

Deep Generative Models

Lecture 14

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Outline

1. Conditional flow matching

Conical gaussian paths (continued)

Link with score-based models

Linear interpolation

Rectified flows

2. Latent space models

Score-based models

Autoregressive models

3. The worst course overview

Recap of previous lecture

Discrete-in-time objective

$$\mathbb{E}_{\pi(\mathbf{x}_0)} \mathbb{E}_{t \sim U\{1, T\}} \mathbb{E}_{q(\mathbf{x}_t | \mathbf{x}_0)} \| \mathbf{s}_{\theta, t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x}_0) \|_2^2$$

Continuous-in-time objective

$$\mathbb{E}_{\pi(\mathbf{x}(0))} \mathbb{E}_{t \sim U[0, 1]} \mathbb{E}_{q(\mathbf{x}(t) | \mathbf{x}(0))} \| \mathbf{s}_{\theta}(\mathbf{x}(t), t) - \nabla_{\mathbf{x}(t)} \log q(\mathbf{x}(t) | \mathbf{x}(0)) \|_2^2$$

NCSN

$$q(\mathbf{x}(t) | \mathbf{x}(0)) = \mathcal{N} (\mathbf{x}(0), [\sigma^2(t) - \sigma^2(0)] \cdot \mathbf{I})$$

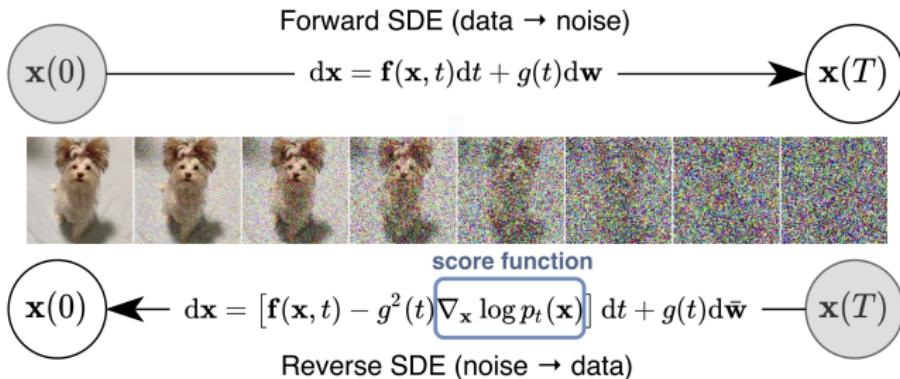
DDPM

$$q(\mathbf{x}(t) | \mathbf{x}(0)) = \mathcal{N} \left(\mathbf{x}(0) e^{-\frac{1}{2} \int_0^t \beta(s) ds}, \left(1 - e^{-\int_0^t \beta(s) ds} \right) \cdot \mathbf{I} \right)$$

Recap of previous lecture

Sampling

Solve reverse SDE using numerical solvers (SDESolve).



- ▶ Discretization of the reverse SDE gives us the ancestral sampling.
- ▶ If we use probability flow instead of SDE than the reverse ODE gives us the DDIM sampling.

Recap of previous lecture

Let consider ODE dynamic $\mathbf{x}(t)$ in time interval $t \in [0, 1]$ with $\mathbf{x}_0 \sim p_0(\mathbf{x}) = p(\mathbf{x})$, $\mathbf{x}_1 \sim p_1(\mathbf{x}) = \pi(\mathbf{x})$.

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t), \quad \text{with initial condition } \mathbf{x}(0) = \mathbf{x}_0.$$

KFP theorem (continuity equation)

$$\frac{\partial p_t(\mathbf{x})}{\partial t} = -\operatorname{div}(\mathbf{f}(\mathbf{x}, t)p_t(\mathbf{x})) \Leftrightarrow \frac{d \log p_t(\mathbf{x}(t))}{dt} = -\operatorname{tr}\left(\frac{\partial \mathbf{f}(\mathbf{x}(t), t)}{\partial \mathbf{x}(t)}\right)$$

Solving the continuity equation using the adjoint method is complicated and unstable process.

Flow Matching

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

Recap of previous lecture

Let's introduce the latent variable \mathbf{z} :

$$p_t(\mathbf{x}) = \int p_t(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z}$$
$$\frac{\partial p_t(\mathbf{x}|\mathbf{z})}{\partial t} = -\text{div}(\mathbf{f}(\mathbf{x}, \mathbf{z}, t)p_t(\mathbf{x}|\mathbf{z})).$$

- ▶ $p_t(\mathbf{x}|\mathbf{z})$ is a **conditional probability path**;
- ▶ $\mathbf{f}(\mathbf{x}, \mathbf{z}, t)$ is a **conditional vector field**.

