

Deep Generative Models

Lecture 10

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Recap of Previous Lecture

Forward Process: Converts an arbitrary distribution $\pi(\mathbf{x})$ into the standard normal $\mathcal{N}(0, \mathbf{I})$ by incrementally adding noise.

$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\sqrt{1 - \beta_t} \mathbf{x}_{t-1}, \beta_t \mathbf{I});$$
$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0, (1 - \bar{\alpha}_t) \mathbf{I}).$$

Reverse Process: This intractable distribution can be well-approximated by a Gaussian (with unknown parameters) when β_t is sufficiently small.

$$q(\mathbf{x}_{t-1} | \mathbf{x}_t) = \frac{q(\mathbf{x}_t | \mathbf{x}_{t-1}) q(\mathbf{x}_{t-1})}{q(\mathbf{x}_t)} \approx \mathcal{N}(\boldsymbol{\mu}_{\theta,t}(\mathbf{x}_t), \sigma_{\theta,t}^2(\mathbf{x}_t))$$

Conditioned Reverse Process: This Gaussian, with known parameters, describes how to denoise a noisy image \mathbf{x}_t when the final clean image \mathbf{x}_0 is known.

$$q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I})$$

Recap of Previous Lecture

- ▶ $\mathbf{z} = (\mathbf{x}_1, \dots, \mathbf{x}_T)$ represents the latent variables.
- ▶ Variational posterior distribution:

$$q(\mathbf{z}|\mathbf{x}) = q(\mathbf{x}_1, \dots, \mathbf{x}_T|\mathbf{x}_0) = \prod_{t=1}^T q(\mathbf{x}_t|\mathbf{x}_{t-1}).$$

- ▶ Generative model and prior:

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = p(\mathbf{x}_0|\mathbf{x}_1, \boldsymbol{\theta}); \quad p(\mathbf{z}|\boldsymbol{\theta}) = \prod_{t=2}^T p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta}) \cdot p(\mathbf{x}_T)$$

ELBO

$$\log p(\mathbf{x}|\boldsymbol{\theta}) \geq \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})} = \mathcal{L}_{\phi, \boldsymbol{\theta}}(\mathbf{x}) \rightarrow \max_{q, \boldsymbol{\theta}}$$

$$\begin{aligned} \mathcal{L}_{\phi, \boldsymbol{\theta}}(\mathbf{x}) &= \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p(\mathbf{x}_0|\mathbf{x}_1, \boldsymbol{\theta}) - \text{KL}(q(\mathbf{x}_T|\mathbf{x}_0) \| p(\mathbf{x}_T)) - \\ &\quad - \sum_{t=2}^T \underbrace{\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) \| p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta}))}_{\mathcal{L}_t} \end{aligned}$$

Recap of Previous Lecture

ELBO of the Gaussian Diffusion Model

$$\begin{aligned}\mathcal{L}_{\phi, \theta}(\mathbf{x}) = & \mathbb{E}_{q(\mathbf{x}_1|\mathbf{x}_0)} \log p(\mathbf{x}_0|\mathbf{x}_1, \theta) - \text{KL}(q(\mathbf{x}_T|\mathbf{x}_0)\|p(\mathbf{x}_T)) - \\ & - \sum_{t=2}^T \underbrace{\mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \text{KL}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)\|p(\mathbf{x}_{t-1}|\mathbf{x}_t, \theta))}_{\mathcal{L}_t}\end{aligned}$$

$$\begin{aligned}q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) &= \mathcal{N}(\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I}), \\ p(\mathbf{x}_{t-1}|\mathbf{x}_t, \theta) &= \mathcal{N}(\mu_{\theta,t}(\mathbf{x}_t), \sigma_{\theta,t}^2(\mathbf{x}_t))\end{aligned}$$

It is assumed that $\sigma_{\theta,t}^2(\mathbf{x}_t) = \tilde{\beta}_t \mathbf{I}$.

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \left[\frac{1}{2\tilde{\beta}_t} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_{\theta,t}(\mathbf{x}_t)\|^2 \right]$$

Recap of Previous Lecture

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t | \mathbf{x}_0)} \left[\frac{1}{2\tilde{\beta}_t} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_{\theta,t}(\mathbf{x}_t)\|^2 \right]$$

Reparameterization

$$\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) = \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \boldsymbol{\epsilon}$$

$$\mu_{\theta,t}(\mathbf{x}_t) = \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \boldsymbol{\epsilon}_{\theta,t}(\textcolor{teal}{x_t})$$

$$\mathcal{L}_t = \mathbb{E}_{\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t (1 - \bar{\alpha}_t)} \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\theta,t}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}) \right\|^2 \right]$$

At each step in the reverse diffusion process, our goal is to predict the noise $\boldsymbol{\epsilon}$ added by the forward process!

