

Deep Generative Models

Lecture 13

Roman Isachenko

Moscow Institute of Physics and Technology
Yandex School of Data Analysis

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Outline

1. Flow Matching

- Endpoint conditioning
- Pair conditioning

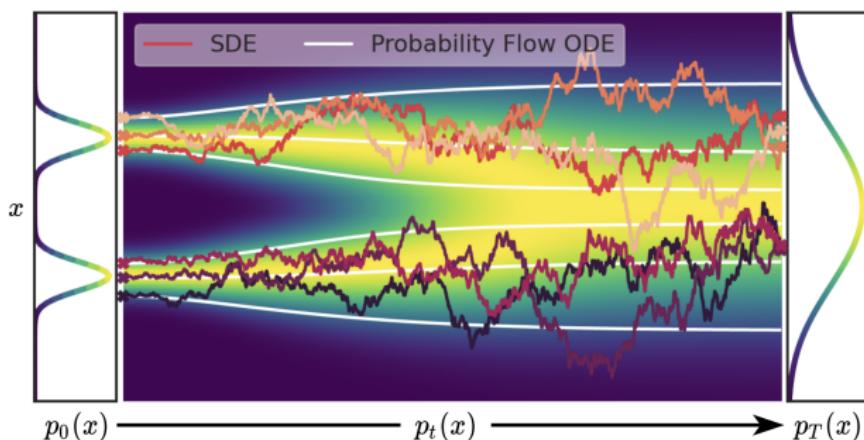
Recap of previous lecture

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w} - \text{SDE with the probability path } p_t(\mathbf{x})$$

Probability flow ODE

There exists ODE with identical the probability path $p_t(\mathbf{x})$ of the form

$$d\mathbf{x} = \left[\mathbf{f}(\mathbf{x}, t) - \frac{1}{2}g^2(t)\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x}) \right] dt$$



Recap of previous lecture

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt, \quad \mathbf{x}(t + dt) = \mathbf{x}(t) + \mathbf{f}(\mathbf{x}, t)dt$$

Reverse ODE

Let $\tau = 1 - t$ ($d\tau = -dt$).

$$d\mathbf{x} = -\mathbf{f}(\mathbf{x}, 1 - \tau)d\tau$$

Reverse SDE

There exists the reverse SDE for the SDE $d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$ that has the following form

$$d\mathbf{x} = \left(\mathbf{f}(\mathbf{x}, t) - g^2(t) \frac{\partial \log p_t(\mathbf{x})}{\partial \mathbf{x}} \right) dt + g(t)d\mathbf{w}, \quad dt < 0$$

Sketch of the proof

- ▶ Convert initial SDE to probability flow ODE.
- ▶ Revert probability flow ODE.
- ▶ Convert reverse probability flow ODE to reverse SDE.

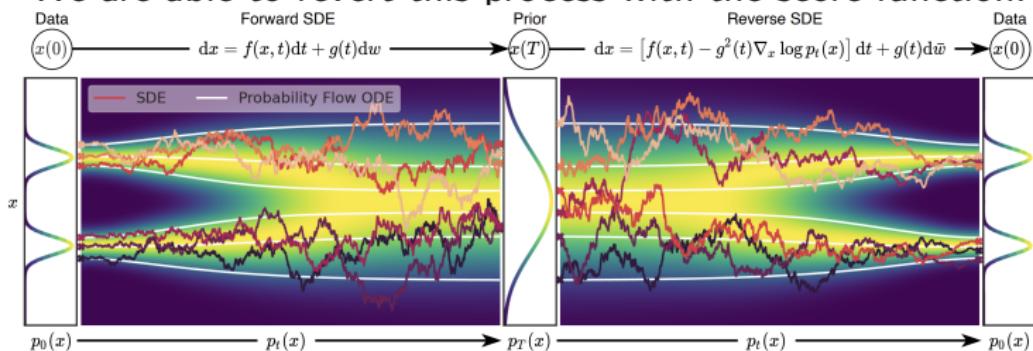
Recap of previous lecture

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w} - \text{SDE}$$

$$d\mathbf{x} = \left[\mathbf{f}(\mathbf{x}, t) - \frac{1}{2}g^2(t)\frac{\partial}{\partial \mathbf{x}} \log p_t(\mathbf{x}) \right] dt - \text{probability flow ODE}$$

$$d\mathbf{x} = \left(\mathbf{f}(\mathbf{x}, t) - g^2(t)\frac{\partial \log p_t(\mathbf{x})}{\partial \mathbf{x}} \right) dt + g(t)d\mathbf{w} - \text{reverse SDE}$$