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

Theorem

The following vector field generates the probability path $p_t(\mathbf{x})$.

$$\mathbf{f}(\mathbf{x}, t) = \mathbb{E}_{p_t(\mathbf{z}|\mathbf{x})}\mathbf{f}(\mathbf{x}, \mathbf{z}, t) = \int \mathbf{f}(\mathbf{x}, \mathbf{z}, t) \frac{p_t(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{p_t(\mathbf{x})} d\mathbf{z}$$

Recap of previous lecture

Flow Matching (FM)

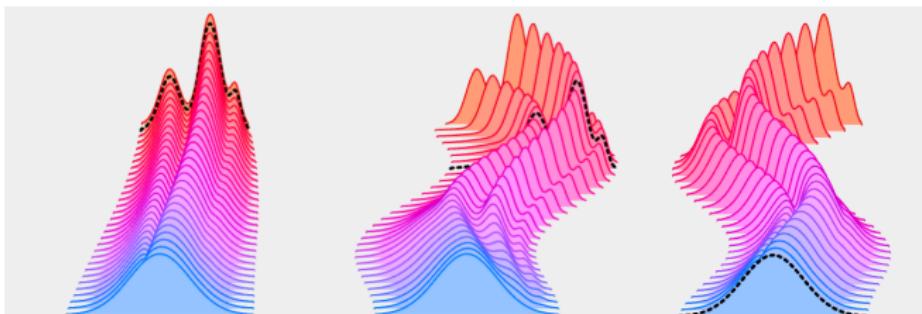
$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x})} \|\mathbf{f}(\mathbf{x}, t) - \mathbf{f}_\theta(\mathbf{x}, t)\|^2 \rightarrow \min_{\theta}$$

Conditional Flow Matching (CFM)

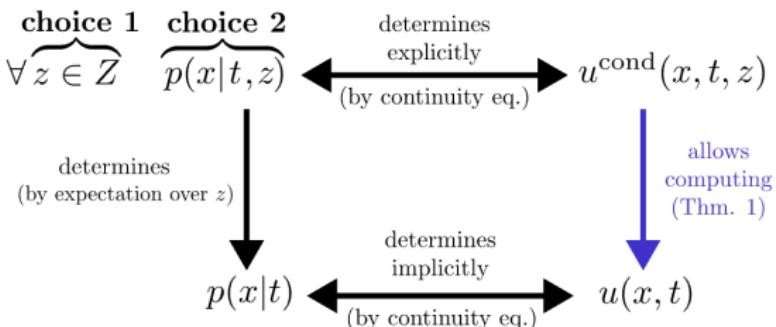
$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x}|\mathbf{z})} \|\mathbf{f}(\mathbf{x}, \mathbf{z}, t) - \mathbf{f}_\theta(\mathbf{x}, t)\|^2 \rightarrow \min_{\theta}$$

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.



Recap of previous lecture



Constraints

$$p(\mathbf{x}) = \mathcal{N}(0, \mathbf{I}) = \mathbb{E}_{p(z)} p_0(\mathbf{x}|z); \quad \pi(\mathbf{x}) = \mathbb{E}_{p(z)} p_1(\mathbf{x}|z).$$

- ▶ How to choose the conditioning latent variable z ?
- ▶ How to define $p_t(\mathbf{x}|z)$ which follows the constraints?

Gaussian conditional probability path

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

$$\mathbf{x}_t = \boldsymbol{\mu}_t(z) + \boldsymbol{\sigma}_t(z) \odot \mathbf{x}_0, \quad \mathbf{x}_0 \sim p_0(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$$

Recap of previous lecture

Gaussian conditional probability path

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

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

Conditioning latent variable

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 constraints:

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

Recap of previous lecture

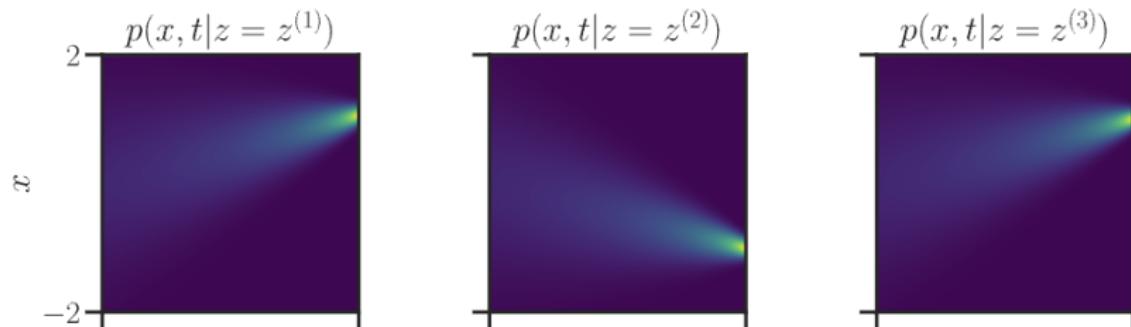
$$p_0(\mathbf{x}|\mathbf{x}_1) = \mathcal{N}(0, \mathbf{I}); \quad p_1(\mathbf{x}|\mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1).$$

Gaussian conditional probability path

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

Let consider straight conditional paths

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



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Conical gaussian paths (continued)