Simplified Objective

$$\mathcal{L}_{\text{simple}} = \mathbb{E}_{t \sim U\{2, T\}} \mathbb{E}_{\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})} \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\theta,t}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}) \right\|^2$$

Recap of Previous Lecture

Training DDPM

1. Draw a sample $\mathbf{x}_0 \sim \pi(\mathbf{x})$.
2. Sample a timestep $t \sim U\{1, T\}$ and noise $\epsilon \sim \mathcal{N}(0, \mathbf{I})$.
3. Obtain the noisy image: $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \epsilon$.
4. Compute the loss: $\mathcal{L}_{\text{simple}} = \|\epsilon - \epsilon_{\theta,t}(\mathbf{x}_t)\|^2$.

Sampling with DDPM

1. Sample $\mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$.
2. Compute the mean of $p(\mathbf{x}_{t-1} | \mathbf{x}_t, \theta) = \mathcal{N}(\mu_{\theta,t}(\mathbf{x}_t), \sigma_t^2 \cdot \mathbf{I})$:

$$\mu_{\theta,t}(\mathbf{x}_t) = \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \epsilon_{\theta,t}(\mathbf{x}_t)$$

3. Generate a denoised image: $\mathbf{x}_{t-1} = \mu_{\theta,t}(\mathbf{x}_t) + \sigma_t \cdot \epsilon$, where $\epsilon \sim \mathcal{N}(0, \mathbf{I})$.

Outline

1. DDPM as a Score-Based Generative Model
2. Guidance
 - Classifier Guidance
 - Classifier-Free Guidance
3. Continuous-Time Normalizing Flows

Outline

1. DDPM as a Score-Based Generative Model

2. Guidance

Classifier Guidance

Classifier-Free Guidance

3. Continuous-Time Normalizing Flows

Denoising Diffusion as a Score-Based Generative Model

DDPM Objective

$$\mathcal{L}_t = \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t (1 - \bar{\alpha}_t)} \|\epsilon_{\theta, t}(\mathbf{x}_t) - \epsilon\|_2^2 \right]$$

Denoising Diffusion as a Score-Based Generative Model

DDPM Objective

$$\begin{aligned}\mathcal{L}_t &= \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t (1 - \bar{\alpha}_t)} \|\epsilon_{\theta, t}(\mathbf{x}_t) - \epsilon\|_2^2 \right] \\ &= \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t} \left\| \frac{\epsilon_{\theta, t}(\mathbf{x}_t)}{\sqrt{1 - \bar{\alpha}_t}} - \frac{\epsilon}{\sqrt{1 - \bar{\alpha}_t}} \right\|_2^2 \right]\end{aligned}$$

Denoising Diffusion as a Score-Based Generative Model

DDPM Objective

$$\begin{aligned}\mathcal{L}_t &= \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t (1 - \bar{\alpha}_t)} \|\epsilon_{\theta, t}(\mathbf{x}_t) - \epsilon\|_2^2 \right] \\ &= \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t} \left\| \frac{\epsilon_{\theta, t}(\mathbf{x}_t)}{\sqrt{1 - \bar{\alpha}_t}} - \frac{\epsilon}{\sqrt{1 - \bar{\alpha}_t}} \right\|_2^2 \right]\end{aligned}$$

$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0, (1 - \bar{\alpha}_t) \cdot \mathbf{I})$$

Denoising Diffusion as a Score-Based Generative Model

DDPM Objective

$$\begin{aligned}\mathcal{L}_t &= \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t (1 - \bar{\alpha}_t)} \|\epsilon_{\theta, t}(\mathbf{x}_t) - \epsilon\|_2^2 \right] \\ &= \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t} \left\| \frac{\epsilon_{\theta, t}(\mathbf{x}_t)}{\sqrt{1 - \bar{\alpha}_t}} - \frac{\epsilon}{\sqrt{1 - \bar{\alpha}_t}} \right\|_2^2 \right]\end{aligned}$$

$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0, (1 - \bar{\alpha}_t) \cdot \mathbf{I})$$

$$\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x}_0) = -\frac{\mathbf{x}_t - \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0}{1 - \bar{\alpha}_t} = -\frac{\epsilon}{\sqrt{1 - \bar{\alpha}_t}}.$$

Denoising Diffusion as a Score-Based Generative Model

DDPM Objective

$$\begin{aligned}\mathcal{L}_t &= \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t (1 - \bar{\alpha}_t)} \|\epsilon_{\theta, t}(\mathbf{x}_t) - \epsilon\|_2^2 \right] \\ &= \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t} \left\| \frac{\epsilon_{\theta, t}(\mathbf{x}_t)}{\sqrt{1 - \bar{\alpha}_t}} - \frac{\epsilon}{\sqrt{1 - \bar{\alpha}_t}} \right\|_2^2 \right]\end{aligned}$$

