

Deep Generative Models

Lecture 9

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Recap of Previous Lecture

Forward Process: Converts an arbitrary distribution $p_{\text{data}}(\mathbf{x})$ 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.

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

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:

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

ELBO

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

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

Recap of Previous Lecture

ELBO of the Gaussian Diffusion Model

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

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

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

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

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

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

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

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

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

At each step in the reverse diffusion process, our goal is to predict the noise ϵ added by the forward process!

Simplified Objective

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

Recap of Previous Lecture

Training DDPM

1. Draw a sample $\mathbf{x}_0 \sim p_{\text{data}}(\mathbf{x})$.
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 $p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_t) = \mathcal{N}(\mu_{\theta,t}(\mathbf{x}_t), \sigma_t^2 \cdot \mathbf{I})$:

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

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

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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

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

Denoising Diffusion as a Score-Based Generative Model

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

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

Denoising Diffusion as a Score-Based Generative Model

DDPM Objective

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

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We can reparameterize the model as:

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

Denoising Diffusion as a Score-Based Generative Model

DDPM Objective

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

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

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

DDPM vs NCSN: Objectives

DDPM Objective

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

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

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

In practice, this coefficient is often omitted.

DDPM vs NCSN: Objectives

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

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

In practice, this coefficient is often omitted.

NCSN Objective

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

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

DDPM vs NCSN: Objectives

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

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In practice, this coefficient is often omitted.

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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

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

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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:
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 - ▶ 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 $p_\theta(\mathbf{x})$.
- ▶ In practice, most generative models are **conditional** (in diffusion era it is called guided): $p_\theta(\mathbf{x}|\mathbf{y})$.
- ▶ 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

Conditional Models

In practice, we're typically interested in learning conditional models (sampling from conditional distribution $p_{\text{data}}(\mathbf{x}|\mathbf{y})$).

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

Label Guidance

Label: Ostrich (10th ImageNet class)



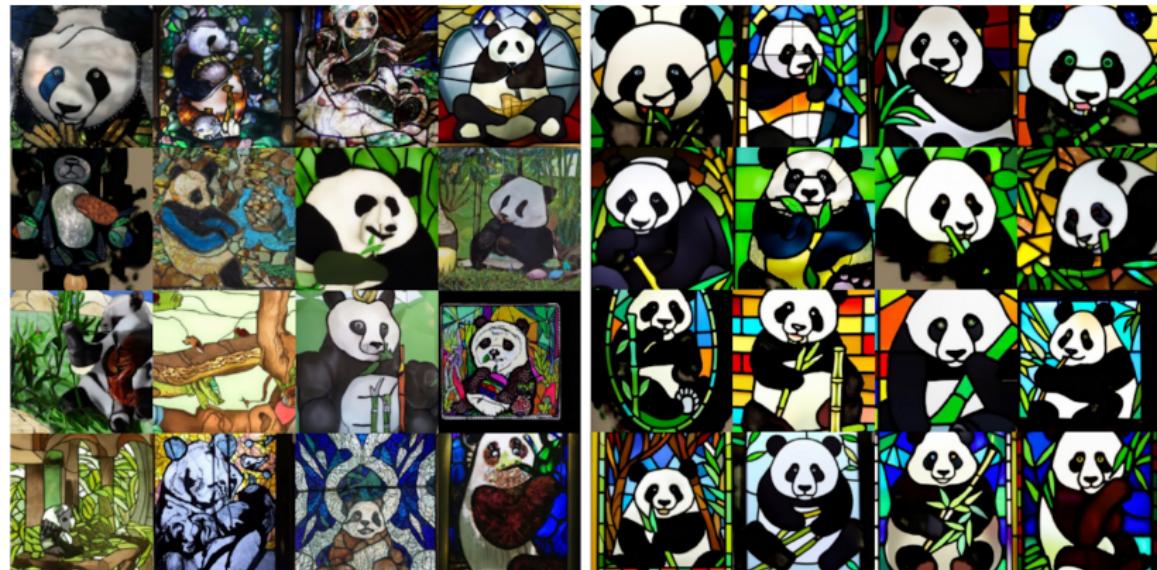
VQ-VAE (Proposed)

BigGAN deep

Text Guidance

Prompt: a stained glass window of a panda eating bamboo

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



Guidance in Generative Models

How to make guided model?