- ▶ We got the way to transform one distribution to another via SDE with some probability path $p_t(\mathbf{x})$.
- ▶ We are able to revert this process with the score function.



Recap of previous lecture

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$$

Variance Exploding SDE (NCSN)

$$d\mathbf{x} = \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}, \quad \mathbf{f}(\mathbf{x}, t) = 0, \quad g(t) = \sqrt{\frac{d[\sigma^2(t)]}{dt}}$$

Variance grows since $\sigma(t)$ is a monotonically increasing function.

Variance Preserving SDE (DDPM)

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}(t)dt + \sqrt{\beta(t)} \cdot d\mathbf{w}$$

$$\mathbf{f}(\mathbf{x}, t) = -\frac{1}{2}\beta(t)\mathbf{x}(t), \quad g(t) = \sqrt{\beta(t)}$$

Variance is preserved if $\mathbf{x}(0)$ has a unit variance.

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Flow Matching

Let consider ODE dynamic $\mathbf{x}_t = \mathbf{x}(t)$ in time interval $t \in [0, 1]$

- ▶ $\mathbf{x}_0 \sim p_0(\mathbf{x}) = p(\mathbf{x})$, $\mathbf{x}_1 \sim p_1(\mathbf{x}) = \pi(\mathbf{x})$;
- ▶ $p(\mathbf{x})$ is a base distribution ($\mathcal{N}(0, \mathbf{I})$) and $\pi(\mathbf{x})$ is a true data distribution.

Note: the difference with diffusion models in time direction.

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, t),$$

$\mathbf{u}(\mathbf{x}, t) : \mathbb{R}^m \times [0, 1] \rightarrow \mathbb{R}^m$ is a vector field.

$$\frac{\partial p_t(\mathbf{x})}{\partial t} = -\text{div}(\mathbf{u}(\mathbf{x}, t)p_t(\mathbf{x}))$$

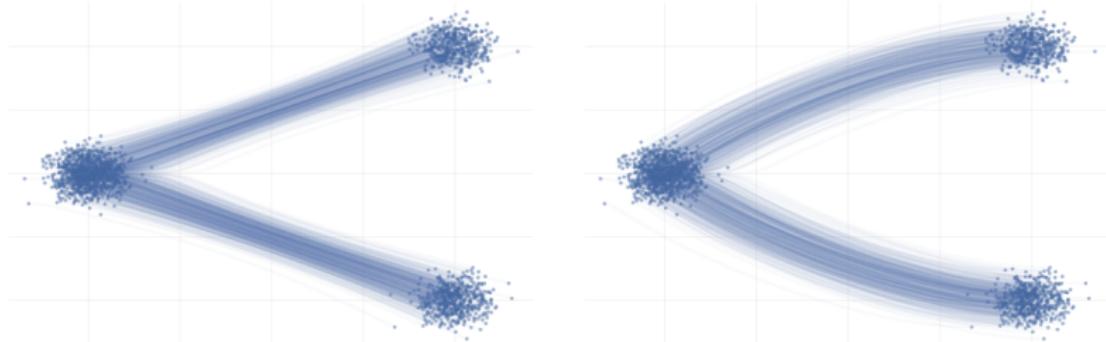
If we know the true vector field $\mathbf{u}(\mathbf{x}, t)$, then KFP equation gives us the way to compute the density $p_t(\mathbf{x})$.

Flow Matching

Flow Matching

$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x})} \|\mathbf{u}(\mathbf{x}, t) - \mathbf{u}_\theta(\mathbf{x}, t)\|^2 \rightarrow \min_{\theta}$$

There exists infinite number of possible $\mathbf{u}(\mathbf{x}, t)$ between $\pi(\mathbf{x})$ and $p(\mathbf{x})$.