$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0, (1 - \bar{\alpha}_t) \cdot \mathbf{I})$$

$$\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x}_0) = -\frac{\mathbf{x}_t - \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0}{1 - \bar{\alpha}_t} = -\frac{\epsilon}{\sqrt{1 - \bar{\alpha}_t}}.$$

We can reparameterize the model as:

$$\mathbf{s}_{\theta, t}(\mathbf{x}_t) = -\frac{\epsilon_{\theta, t}(\mathbf{x}_t)}{\sqrt{1 - \bar{\alpha}_t}} = \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \theta).$$

Denoising Diffusion as a Score-Based Generative Model

DDPM Objective

$$\begin{aligned}\mathcal{L}_t &= \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t (1 - \bar{\alpha}_t)} \|\epsilon_{\theta, t}(\mathbf{x}_t) - \epsilon\|_2^2 \right] \\ &= \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t} \left\| \frac{\epsilon_{\theta, t}(\mathbf{x}_t)}{\sqrt{1 - \bar{\alpha}_t}} - \frac{\epsilon}{\sqrt{1 - \bar{\alpha}_t}} \right\|_2^2 \right]\end{aligned}$$

$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0, (1 - \bar{\alpha}_t) \cdot \mathbf{I})$$

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We can reparameterize the model as:

$$\mathbf{s}_{\theta, t}(\mathbf{x}_t) = \frac{\epsilon_{\theta, t}(\mathbf{x}_t)}{\sqrt{1 - \bar{\alpha}_t}} = \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \theta).$$

$$\mathcal{L}_t = \mathbb{E}_{q(\mathbf{x}_t | \mathbf{x}_0)} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t} \left\| \mathbf{s}_{\theta, t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x}_0) \right\|_2^2 \right]$$

DDPM vs NCSN: Objectives

DDPM Objective

$$\mathbb{E}_{\pi(\mathbf{x}_0)} \mathbb{E}_{t \sim U\{1, T\}} \mathbb{E}_{q(\mathbf{x}_t | \mathbf{x}_0)} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t} \left\| \mathbf{s}_{\theta, t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x}_0) \right\|_2^2 \right]$$

$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}$$

DDPM vs NCSN: Objectives

DDPM Objective

$$\mathbb{E}_{\pi(\mathbf{x}_0)} \mathbb{E}_{t \sim U\{1, T\}} \mathbb{E}_{q(\mathbf{x}_t | \mathbf{x}_0)} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t} \left\| \mathbf{s}_{\theta, t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x}_0) \right\|_2^2 \right]$$

$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}$$

In practice, this coefficient is often omitted.

DDPM vs NCSN: Objectives

DDPM Objective

$$\mathbb{E}_{\pi(\mathbf{x}_0)} \mathbb{E}_{t \sim U\{1, T\}} \mathbb{E}_{q(\mathbf{x}_t | \mathbf{x}_0)} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t} \left\| \mathbf{s}_{\theta, t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x}_0) \right\|_2^2 \right]$$

$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}$$

In practice, this coefficient is often omitted.

NCSN Objective

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

$$\mathbf{x}_t = \mathbf{x}_0 + \sigma_t \cdot \boldsymbol{\epsilon}$$

DDPM vs NCSN: Objectives

DDPM Objective

$$\mathbb{E}_{\pi(\mathbf{x}_0)} \mathbb{E}_{t \sim U\{1, T\}} \mathbb{E}_{q(\mathbf{x}_t | \mathbf{x}_0)} \left[\frac{(1 - \alpha_t)^2}{2\tilde{\beta}_t \alpha_t} \left\| \mathbf{s}_{\theta, t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x}_0) \right\|_2^2 \right]$$

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In practice, this coefficient is often omitted.

NCSN Objective

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$$\mathbf{x}_t = \mathbf{x}_0 + \sigma_t \cdot \boldsymbol{\epsilon}$$

Maximizing the ELBO leads to the same objective as denoising score matching!

DDPM vs NCSN: Sampling

DDPM Sampling (Ancestral Sampling)

$$\mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$$

$$\mathbf{x}_{t-1} = \mu_{\theta,t}(\mathbf{x}_t) + \sigma_t \cdot \epsilon$$

DDPM vs NCSN: Sampling

DDPM Sampling (Ancestral Sampling)

$$\mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$$

$$\begin{aligned}\mathbf{x}_{t-1} &= \boldsymbol{\mu}_{\theta,t}(\mathbf{x}_t) + \sigma_t \cdot \boldsymbol{\epsilon} \\ &= \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \boldsymbol{\epsilon}_{\theta,t}(\mathbf{x}_t) + \sigma_t \cdot \boldsymbol{\epsilon}\end{aligned}$$

DDPM vs NCSN: Sampling

DDPM Sampling (Ancestral Sampling)

$$\mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$$

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DDPM vs NCSN: Sampling

DDPM Sampling (Ancestral Sampling)