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Conical gaussian paths

$$p_t(\mathbf{x}|\mathbf{x}_1) = \mathcal{N} \left(t\mathbf{x}_1, (1-t)^2 \mathbf{I} \right); \quad \mathbf{x}_t = t\mathbf{x}_1 + (1-t)\mathbf{x}_0.$$

Conditional vector field

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

$$\begin{aligned} \mathbf{f}(\mathbf{x}, \mathbf{x}_1, t) &= \mathbf{x}_1 - \frac{1}{1-t} \cdot (\mathbf{x} - t\mathbf{x}_1) = \frac{\mathbf{x}_1 - \mathbf{x}}{1-t} = \\ &= \frac{\mathbf{x}_1 - t\mathbf{x}_1 + (1-t)\mathbf{x}_0}{1-t} = \mathbf{x}_1 - \mathbf{x}_0 \end{aligned}$$

Conditional Flow Matching

$$\begin{aligned} \mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x}|\mathbf{z})} \|\mathbf{f}(\mathbf{x}, \mathbf{z}, t) - \mathbf{f}_\theta(\mathbf{x}, t)\|^2 &= \\ \mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{x}_1 \sim \pi(\mathbf{x})} \mathbb{E}_{\mathbf{x} \sim p_t(\mathbf{x}|\mathbf{x}_1)} \left\| \left(\frac{\mathbf{x}_1 - \mathbf{x}}{1-t} \right) - \mathbf{f}_\theta(\mathbf{x}, t) \right\|^2 &= \\ \mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{x}_1 \sim \pi(\mathbf{x})} \mathbb{E}_{\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})} \|(\mathbf{x}_1 - \mathbf{x}_0) - \mathbf{f}_\theta(t\mathbf{x}_1 + (1-t)\mathbf{x}_0, t)\|^2 \end{aligned}$$

Conditional Flow Matching

$$\mathbb{E}_{t \sim U[0,1]} \mathbb{E}_{\mathbf{x}_1 \sim \pi(\mathbf{x})} \mathbb{E}_{\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})} \|(\mathbf{x}_1 - \mathbf{x}_0) - \mathbf{f}_\theta(\mathbf{x}, t)\|^2 \rightarrow \min_{\theta}$$

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

Training

1. Get the sample $\mathbf{x}_1 \sim \pi(\mathbf{x})$.
2. Sample timestamp $t \sim U\{1, T\}$ and $\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})$.
3. Get noisy image $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}$.
4. Compute loss $\mathcal{L} = \|(\mathbf{x}_1 - \mathbf{x}_0) - \mathbf{f}_\theta(\mathbf{x}, t)\|^2$.

Sampling

1. Sample $\mathbf{x}_0 \sim \mathcal{N}(0, \mathbf{I})$.
2. Solve the ODE to get \mathbf{x}_1 :

$$\mathbf{x}_1 = \text{ODESolve}_f(\mathbf{x}_0, \theta, t_0 = 0, t_1 = 1).$$

Flow Matching

$$\mathbf{x}_t = t\mathbf{x}_1 + (1 - t)\mathbf{x}_0$$

- ▶ The conditional probability path $p_t(\mathbf{x}|\mathbf{z})$ is an **optimal transport path** from $p_0(\mathbf{x}|\mathbf{z})$ to $p_1(\mathbf{x}|\mathbf{z})$ (in terms of the conditional trajectories straightness).
- ▶ 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 $p_1(\mathbf{x})$.



image credit: <https://mlg.eng.cam.ac.uk/blog/2024/01/20/flow-matching.html>

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Conical gaussian paths (continued)

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Flow matching vs score-based SDE models

Flow matching probability path

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

Variance Exploding SDE probability path

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

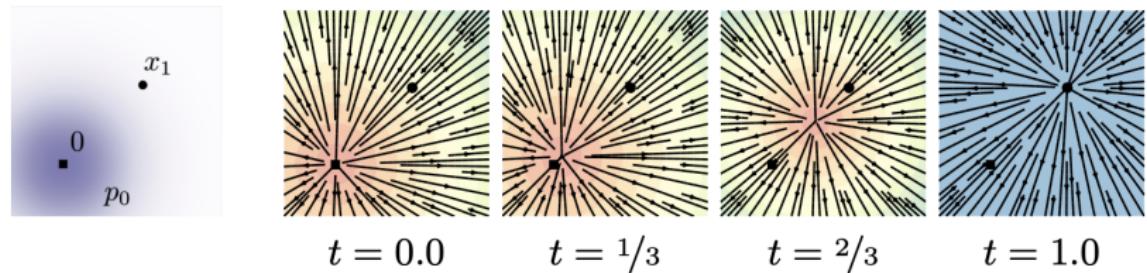
Variance Preserving SDE probability path

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

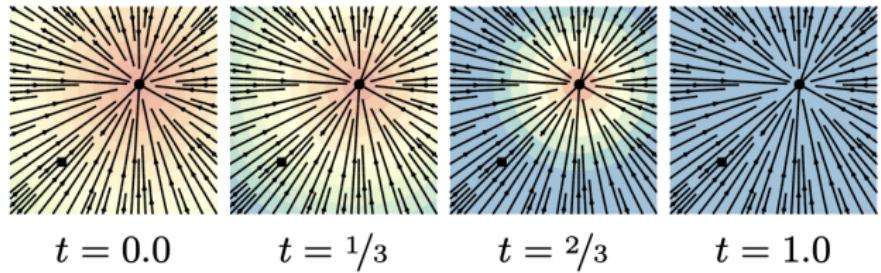
Here $\alpha_t = \exp\left(-\frac{1}{2} \int_0^t \beta(s)ds\right)$.