Flow Matching

$$p_t(\mathbf{x}) = \int p_t(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z}$$

Here $p_t(\mathbf{x}|\mathbf{z})$ is a **conditional probability path**.

The conditional probability path $p_t(\mathbf{x}|\mathbf{z})$ satisfies KFP theorem

$$\frac{\partial p_t(\mathbf{x}|\mathbf{z})}{\partial t} = -\text{div}(\mathbf{u}(\mathbf{x}, \mathbf{z}, t)p_t(\mathbf{x}|\mathbf{z})),$$

where $\mathbf{u}(\mathbf{x}, \mathbf{z}, t)$ is a **conditional vector field**.

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, t) \quad \Rightarrow \quad \frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, \mathbf{z}, t)$$

Flow Matching

$$\frac{\partial p_t(\mathbf{x}|\mathbf{z})}{\partial t} = -\operatorname{div}(\mathbf{u}(\mathbf{x}, \mathbf{z}, t) p_t(\mathbf{x}|\mathbf{z})),$$

Theorem

$$\mathbf{u}(\mathbf{x}, t) = \int \mathbf{u}(\mathbf{x}, \mathbf{z}, t) \frac{p_t(\mathbf{x}|\mathbf{z}) p(\mathbf{z})}{p_t(\mathbf{x})} d\mathbf{z}$$

Proof

$$\begin{aligned}\frac{\partial p_t(\mathbf{x})}{\partial t} &= \frac{\partial}{\partial t} \int p_t(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z} = \int \left(\frac{\partial p_t(\mathbf{x}|\mathbf{z})}{\partial t} \right) p(\mathbf{z}) d\mathbf{z} = \\ &= \int (-\operatorname{div}(\mathbf{u}(\mathbf{x}, \mathbf{z}, t) p_t(\mathbf{x}|\mathbf{z}))) p(\mathbf{z}) d\mathbf{z} = \\ &= -\operatorname{div} \left(\int \mathbf{u}(\mathbf{x}, \mathbf{z}, t) p_t(\mathbf{x}|\mathbf{z}) p(\mathbf{z}) d\mathbf{z} \right) = -\operatorname{div}(\mathbf{u}(\mathbf{x}, t) p_t(\mathbf{x}))\end{aligned}$$

Flow Matching

Flow Matching

$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x})} \|\mathbf{u}(\mathbf{x}, t) - \mathbf{u}_\theta(\mathbf{x}, t)\|^2 \rightarrow \min_{\theta}$$

Conditional Flow Matching

$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x}|\mathbf{z})} \|\mathbf{u}(\mathbf{x}, \mathbf{z}, t) - \mathbf{u}_\theta(\mathbf{x}, t)\|^2 \rightarrow \min_{\theta}$$

Theorem

If $\text{supp}(p_t(\mathbf{x})) = \mathbb{R}^m$, then the optimal value of FM objective is equal to the optimal value of CFM objective.

Proof

It is proved similarly with the denoising score matching theorem.

Flow Matching

Gaussian conditional probability path

$$p_t(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\boldsymbol{\mu}_t(\mathbf{z}), \boldsymbol{\sigma}_t^2(\mathbf{z}))$$

- ▶ There is an infinite number of vector fields that generate any particular probability path.
- ▶ Let consider the following dynamics:

$$\mathbf{x}_t = \boldsymbol{\mu}_t(\mathbf{z}) + \boldsymbol{\sigma}_t(\mathbf{z}) \odot \mathbf{x}_0$$

Flow Matching

Theorem

$$\mathbf{u}(\mathbf{x}, \mathbf{z}, t) = \boldsymbol{\mu}'_t(\mathbf{z}) + \frac{\boldsymbol{\sigma}'_t(\mathbf{z})}{\boldsymbol{\sigma}_t(\mathbf{z})} \odot (\mathbf{x} - \boldsymbol{\mu}_t(\mathbf{z}))$$

