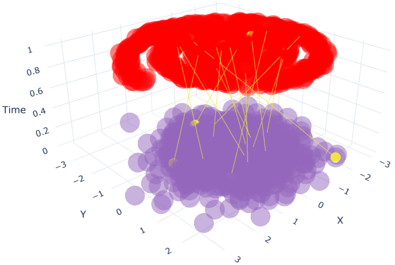

Figure 2: 3D View.

Problems with Straight Paths

- Despite its simplicity, this approach encounters several fundamental challenges:
  - **Crossings:** The interpolation paths X_t can intersect, resulting in non-unique solutions, as shown in Figure 3.
  - **Non-causality:** These paths are constructed using both starting and ending points, but in reality, the true endpoints (samples) are unknown during inference.

Figure 3: Linear Interpolation. Source: [Liu et al., 2022]

Intuition of Rectified Flow

- In rectified flow, data points evolve according to an ODE:

$$\mathrm{d}Z_t = v(Z_t, t)\,\mathrm{d}t, \qquad t \in [0, 1] \tag{1}$$

  where velocity field v is a **parameterized network**, ensuring that the ODE trajectory closely follows the **imagined** straight path.
- ODEs inherently prevent trajectory crossings: by the **Picard–Lindelöf theorem**, each starting point generates a unique path, provided v is Lipschitz continuous.
- The resulting flow can be seen as an “average” of many particles traveling along these imagined straight lines, blending their crossings into a smooth, non-crossing transformation.

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Model

- Given X_0 and X_1, we have the **non-causal** linear interpolation:

$$X_t = tX_1 + (1-t)X_0, \qquad t \in [0,1] \tag{2}$$

- The **rectified flow** induced from empirical observations (X_0, X_1) is an ODE:

$$\mathrm{d}Z_t = v(Z_t, t)\,\mathrm{d}t, \qquad t \in [0,1] \tag{3}$$

  which converts Z_0 from π_0 to Z_1 following π_1.

- $v : \mathbb{R}^d \times [0,1] \to \mathbb{R}^d$ is trained to drive the flow to follow the direction $(X_1 - X_0)$ of the linear path pointing from X_0 to X_1, by solving a least squares regression problem:

$$\min_v \int_0^1 \mathbb{E}\left[\|(X_1 - X_0) - v(X_t, t)\|^2\right] \mathrm{d}t, \qquad X_t = tX_1 + (1-t)X_0 \tag{4}$$

  which is estimated by randomly samplings pairs of (X_0, X_1) and t, and optimized using SGD.

Algorithm

- **Procedure:** $\boldsymbol{Z} = \mathrm{RectFlow}((X_0, X_1)):$
  - **Inputs:** Velocity model $v_\theta : \mathbb{R}^d \to \mathbb{R}^d$ with parameter θ.
  - **Training:** $\hat{\theta} = \arg\min_\theta \mathbb{E}\left[\left\| X_1 - X_0 - v\big(tX_1 + (1-t)X_0, t\big)\right\|^2\right]$, where $t \sim \mathrm{Uniform}([0,1])$, $(X_0, X_1) \sim \pi_0 \times \pi_1$.
  - **Sampling:** Draw (Z_0, Z_1) following $\mathrm{d}Z_t = v_{\hat{\theta}}(Z_t, t)\mathrm{d}t$ starting from $Z_0 \sim \pi_0$ (or $Z_1 \sim \pi_1$).
  - **Return:** $\boldsymbol{Z} = \{Z_t : t \in [0,1]\}$.
- **Reflow (optional):** $\boldsymbol{Z}^{k+1} = \mathrm{RectFlow}((Z_0^k, Z_1^k))$, starting from $(Z_0^0, Z_1^0) = (X_0, X_1)$, where $(X_0, X_1) \sim \pi_0 \times \pi_1$.
- **Distill (optional):** Learn a neural network $\hat{T}$ to distill the k-rectified flow, such that $Z_1^k \approx \hat{T}(Z_0^k)$.

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Flows Avoid Crossing

- A well-defined ODE yields unique solutions: **the trajectories cannot cross at any time** $t \in [0, 1]$.
- This uniqueness prevents multiple paths from passing through the same point at the same time in different directions (Figure 4).
- Think of linear interpolation X_t as "building roads" between π_0 and π_1, while rectified flow finds an **averaged** path without crossing (Figure 5).

Figure 4: Crossings.

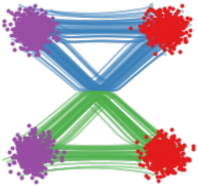

Figure 5: No Crossings.

Minimizer of Objective

Important note: in all context, a **coupling** (X_0, X_1) where $X_0 \sim \pi_0, X_1 \sim \pi_1$, stands for a **joint distribution** $\gamma(X_0, X_1)$, whose marginal distribution are π_0, π_1 respectively.

Theorem 1

For a given input coupling (X_0, X_1), the exact minimum of (4) is achieved by

$$v^X(x,t) = \mathbb{E}[X_1 - X_0 \mid X_t = x] = \int (X_1 - X_0)\, P_{(X_0,X_1)|X_t=x}(dX_0, dX_1) \tag{5}$$

which is the expectation of the line directions $X_1 - X_0$ that pass through x at time t.

This is based on **the following result:** Let $\hat{X} = g(Y)$ be an estimator of the random variable X. The MSE of this estimator is defined as

$$E[(X - \hat{X})^2] = E\left[(X - g(Y))^2\right]. \tag{6}$$

The MMSE (Minimum Mean Squared Error) estimator of X,

$$\hat{X}_M = E[X \mid Y], \tag{7}$$

has the lowest MSE among all possible estimators.

Nonlinear Extension of Rectified Flow

- We consider a nonlinear extension of rectified flow, where the linear interpolation X_t is replaced by any time-differentiable curve connecting X_0 and X_1.
- Let $\boldsymbol{X} = \{X_t : t \in [0,1]\}$ be any time-differentiable random process connecting X_0 and X_1, with time derivative $\frac{\mathrm{d}X_t}{\mathrm{d}t} := \dot{X}_t$. The nonlinear rectified flow induced from $\boldsymbol{X}$ is defined as:

$$\mathrm{d}Z_t = v^{\boldsymbol{X}}(Z_t, t)\,\mathrm{d}t, \text{ with } Z_0 = X_0, \qquad v^{\boldsymbol{X}}(z,t) = \mathbb{E}[\dot{X}_t \mid X_t = z]. \tag{8}$$

- $v^{\boldsymbol{X}}$ can be considered as the **optimization goal**, and we find it by solving:

$$\min_v \int_0^1 \mathbb{E}\left[w_t \left\|\dot{X}_t - v(X_t,t)\right\|^2\right]\mathrm{d}t, \tag{9}$$

  where $w_t : (0,1) \to (0,+\infty)$ is a positive weighting sequence ($w_t = 1$ by default). When $X_t = tX_1 + (1-t)X_0$ and $w_t = 1$, (9) becomes (4).
- This is a reasonable objective, as it encourages the velocity field v to closely match the **instantaneous rate of change** $\dot{X}_t$ of the process at every moment in time.

Marginal Preserving Property

The marginal preserving property that $\mathrm{Law}(Z_t) = \mathrm{Law}(X_t) \quad \forall t$ is a general property of the nonlinear rectified flow in (8). **This is why we need to find** $v^{\boldsymbol{X}}$.

Definition 1

For a path-wise continuously differentiable random process $\boldsymbol{X} = \{X_t : t \in [0,1]\}$, its *expected velocity* $v^{\boldsymbol{X}}$ is defined as

$$v^{\boldsymbol{X}}(x,t) = \mathbb{E}[\dot{X}_t \mid X_t = x], \qquad \forall x \in \mathrm{supp}(X_t). \tag{10}$$

For $x \notin \mathrm{supp}(X_t)$, the conditional expectation is not defined and we set $v^{\boldsymbol{X}}$ arbitrarily, say $v^{\boldsymbol{X}}(x,t) = 0$.

Definition 2

We call that $\boldsymbol{X}$ is *rectifiable* if $v^{\boldsymbol{X}}$ is locally bounded and the solution of the integral equation below exists and is unique:

$$Z_t = Z_0 + \int_0^t v^{\boldsymbol{X}}(Z_t, t)\mathrm{d}t, \qquad \forall t \in [0,1], \qquad Z_0 = X_0. \tag{11}$$

In this case, $\boldsymbol{Z} = \{Z_t : t \in [0,1]\}$ is called the *rectified flow induced from* $\boldsymbol{X}$.