Instead of sampling from $p_{\theta}(\mathbf{x})$, we sample from $p_{\theta}(\mathbf{x}|\mathbf{y})$.

Guidance in Generative Models

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Given **supervised** data $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n$, we can treat \mathbf{y} as an additional model input:

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- ▶ $p_{\theta}(x_j | \mathbf{x}_{1:j-1}, \mathbf{y})$ for AR models;

Guidance in Generative Models

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Instead of sampling from $p_\theta(\mathbf{x})$, we sample from $p_\theta(\mathbf{x}|\mathbf{y})$.

Given **supervised** data $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n$, we can treat \mathbf{y} as an additional model input:

- ▶ $p_\theta(x_j|\mathbf{x}_{1:j-1}, \mathbf{y})$ for AR models;
- ▶ Encoder $q_\phi(\mathbf{z}|\mathbf{x}, \mathbf{y})$ and decoder $p_\theta(\mathbf{x}|\mathbf{z}, \mathbf{y})$ for VAEs;

Guidance in Generative Models

How to make guided model?

Instead of sampling from $p_\theta(\mathbf{x})$, we sample from $p_\theta(\mathbf{x}|\mathbf{y})$.

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- ▶ $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{y})$ for DDPMs.

Challenge

- ▶ Empirically, images sampled with this procedure do not fit well enough to the desired label \mathbf{y} .
- ▶ Being able to control the strength of guidance is especially valuable.

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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What is the link between $\nabla_{\mathbf{x}_t} \log p_{\theta}(\mathbf{x}_t)$ and $\nabla_{\mathbf{x}_t} \log p_{\theta}(\mathbf{x}_t | \mathbf{y})$?

Classifier Guidance: Guided Score Function

Guided Generation

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Classifier Guidance: Guidance Scale

Guided Score Function

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Guidance Scale

It is a natural idea to scale up the contribution of the guidance

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

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- ▶ The **guidance scale** γ adjusts the strength of classifier guidance.
- ▶ $\mathbf{s}_{\theta,t}^{\gamma}(\mathbf{x}_t, \mathbf{y})$ is not the true guided score function $\mathbf{s}_{\theta,t}(\mathbf{x}_t, \mathbf{y})$.

Classifier Guidance: Distribution Sharpening

Scaled Guided Score Function

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Classifier Guidance: Distribution Sharpening

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Note: Increasing γ sharpens $p(\mathbf{y}|\mathbf{x}_t)$, making it more contrast

$$\hat{p}(\mathbf{y}|\mathbf{x}_t) \propto p(\mathbf{y}|\mathbf{x}_t)^{\gamma}.$$

Classifier Guidance: Overview

Training

- ▶ Train the DDPM as before.
- ▶ Train an additional classifier $p(\mathbf{y}|\mathbf{x}_t)$ on noisy data (note that it is dependent on time t).

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Guided DDPM Sampling

1. Sample $\mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$.
2. Generate the denoised image (using scaled guided score function):

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Classifier-Free Guidance

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Bayes theorem

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Scaled Guided Score Function

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Classifier-Free Guidance: Formulation

Scaled Guided Score Function

$$\nabla_{\mathbf{x}_t}^{\gamma} \log p_{\theta}(\mathbf{x}_t | \mathbf{y}) = (1 - \gamma) \cdot \nabla_{\mathbf{x}_t} \log p_{\theta}(\mathbf{x}_t) + \gamma \cdot \nabla_{\mathbf{x}_t} \log p_{\theta}(\mathbf{x}_t | \mathbf{y})$$

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

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Naive training approach

- ▶ Train an unguided score function model $\mathbf{s}_{\theta,t}(\mathbf{x}_t)$.
- ▶ Train a guided score function model $\mathbf{s}_{\theta,t}(\mathbf{x}_t, \mathbf{y})$.

Classifier-Free Guidance: Formulation

Scaled Guided Score Function

$$\nabla_{\mathbf{x}_t}^{\gamma} \log p_{\theta}(\mathbf{x}_t | \mathbf{y}) = (1 - \gamma) \cdot \nabla_{\mathbf{x}_t} \log p_{\theta}(\mathbf{x}_t) + \gamma \cdot \nabla_{\mathbf{x}_t} \log p_{\theta}(\mathbf{x}_t | \mathbf{y})$$

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

Naive training approach

- ▶ Train an unguided score function model $\mathbf{s}_{\theta,t}(\mathbf{x}_t)$.
- ▶ Train a guided score function model $\mathbf{s}_{\theta,t}(\mathbf{x}_t, \mathbf{y})$.
- ▶ Use their convex combination at inference.