Flow matching vs score-based SDE models

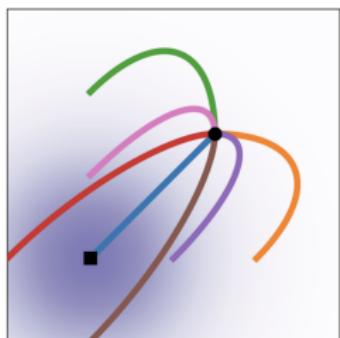
Diffusion vector field



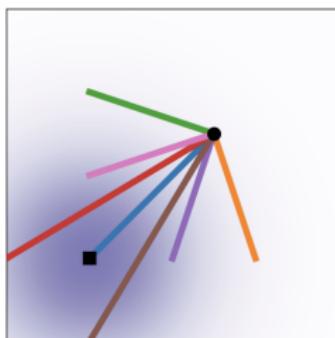
Flow matching vector field



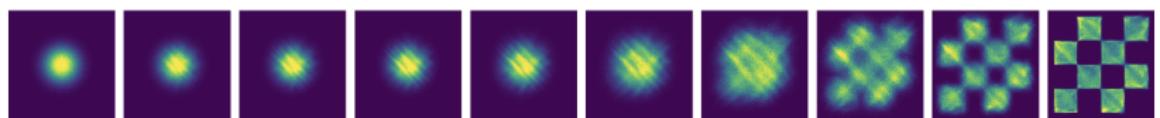
Flow matching vs score-based SDE models



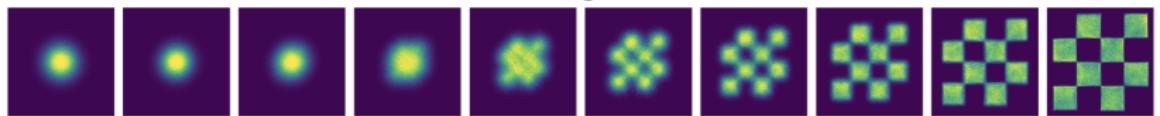
Diffusion



OT



Score matching w/ Diffusion



Flow Matching w/ OT

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Flow Matching

Conditional Flow Matching

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

Let choose $\mathbf{z} = (\mathbf{x}_0, \mathbf{x}_1)$. Then $p(\mathbf{z}) = p_0(\mathbf{x}_0)p_1(\mathbf{x}_1)$.

$$p_t(\mathbf{x}) = \int p_t(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) p_0(\mathbf{x}_0) p_1(\mathbf{x}_1) d\mathbf{x}_0 d\mathbf{x}_1$$

We need to ensure boundary conditions:

$$\begin{cases} p_0(\mathbf{x}) = p(\mathbf{x}) = \mathcal{N}(0, \mathbf{I}); \\ p_1(\mathbf{x}) = \pi(\mathbf{x}). \end{cases} \Rightarrow \begin{cases} p_0(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_0); \\ p_1(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1). \end{cases}$$

Gaussian conditional probability path

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

Flow Matching

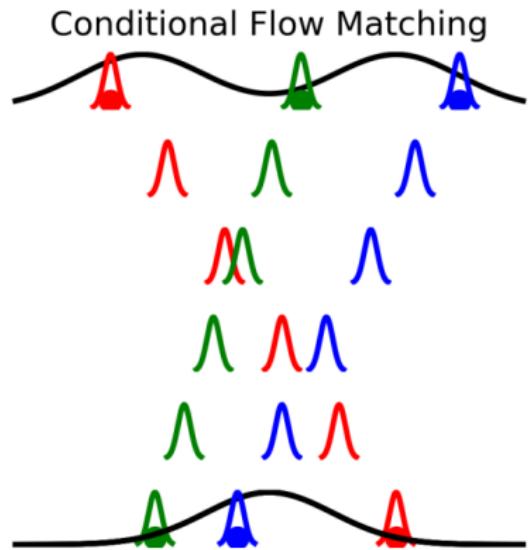
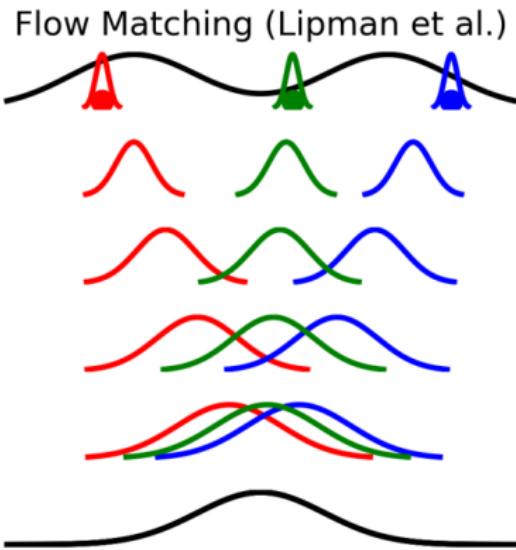
$$\begin{cases} p_0(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_0); \\ p_1(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \delta(\mathbf{x} - \mathbf{x}_1). \end{cases} \Rightarrow \begin{cases} \mu_0(\mathbf{x}_0, \mathbf{x}_1) = \mathbf{x}_0, & \sigma_0(\mathbf{x}_0, \mathbf{x}_1) = 0 \\ \mu_1(\mathbf{x}_0, \mathbf{x}_1) = \mathbf{x}_1, & \sigma_1(\mathbf{x}_0, \mathbf{x}_1) = 0 \end{cases}$$