Marginal Preserving Property (cont'd)

Theorem 2

Assume $\boldsymbol{X}$ is rectifiable and $\boldsymbol{Z}$ is its rectified flow. Then $\mathrm{Law}(Z_t) = \mathrm{Law}(X_t) \quad \forall t \in [0,1]$.

Proof.
For any compactly supported continuously differentiable test function $h : \mathbb{R}^d \to \mathbb{R}$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}[h(X_t)] = \mathbb{E}[\nabla h(X_t)^\top \dot{X}_t] \tag{12}$$

$$= \mathbb{E}\left[\mathbb{E}\left[\nabla h(X_t)^\top \dot{X}_t \mid X_t\right]\right] \tag{13}$$

$$= \mathbb{E}\left[\nabla h(X_t)^\top \mathbb{E}\left[\dot{X}_t \mid X_t\right]\right] \tag{14}$$

$$= \mathbb{E}[\nabla h(X_t)^\top v^{\boldsymbol{X}}(X_t, t)] \tag{15}$$

where in (12) we used chain rule and in (15) we used the definition of $v^{\boldsymbol{X}}(X_t, t)$.
This is equivalent to that $\pi_t := \mathrm{Law}(X_t)$ solves the continuity equation (FP equation) with drift $v_t^{\boldsymbol{X}} := v^{\boldsymbol{X}}(\cdot, t)$:

$$\dot{\pi}_t + \nabla \cdot (v_t^{\boldsymbol{X}} \pi_t) = 0. \tag{16}$$

Marginal Preserving Property (cont'd)

To see this, we can multiply (16) with h and integrate both sides:

$$0 = \int h\big(\dot{\pi}_t + \nabla \cdot (v_t^{\boldsymbol{X}} \pi_t)\big)\mathrm{d}x \tag{17}$$

$$= \int (h\,\dot{\pi}_t - \nabla h^\top v_t^{\boldsymbol{X}} \pi_t)\mathrm{d}x \tag{18}$$

$$= \frac{\mathrm{d}}{\mathrm{d}t}\mathbb{E}[h(X_t)] - \mathbb{E}[\nabla h(X_t)^\top v^{\boldsymbol{X}}(X_t, t)], \tag{19}$$

where we use integration by parts that $\int h\,\nabla \cdot (v_t^{\boldsymbol{X}} \pi_t)\mathrm{d}x = -\int \nabla h^\top (v_t^{\boldsymbol{X}} \pi_t)\mathrm{d}x$. $\square$

Because Z_t is driven by the same velocity field $v^{\boldsymbol{X}}$, its marginal law $\mathrm{Law}(Z_t)$ **solves the same equation with the same initial condition** $(Z_0 = X_0)$**.**

Hence, the equivalence of $\mathrm{Law}(Z_t)$ and $\mathrm{Law}(X_t)$ follows if the solution of (16) is unique, which is equivalent to the uniqueness of the solution of $\mathrm{d}Z_t = v^{\boldsymbol{X}}(Z_t, t)\,\mathrm{d}t$.

However, the **joint distributions** of the whole trajectory of Z_t and that of X_t are different in general.

Reducing Convex Transport Costs

- This property only holds for **linear** rectified flow.
- Monge's Optimal Transport problem ([Monge, 1781]):

$$\min_T \mathbb{E}\left[c(Z_1 - Z_0)\right] \qquad \text{s.t.} \qquad Z_1 = T(Z_0),\ \mathrm{Law}(Z_0) = \pi_0,\ \mathrm{Law}(Z_1) = \pi_1 \tag{20}$$

where $c : \mathbb{R}^d \to \mathbb{R}$ is a cost function, e.g., $c(x) = \frac{1}{2}\|x\|^2$.

Definition 3

A coupling (X_0, X_1) is called *rectifiable* if its linear interpolation process $\boldsymbol{X} = \{tX_1 + (1-t)X_0 : t \in [0,1]\}$ is rectifiable.
In this case, the $\boldsymbol{Z} = \{Z_t : t \in [0,1]\}$ in (11) is called the *rectified flow* of coupling (X_0, X_1), denoted as $\boldsymbol{Z} = \mathrm{RectFlow}((X_0, X_1))$, and (Z_0, Z_1) is called the *rectified coupling* of (X_0, X_1), denoted as $(Z_0, Z_1) = \mathrm{RectFlow}((X_0, X_1))$.

Theorem 3

Assume (X_0, X_1) is rectifiable and $(Z_0, Z_1) = \mathrm{RectFlow}((X_0, X_1))$. Then for any convex function $c : \mathbb{R}^d \to \mathbb{R}$, we have

$$\mathbb{E}[c(Z_1 - Z_0)] \leq \mathbb{E}[c(X_1 - X_0)]. \tag{21}$$

Reducing Convex Transport Costs (cont'd)

Proof.

$$\mathbb{E}\left[c(Z_1 - Z_0)\right] = \mathbb{E}\left[c\left(\int_0^1 v^{\boldsymbol{X}}(Z_t, t)\,\mathrm{d}t\right)\right] \tag{22}$$

$$\leq \mathbb{E}\left[\int_0^1 c\left(v^{\boldsymbol{X}}(Z_t, t)\right)\mathrm{d}t\right] \tag{23}$$

$$= \mathbb{E}\left[\int_0^1 c\left(v^{\boldsymbol{X}}(X_t, t)\right)\mathrm{d}t\right] \tag{24}$$

$$= \mathbb{E}\left[\int_0^1 c\left(\mathbb{E}[X_1 - X_0 \mid X_t]\right)\mathrm{d}t\right] \tag{25}$$

$$\leq \mathbb{E}\left[\int_0^1 \mathbb{E}\left[c(X_1 - X_0) \mid X_t\right]\mathrm{d}t\right] \tag{26}$$

$$= \int_0^1 \mathbb{E}\left[c(X_1 - X_0)\right]\mathrm{d}t \tag{27}$$

$$= \mathbb{E}\left[c(X_1 - X_0)\right]. \tag{28}$$

where the two inequalities follow from Jensen's inequality. □

Straightening Effect of Reflow

- This property also holds for **linear** rectified flow only.
- $\boldsymbol{Z} = \text{RectFlow}((X_0, X_1))$ denotes the rectified flow induced from (X_0, X_1). **Applying the algorithm recursively** yields a sequence of rectified flows $\boldsymbol{Z}^{k+1} = \text{RectFlow}\big((Z_0^k, Z_1^k)\big)$ with $(Z_0^0, Z_1^0) = (X_0, X_1)$.
- The reflow procedure not only decreases transport cost, but can also **straighten the paths of rectified flows** (Figure 6).
- This is a nice property since perfectly straight paths can be simulated exactly with a single Euler step.

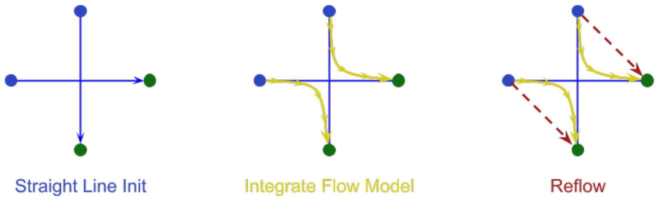

Figure 6: Straightening Effect of Reflow. Source: [Hawley, 2024]

Straightening Effect of Reflow (cont'd)

- The straightness of any smooth process $\boldsymbol{Z} = \{Z_t\}$ can be measured by

$$S(\boldsymbol{Z}) = \int_0^1 \mathbb{E}\left[\left\|(Z_1 - Z_0) - \dot{Z}_t\right\|^2\right] \mathrm{d}t. \tag{29}$$

  $S(\boldsymbol{Z}) = 0$ implies exact straightness, since now $v(Z_t, t) = \dot{Z}_t = Z_1 - Z_0$, meaning that $Z_t = tZ_1 + (1-t)Z_0, \quad \forall t.$ A flow with a small $S(\boldsymbol{Z})$ has nearly straight paths.
- It is not recommended to apply too many reflow steps as it may accumulate estimation error on $v^{\boldsymbol{X}}$.

Straightening Effect of Reflow (cont'd)

A coupling (X_0, X_1) is said to be straight (or fully rectified) if it is a fixed point of the $\text{RectFlow}(\cdot)$ mapping, i.e., $(X_0, X_1) = \text{RectFlow}\big((X_0, X_1)\big)$. It is desirable to obtain a straight coupling because its rectified flow is straight.

