Deep Generative Models

Lecture 10

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AI Masters

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Recap of previous lecture

Forward process goes from any distribution $\pi(\mathbf{x})$ to $\mathcal{N}(0, \mathbf{I})$ via noise injection.

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

Reverse process is Intractable distribution that is able to be approximated by Normal (with unknown parameters) for small β_t.

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

Conditioned reverse process is Normal with the known parameters, which defines how to denoise a noisy image $\mathbf{x}_t$ with access to what the final, completely denoised image $\mathbf{x}_0$ should be.

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

Recap of previous lecture

- $\mathbf{z} = (\mathbf{x}_1, \ldots, \mathbf{x}_T)$ is a latent variable.
- Variational posterior distribution

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

- Generative distribution 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

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

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

Das A. An introduction to Diffusion Probabilistic Models, blog post, 2021

Recap of previous lecture

ELBO of Gaussian diffusion model

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

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t \mathbf{I}),$$
$$p(\mathbf{x}_{t-1}|\mathbf{x}_t, \theta) = \mathcal{N}\big(\boldsymbol{\mu}_{\theta,t}(\mathbf{x}_t), \boldsymbol{\sigma}^2_{\theta,t}(\mathbf{x}_t)\big)$$

Our assumption: $\boldsymbol{\sigma}^2_{\theta,t}(\mathbf{x}_t) = \tilde{\beta}_t \mathbf{I}$.

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

Recap of previous lecture

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

Reparametrization

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

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

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

At each step of reverse diffusion process we try to predict the noise ϵ that we used in the forward diffusion process!

Simplified objective

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

Recap of previous lecture

Training of DDPM

1. Get the sample $\mathbf{x}_0 \sim \pi(\mathbf{x})$.
2. Sample timestamp $t \sim U\{1, T\}$ and the noise $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.
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 $\mathcal{L}_{\text{simple}} = \|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t)\|^2$.

Sampling of DDPM

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

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

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

Outline

1. DDPM as score-based generative model

2. Guidance
   - Classifier guidance
   - Classifier-free guidance

3. Continuous-in-time normalizing flows

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Denosing diffusion as score-based generative model

DDPM objective

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

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

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

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

Let reparametrize our model:

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

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

DDPM vs NCSN: objectives

DDPM objective

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

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

In practice the coefficient is omitted.

NCSN objective

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

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

ELBO maximization approach gives the same objective as denoising score-matching approach!

Ho J. Denoising Diffusion Probabilistic Models, 2020

DDPM vs NCSN: sampling

DDPM sampling (ancestral sampling)

$$
\begin{aligned}
\mathbf{x}_T &\sim \mathcal{N}(0, \mathbf{I}) \\
\mathbf{x}_{t-1} &= \boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t) + \sigma_t \cdot \boldsymbol{\epsilon} \\
&= \frac{1}{\sqrt{\alpha_t}} \cdot \mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{\alpha_t(1-\bar{\alpha}_t)}} \cdot \boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t) + \sigma_t \cdot \boldsymbol{\epsilon} \\
&= \frac{1}{\sqrt{1-\beta_t}} \cdot \mathbf{x}_t + \frac{\beta_t}{\sqrt{1-\beta_t}} \cdot \mathbf{s}_{\boldsymbol{\theta},t}(\mathbf{x}_t) + \sigma_t \cdot \boldsymbol{\epsilon}
\end{aligned}
$$

NCSN sampling (annealed Langevin dynamics)

- Sample $\mathbf{x}_T^0 \sim \mathcal{N}(0, \sigma_T^2 \cdot \mathbf{I}) \approx q(\mathbf{x}_T)$.
- Apply L steps of Langevin dynamic

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

- Update $\mathbf{x}_{t-1}^0 = \mathbf{x}_t^L$ and choose the next σ_t.

Ho J. Denoising Diffusion Probabilistic Models, 2020

DDPM vs NCSN

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: $\mathbf{x}_t = \mathbf{x}_0 + \sigma_t \cdot \boldsymbol{\epsilon}$.
  - It is possible to consider the more general framework $q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\alpha_t \cdot \mathbf{x}_0, \sigma_t^2 \cdot \mathbf{I})$
- Identical objectives: ELBO $\equiv$ score-matching.
- Different sampling schemes:
  - ancestral sampling for DDPM;
  - annealed Langevin dynamics for NCSN;
  - there is a combined approach with alternating updates of DDPM and NCSN.