Let consider straight conditional paths

$$\begin{cases} \mu_t(\mathbf{x}_0, \mathbf{x}_1) = t\mathbf{x}_1 + (1 - t)\mathbf{x}_0; \\ \sigma_t(\mathbf{x}_0, \mathbf{x}_1) = 0. \end{cases} \Rightarrow \begin{cases} p_t(\mathbf{x}|\mathbf{x}_0, \mathbf{x}_1) = \mathcal{N}(t\mathbf{x}_1 + (1 - t)\mathbf{x}_0, 0) \\ \mathbf{x}_t = t\mathbf{x}_1 + (1 - t)\mathbf{x}_0. \end{cases}$$

$$\frac{d\mathbf{x}}{dt} = \mathbf{x}_1 - \mathbf{x}_0.$$

Flow Matching



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Conical gaussian paths (continued)

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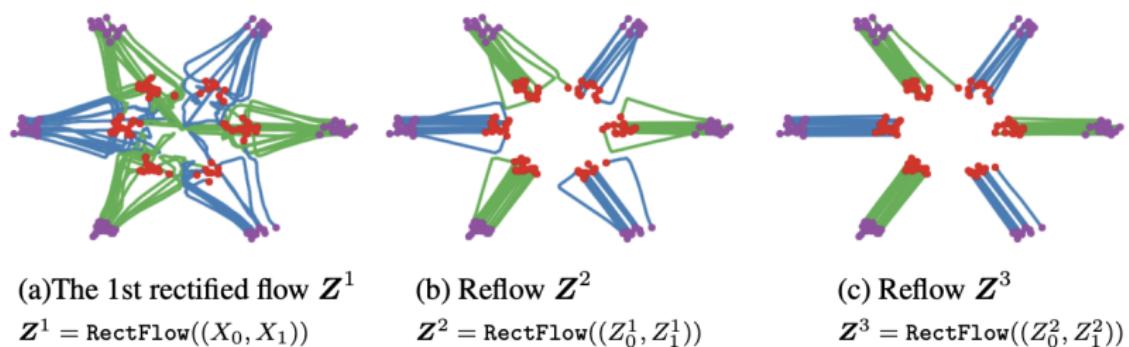
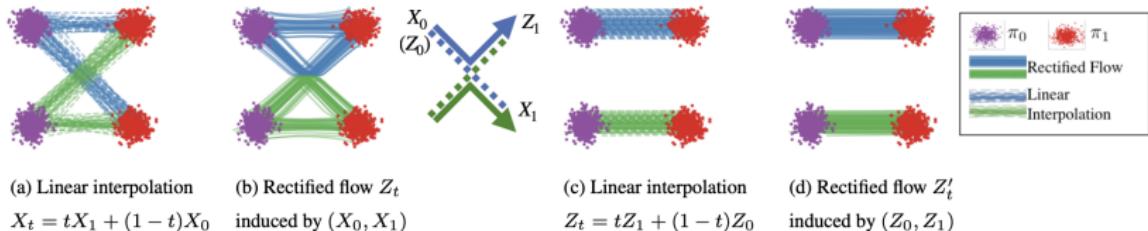
2. Latent space models