Theorem 4

Assume (X_0, X_1) is rectifiable. Let $X_t = tX_1 + (1-t)X_0$ and $\boldsymbol{Z} = \text{RectFlow}((X_0, X_1))$. Then (X_0, X_1) is a straight coupling iff the following equivalent statements hold.

1. There exists a strictly convex function $c : \mathbb{R}^d \to \mathbb{R}$, such that $\mathbb{E}[c(Z_1 - Z_0)] = \mathbb{E}[c(X_1 - X_0)]$.
2. (X_0, X_1) is a fixed point of $\text{RectFlow}(\cdot)$, i.e., $(X_0, X_1) = (Z_0, Z_1)$. This is the definition of being straight.
3. The rectified flow coincides with the linear interpolation process: $\boldsymbol{X} = \boldsymbol{Z}$.
4. The paths of the linear interpolation $\boldsymbol{X}$ do not intersect:

$$V((X_0, X_1)) := \int_0^1 \mathbb{E}\left[\|X_1 - X_0 - \mathbb{E}[X_1 - X_0 \mid X_t]\|^2\right] \mathrm{d}t = 0, \tag{30}$$

where $V((X_0, X_1)) = 0$ indicates that $X_1 - X_0 = \mathbb{E}[X_1 - X_0 \mid X_t]$ almost surely when $t \sim \text{Uniform}([0, 1])$, meaning that the direction $X_1 - X_0$ for lines passing through each X_t is unique, and hence no linear interpolation paths intersect.

Straightening Effect of Reflow (cont'd)

Proof.

- $3 \to 2 \to 1$: obvious.
- $1 \to 4$: if $\mathbb{E}[c(Z_1 - Z_0)] = \mathbb{E}[c(X_1 - X_0)]$, the two applications of Jensen's inequality in the proof of Theorem 3 are tight. Since c is strictly convex, for any $x \neq y$ and $\lambda \in (0, 1)$ we have

$$c(\lambda x + (1-\lambda)y) < \lambda c(x) + (1-\lambda)c(y) \tag{31}$$

  So the second Jensen's inequality in the proof implies that $X_1 - X_0 = \mathbb{E}[X_1 - X_0 \mid X_t]$ almost surely w.r.t. X and $t \sim \text{Uniform}([0, 1])$, which implies that $V(\boldsymbol{X}) = 0$.
- $4 \to 3$: if $V(\boldsymbol{X}) = 0$, we have $\int_0^s (X_1 - X_0)\mathrm{d}t = \int_0^s \mathbb{E}[X_1 - X_0 \mid X_t]\mathrm{d}t = \int_0^s v^{\boldsymbol{X}}(X_t, t)\mathrm{d}t$ for $s \in (0, 1]$. Hence

$$X_t = X_0 + \int_0^t (X_1 - X_0)\mathrm{d}t = X_0 + \int_0^t v^{\boldsymbol{X}}(X_t, t)\mathrm{d}t. \tag{32}$$

  Because $\boldsymbol{Z}$ satisfies the same equation (11), we have $\boldsymbol{X} = \boldsymbol{Z}$ by the uniqueness of the solution. □

Straightening Effect of Reflow (cont'd)

Theorem 5

Let $\boldsymbol{Z}^k$ be the k-th rectified flow of (X_0, X_1), that is, $\boldsymbol{Z}^{k+1} = \mathrm{RectFlow}((Z_0^k, Z_1^k))$ and $(Z_0^0, Z_1^0) = (X_0, X_1)$. Assume each (Z_0^k, Z_1^k) is rectifiable for $k = 0, \ldots, K$.
Then

$$\sum_{k=0}^{K} \left[S(\boldsymbol{Z}^{k+1}) + V((Z_0^k, Z_1^k)) \right] \leq \mathbb{E}\left[\|X_1 - X_0\|^2 \right]. \tag{33}$$

So we have $\min_{k \leq K} \left(S(\boldsymbol{Z}^{k+1}) + V((Z_0^k, Z_1^k)) \right) = O(1/K)$.

Straightening Effect of Reflow (cont'd)

Proof.
We have

$$\mathbb{E}\left[\|X_1 - X_0\|^2\right] - \mathbb{E}\left[\|Z_1 - Z_0\|^2\right] = S(\boldsymbol{Z}) + V((X_0, X_1)). \tag{34}$$

Applying it to each rectification step yields

$$\mathbb{E}\left[\|Z_1^k - Z_0^k\|^2\right] - \mathbb{E}\left[\|Z_1^{k+1} - Z_0^{k+1}\|^2\right] = S(\boldsymbol{Z}^{k+1}) + V((Z_0^k, Z_1^k)). \tag{35}$$

Take the sum over $k = 0, 1, \ldots, K$

$$\sum_{k=0}^{K}\left[\mathbb{E}\left[\|Z_1^k - Z_0^k\|^2\right] - \mathbb{E}\left[\|Z_1^{k+1} - Z_0^{k+1}\|^2\right]\right] = \sum_{k=0}^{K}\left[S(\boldsymbol{Z}^{k+1}) + V((Z_0^k, Z_1^k))\right] \tag{36}$$

The left side is a telescoping sum, so only the first and last terms remain:

$$\mathbb{E}\left[\|Z_1^0 - Z_0^0\|^2\right] - \mathbb{E}\left[\|Z_1^{K+1} - Z_0^{K+1}\|^2\right] = \sum_{k=0}^{K}\left[S(\boldsymbol{Z}^{k+1}) + V((Z_0^k, Z_1^k))\right] \tag{37}$$

Since $Z_0^0 = X_0$, $Z_1^0 = X_1$, we have

$$\mathbb{E}\left[\|X_1 - X_0\|^2\right] \geq \sum_{k=0}^{K}\left[S(\boldsymbol{Z}^{k+1}) + V((Z_0^k, Z_1^k))\right] \tag{38}$$

which is exactly the conclusion stated in the theorem.

Straightening Effect of Reflow (cont'd)

Next, we show that $\min_{k \le K} \left(S(\boldsymbol{Z}^{k+1}) + V((Z_0^k, Z_1^k)) \right) = O(1/K)$.
From last page we have:

$$\sum_{k=0}^{K} \left[S(\boldsymbol{Z}^{k+1}) + V((Z_0^k, Z_1^k)) \right] \le \mathbb{E}\left[\|X_1 - X_0\|^2 \right] \tag{39}$$

Let $C := \mathbb{E}\left[\|X_1 - X_0\|^2 \right], a_k := S(\boldsymbol{Z}^{k+1}) + V((Z_0^k, Z_1^k))$, so

$$\sum_{k=0}^{K} a_k \le C \tag{40}$$

Since minimum is less than the average,

$$\min_{0 \le k \le K} a_k \le \frac{1}{K+1} \sum_{k=0}^{K} a_k \le \frac{C}{K+1} = O(1/K) \tag{41}$$

Straightening Effect of Reflow (cont'd)

Finally, we will prove that (34) holds.

$$\mathbb{E}\left[\|X_1 - X_0\|^2\right] = \int_0^1 \mathbb{E}\left[\|X_1 - X_0\|^2\right] \mathrm{d}t \tag{42}$$

$$= \int_0^1 \mathbb{E}\left[\left\|(X_1 - X_0) - v^{\boldsymbol{X}}(X_t, t) + v^{\boldsymbol{X}}(X_t, t)\right\|^2\right] \mathrm{d}t \tag{43}$$

$$= \int_0^1 \mathbb{E}\left[\left\|(X_1 - X_0) - v^{\boldsymbol{X}}(X_t, t)\right\|^2\right] \mathrm{d}t \tag{44}$$

$$+ \int_0^1 \mathbb{E}\left[\|v^{\boldsymbol{X}}(X_t, t)\|^2\right] \mathrm{d}t$$

$$+ 2\int_0^1 \mathbb{E}\left[\left\langle (X_1 - X_0) - v^{\boldsymbol{X}}(X_t, t), v^{\boldsymbol{X}}(X_t, t)\right\rangle\right] \mathrm{d}t$$

where $v^{\boldsymbol{X}}(x, t) = \mathbb{E}[X_1 - X_0 \mid X_t = x]$.