Kingma D. et al. Variational Diffusion Models, 2021
Song Y. et al. Score-Based Generative Modeling through Stochastic Differential Equations, 2020

Outline

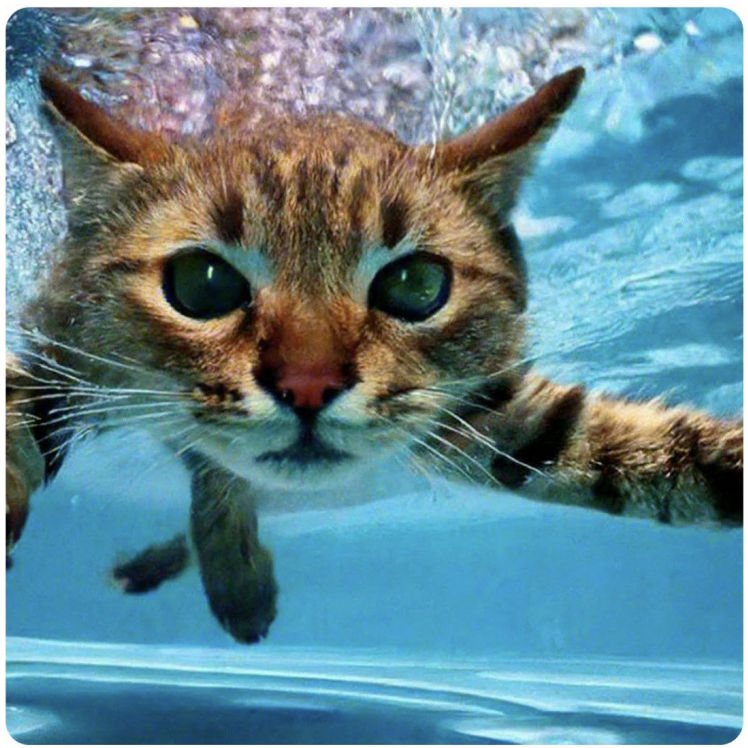
1. DDPM as score-based generative model

2. Guidance
   - Classifier guidance
   - Classifier-free guidance

3. Continuous-in-time normalizing flows

Guidance

- Throughout the whole course we have discussed unconditional generative models $p(\mathbf{x}|\boldsymbol{\theta})$.
- In practice the majority of the generative models are **conditional**: $p(\mathbf{x}|\mathbf{y}, \boldsymbol{\theta})$.
- Here $\mathbf{y}$ could be the class label or **text** (for text-to-image models).



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

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

Taxonomy of conditional tasks

In practice the popular task is to create a conditional model $\pi(\mathbf{x}|\mathbf{y})$.

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

Label guidance

Label: Ostrich (10th ImageNet class)

VQ-VAE (Proposed) **BigGAN deep**

Razavi A., Oord A., et al. Generating Diverse High-Fidelity Images with VQ-VAE-2, 2019

Text guidance

Prompt: a stained glass window of a panda eating bamboo
Left: $\gamma = 1$, Right: $\gamma = 3$.

Nichol A., et al. GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models, 2022

Guidance

- If we have **supervised** data $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^n$ we could theat $\mathbf{y}$ as additional model input:
  - $p(x_j|\mathbf{x}_{1:j-1}, \mathbf{y}, \boldsymbol{\theta})$ for AR;
  - Encoder $q(\mathbf{z}|\mathbf{x}, \mathbf{y}, \boldsymbol{\phi})$ and decoder $p(\mathbf{x}|\mathbf{z}, \mathbf{y}, \boldsymbol{\theta})$ for VAE;
  - $G_{\boldsymbol{\theta}}(\mathbf{z}, \mathbf{y})$ for NF and GAN;
  - $p(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{y}, \boldsymbol{\theta})$ for DDPM.
- If we have **unsupervised** data $\{\mathbf{x}_i\}_{i=1}^n$ we need to create the way to convert unconditional model $p(\mathbf{x}|\boldsymbol{\theta})$ to the conditional.
- It is really helpful to have the way to control the power of guidance.

