Deep Generative Models

Lecture 14

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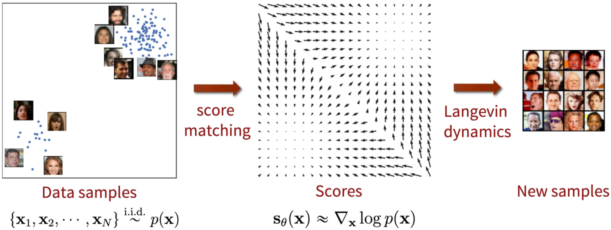
2023, Autumn

Recap of previous lecture



Theorem (implicit score matching)

$$\frac{1}{2}\mathbb{E}_\pi \left\| \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}) - \nabla_\mathbf{x} \log \pi(\mathbf{x}) \right\|_2^2 = \mathbb{E}_\pi \left[\frac{1}{2} \|\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\|_2^2 + \text{tr}\left(\nabla_\mathbf{x} \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x})\right) \right] + \text{const}$$

1. The left hand side is intractable due to unknown $\pi(\mathbf{x})$ – **denoising score matching**.
2. The right hand side is complex due to Hessian matrix – **sliced score matching (Hutchinson's trace estimation)**.

Song Y. Generative Modeling by Estimating Gradients of the Data Distribution, blog post, 2021

Recap of previous lecture

Let perturb original data by normal noise $p(\mathbf{x}'|\mathbf{x}, \sigma) = \mathcal{N}(\mathbf{x}'|\mathbf{x}, \sigma^2 \mathbf{I})$

$$\pi(\mathbf{x}'|\sigma) = \int \pi(\mathbf{x}) p(\mathbf{x}'|\mathbf{x}, \sigma) d\mathbf{x}.$$

Then the solution of

$$\frac{1}{2} \mathbb{E}_{\pi(\mathbf{x}'|\sigma)} \big\| \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma) - \nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma) \big\|_2^2 \rightarrow \min_{\boldsymbol{\theta}}$$

satisfies $\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma) \approx \mathbf{s}(\mathbf{x}', \boldsymbol{\theta}, 0) = \mathbf{s}(\mathbf{x}', \boldsymbol{\theta})$ if σ is small enough.

Theorem (denoising score matching)

$$\mathbb{E}_{\pi(\mathbf{x}'|\sigma)} \big\| \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma) - \nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma) \big\|_2^2 =$$
$$= \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{p(\mathbf{x}'|\mathbf{x}, \sigma)} \big\| \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma) - \nabla_{\mathbf{x}'} \log p(\mathbf{x}'|\mathbf{x}, \sigma) \big\|_2^2 + \text{const}(\boldsymbol{\theta})$$

Here $\nabla_{\mathbf{x}'} \log p(\mathbf{x}'|\mathbf{x}, \sigma) = -\frac{\mathbf{x}' - \mathbf{x}}{\sigma^2}$.

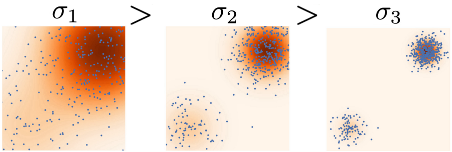
- The RHS does not need to compute $\nabla_{\mathbf{x}'} \log \pi(\mathbf{x}'|\sigma)$ and even more $\nabla_{\mathbf{x}'} \log \pi(\mathbf{x}')$.
- $\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma)$ tries to **denoise** a corrupted sample.
- Score function $\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma)$ parametrized by σ.

Vincent P. A Connection Between Score Matching and Denoising Autoencoders, 2010

Recap of previous lecture

Noise conditioned score network

- Define the sequence of noise levels: $\sigma_1 > \sigma_2 > \dots > \sigma_L$.
- Train denoised score function $\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma)$ for each noise level:
$$\sum_{l=1}^{L} \sigma_l^2 \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{p(\mathbf{x}'|\mathbf{x}, \sigma_l)} \big\| \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma_l) - \nabla'_{\mathbf{x}} \log p(\mathbf{x}'|\mathbf{x}, \sigma_l) \big\|_2^2 \to \min_{\boldsymbol{\theta}}$$
- Sample from **annealed** Langevin dynamics (for $l = 1, \dots, L$).