Score-based models

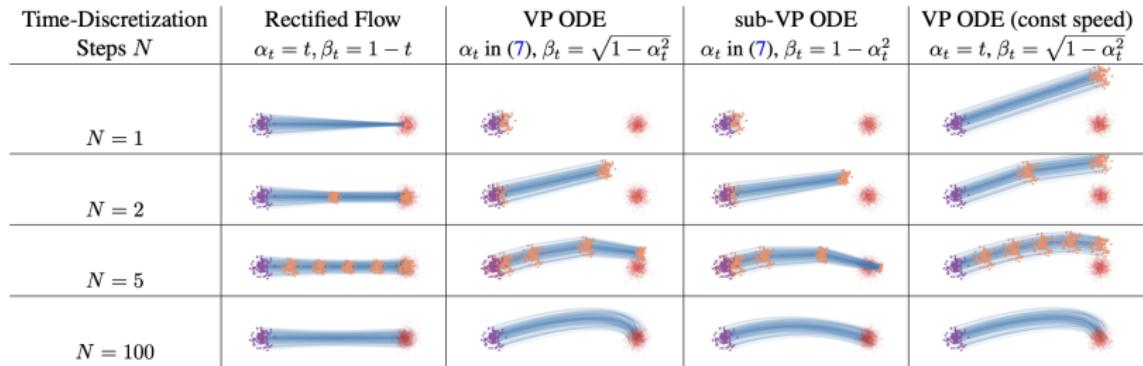
Autoregressive models

3. The worst course overview

Rectified flows



Rectified flows



Rectified flows



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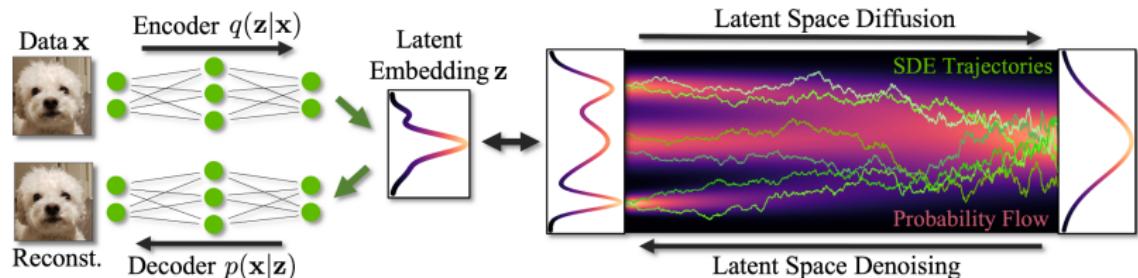
Score-based models

Autoregressive models

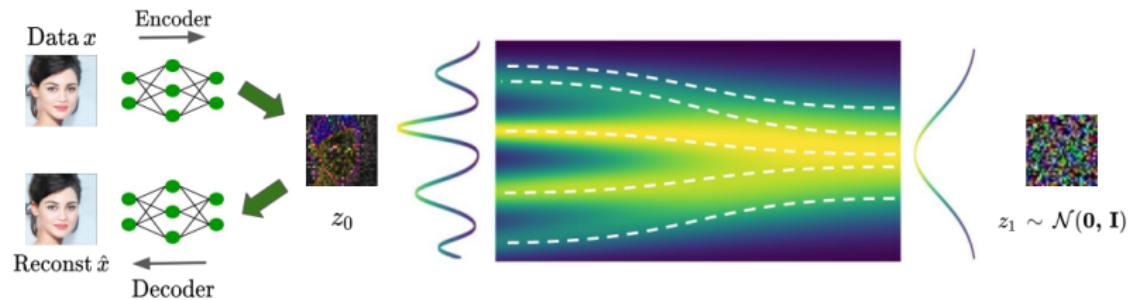
3. The worst course overview

Latent space models

Score-based models (diffusion)



Flow matching



Dao Q. et al. *Flow Matching in Latent Space*, 2023

NeurIPS 2023 Tutorial: Latent Diffusion Models: Is the Generative AI Revolution Happening in Latent Space?

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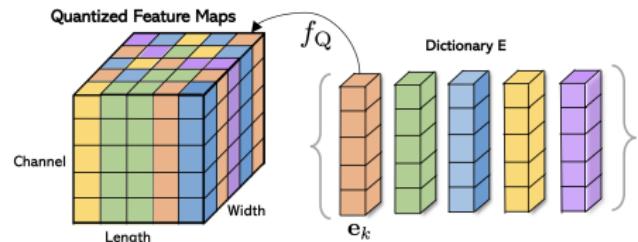
Vector Quantized VAE (VQ-VAE)

Vector quantization

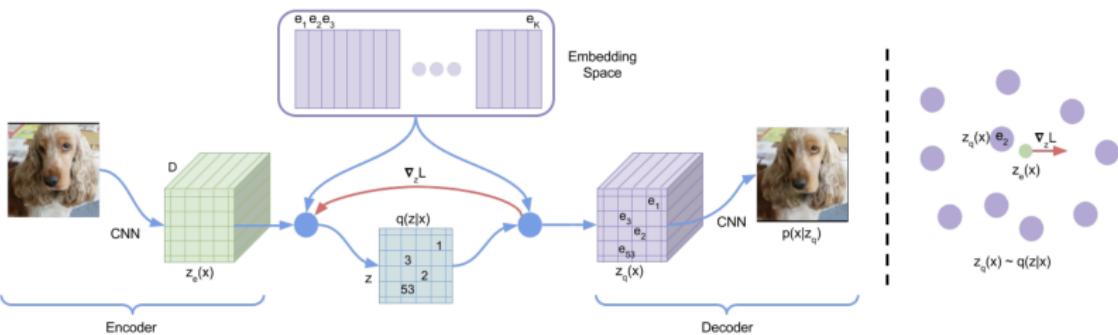
Define the dictionary space $\{\mathbf{e}_k\}_{k=1}^K$, where $\mathbf{e}_k \in \mathbb{R}^C$, K is the size of the dictionary.