Straightening Effect of Reflow (cont'd)

$$\mathbb{E}\left[\left\langle (X_1 - X_0) - v^{\boldsymbol{X}}(X_t, t), v^{\boldsymbol{X}}(X_t, t)\right\rangle\right] \tag{45}$$

$$= \mathbb{E}\left[\left\langle X_1 - X_0,\, v^{\boldsymbol{X}}(X_t, t)\right\rangle\right] - \mathbb{E}\left[\left\langle v^{\boldsymbol{X}}(X_t, t),\, v^{\boldsymbol{X}}(X_t, t)\right\rangle\right] \tag{46}$$

$$= \mathbb{E}\left[\left\langle X_1 - X_0,\, v^{\boldsymbol{X}}(X_t, t)\right\rangle\right] - \mathbb{E}\left[\|v^{\boldsymbol{X}}(X_t, t)\|^2\right] \tag{47}$$

$$\mathbb{E}\left[\left\langle X_1 - X_0,\, v^X(X_t, t)\right\rangle\right] = \mathbb{E}\left[\mathbb{E}\left[\left\langle X_1 - X_0,\, v^X(X_t, t)\right\rangle \mid X_t\right]\right] \tag{48}$$

$$= \mathbb{E}\left[\left\langle\, \mathbb{E}[X_1 - X_0 \mid X_t],\, v^X(X_t, t)\right\rangle\right] \tag{49}$$

$$= \mathbb{E}\left[\left\langle v^X(X_t, t),\, v^X(X_t, t)\right\rangle\right] \tag{50}$$

$$= \mathbb{E}\left[\|v^X(X_t, t)\|^2\right] \tag{51}$$

So we have

$$\mathbb{E}\left[\left\langle (X_1 - X_0) - v^{\boldsymbol{X}}(X_t, t), v^{\boldsymbol{X}}(X_t, t)\right\rangle\right] = 0 \tag{52}$$

Straightening Effect of Reflow (cont'd)

After simplification:

$$\mathbb{E}\left[\|X_1 - X_0\|^2\right] = \underbrace{\int_0^1 \mathbb{E}\left[\left\|(X_1 - X_0) - v^X(X_t, t)\right\|^2\right] \mathrm{d}t}_{V((X_0, X_1))} + \int_0^1 \mathbb{E}\left[\|v^X(X_t, t)\|^2\right] \mathrm{d}t \tag{53}$$

$$S(\boldsymbol{Z}) = \int_0^1 \mathbb{E}\left[\left\|(Z_1 - Z_0) - \dot{Z}_t\right\|^2\right] \mathrm{d}t \tag{54}$$

$$= \int_0^1 \mathbb{E}\left[\|Z_1 - Z_0\|^2 - 2\langle Z_1 - Z_0,\, \dot{Z}_t\rangle + \|\dot{Z}_t\|^2\right] \mathrm{d}t \tag{55}$$

$$= \mathbb{E}\left[\|Z_1 - Z_0\|^2\right] - 2\mathbb{E}\left[\left\langle Z_1 - Z_0,\, \int_0^1 \dot{Z}_t \mathrm{d}t\right\rangle\right] + \int_0^1 \mathbb{E}\left[\|\dot{Z}_t\|^2\right] \mathrm{d}t \tag{56}$$

$$= \mathbb{E}\left[\|Z_1 - Z_0\|^2\right] - 2\mathbb{E}\left[\|Z_1 - Z_0\|^2\right] + \int_0^1 \mathbb{E}\left[\|v^X(Z_t, t)\|^2\right] \mathrm{d}t \tag{57}$$

$$= \int_0^1 \mathbb{E}\left[\|v^X(X_t, t)\|^2\right] \mathrm{d}t - \mathbb{E}\left[\|Z_1 - Z_0\|^2\right] \tag{58}$$

So (34) is proven. □

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Reformulate the Transport Mapping Problem

- Let $\rho_0 :=$ prior density and $\rho_1 :=$ target density, both supported on $\Omega \subseteq \mathbb{R}^d$. The problem can be formulated as constructing a map $X_t : \Omega \to \Omega$ with $t \in [0, 1]$, such that

$$\text{if } x \sim \rho_0 \text{ then } X_t(x) \sim \rho_t \text{ with } \rho_{t=0} = \rho_0 \text{ and } \rho_{t=1} = \rho_1 \tag{59}$$

  where ρ_t is some density.

- Represent this map as the flow associated with the ODE

$$\dot{X}_t(x) = v_t(X_t(x)), \qquad X_{t=0}(x) = x. \tag{60}$$

  Here, v_t is the same as $v^{\boldsymbol{X}}$ in (10).

- This is equivalent to saying that $\rho_t(x)$ and $v_t(x)$ satisfies the continuity equation

$$\partial_t \rho_t + \nabla \cdot (v_t \rho_t) = 0 \text{ with } \rho_{t=0} = \rho_0 \qquad \text{and} \qquad \rho_{t=1} = \rho_1, \tag{61}$$

  and the problem becomes estimating v_t satisfying the equation.

Stochastic Interpolant

- Introduce a time-differentiable interpolant

$$I_t : \Omega \times \Omega \to \Omega \text{ with } I_{t=0}(x_0, x_1) = x_0 \text{ and } I_{t=1}(x_0, x_1) = x_1 \quad (62)$$

  E.g., linear interpolant $I_t(x_0, x_1) = tx_1 + (1-t)x_0$ in rectified flow.

- Given this interpolant, we then construct the stochastic process x_t by sampling independently x_0 from ρ_0 and x_1 from ρ_1, and passing them through I_t:

$$x_t = I_t(x_0, x_1), \qquad x_0 \sim \rho_0, \qquad x_1 \sim \rho_1 \qquad \text{independent.} \quad (63)$$

  We refer to the process x_t as a **stochastic interpolant**.

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Minimizer of Objective

Theorem 6

The stochastic interpolant x_t defined in (63) with $I_t(x_0, x_1)$ satisfying (62) has a probability density $\rho_t(x)$ that satisfies the continuity equation (61) with a velocity $v_t(x)$ which is the unique minimizer over $\hat{v}_t(x)$ of the objective

$$G(\hat{v}) = \mathbb{E}\left[|\hat{v}_t(I_t(x_0, x_1))|^2 - 2\partial_t I_t(x_0, x_1) \cdot \hat{v}_t(I_t(x_0, x_1))\right] \tag{64}$$

where $\cdot$ denotes vector inner product.
In addition, the minimum value of this objective is given by

$$G(v) = -\mathbb{E}\left[|v_t(I_t(x_0, x_1))|^2\right] = -\int_0^1 \int_{\mathbb{R}^d} |v_t(x)|^2 \rho_t(x) \mathrm{d}x \mathrm{d}t > -\infty \tag{65}$$

Equivalent Objective

- By definition of the stochastic interpolant x_t we can express its density $\rho_t(x)$ using the Dirac delta function as

$$\rho_t(x) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \delta\big(x - I_t(x_0, x_1)\big)\, \rho_0(x_0)\, \rho_1(x_1)\, \mathrm{d}x_0\, \mathrm{d}x_1. \tag{66}$$

- Take derivative w.r.t t using chain rule, we have:

$$\partial_t \rho_t(x) = -\int_{\mathbb{R}^d \times \mathbb{R}^d} \partial_t I_t(x_0, x_1) \cdot \nabla \delta\big(x - I_t(x_0, x_1)\big)\, \rho_0(x_0) \rho_1(x_1) \mathrm{d}x_0 \mathrm{d}x_1 \equiv -\nabla \cdot j_t(x) \tag{67}$$

where

$$j_t(x) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \partial_t I_t(x_0, x_1)\, \delta\big(x - I_t(x_0, x_1)\big)\, \rho_0(x_0)\, \rho_1(x_1)\, \mathrm{d}x_0\, \mathrm{d}x_1. \tag{68}$$

- Introduce $v_t(x)$ via

$$v_t(x) = \begin{cases} j_t(x)/\rho_t(x) & \text{if } \rho_t(x) > 0, \\ 0 & \text{else} \end{cases} \tag{69}$$

then we can write (67) as the continuity equation in (61).