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NCSN Sampling (Annealed Langevin Dynamics)

- ▶ Sample $\mathbf{x}_T^0 \sim \mathcal{N}(0, \sigma_T^2 \mathbf{I}) \approx q(\mathbf{x}_T)$.
- ▶ Perform L steps of Langevin dynamics:

$$\mathbf{x}_t^l = \mathbf{x}_t^{l-1} + \frac{\eta_t}{2} \cdot \mathbf{s}_{\theta,\sigma_t}(\mathbf{x}_t^{l-1}) + \sqrt{\eta_t} \cdot \boldsymbol{\epsilon}_t^l.$$

- ▶ Set $\mathbf{x}_{t-1}^0 = \mathbf{x}_t^L$ and move to the next σ_t .

DDPM vs NCSN: Summary

Summary

- ▶ Different Markov chains:
 - ▶ DDPM: $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon};$
 - ▶ NCSN: $\mathbf{x}_t = \mathbf{x}_0 + \sigma_t \cdot \boldsymbol{\epsilon}.$
 - ▶ One can generalize to $q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\alpha_t \cdot \mathbf{x}_0, \sigma_t^2 \mathbf{I}).$

Kingma D. et al. *Variational Diffusion Models*, 2021

Song Y. et al. *Score-Based Generative Modeling through Stochastic Differential Equations*, 2020

DDPM vs NCSN: Summary

Summary

- ▶ Different Markov chains:
 - ▶ DDPM: $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon};$
 - ▶ NCSN: $\mathbf{x}_t = \mathbf{x}_0 + \sigma_t \cdot \boldsymbol{\epsilon}.$
 - ▶ One can generalize to $q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\alpha_t \cdot \mathbf{x}_0, \sigma_t^2 \mathbf{I}).$
- ▶ The objectives coincide: ELBO \equiv score-matching.

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DDPM vs NCSN: Summary

Summary

- ▶ Different Markov chains:
 - ▶ DDPM: $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}$;
 - ▶ NCSN: $\mathbf{x}_t = \mathbf{x}_0 + \sigma_t \cdot \boldsymbol{\epsilon}$.
 - ▶ One can generalize to $q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\alpha_t \cdot \mathbf{x}_0, \sigma_t^2 \mathbf{I})$.
- ▶ The objectives coincide: ELBO \equiv score-matching.
- ▶ The sampling procedures differ:
 - ▶ Ancestral sampling in DDPM;
 - ▶ Annealed Langevin dynamics for NCSN;
 - ▶ Hybrid approaches that combine both updates are possible.

Kingma D. et al. *Variational Diffusion Models*, 2021

Song Y. et al. *Score-Based Generative Modeling through Stochastic Differential Equations*, 2020

Outline

1. DDPM as a Score-Based Generative Model

2. Guidance

Classifier Guidance

Classifier-Free Guidance

3. Continuous-Time Normalizing Flows

Guidance

- ▶ Up to now, we have focused on **unconditional** generative models $p(\mathbf{x}|\theta)$.
- ▶ In practice, most generative models are **conditional**: $p(\mathbf{x}|\mathbf{y}, \theta)$.
- ▶ Here, \mathbf{y} might denote a class label or **text** (as in text-to-image tasks).



Кот ныряет в бассейн, как ребенок на обложке альбома Nevermind, реалистично



рука человека с пятью пальцами, ни четырьмя, ни шестью, а с 5 (пять) пальцами

Taxonomy of Conditional Tasks

In practice, an important task is to construct a conditional model $\pi(\mathbf{x}|\mathbf{y})$.

- ▶ $\mathbf{y} = \emptyset$, \mathbf{x} – image \Rightarrow unconditional image model.
- ▶ \mathbf{y} – class label, \mathbf{x} – image \Rightarrow class-conditional image model.
- ▶ \mathbf{y} – text prompt, \mathbf{x} – image \Rightarrow text-to-image model.
- ▶ \mathbf{y} – image, \mathbf{x} – image \Rightarrow image-to-image model.
- ▶ \mathbf{y} – image, \mathbf{x} – text \Rightarrow image-to-text model (image captioning).
- ▶ \mathbf{y} – English text, \mathbf{x} – Russian text \Rightarrow sequence-to-sequence model (machine translation).
- ▶ \mathbf{y} – sound, \mathbf{x} – text \Rightarrow speech-to-text model (automatic speech recognition).
- ▶ \mathbf{y} – text, \mathbf{x} – sound \Rightarrow text-to-speech model.