$$\mathbf{z}_q = \mathbf{q}(\mathbf{z}) = \mathbf{e}_{k^*}$$

$$\text{Here } k^* = \arg \min_k \|\mathbf{z} - \mathbf{e}_k\|.$$



$$\mathcal{L}_{\phi, \theta}(\mathbf{x}) = \log p(\mathbf{x} | \mathbf{z}_q, \theta) - \log K$$

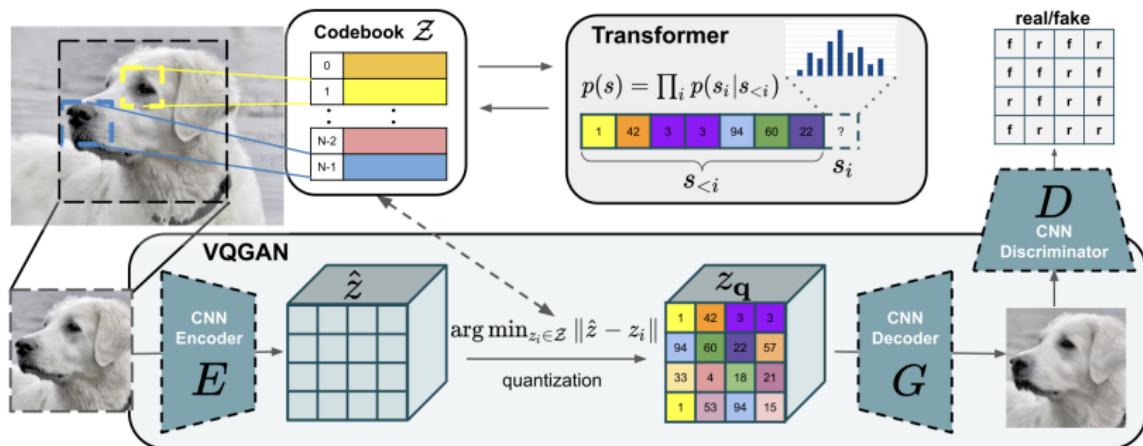


Zhao Y. et al. Feature Quantization Improves GAN Training, 2020

Oord A., Vinyals O., Kavukcuoglu K. Neural Discrete Representation Learning, 2017

Vector Quantized GAN

- ▶ Use VQVAE model and objective.
- ▶ Add adversarial loss between generated and real images to improve the visual quality of the reconstructions.

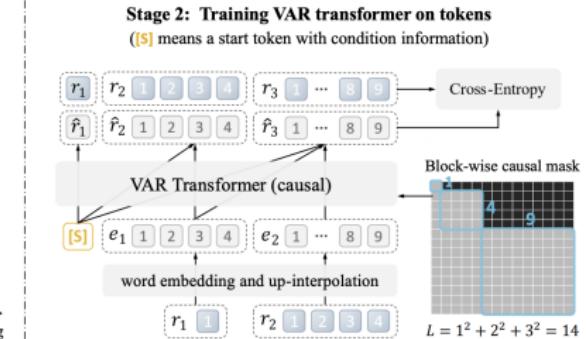
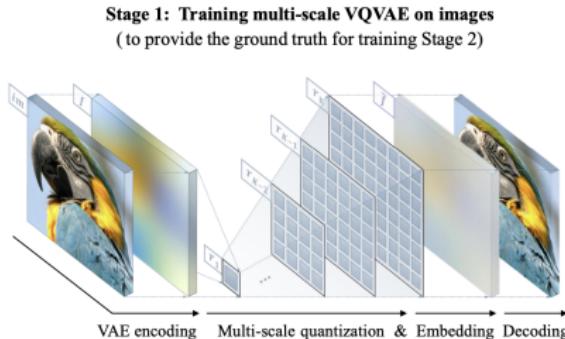
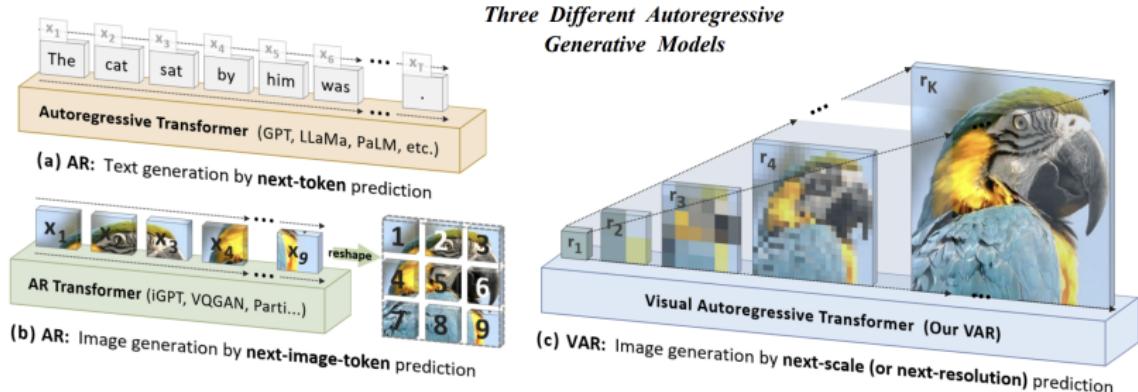