Equivalent Objective (cont'd)

- Write (64) explicitly:

$$G(\hat{v}) = \int \mathrm{d}t \int \mathrm{d}x_0 \mathrm{d}x_1 \left(|\hat{v}_t(I_t(x_0, x_1))|^2 - 2\, \partial_t I_t(x_0, x_1) \cdot \hat{v}_t(I_t(x_0, x_1)) \right) \rho_0(x_0) \rho_1(x_1) \tag{70}$$

- Handle the two terms separately:

$$\int \mathrm{d}x_0 \, \mathrm{d}x_1 \; |\hat{v}_t(I_t(x_0, x_1))|^2 \; \rho_0(x_0)\rho_1(x_1) \tag{71}$$

$$= \int \mathrm{d}x_0 \, \mathrm{d}x_1 \int \mathrm{d}x \; |\hat{v}_t(I_t(x_0, x_1))|^2 \, \delta\big(x - I_t(x_0, x_1)\big) \rho_0(x_0)\rho_1(x_1) \tag{72}$$

$$= \int \mathrm{d}x \, \big|\hat{v}_t(x)\big|^2 \int \mathrm{d}x_0 \, \mathrm{d}x_1 \, \delta\big(x - I_t(x_0, x_1)\big) \rho_0(x_0)\rho_1(x_1) \tag{73}$$

$$= \int \mathrm{d}x \, \big|\hat{v}_t(x)\big|^2 \, \rho_t(x) \tag{74}$$

Similarly, we have:

$$\int \mathrm{d}x_0 \, \mathrm{d}x_1 \; (-2\, \partial_t I_t(x_0, x_1) \cdot \hat{v}_t(I_t(x_0, x_1))) \, \rho_0(x_0)\rho_1(x_1) = \int \mathrm{d}x \; (-2\hat{v}_t(x) \cdot j_t(x)) \tag{75}$$

Equivalent Objective (cont'd)

- Finally (64) becomes:

$$G(\hat{v}) = \int_0^1 \int_{\mathbb{R}^d} \left(|\hat{v}_t(x)|^2 \rho_t(x) - 2\hat{v}_t(x) \cdot j_t(x) \right) \mathrm{d}x \, \mathrm{d}t \tag{76}$$

- Consider the alternative objective which directly measures the distance between model and goal:

$$H(\hat{v}) = \int_0^1 \int_{\mathbb{R}^d} |\hat{v}_t(x) - v_t(x)|^2 \, \rho_t(x) \, \mathrm{d}x \, \mathrm{d}t \tag{77}$$

$$= \int_0^1 \int_{\mathbb{R}^d} \left(|\hat{v}_t(x)|^2 \rho_t(x) - 2\hat{v}_t(x) \cdot j_t(x) + |v_t(x)|^2 \rho_t(x) \right) \mathrm{d}x \, \mathrm{d}t \tag{78}$$

- It follows that

$$G(\hat{v}) = H(\hat{v}) - \int_0^1 \int_{\mathbb{R}^d} |v_t(x)|^2 \rho_t(x) \, \mathrm{d}x \, \mathrm{d}t = H(\hat{v}) - \mathbb{E}\left[|v_t(I_t(x_0, x_1))|^2 \right] \tag{79}$$

- Clearly, (77) is equivalent to (9).

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Notations

Standard notation for function spaces:

- $C^1([0,1])$: The space of continuously differentiable functions from $[0,1]$ to $\mathbb{R}$.
- $(C^2(\mathbb{R}^d))^d$: The space of twice continuously differentiable functions from $\mathbb{R}^d$ to $\mathbb{R}^d$.
- $C_0^p(\mathbb{R}^d)$: The space of compactly supported functions from $\mathbb{R}^d$ to $\mathbb{R}$ that are continuously differentiable p times.
- Given a function $b : [0,1] \times \mathbb{R}^d \to \mathbb{R}^d$ with value $b(t,x)$ at (t,x), $b \in C^1([0,1], (C^2(\mathbb{R}^d))^d)$ indicates that b is continuously differentiable in t for all $(t,x) \in [0,1] \times \mathbb{R}^d$ and that $b(t,\cdot)$ is an element of $(C^2(\mathbb{R}^d))^d$ for all $t \in [0,1]$.

(New) Stochastic Interpolant

- Given two probability density functions $\rho_0, \rho_1 : \mathbb{R}^d \to \mathbb{R}_{\geq 0}$, a stochastic interpolant between ρ_0 and ρ_1 is a stochastic process x_t defined as

$$x_t = I(t, x_0, x_1) + \gamma(t)z, \qquad t \in [0, 1], \tag{80}$$

where:

  - $I \in C^2([0,1]; (C^2(\mathbb{R}^d \times \mathbb{R}^d))^d)$ satisfies the boundary conditions $I(0, x_0, x_1) = x_0$ and $I(1, x_0, x_1) = x_1$, as well as

$$\exists C_1 < \infty : |\partial_t I(t, x_0, x_1)| \leq C_1 |x_0 - x_1| \qquad \forall (t, x_0, x_1) \in [0,1] \times \mathbb{R}^d \times \mathbb{R}^d. \tag{81}$$

  - $\gamma : [0,1] \to \mathbb{R}$ satisfies $\gamma(0) = \gamma(1) = 0$, $\gamma(t) > 0$ for all $t \in (0,1)$, and $\gamma^2 \in C^2([0,1])$.
  - The pair (x_0, x_1) is drawn from a probability measure ν that marginalizes on ρ_0 and ρ_1, i.e.

$$\int \nu(x_0, x_1)\, \mathrm{d}x_1 = \rho_0(x_0), \int \nu(x_0, x_1)\, \mathrm{d}x_0 = \rho_1(x_1). \tag{82}$$

  - z is a Gaussian random variable independent of (x_0, x_1), i.e. $z \sim \mathcal{N}(0, I_d)$ and $z \perp (x_0, x_1)$.

Details

- (81) restricts the speed of the interpolation trajectory, and prevents the trajectory from deviation.
- A simple choice of ν is the product measure $\nu(\mathrm{d}x_0, \mathrm{d}x_1) = \rho_0(x_0)\rho_1(x_1)\,\mathrm{d}x_0\mathrm{d}x_1$, where $x_0 \perp x_1$.
- We will see the advantage of the **additional term** $\gamma(t)z$, compared with (62).
- Another way to define the stochastic interpolant is via

$$x_t^{\mathrm{d}} = I(t, x_0, x_1) + N_t \tag{83}$$

where $N : [0,1] \to \mathbb{R}^d$ is a zero-mean Gaussian stochastic process satisfying $N_{t=0} = N_{t=1} = 0$, so we only need to know the covariance matrix $\mathbb{E}[N_t N_t^\top]$ at each timestep.

Transport Equation

Theorem 7

The probability distribution of the stochastic interpolant x_t defined in (80) is absolutely continuous with respect to the Lebesgue measure at all times $t \in [0,1]$ and its time-dependent density $\rho(t)$ satisfies $\rho(0) = \rho_0$, $\rho(1) = \rho_1$, $\rho \in C^1([0,1]; C^p(\mathbb{R}^d))$ for any $p \in \mathbb{N}$, and $\rho(t,x) > 0$ for all $(t,x) \in [0,1] \times \mathbb{R}^d$. In addition, ρ solves the transport equation

$$\partial_t \rho + \nabla \cdot (b\rho) = 0, \tag{84}$$

where we defined the velocity

$$b(t,x) = \mathbb{E}[\dot{x}_t \mid x_t = x] = \mathbb{E}[\partial_t I(t, x_0, x_1) + \dot{\gamma}(t) z \mid x_t = x]. \tag{85}$$

This velocity is in $C^0([0,1]; (C^p(\mathbb{R}^d))^d)$ for any $p \in \mathbb{N}$, and such that

$$\forall t \in [0,1] : \int_{\mathbb{R}^d} |b(t,x)|^2 \rho(t,x) \mathrm{d}x < \infty. \tag{86}$$

Objective

Theorem 8

The velocity b defined in (85) is the unique minimizer in $C^0([0,1];(C^1(\mathbb{R}^d))^d)$ of the quadratic objective

$$\mathcal{L}_b[\hat{b}] = \int_0^1 \mathbb{E}\left(\frac{1}{2}|\hat{b}(t,x_t)|^2 - (\partial_t I(t,x_0,x_1) + \dot{\gamma}(t)z)\cdot \hat{b}(t,x_t)\right)\mathrm{d}t \qquad (87)$$

where x_t is defined in (80) and the expectation is taken independently over $(x_0,x_1) \sim \nu$ and $z \sim \mathcal{N}(0, I_d)$.