Label Guidance

Label: Ostrich (10th ImageNet class)



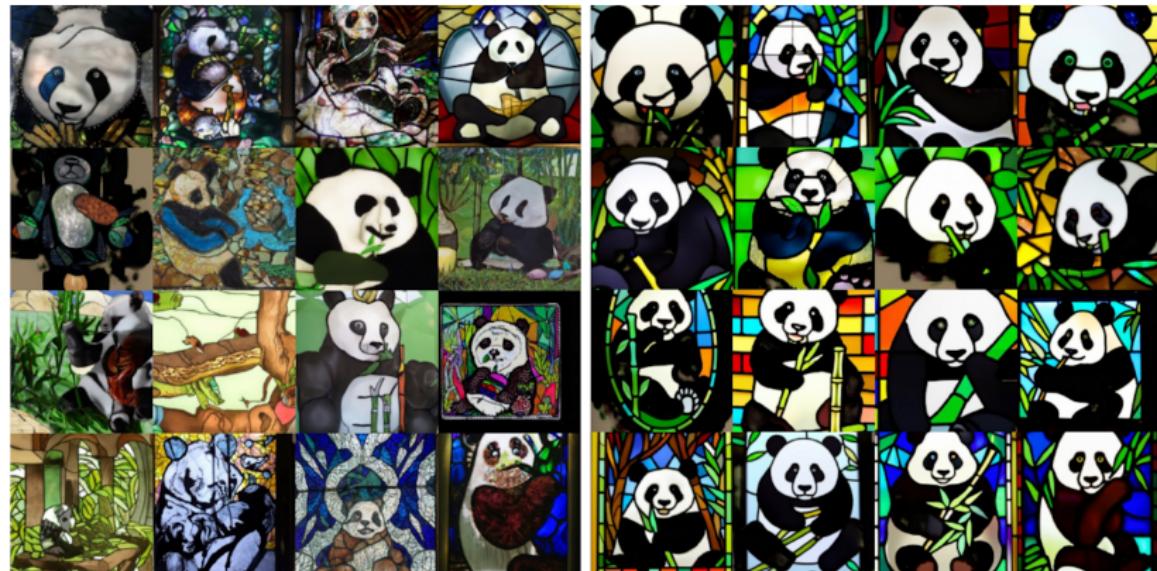
VQ-VAE (Proposed)

BigGAN deep

Text Guidance

Prompt: a stained glass window of a panda eating bamboo

Left: $\gamma = 1$, Right: $\gamma = 3$.



Guidance in Generative Models

- ▶ Given **supervised** data $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n$, we can treat \mathbf{y} as an additional input:
 - ▶ $p(x_j | \mathbf{x}_{1:j-1}, \mathbf{y}, \theta)$ for AR models;
 - ▶ Encoder $q(\mathbf{z} | \mathbf{x}, \mathbf{y}, \phi)$ and decoder $p(\mathbf{x} | \mathbf{z}, \mathbf{y}, \theta)$ for VAEs;
 - ▶ $G_\theta(\mathbf{z}, \mathbf{y})$ for NFs and GANs;
 - ▶ $p(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{y}, \theta)$ for DDPMs.

Guidance in Generative Models

- ▶ Given **supervised** data $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n$, we can treat \mathbf{y} as an additional input:
 - ▶ $p(x_j | \mathbf{x}_{1:j-1}, \mathbf{y}, \theta)$ for AR models;
 - ▶ Encoder $q(\mathbf{z}|\mathbf{x}, \mathbf{y}, \phi)$ and decoder $p(\mathbf{x}|\mathbf{z}, \mathbf{y}, \theta)$ for VAEs;
 - ▶ $G_\theta(\mathbf{z}, \mathbf{y})$ for NFs and GANs;
 - ▶ $p(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{y}, \theta)$ for DDPMs.
- ▶ For **unsupervised** data $\{\mathbf{x}_i\}_{i=1}^n$, it becomes necessary to devise a way to transform the unconditional model $p(\mathbf{x}|\theta)$ into a conditional version.

Guidance in Generative Models

- ▶ Given **supervised** data $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n$, we can treat \mathbf{y} as an additional input:
 - ▶ $p(x_j | \mathbf{x}_{1:j-1}, \mathbf{y}, \theta)$ for AR models;
 - ▶ Encoder $q(\mathbf{z}|\mathbf{x}, \mathbf{y}, \phi)$ and decoder $p(\mathbf{x}|\mathbf{z}, \mathbf{y}, \theta)$ for VAEs;
 - ▶ $G_\theta(\mathbf{z}, \mathbf{y})$ for NFs and GANs;
 - ▶ $p(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{y}, \theta)$ for DDPMs.
- ▶ For **unsupervised** data $\{\mathbf{x}_i\}_{i=1}^n$, it becomes necessary to devise a way to transform the unconditional model $p(\mathbf{x}|\theta)$ into a conditional version.
- ▶ Being able to control the strength of guidance is especially valuable.