Guidance types

- **Classifier guidance:**
  - suitable for unsupervised data;
  - uses the additional classifier model (we need supervised data to train the classifier).
- **Classifier-free guidance:**
  - suitable for supervised data;
  - get rid of the additional classifier model.

Outline

Classifier guidance

DDPM sampling

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

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

Conditional generation

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

- Assume for simplicity $\mathbf{y}$ is a class labels.
- Suppose that we have the distribution $p(\mathbf{y}|\mathbf{x}_t)$ – classifier on noisy samples.

Dhariwal P., Nichol A. Diffusion Models Beat GANs on Image Synthesis, 2021

Classifier guidance

Conditional generation

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

Conditional distribution

$$\begin{aligned}
\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}, \boldsymbol{\theta}) &= \nabla_{\mathbf{x}_t} \log \left(\frac{p(\mathbf{y}|\mathbf{x}_t) p(\mathbf{x}_t|\boldsymbol{\theta})}{p(\mathbf{y})} \right) \\
&= \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t) + \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\boldsymbol{\theta}) \\
&= \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t) - \frac{\boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t)}{\sqrt{1-\bar{\alpha}_t}}
\end{aligned}$$

Let parametetrize $\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}, \boldsymbol{\theta}) = -\frac{\boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t, \mathbf{y})}{\sqrt{1-\bar{\alpha}_t}}$.

Classifier-corrected noise prediction

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

Dhariwal P., Nichol A. Diffusion Models Beat GANs on Image Synthesis, 2021

Classifier guidance

Classifier-corrected noise prediction

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

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 we introduce guidance scale γ that controls the magnitude of the classifier guidance.

Training

- Train DDPM as usual.
- Train the additional classifier $p(\mathbf{y}|\mathbf{x}_t)$ on the noisy samples $\mathbf{x}_t$.

Guided sampling

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

Dhariwal P., Nichol A. Diffusion Models Beat GANs on Image Synthesis, 2021

Classifier guidance

Classifier-corrected noise prediction

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

Guidance-scaled conditional distribution

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

$$\begin{aligned}
\nabla^{\gamma}_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}, \boldsymbol{\theta}) &= \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\boldsymbol{\theta}) + \gamma \cdot \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t) \\
&= \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\boldsymbol{\theta}) + \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t)^{\gamma} \\
&= \nabla_{\mathbf{x}_t} \log \left(\frac{p(\mathbf{y}|\mathbf{x}_t)^{\gamma} p(\mathbf{x}_t|\boldsymbol{\theta})}{Z} \right)
\end{aligned}$$

Note: Guidance scale γ tries to sharpen the distribution $p(\mathbf{y}|\mathbf{x}_t)$ (in this case Z should not depend on $\mathbf{x}_t$).

Dhariwal P., Nichol A. Diffusion Models Beat GANs on Image Synthesis, 2021

Outline

Classifier-free guidance

- Previous method requires training the additional classifier model $p(\mathbf{y}|\mathbf{x}_t)$ on the noisy data.
- Let try to avoid this requirement.

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

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

$$= \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}, \boldsymbol{\theta}) - \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\boldsymbol{\theta})$$

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

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

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

Note: In the case of $\gamma = 1$ we will get the identity statement.

Ho J., Salimans T. Classifier-Free Diffusion Guidance, 2022

Classifier-free guidance

$$\nabla^{\gamma}_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y},\boldsymbol{\theta}) = (1-\gamma)\cdot\nabla_{\mathbf{x}_t}\log p(\mathbf{x}_t|\boldsymbol{\theta}) + \gamma\cdot\nabla_{\mathbf{x}_t}\log p(\mathbf{x}_t|\mathbf{y},\boldsymbol{\theta})$$

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

Classifier-free-corrected noise prediction

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

- Train the single model $\boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t,\mathbf{y})$ on **supervised** data alternating with real conditioning $\mathbf{y}$ and empty conditioning $\mathbf{y}=\emptyset$.
- Apply the model twice during inference.