Proof

$$\mathbf{x}_t = \boldsymbol{\mu}_t(\mathbf{z}) + \boldsymbol{\sigma}_t(\mathbf{z}) \odot \mathbf{x}_0 \quad \Rightarrow \quad \mathbf{x}_0 = \frac{1}{\boldsymbol{\sigma}_t(\mathbf{z})} \odot (\mathbf{x}_t - \boldsymbol{\mu}_t(\mathbf{z}))$$

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, \mathbf{z}, t)$$

$$\frac{d\mathbf{x}}{dt} = \boldsymbol{\mu}'_t(\mathbf{z}) + \boldsymbol{\sigma}'_t(\mathbf{z}) \odot \mathbf{x}_0 = \boldsymbol{\mu}'_t(\mathbf{z}) + \frac{\boldsymbol{\sigma}'_t(\mathbf{z})}{\boldsymbol{\sigma}_t(\mathbf{z})} \odot (\mathbf{x} - \boldsymbol{\mu}_t(\mathbf{z}))$$

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Pair conditioning

Flow Matching

Conditional Flow Matching

$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x}|\mathbf{z})} \|\mathbf{u}(\mathbf{x}, \mathbf{z}, t) - \mathbf{u}_\theta(\mathbf{x}, t)\|^2 \rightarrow \min_{\theta}$$

Let choose $\mathbf{z} = \mathbf{x}_1$. Then $p(\mathbf{z}) = p_1(\mathbf{x}_1)$.

$$p_t(\mathbf{x}) = \int p_t(\mathbf{x}|\mathbf{x}_1) p_1(\mathbf{x}_1) d\mathbf{x}_1$$

We need to ensure boundary conditions:

$$\begin{cases} p_0(\mathbf{x}) = p(\mathbf{x}) = \mathcal{N}(0, \mathbf{I}); \\ p_1(\mathbf{x}) = \pi(\mathbf{x}). \end{cases} \Rightarrow \begin{cases} p_0(\mathbf{x}|\mathbf{x}_1) = p_0(\mathbf{x}); \\ p_1(\mathbf{x}|\mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1). \end{cases}$$

Gaussian conditional probability path

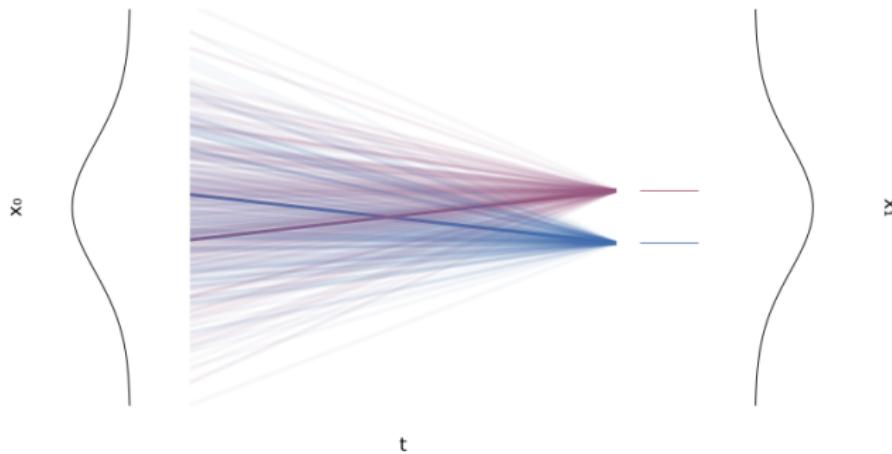
$$p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(\boldsymbol{\mu}_t(\mathbf{x}_1), \boldsymbol{\sigma}_t^2(\mathbf{x}_1)); \quad \mathbf{x}_t = \boldsymbol{\mu}_t(\mathbf{x}_1) + \boldsymbol{\sigma}_t^2(\mathbf{x}_1) \odot \mathbf{x}_0.$$