Types of Guidance

► **Classifier Guidance:**

- ▶ Suitable for unsupervised data;
- ▶ Utilizes an auxiliary classifier (which still requires supervision for classifier training).

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- ▶ **Classifier Guidance:**

- ▶ Suitable for unsupervised data;
- ▶ Utilizes an auxiliary classifier (which still requires supervision for classifier training).

- ▶ **Classifier-Free Guidance:**

- ▶ Best suited for supervised data;
- ▶ Does not rely on an additional classifier.

Outline

1. DDPM as a Score-Based Generative Model

2. Guidance

Classifier Guidance

Classifier-Free Guidance

3. Continuous-Time Normalizing Flows

Classifier Guidance

DDPM Sampling

1. Sample $\mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$.
2. Generate the denoised image (unconditional generation):

$$\mathbf{x}_{t-1} = \frac{1}{\sqrt{1 - \beta_t}} \cdot \mathbf{x}_t + \frac{\beta_t}{\sqrt{1 - \beta_t}} \cdot \mathbf{s}_{\theta, t}(\mathbf{x}_t) + \sigma_t \cdot \boldsymbol{\epsilon}$$

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Conditional Generation

$$\mathbf{x}_{t-1} = \frac{1}{\sqrt{1 - \beta_t}} \cdot \mathbf{x}_t + \frac{\beta_t}{\sqrt{1 - \beta_t}} \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \mathbf{y}, \theta) + \sigma_t \cdot \epsilon$$

- ▶ Let us assume \mathbf{y} is a class label.
- ▶ Suppose $p(\mathbf{y}|\mathbf{x}_t)$ (a classifier for noisy inputs) is available.

Classifier Guidance: Conditional Update

Conditional Generation

$$\mathbf{x}_{t-1} = \frac{1}{\sqrt{1 - \beta_t}} \cdot \mathbf{x}_t + \frac{\beta_t}{\sqrt{1 - \beta_t}} \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \mathbf{y}, \theta) + \sigma_t \cdot \epsilon$$

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Conditional Distribution

$$\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \mathbf{y}, \theta) = \nabla_{\mathbf{x}_t} \log \left(\frac{p(\mathbf{y} | \mathbf{x}_t) p(\mathbf{x}_t | \theta)}{p(\mathbf{y})} \right)$$

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Let's reparameterize: $\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \mathbf{y}, \theta) = -\frac{\epsilon_{\theta, t}(\mathbf{x}_t, \mathbf{y})}{\sqrt{1 - \bar{\alpha}_t}}$.

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Classifier-Corrected Noise Prediction

$$\epsilon_{\theta, t}(\mathbf{x}_t, \mathbf{y}) = \epsilon_{\theta, t}(\mathbf{x}_t) - \sqrt{1 - \bar{\alpha}_t} \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{y} | \mathbf{x}_t)$$

Classifier Guidance: Practical Implementation

Classifier-Corrected Noise Prediction

$$\epsilon_{\theta,t}(\mathbf{x}_t, \mathbf{y}) = \epsilon_{\theta,t}(\mathbf{x}_t) - \sqrt{1 - \bar{\alpha}_t} \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t)$$

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Guidance Scale

$$\epsilon_{\theta,t}(\mathbf{x}_t, \mathbf{y}) = \epsilon_{\theta,t}(\mathbf{x}_t) - \gamma \cdot \sqrt{1 - \bar{\alpha}_t} \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t)$$

Here, the **guidance scale** γ adjusts the strength of classifier guidance.

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Training

- ▶ Train the DDPM as before.
- ▶ Train an additional classifier $p(\mathbf{y}|\mathbf{x}_t)$ on noisy data.

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Guided Sampling

$$\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \epsilon_{\theta,t}(\mathbf{x}_t, \mathbf{y}) + \sigma_t \cdot \epsilon$$

Classifier Guidance: Distribution Sharpening

Classifier-Corrected Noise Prediction, with Scaling

$$\epsilon_{\theta,t}(\mathbf{x}_t, \mathbf{y}) = \epsilon_{\theta,t}(\mathbf{x}_t) - \gamma \cdot \sqrt{1 - \bar{\alpha}_t} \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t)$$

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$$\nabla_{\mathbf{x}_t}^{\gamma} \log p(\mathbf{x}_t|\mathbf{y}, \theta) = \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\theta) + \gamma \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t)$$

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Classifier Guidance: Distribution Sharpening

Classifier-Corrected Noise Prediction, with Scaling

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Note: Increasing γ sharpens $p(\mathbf{y}|\mathbf{x}_t)$ (with Z independent of \mathbf{x}_t).

Outline

1. DDPM as a Score-Based Generative Model

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Classifier Guidance

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3. Continuous-Time Normalizing Flows

Classifier-Free Guidance

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Note: When $\gamma = 1$, the original identity is restored.