Guided sampling

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

Ho J., Salimans T. Classifier-Free Diffusion Guidance, 2022

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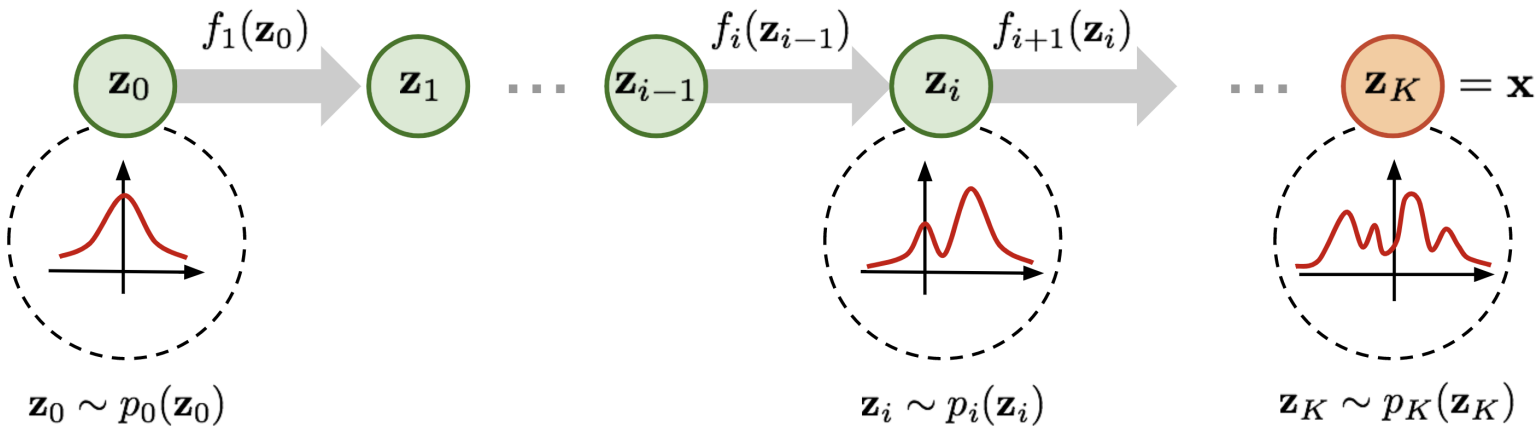
3. Continuous-in-time normalizing flows

Discrete-in-time NF

Change of variable theorem (CoV)

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

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



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

https://lilianweng.github.io/lil-log/2018/10/13/flow-based-deep-generative-models.html

Discrete-in-time NF

- Previously we assumed that the time axis is discrete:

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

- Let consider the more general case of continuous time. It means that we will have the function $\mathbf{x}(t) : \mathbb{R} \to \mathbb{R}^m$ of continuous dynamic.

Continuous-in-time dynamics

Consider Ordinary Differential Equation (ODE)

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

$$\mathbf{x}(t_1) = \int_{t_0}^{t_1} \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}(t), t) dt + \mathbf{x}_0$$

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

Numerical solution of ODE

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

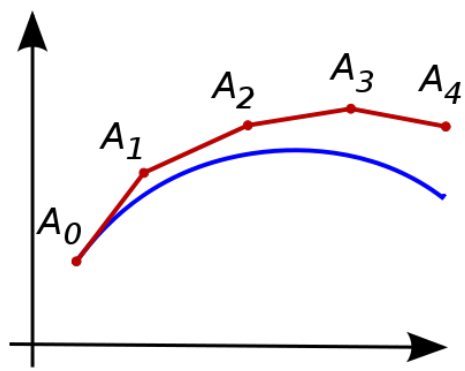
$$\mathbf{x}(t_1) = \int_{t_0}^{t_1} \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}(t), t)dt + \mathbf{x}_0 \approx \text{ODESolve}_f(\mathbf{x}_0, \boldsymbol{\theta}, t_0, t_1).$$

Here we need to define the computational procedure $\text{ODESolve}_f(\mathbf{x}_0, \boldsymbol{\theta}, t_0, t_1)$.

Euler update step

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

$$\mathbf{x}(t + \Delta t) = \mathbf{x}(t) + \Delta t \cdot \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}(t), t)$$



Note: Euler method is the simplest version of the ODESolve that is unstable in practice. It is possible to use more sophisticated numerical methods instead if Euler (e.x. Runge-Kutta methods).