This is a generalization of (64). An equivalent objective is
$\mathbb{E}\left(\frac{1}{2}|\hat{b}(t,x_t)|^2 - (\partial_t I(t,x_0,x_1) + \dot{\gamma}(t)z)\cdot \hat{b}(t,x_t)\right), \quad t \in [0,1].$

Theorem 9

The score of the probability density ρ specified in Theorem 7 is in $C^1([0,1];(C^p(\mathbb{R}^d))^d)$ for any $p \in \mathbb{N}$ and given by

$$s(t,x) = \nabla \log \rho(t,x) = -\gamma^{-1}(t)\mathbb{E}(z \mid x_t = x) \qquad \forall (t,x) \in (0,1) \times \mathbb{R}^d \tag{88}$$

In addition it satisfies

$$\forall t \in [0,1] : \int_{\mathbb{R}^d} |s(t,x)|^2 \rho(t,x) \mathrm{d}x < \infty, \tag{89}$$

and is the unique minimizer in $C^1([0,1];(C^1(\mathbb{R}^d))^d)$ of the quadratic objective

$$\mathcal{L}_s[\hat{s}] = \int_0^1 \mathbb{E}\left(\frac{1}{2}|\hat{s}(t,x_t)|^2 + \gamma^{-1}(t) z \cdot \hat{s}(t,x_t)\right) \mathrm{d}t \tag{90}$$

where x_t is defined in (80) and the expectation is taken independently over $(x_0, x_1) \sim \nu$ and $z \sim \mathcal{N}(0, I_d)$.

An equivalent objective is $\mathbb{E}\left(\frac{1}{2}|\hat{s}(t,x_t)|^2 + \gamma^{-1}(t) z \cdot \hat{s}(t,x_t)\right), \quad t \in (0,1).$

Denoiser

- The quantity

$$\eta_z(t,x) = \mathbb{E}(z \mid x_t = x), \tag{91}$$

  is defined as the denoiser.
- We can rewrite score on $t \in (0,1)$ (where $\gamma(t) > 0$) as:

$$s(t,x) = -\gamma^{-1}(t)\eta_z(t,x). \tag{92}$$

- This denoiser is the minimizer of an equivalent expression to (90),

$$\mathcal{L}_{\eta_z}[\hat{\eta}_z] = \int_0^1 \mathbb{E}\left(\frac{1}{2}\left|\hat{\eta}_z(t,x_t)\right|^2 - z \cdot \hat{\eta}_z(t,x_t)\right) \mathrm{d}t. \tag{93}$$

FP Equations

For any $\epsilon \in C^0([0,1])$ with $\epsilon(t) \geq 0$ for all $t \in [0,1]$, the probability density ρ specified in Theorem 7 satisfies:

- The forward Fokker-Planck equation

$$\partial_t \rho + \nabla \cdot (b_{\mathrm{F}} \rho) = \epsilon(t) \Delta \rho, \qquad \rho(0) = \rho_0, \tag{94}$$

  where we defined the forward drift

$$b_{\mathrm{F}}(t,x) = b(t,x) + \epsilon(t) s(t,x). \tag{95}$$

  (94) is solved **forward in time** from $t = 0$ to $t = 1$, and its solution for the initial condition $\rho(0) = \rho_0$ satisfies $\rho(1) = \rho_1$.

- The backward Fokker-Planck equation

$$\partial_t \rho + \nabla \cdot (b_{\mathrm{B}} \rho) = -\epsilon(t) \Delta \rho, \qquad \rho(1) = \rho_1, \tag{96}$$

  where we defined the backward drift

$$b_{\mathrm{B}}(t,x) = b(t,x) - \epsilon(t) s(t,x). \tag{97}$$

  (96) is solved **backward in time** from $t = 1$ to $t = 0$, and its solution for the final condition $\rho(1) = \rho_1$ satisfies $\rho(0) = \rho_0$.

To verify these two equations, just plug in definition of b_{F} or b_{B}, and note that $sp = (\nabla \log \rho)\rho = \nabla \rho$, so $\nabla \cdot (s\rho) = \nabla \cdot (\nabla \rho) = \Delta \rho$.

Velocity Field

- From (85) we can write

$$b(t,x) = v(t,x) - \dot{\gamma}(t)\gamma(t)s(t,x), \tag{98}$$

where s is the score given in (88) and we define the velocity field

$$v(t,x) = \mathbb{E}\big(\partial_t I(t,x_0,x_1) \mid x_t = x\big). \tag{99}$$

- The velocity field $v \in C^0([0,1];(C^p(\mathbb{R}^d))^d)$ for any $p \in \mathbb{N}$ and can be characterized as the unique minimizer of

$$\mathcal{L}_v[\hat{v}] = \int_0^1 \mathbb{E}\left(\frac{1}{2}|\hat{v}(t,x_t)|^2 - \partial_t I(t,x_0,x_1)\cdot\hat{v}(t,x_t)\right)\mathrm{d}t \tag{100}$$

Generative Models

At any time $t \in [0, 1]$, the law of the stochastic interpolant x_t coincides with the law of the three processes X_t, X_t^{F}, and X_t^{B}, respectively defined as:

1. The solutions of the probability flow associated with the transport equation (84)

$$\frac{\mathrm{d}}{\mathrm{d}t} X_t = b(t, X_t), \tag{101}$$

   solved either forward in time from the initial data $X_{t=0} \sim \rho_0$ or backward in time from the final data $X_{t=1} = x_1 \sim \rho_1$.

2. The solutions of the forward SDE associated with the FPE (94)

$$\mathrm{d}X_t^{\mathrm{F}} = b_{\mathrm{F}}(t, X_t^{\mathrm{F}})\mathrm{d}t + \sqrt{2\epsilon(t)}\,\mathrm{d}W_t, \tag{102}$$

   solved forward in time from the initial data $X_{t=0}^{\mathrm{F}} \sim \rho_0$ independent of W.

3. The solutions of the backward SDE associated with the backward FPE (96)

$$\mathrm{d}X_t^{\mathrm{B}} = b_{\mathrm{B}}(t, X_t^{\mathrm{B}})\mathrm{d}t + \sqrt{2\epsilon(t)}\,\mathrm{d}W_t^{\mathrm{B}}, \qquad W_t^{\mathrm{B}} = -W_{1-t}, \tag{103}$$

   solved backward in time from the final data $X_{t=1}^{\mathrm{B}} \sim \rho_1$ independent of W^{B}. Alternatively, solution of (103) is given by $X_t^{\mathrm{B}} = Z_{1-t}^{\mathrm{F}}$ where Z_t^{F} satisfies

$$\mathrm{d}Z_t^{\mathrm{F}} = -b_{\mathrm{B}}(1-t, Z_t^{\mathrm{F}})\mathrm{d}t + \sqrt{2\epsilon(t)}\,\mathrm{d}W_t, \tag{104}$$

   solved forward in time from the initial data $Z_{t=0}^{\mathrm{F}} \sim \rho_1$ independent of W.

$x_t, X_t, X_t^{\mathrm{F}}$ and X_t^{B} are different stochastic processes, but their **laws all coincide with** $\rho(t)$ **at any time** $t \in [0, 1]$.

Likelihood Control

Theorem 10

Let ρ denote the solution of the FP equation (94) with $\epsilon(t) = \epsilon > 0$. Given two velocity fields $\hat{b}, \hat{s} \in C^0([0,1]; (C^1(\mathbb{R}^d))^d)$, define

$$\hat{b}_{\mathrm{F}}(t,x) = \hat{b}(t,x) + \epsilon \hat{s}(t,x), \qquad \hat{v}(t,x) = \hat{b}(t,x) + \gamma(t)\dot{\gamma}(t)\hat{s}(t,x) \tag{105}$$

Let $\hat{\rho}$ denote the solution to the FP equation

$$\partial_t \hat{\rho} + \nabla \cdot (\hat{b}_{\mathrm{F}} \hat{\rho}) = \epsilon \Delta \hat{\rho}, \qquad \hat{\rho}(0) = \rho_0. \tag{106}$$

Then,

$$\mathrm{KL}(\rho_1 \| \hat{\rho}(1)) \leq \frac{1}{2\epsilon} \left(\mathcal{L}_b[\hat{b}] - \min_{\hat{b}} \mathcal{L}_b[\hat{b}] \right) + \frac{\epsilon}{2} \left(\mathcal{L}_s[\hat{s}] - \min_{\hat{s}} \mathcal{L}_s[\hat{s}] \right), \tag{107}$$

and

$$\mathrm{KL}(\rho_1 \| \hat{\rho}(1)) \leq \frac{1}{2\epsilon} \left(\mathcal{L}_v[\hat{v}] - \min_{\hat{v}} \mathcal{L}_v[\hat{v}] \right) + \frac{\sup_{t\in[0,1]} (\gamma(t)\dot{\gamma}(t) - \epsilon)^2}{2\epsilon} \left(\mathcal{L}_s[\hat{s}] - \min_{\hat{s}} \mathcal{L}_s[\hat{s}] \right). \tag{108}$$

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Diffusive Interpolants

Given two probability density functions $\rho_0, \rho_1 : \mathbb{R}^d \to \mathbb{R}_{\geq 0}$, a diffusive interpolant between ρ_0 and ρ_1 is a stochastic process x_t^{d} defined as

$$x_t^{\mathrm{d}} = I(t, x_0, x_1) + \sqrt{2a(t)} B_t, \qquad t \in [0,1], \tag{109}$$

where:

- $I(t, x_0, x_1)$ is as in (80).
- $(x_0, x_1) \sim \nu$ with ν satisfying (82).
- $a(t) \in C^2([0,1])$ with $a(0) > 0$ and $a(t) \geq 0$ for all $t \in [0,1]$.
- B_t is a standard **Brownian bridge process**, independent of x_0 and x_1.