LlamaGen: pure autoregression

- ▶ Use VQGAN encoder to map images to the discrete latent space of the codebook vectors.
- ▶ Learn the pure autoregression model (Llama-based) in the latent space.
- ▶ Use VQGAN decoder to map the discrete space tokens to the image space.



Visual Autoregressive Modeling (VAR)



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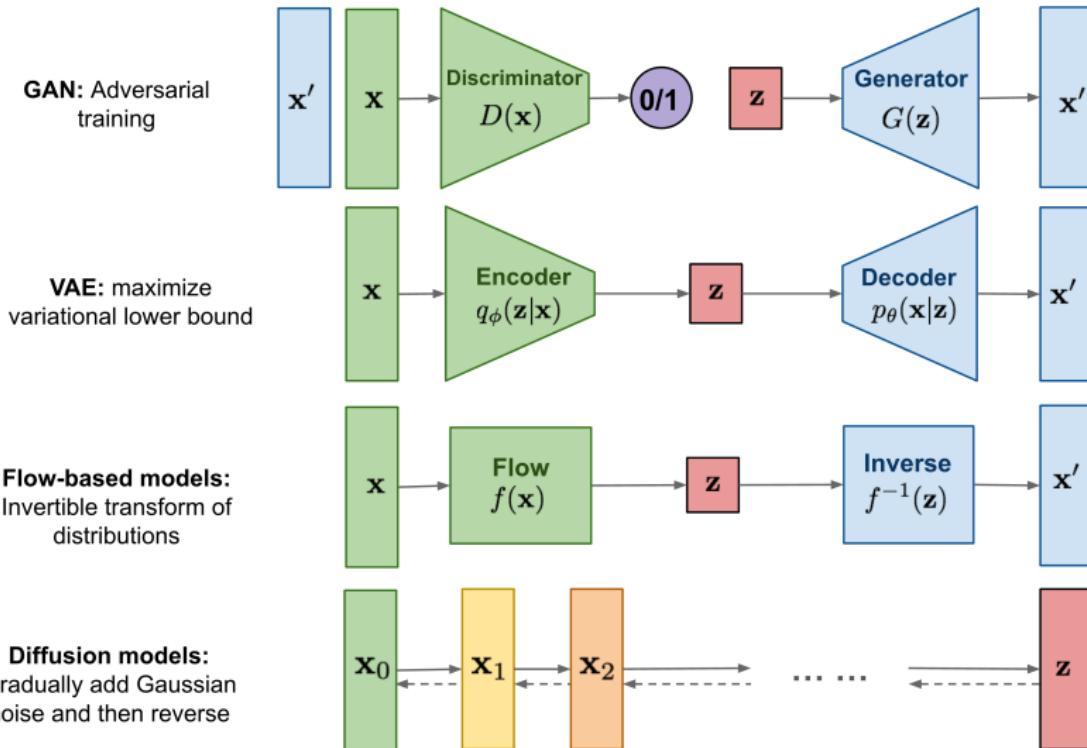
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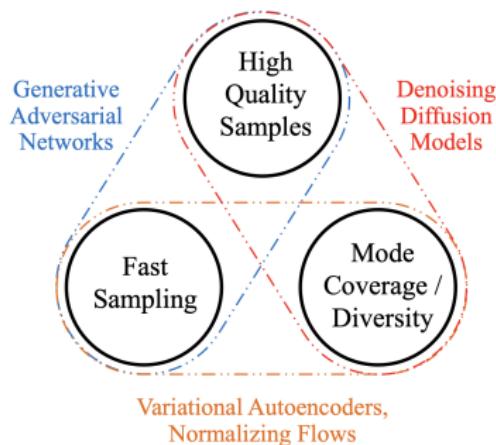
Autoregressive models

3. The worst course overview

The worst course overview :)



The worst course overview :)



Model	Efficient	Sample quality	Coverage	Well-behaved latent space	Disentangled latent space	Efficient likelihood
GANs	✓	✓	✗	✓	?	n/a
VAEs	✓	✗	?	✓	?	✗
Flows	✓	✗	?	✓	?	✓
Diffusion	✗	✓	?	✗	✗	✗

Xiao Z., Kreis K., Vahdat A. *Tackling the generative learning trilemma with denoising diffusion GANs*, 2021

Simon J.D. Prince. *Understanding Deep Learning*, 2023

Summary

- ▶ Conical gaussian paths is the example of the effective FM technique.
- ▶