Flow Matching

Gaussian conditional probability path

$$p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(\boldsymbol{\mu}_t(\mathbf{x}_1), \boldsymbol{\sigma}_t^2(\mathbf{x}_1)); \quad \mathbf{x}_t = \boldsymbol{\mu}_t(\mathbf{x}_1) + \boldsymbol{\sigma}_t^2(\mathbf{x}_1)\mathbf{x}_0.$$

$$p_0(\mathbf{x}|\mathbf{x}_1) = p_0(\mathbf{x}) \quad p_1(\mathbf{x}|\mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1)$$



Flow Matching

$$\begin{cases} p_0(\mathbf{x}|\mathbf{x}_1) = p_0(\mathbf{x}); \\ p_1(\mathbf{x}|\mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1). \end{cases} \Rightarrow \begin{cases} \mu_0(\mathbf{x}_1) = 0, & \sigma_0(\mathbf{x}_1) = 1; \\ \mu_1(\mathbf{x}_1) = \mathbf{x}_1, & \sigma_1(\mathbf{x}_1) = 0. \end{cases}$$

Let consider straight conditional paths

$$\begin{cases} \mu_t(\mathbf{x}_1) = t\mathbf{x}_1; \\ \sigma_t(\mathbf{x}_1) = (1-t). \end{cases} \Rightarrow \begin{cases} p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(t\mathbf{x}_1, (1-t)^2); \\ \mathbf{x}_t = t\mathbf{x}_1 + (1-t)\mathbf{x}_0. \end{cases}$$

$$\mathbf{u}(\mathbf{x}, \mathbf{x}_1, t) = \mu'_t(\mathbf{x}_1) + \frac{\sigma'_t(\mathbf{x}_1)}{\sigma_t(\mathbf{x}_1)} \odot (\mathbf{x} - \mu_t(\mathbf{x}_1))$$

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, \mathbf{z}, t); \quad \mathbf{u}(\mathbf{x}, \mathbf{x}_1, t) = \frac{\mathbf{x}_1 - \mathbf{x}}{1-t}; \quad \frac{d\mathbf{x}}{dt} = \mathbf{x}_1 - \mathbf{x}_0.$$

Flow Matching

Conditional Flow Matching

$$\begin{aligned} \mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x}|\mathbf{z})} \| \mathbf{u}(\mathbf{x}, \mathbf{z}, t) - \mathbf{u}_\theta(\mathbf{x}, t) \|^2 = \\ \mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{x}_1 \sim \pi(\mathbf{x})} \mathbb{E}_{\mathbf{x}_0 \sim p(\mathbf{x})} \| (\mathbf{x}_1 - \mathbf{x}_0) - \mathbf{u}_\theta(\mathbf{x}, t) \|^2 \rightarrow \min_{\theta} \end{aligned}$$

We fit straight lines between noise distribution $p(\mathbf{x})$ and the data distribution $\pi(\mathbf{x})$.

Flow Matching

- ▶ The conditional probability path $p_t(\mathbf{x}|\mathbf{z})$ is an optimal transport path from $p_0(\mathbf{x}|\mathbf{z})$ to $p_1(\mathbf{x}|\mathbf{z})$.
- ▶ The marginal path $p_t(\mathbf{x})$ is not in general an optimal transport path from the standard normal $p_0(\mathbf{x})$ to the data distribution $p_1(\mathbf{x})$.



Flow Matching

Flow matching probability path

$$p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(t\mathbf{x}_1, (1-t)^2); \quad \mathbf{u}(\mathbf{x}, \mathbf{x}_1, t) = \frac{\mathbf{x}_1 - \mathbf{x}}{1-t}$$

Variance Exploding SDE probability path

$$d\mathbf{x} = \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}; \quad \Rightarrow \quad \begin{cases} p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(\mathbf{x}_1, \sigma_{1-t}^2 \mathbf{I}) \\ \mathbf{u}(\mathbf{x}, \mathbf{x}_1, t) = -\frac{\sigma'_{1-t}}{\sigma_{1-t}} \cdot (\mathbf{x} - \mathbf{x}_1) \end{cases}$$