(109) has the same single-time statistics and time-dependent density $\rho(t,x)$ as the following stochastic interpolant:

$$x_t = I(t, x_0, x_1) + \sqrt{2a(t)t(1-t)}\, z \qquad \text{with} \qquad (x_0, x_1) \sim \nu,\ z \sim \mathcal{N}(0, I_d),\ (x_0, x_1) \perp z. \tag{110}$$

One-sided Interpolants for Gaussian ρ_0

Given a probability density function $\rho_1 : \mathbb{R}^d \to \mathbb{R}_{\geq 0}$, a one-sided stochastic interpolant **between** $\mathcal{N}(0, I_d)$ **and** ρ_1 is a stochastic process x_t^{os}

$$x_t^{\mathrm{os}} = \alpha(t)z + J(t, x_1), \qquad t \in [0, 1] \tag{111}$$

where:

- $J \in C^2([0,1]; C^2((\mathbb{R}^d)^d))$ satisfies the boundary conditions $J(0, x_1) = 0$ and $J(1, x_1) = x_1$.
- x_1 and z are independent random variables drawn from ρ_1 and $\mathcal{N}(0, I_d)$, respectively.
- $\alpha : [0,1] \to \mathbb{R}$ satisfies $\alpha(0) = 1$, $\alpha(1) = 0$, $\alpha(t) > 0$ for all $t \in [0, 1)$, and $\alpha^2 \in C^2([0,1])$.

By construction, $x_{t=0}^{\mathrm{os}} = z \sim \mathcal{N}(0, I_d)$ and $x_{t=1}^{\mathrm{os}} = x_1 \sim \rho_1$, so that the distribution of the stochastic process x_t^{os} **bridges** $\mathcal{N}(0, I_d)$ **and** ρ_1.

One-sided Interpolants for Gaussian ρ_0 (cont'd)

- (111) has the same density as the stochastic interpolant defined in (80) if we set $I(t, x_0, x_1) = J_t(x_1) + \delta(t)x_0$ and take $\delta^2(t) + \gamma^2(t) = \alpha^2(t)$, since $x_0 \sim \mathcal{N}(0, I_d)$.
- Velocity field b becomes

$$b(t, x) = \mathbb{E}(\dot{\alpha}(t)z + \partial_t J(t, x_1) \mid x_t^{\mathrm{os}} = x), \tag{112}$$

- Quadratic objective becomes

$$\mathcal{L}_b[\hat{b}] = \int_0^1 \mathbb{E}\left(\frac{1}{2}|\hat{b}(t, x_t^{\mathrm{os}})|^2 - (\dot{\alpha}(t)z + \partial_t J(t, x_1)) \cdot \hat{b}(t, x_t^{\mathrm{os}})\right) \mathrm{d}t. \tag{113}$$

  The expectation $\mathbb{E}$ is taken independently over $x_1 \sim \rho_1$ and $z \sim \mathcal{N}(0, I_d)$.
- The score is given by

$$s(t, x) = -\alpha^{-1}(t)\eta_z(t, x), \qquad \eta_z(t, x) = \mathbb{E}(z \mid x_t^{\mathrm{os}} = x), \tag{114}$$

- These functions are the unique minimizers of the objectives

$$\mathcal{L}_s[\hat{s}] = \int_0^1 \mathbb{E}\left(\frac{1}{2}|\hat{s}(t, x_t^{\mathrm{os}})|^2 + \gamma^{-1}(t)z \cdot \hat{s}(t, x_t^{\mathrm{os}})\right) \mathrm{d}t, \tag{115}$$

$$\mathcal{L}_{\eta_z}[\hat{\eta}_z] = \int_0^1 \mathbb{E}\left(\frac{1}{2}|\hat{\eta}_z(t, x_t^{\mathrm{os}})|^2 - z \cdot \hat{\eta}_z(t, x_t^{\mathrm{os}})\right) \mathrm{d}t. \tag{116}$$

Mirror Interpolants

Given a probability density function $\rho_1 : \mathbb{R}^d \to \mathbb{R}_{\geq 0}$, a mirror stochastic interpolant **between ρ_1 and itself** is a stochastic process x_t^{mir}

$$x_t^{\text{mir}} = K(t, x_1) + \gamma(t) z, \qquad t \in [0, 1] \tag{117}$$

where:

- $K \in C^2([0, 1]; C^2((\mathbb{R}^d)^d))$ satisfies the boundary conditions $K(0, x_1) = x_1$ and $K(1, x_1) = x_1$.
- x_1 and z are random variables drawn independently from ρ_1 and $\mathcal{N}(0, I_d)$, respectively.
- $\gamma : [0, 1] \to \mathbb{R}$ satisfies $\gamma(0) = \gamma(1) = 0$, $\gamma(t) > 0$ for all $t \in (0, 1)$, and $\gamma^2 \in C^1([0, 1])$.

By construction, $x_{t=0}^{\text{mir}} = x_{t=1}^{\text{mir}} = x_1 \sim \rho_1$, so that the distribution of the stochastic process x_t^{mir} **bridges ρ_1 to itself**.

Mirror Interpolants (cont'd)

- Velocity field b becomes

$$b(t, x) = \mathbb{E}(\partial_t K(t, x_1) + \dot{\gamma}(t) z \mid x_t^{\text{mir}} = x). \tag{118}$$

- Quadratic objective becomes

$$\mathcal{L}_b[\hat{b}] = \int_0^1 \mathbb{E}\left(\frac{1}{2}|\hat{b}(t, x_t^{\text{mir}})|^2 - (\partial_t K(t, x_1) + \dot{\gamma}(t) z) \cdot \hat{b}(t, x_t^{\text{mir}})\right) \mathrm{d}t. \tag{119}$$

The expectation $\mathbb{E}$ is taken independently over $x_1 \sim \rho_1$ and $z \sim \mathcal{N}(0, I_d)$.

- The score is given by

$$s(t, x) = -\gamma^{-1}(t) \eta_z(t, x), \qquad \eta_z(t, x) = \mathbb{E}(z \mid x_t^{\text{mir}} = x). \tag{120}$$

- These functions are the unique minimizers of the objectives

$$\mathcal{L}_s[\hat{s}] = \int_0^1 \mathbb{E}\left(\frac{1}{2}|\hat{s}(t, x_t^{\text{mir}})|^2 + \gamma^{-1}(t) z \cdot \hat{s}(t, x_t^{\text{mir}})\right) \mathrm{d}t, \tag{121}$$

$$\mathcal{L}_{\eta_z}[\hat{\eta}_z] = \int_0^1 \mathbb{E}\left(\frac{1}{2}|\hat{\eta}_z(t, x_t^{\text{mir}})|^2 - z \cdot \hat{\eta}_z(t, x_t^{\text{mir}})\right) \mathrm{d}t. \tag{122}$$

Spatially Linear Interpolants

Specialize the function I to be linear in both x_0 and x_1, i.e., we consider

$$x_t^{\text{lin}} = \alpha(t)x_0 + \beta(t)x_1 + \gamma(t)z, \tag{123}$$

where:

- $(x_0, x_1) \sim \nu$.
- $z \sim \mathcal{N}(0, I_d)$ with $(x_0, x_1) \perp z$.
- $\alpha, \beta, \gamma^2 \in C^2([0,1])$ satisfy the conditions

$$\alpha(0) = \beta(1) = 1; \qquad \alpha(1) = \beta(0) = \gamma(0) = \gamma(1) = 0; \qquad \forall t \in (0,1):\ \gamma(t) > 0. \tag{124}$$