Guided Sampling

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

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How to avoid training two separate score function models?

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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

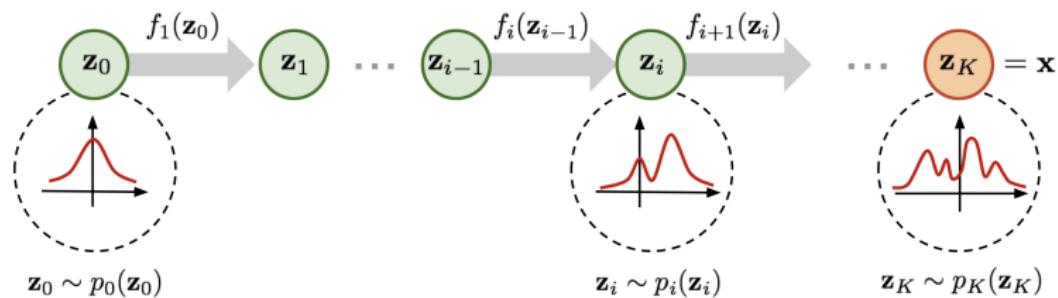
$$p(\mathbf{x}) = p(\mathbf{z}) |\det(\mathbf{J}_f)| = p(\mathbf{z}) \left| \det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) \right| = p(\mathbf{f}(\mathbf{x})) \left| \det \left(\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} \right) \right|$$

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

Towards Continuous-Time Normalizing Flows

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

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

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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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Heun's Update Step

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

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

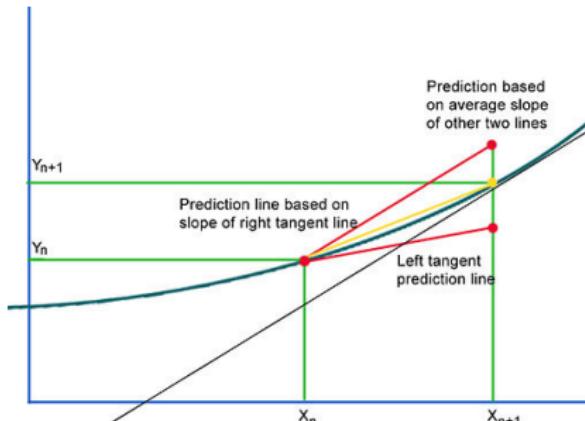


Image credit: https://en.wikipedia.org/wiki/Heun's_method

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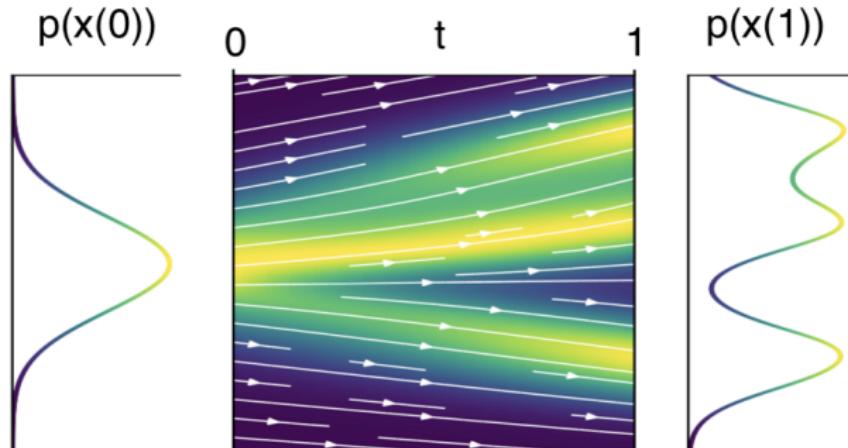
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- ▶ $p_t(\mathbf{x}) = p(\mathbf{x}, t)$ describes the **probability path** interpolating between $p_0(\mathbf{x})$ and $p_1(\mathbf{x})$.
- ▶ What is the difference between $p_t(\mathbf{x}(t))$ and $p_t(\mathbf{x})$?

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

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Note: Unlike discrete-time flows, \mathbf{f} need not be invertible (uniqueness ensures bijection). How can we compute $p_t(\mathbf{x})$ at arbitrary t ?

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.