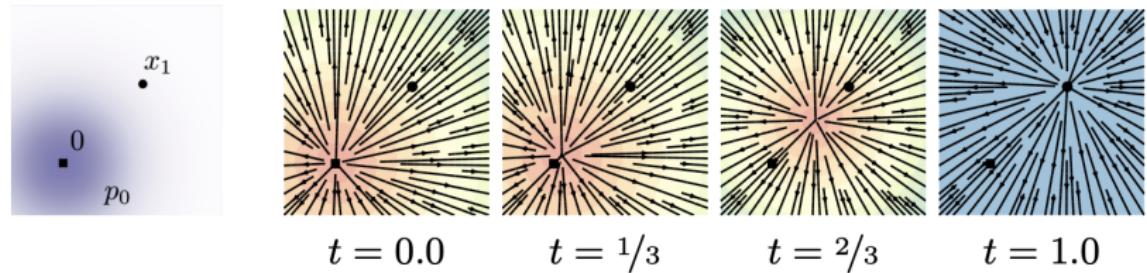
Variance Preserving SDE probability path

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}(t)dt + \sqrt{\beta(t)}d\mathbf{w}; \Rightarrow \begin{cases} p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(\alpha_{1-t}\mathbf{x}_1, (1-\alpha_{1-t}^2)\mathbf{I}) \\ \mathbf{u}(\mathbf{x}, \mathbf{x}_1, t) = \frac{\alpha'_{1-t}}{1-\alpha_{1-t}^2} \cdot (\alpha_{1-t}\mathbf{x} - \mathbf{x}_1) \end{cases}$$

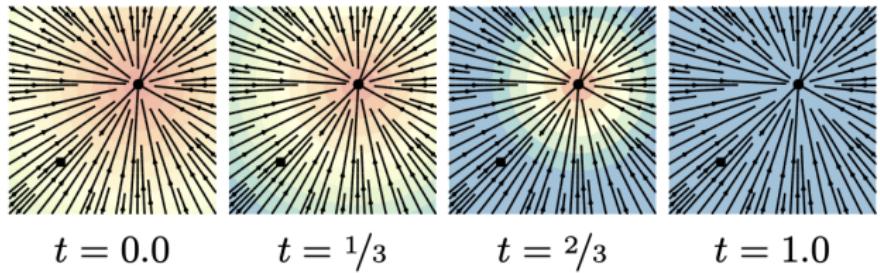
Here $\alpha_t = \exp\left(-\frac{1}{2} \int_0^t \beta(s)ds\right)$.