Classifier-Free Guidance: Formulation

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Classifier-Free Corrected Noise Prediction

$$\hat{\epsilon}_{\theta,t}(\mathbf{x}_t, \mathbf{y}) = \gamma \cdot \epsilon_{\theta,t}(\mathbf{x}_t, \mathbf{y}) + (1 - \gamma) \cdot \epsilon_{\theta,t}(\mathbf{x}_t)$$

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- ▶ Train a single model $\epsilon_{\theta,t}(\mathbf{x}_t, \mathbf{y})$ using **supervised** data, alternating between conditioning and unconditional training (i.e., using $\mathbf{y} = \emptyset$).

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Guided Sampling

$$\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{\alpha_t(1 - \bar{\alpha}_t)}} \cdot \hat{\epsilon}_{\theta,t}(\mathbf{x}_t, \mathbf{y}) + \sigma_t \cdot \epsilon$$

Outline

1. DDPM as a Score-Based Generative Model
2. Guidance
 - Classifier Guidance
 - Classifier-Free Guidance
3. Continuous-Time Normalizing Flows

Discrete-Time Normalizing Flows

Change of Variable Theorem (CoV)

Let \mathbf{x} be a random variable with density $p(\mathbf{x})$, and let $\mathbf{f} : \mathbb{R}^m \rightarrow \mathbb{R}^m$ be a differentiable and **invertible** transformation. If $\mathbf{z} = \mathbf{f}(\mathbf{x})$, $\mathbf{x} = \mathbf{f}^{-1}(\mathbf{z}) = \mathbf{g}(\mathbf{z})$, then

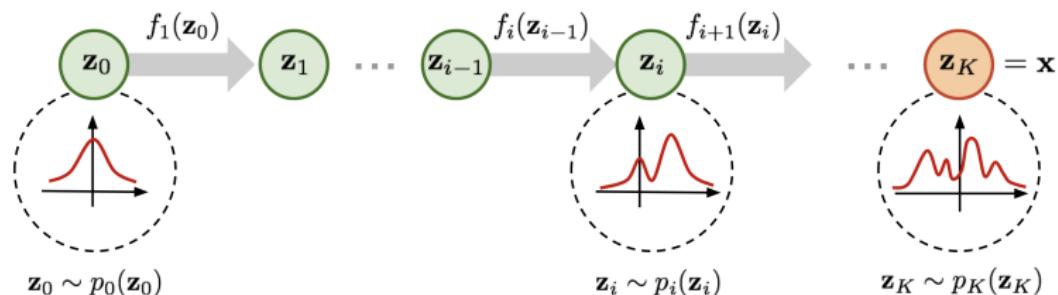
$$p(\mathbf{x}) = p(\mathbf{z}) |\det(\mathbf{J}_\mathbf{f})| = p(\mathbf{z}) \left| \det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) \right| = p(\mathbf{f}(\mathbf{x})) \left| \det \left(\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} \right) \right|$$

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$$\log p(\mathbf{x}|\theta) = \log p(\mathbf{f}_K \circ \dots \circ \mathbf{f}_1(\mathbf{x})) + \sum_{k=1}^K \log \left| \det \left(\frac{\partial \mathbf{f}_k}{\partial \mathbf{f}_{k-1}} \right) \right|.$$

Towards Continuous-Time Normalizing Flows

- ▶ Up to this point, we have considered discrete-time normalizing flows:

$$\mathbf{x}_{t+1} = \mathbf{f}_\theta(\mathbf{x}_t, t); \quad \log p(\mathbf{x}_{t+1}) = \log p(\mathbf{x}_t) - \log \left| \det \frac{\partial \mathbf{f}_\theta(\mathbf{x}_t)}{\partial \mathbf{x}_t} \right|.$$

- ▶ Let us now move to the general case of continuous time, using a mapping $\mathbf{x}(t) : \mathbb{R} \rightarrow \mathbb{R}^m$ to describe continuous dynamics.

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Consider an Ordinary Differential Equation (ODE):

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{f}_\theta(\mathbf{x}(t), t); \quad \text{with initial condition } \mathbf{x}(t_0) = \mathbf{x}_0.$$

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Here, $\mathbf{f}_\theta : \mathbb{R}^m \times [t_0, t_1] \rightarrow \mathbb{R}^m$ is a **vector field**.

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Here, we require the numerical routine $\texttt{ODESolve}_f(\mathbf{x}_0, \theta, t_0, t_1)$.