Spatially Linear Interpolants (cont'd)

- The velocity b and the score s can both be expressed in terms of the following three conditional expectations

$$\eta_0(t,x) = \mathbb{E}(x_0 \mid x_t^{\text{lin}} = x), \qquad \eta_1(t,x) = \mathbb{E}(x_1 \mid x_t^{\text{lin}} = x), \qquad \eta_z(t,x) = \mathbb{E}(z \mid x_t^{\text{lin}} = x). \tag{125}$$

- Velocity field b becomes

$$b(t,x) = \dot{\alpha}(t)\eta_0(t,x) + \dot{\beta}(t)\eta_1(t,x) + \dot{\gamma}(t)\eta_z(t,x). \tag{126}$$

- The score is given by

$$s(t,x) = -\gamma^{-1}(t)\,\eta_z(t,x). \tag{127}$$

- η_0, η_1, η_z are the unique minimizers of the objectives

$$\mathcal{L}_{\eta_0}(\hat{\eta}_0) = \int_0^1 \mathbb{E}\left[\frac{1}{2}|\hat{\eta}_0(t,x_t^{\text{lin}})|^2 - x_0 \cdot \hat{\eta}_0(t,x_t^{\text{lin}})\right] \mathrm{d}t, \tag{128}$$

$$\mathcal{L}_{\eta_1}(\hat{\eta}_1) = \int_0^1 \mathbb{E}\left[\frac{1}{2}|\hat{\eta}_1(t,x_t^{\text{lin}})|^2 - x_1 \cdot \hat{\eta}_1(t,x_t^{\text{lin}})\right] \mathrm{d}t, \tag{129}$$

$$\mathcal{L}_{\eta_z}(\hat{\eta}_z) = \int_0^1 \mathbb{E}\left[\frac{1}{2}|\hat{\eta}_z(t,x_t^{\text{lin}})|^2 - z \cdot \hat{\eta}_z(t,x_t^{\text{lin}})\right] \mathrm{d}t. \tag{130}$$

The expectation is taken independently over $(x_0, x_1) \sim \nu$ and $z \sim \mathcal{N}(0, I_d)$.

Table of Contents

SMLD: Forward Process

- **SMLD** (Score Matching with Langevin Dynamics) uses a **variance exploding** SDE for the forward process:

$$\mathrm{d}x_t = \sqrt{\frac{\mathrm{d}[\sigma^2(t)]}{\mathrm{d}t}}\,\mathrm{d}w_t, \qquad x_0 \sim p_{\text{data}} \tag{131}$$

  where $\sigma^2(t)$ is a non-decreasing noise schedule and $t \in [0, 1]$.
- This SDE has no drift term and can be solved as a variable-variance Brownian motion:

$$x_t = x_0 + \int_0^t \sqrt{\frac{\mathrm{d}[\sigma^2(s)]}{\mathrm{d}s}}\,\mathrm{d}w_s \tag{132}$$

  The increment term is a zero-mean Gaussian with covariance

$$\int_0^t \frac{\mathrm{d}[\sigma^2(s)]}{\mathrm{d}s}\mathrm{d}s = \sigma^2(t) - \sigma^2(0) \tag{133}$$

  Assuming $\sigma^2(0) = 0$, the variance is simply $\sigma^2(t)$.
- Therefore, the solution simplifies to

$$x_t = x_0 + \sigma(t)\,z \tag{134}$$

  where $z \sim \mathcal{N}(0, I_d)$.

SMLD as Stochastic Interpolant

The SMLD forward process is a special case of the stochastic interpolant framework:

$$x_t = I(t, x_0, x_1) + \gamma(t)\, z \tag{135}$$

with

$$I(t, x_0, x_1) = x_0, \qquad \gamma(t) = \sigma(t) \tag{136}$$

- This is a **one-sided stochastic interpolant** from x_0 (data) to noise.
- At $t = 0$, $x_t = x_0$; as t increases, noise is gradually added.

Reverse Process in SMLD and Stochastic Interpolant

The forward process adds noise (no learning). The reverse process requires learning:

$$d\bar{x}_t = -\frac{d[\sigma^2(t)]}{dt} \nabla_x \log q_t(\bar{x}_t)\, dt + \sqrt{\frac{d[\sigma^2(t)]}{dt}}\, d\bar{w}_t \tag{137}$$

- The score function $\nabla_x \log q_t(x)$ is learned by a neural network $\mathbf{s}_\theta(x, t)$.
- Training pairs (x_0, x_t) are generated by the forward SDE.
- Loss: Denoising score matching

$$\min_\theta \mathbb{E}\left[\left\|\mathbf{s}_\theta(x_t, t) + \frac{x_t - x_0}{\sigma^2(t)}\right\|^2\right] \tag{138}$$

Connection to stochastic interpolant:

- Compare with the general framework: $I(t, x_0, x_1) = x_0$, $\gamma(t) = \sigma(t)$.
- The forward drift $b_{\mathrm{F}}(t, x) = 0$, $\epsilon(t) = \frac{1}{2}\frac{d[\sigma^2(t)]}{dt}$, $b(t, x) = -\frac{1}{2}\frac{d[\sigma^2(t)]}{dt} s(t, x)$.
- The backward drift $b_{\mathrm{B}}(t, x) = -\frac{d[\sigma^2(t)]}{dt} s(t, x)$, with $s(t, x) = \nabla_x \log q_t(\bar{x}_t)$.

DDPM: Forward Process

- **DDPM** (Denoising Diffusion Probabilistic Model) uses a **variance preserving** SDE for the forward process:

$$\mathrm{d}x_t = -\frac{1}{2}\beta(t)x_t\,\mathrm{d}t + \sqrt{\beta(t)}\,\mathrm{d}w_t, \tag{139}$$

  where $\beta(t)$ is the noise schedule, and $t \in [0, 1]$.
- The SDE above admits an analytical solution:

$$x_t = \alpha(t)x_0 + \sqrt{1-\alpha(t)^2}\,z, \tag{140}$$

  where $z \sim \mathcal{N}(0, I_d)$ and

$$\alpha(t) = \exp\left(-\frac{1}{2}\int_0^t \beta(s)\mathrm{d}s\right). \tag{141}$$

DDPM as Stochastic Interpolant

The DDPM forward process is a special case of the stochastic interpolant framework:

$$x_t = I(t, x_0, x_1) + \gamma(t)\, z \tag{142}$$

with

$$I(t, x_0, x_1) = \alpha(t)x_0, \qquad \gamma(t) = \sqrt{1 - \alpha(t)^2} \tag{143}$$

- This is a **one-sided stochastic interpolant** from x_0 (data) to noise.
- At $t = 0$, $x_t = x_0$; as t increases, noise is gradually added.

Reverse Process in DDPM and Stochastic Interpolant

The forward process adds noise (no learning). The reverse process requires learning:

$$\mathrm{d}\bar{x}_t = \left(-\frac{1}{2}\beta(t)\,\bar{x}_t - \beta(t)\nabla_x \log q_t(\bar{x}_t)\right)\mathrm{d}t + \sqrt{\beta(t)}\,\mathrm{d}\bar{w}_t \tag{144}$$

- The score function $\nabla_x \log q_t(x)$ is learned by a neural network $\mathbf{s}_\theta(x,t)$.
- Training pairs (x_0, x_t) are generated by the forward SDE.
- Loss: Denoising score matching

$$\min_\theta \mathbb{E}\left[\left\|\mathbf{s}_\theta(x_t,t) + \frac{1}{1-\alpha(t)^2}(x_t - \alpha(t)x_0)\right\|^2\right] \tag{145}$$

Connection to stochastic interpolant:

- Compare with the general framework: $I(t,x_0,x_1) = \alpha(t)x_0$, $\gamma(t) = \sqrt{1-\alpha(t)^2}$.
- The forward drift $b_\mathrm{F}(t,x) = -\frac{1}{2}\beta(t)x, \quad \epsilon(t) = \frac{1}{2}\beta(t)$.
- The backward drift $b_\mathrm{B}(t,x) = -\frac{1}{2}\beta(t)x - \beta(t)s(t,x)$, with $s(t,x) = \nabla_x \log q_t(x)$.

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Thank you!
Any questions?