Flow Matching

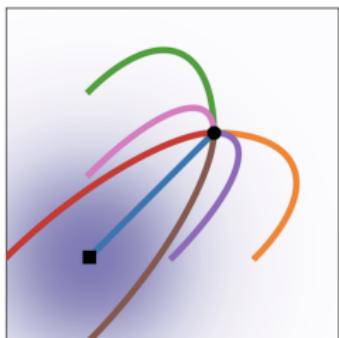
Diffusion vector field



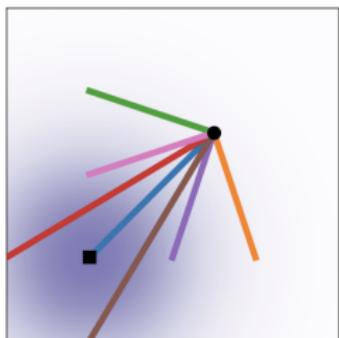
Flow matching vector field



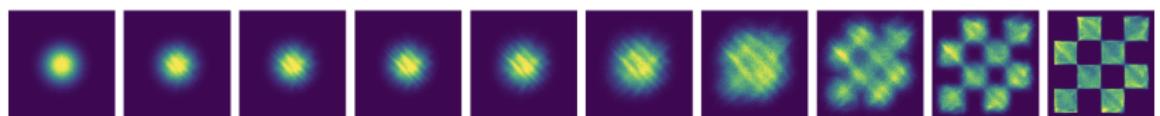
Flow Matching



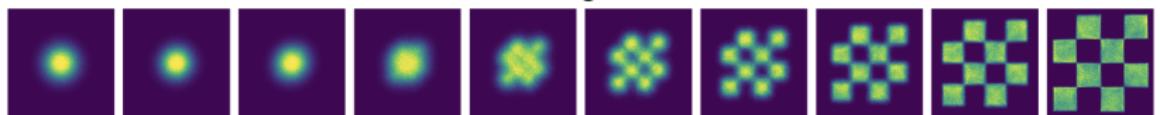
Diffusion



OT



Score matching w/ Diffusion



Flow Matching w/ OT

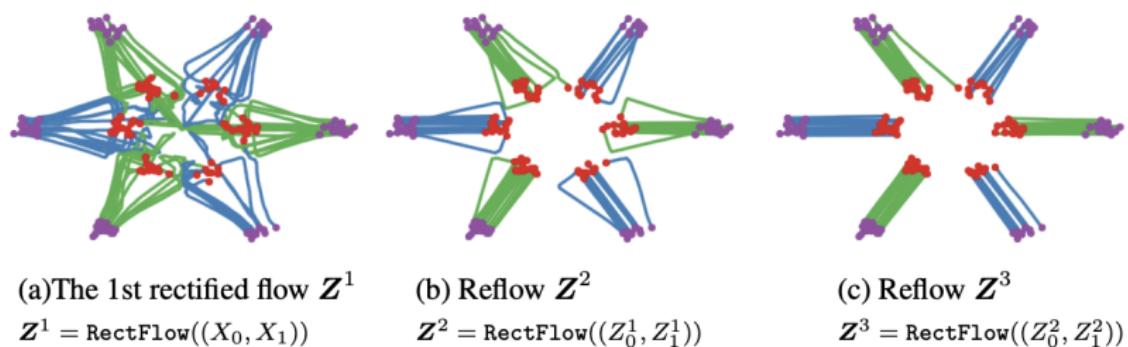
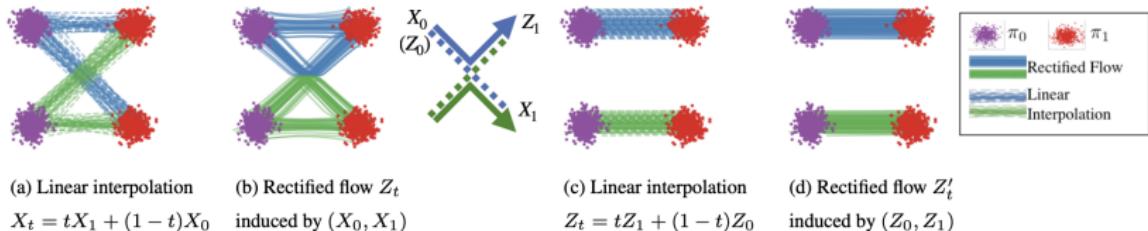
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1. Flow Matching

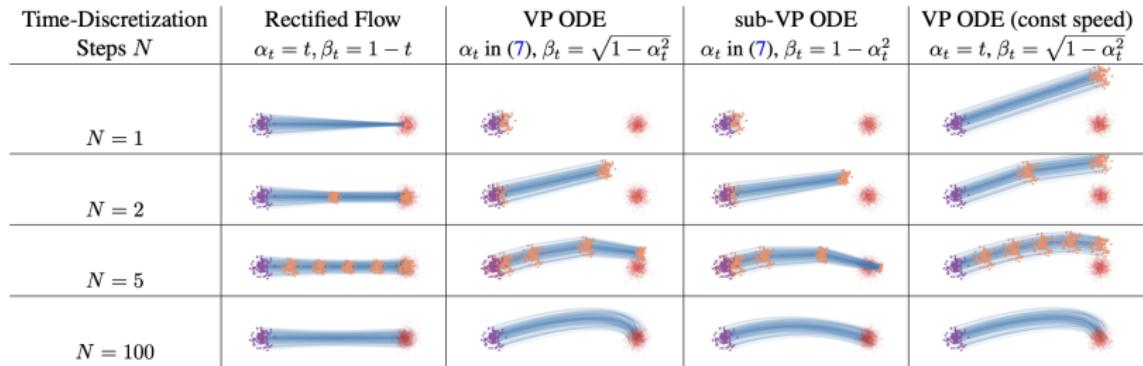
Endpoint conditioning

Pair conditioning

Flow Matching



Flow Matching



Summary