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$$\frac{\mathbf{x}(t+h) - \mathbf{x}(t)}{h} = \mathbf{f}_{\theta}(\mathbf{x}(t), t)$$

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Heun's Update Step

$$\mathbf{x}'(t+h) = \mathbf{x}(t) + h \cdot \mathbf{f}_{\theta}(\mathbf{x}(t), t)$$

$$\mathbf{x}(t+h) = \mathbf{x}(t) + \frac{h}{2} \cdot (\mathbf{f}_{\theta}(\mathbf{x}(t), t) + \mathbf{f}_{\theta}(\mathbf{x}'(t+h), t+h))$$

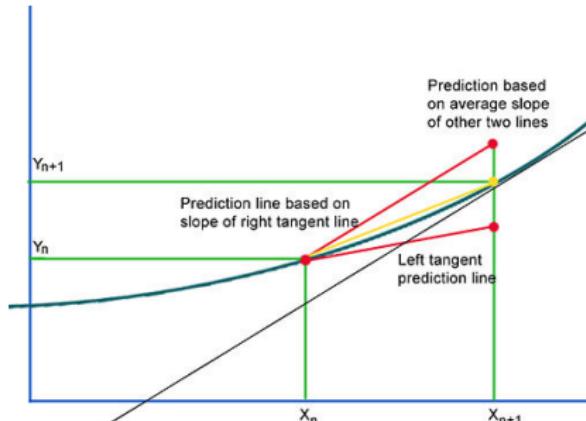


Image credit: https://en.wikipedia.org/wiki/Heun's_method

Continuous-Time Normalizing Flows: Neural ODE

Neural ODE

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{f}_\theta(\mathbf{x}(t), t); \quad \text{with initial condition } \mathbf{x}(t_0) = \mathbf{x}_0$$

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- ▶ Consider $[t_0, t_1] = [0, 1]$ for simplicity.
- ▶ If $\mathbf{x}(0)$ is a random variable with density $p_0(\mathbf{x})$,
- ▶ Then, for any t , $\mathbf{x}(t)$ is a random variable with density $p_t(\mathbf{x})$.

Continuous-Time Normalizing Flows: Intuition

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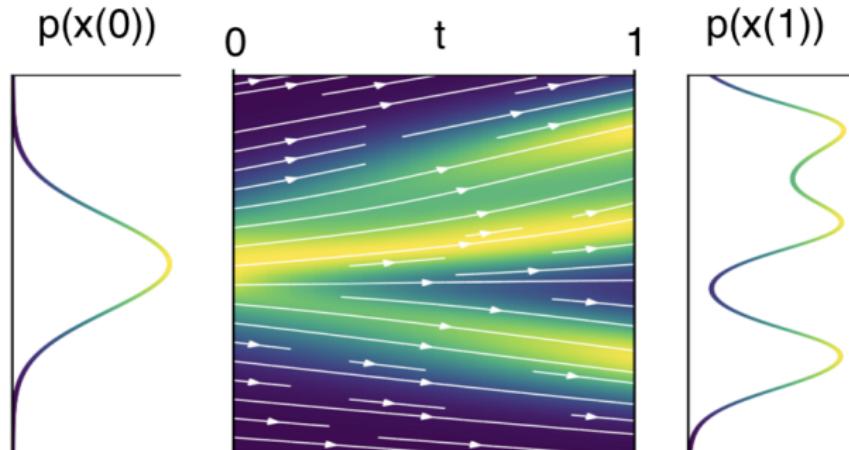
$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{f}_\theta(\mathbf{x}(t), t); \quad \text{with initial condition } \mathbf{x}(t_0) = \mathbf{x}_0$$

- ▶ $p_t(\mathbf{x}) = p(\mathbf{x}, t)$ describes the **probability path** interpolating between $p_0(\mathbf{x})$ and $p_1(\mathbf{x})$.
- ▶ What is the difference between $p_t(\mathbf{x}(t))$ and $p_t(\mathbf{x})$?

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Continuous-Time Normalizing Flows: Reversibility

Theorem (Picard)

If \mathbf{f} is continuously differentiable with a bounded derivative in \mathbf{x} and continuous in t , then the ODE has a **unique solution** given by a flow ψ_t .

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If \mathbf{f} is continuously differentiable with a bounded derivative in \mathbf{x} and continuous in t , then the ODE has a **unique solution** given by a flow ψ_t .

This guarantees the ODE is **uniquely reversible**.

$$\psi_1(\mathbf{x}_0) = \mathbf{x}_0 + \int_0^1 \mathbf{f}_\theta(\psi_t(\mathbf{x}_0), t) dt$$

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Summary

- ▶ DDPM and NCSN are intimately connected at the objective level.
- ▶ Classifier guidance provides a technique to turn an unconditional model into a conditional one by training an auxiliary classifier on noisy data.
- ▶ Classifier-free guidance removes the need for such a classifier, yielding a practical recipe now widely used.
- ▶ Continuous-time normalizing flows leverage neural ODEs to define continuous-time trajectories $\mathbf{x}(t)$, relaxing many constraints of discrete-time flows.
- ▶ If \mathbf{x}_0 is a random variable, this yields a **probability path** $p_t(\mathbf{x})$ as time evolves.