Continuous-in-time NF

Neural ODE

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

Euler ODESolve

$$\mathbf{x}(t + \Delta t) = \mathbf{x}(t) + \Delta t \cdot \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{x}(t), t)$$

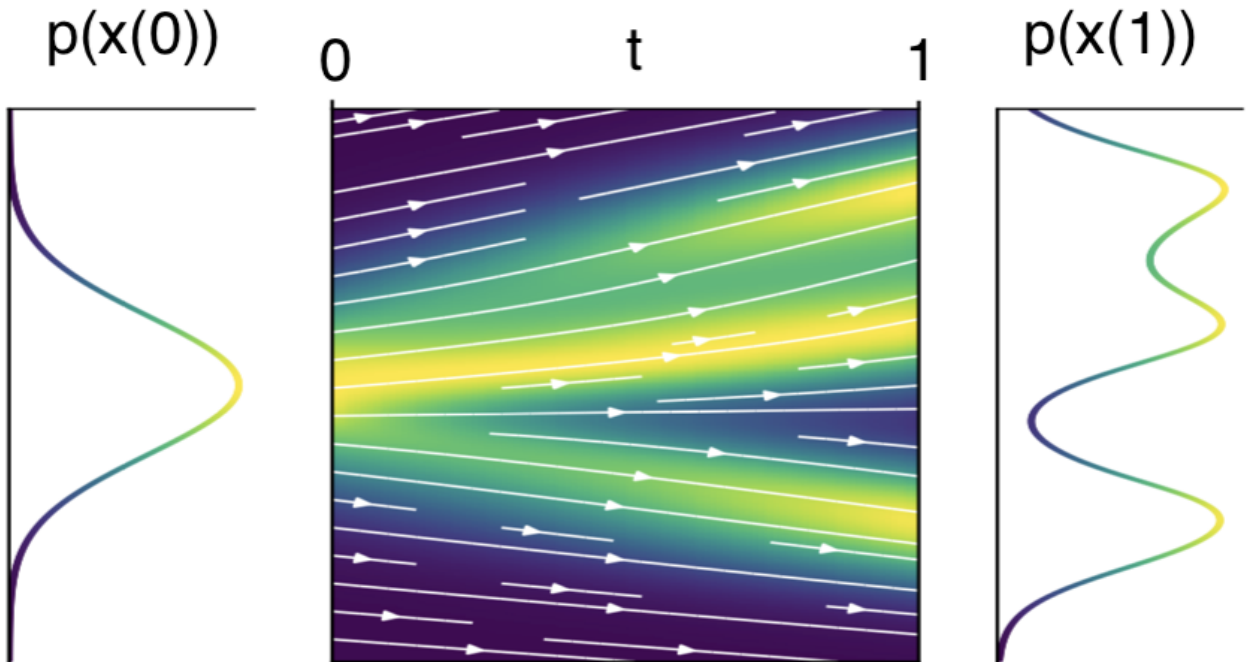
- Let consider time interval $[t_0, t_1] = [0, 1]$ without loss of generality.
- Assume that $\mathbf{x}(0)$ is a random variable with the density function $p_0(\mathbf{x})$.
- Then $\mathbf{x}(t)$ is a random variable with the density function $p_t(\mathbf{x})$.

Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

Continuous-in-time NF

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

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



Grathwohl W. et al. FFJORD: Free-form Continuous Dynamics for Scalable Reversible Generative Models, 2018

Continuous-in-time NF

Theorem (Picard)

If $\mathbf{f}$ is uniformly Lipschitz continuous in $\mathbf{x}$ and continuous in t, then the ODE has a **unique** solution.

It means that we are able **uniquely revert** our ODE.

$$\mathbf{x}(1) = \mathbf{x}(0) + \int_0^1 \mathbf{f}_\theta(\mathbf{x}(t), t)dt$$

$$\mathbf{x}(0) = \mathbf{x}(1) + \int_1^0 \mathbf{f}_\theta(\mathbf{x}(t), t)dt$$

Note: Unlike discrete-in-time NF, $\mathbf{f}$ does not need to be invertible (uniqueness guarantees bijectivity).
How to compute $p_t(\mathbf{x})$ at any moment t?

Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

Summary

- DDPM and NCSN are closely related in terms of objectives.
- Classifier guidance is the way to turn the unconditional model to the conditional one via the training additional classifier on the noisy data.
- Classifier-free guidance allows to avoid the training additional classifier to get the conditional model. It is widely used in practice.
- Continuous-in-time NF uses neural ODE to define continuous dynamic $\mathbf{x}(t)$. It has less functional restrictions.