Song Y. et al. Generative Modeling by Estimating Gradients of the Data Distribution, 2019

Recap of previous lecture

NCSN training

1. Get the sample $\mathbf{x}_0 \sim \pi(\mathbf{x})$.
2. Sample noise level $l \sim U[1, L]$ and the noise $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.
3. Get noisy image $\mathbf{x}' = \mathbf{x}_0 + \sigma_l \cdot \boldsymbol{\epsilon}$.
4. Compute loss $\mathcal{L} = \|\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma_l) + \frac{\boldsymbol{\epsilon}}{\sigma_l}\|^2$.

NCSN sampling (annealed Langevin dynamics)

- Sample $\mathbf{x}_0 \sim \mathcal{N}(0, \sigma_1 \mathbf{I}) \approx \pi(\mathbf{x}|\sigma_L)$.
- Apply T steps of Langevin dynamic

$$\mathbf{x}_t = \mathbf{x}_{t-1} + \frac{1}{2}\alpha_l \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}_{t-1}, \sigma_l) + \sqrt{\alpha_l}\boldsymbol{\epsilon}_t.$$

- Update $\mathbf{x}_0 := \mathbf{x}_T$ and choose the next σ_l.

Song Y. et al. Improved Techniques for Training Score-Based Generative Models, 2020

Recap of previous lecture

NCSN objective

$$\mathbb{E}_{p(\mathbf{x}'|\mathbf{x},\sigma_l)}\left\|\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}', \sigma_l) - \nabla_{\mathbf{x}'} \log p(\mathbf{x}'|\mathbf{x}, \sigma_l)\right\|_2^2 \rightarrow \min_{\boldsymbol{\theta}}$$

DDPM objective

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

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

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

Let reparametrize our model:

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

Outline

1. Classifier guidance

2. The worst course overview

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1. Classifier guidance

2. The worst course overview

Classifier guidance

- Let imagine we are given the distribution $q(\mathbf{y}|\mathbf{x}_0)$.
- Since we have already defined Markov chain, we have $q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{y}) = q(\mathbf{x}_t|\mathbf{x}_{t-1})$.
- Let try to find reverse $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{y})$.
- Helper statement:

$$q(\mathbf{y}|\mathbf{x}_{t-1}, \mathbf{x}_t) = \frac{q(\mathbf{x}_{t-1}, \mathbf{x}_t, \mathbf{y})}{q(\mathbf{x}_{t-1}, \mathbf{x}_t)} =$$
$$= \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{y})q(\mathbf{y}|\mathbf{x}_{t-1})q(\mathbf{x}_{t-1})}{q(\mathbf{x}_t|\mathbf{x}_{t-1})q(\mathbf{x}_{t-1})} = q(\mathbf{y}|\mathbf{x}_{t-1}).$$

Conditional distribution

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{y}) = \frac{q(\mathbf{x}_{t-1}, \mathbf{x}_t, \mathbf{y})}{q(\mathbf{x}_t, \mathbf{y})} =$$
$$= \frac{q(\mathbf{y}|\mathbf{x}_{t-1}, \mathbf{x}_t)q(\mathbf{x}_{t-1}|\mathbf{x}_t)q(\mathbf{x}_t)}{q(\mathbf{y}|\mathbf{x}_t)q(\mathbf{x}_t)} =$$
$$= q(\mathbf{y}|\mathbf{x}_{t-1})q(\mathbf{x}_{t-1}|\mathbf{x}_t) \cdot \text{const}(\mathbf{x}_{t-1}).$$

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

Classifier guidance

Conditional distribution

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{y}) = q(\mathbf{y}|\mathbf{x}_{t-1})q(\mathbf{x}_{t-1}|\mathbf{x}_t) \cdot \text{const}(\mathbf{x}_{t-1}).$$

$$p(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{y}, \boldsymbol{\theta}, \phi) = p(\mathbf{y}|\mathbf{x}_{t-1}, \phi)p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta}) \cdot \text{const}(\mathbf{x}_{t-1}).$$

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

$$\log p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta}) = -\frac{\|\mathbf{x}_{t-1} - \boldsymbol{\mu}\|^2}{2\boldsymbol{\sigma}^2} + \text{const}(\mathbf{x}_{t-1})$$

$$\begin{aligned} \log p(\mathbf{y}|\mathbf{x}_{t-1}, \phi) \approx \log p(\mathbf{y}|\mathbf{x}_{t-1}, \phi)|_{\mathbf{x}_{t-1}=\boldsymbol{\mu}} + \\ + (\mathbf{x}_{t-1} - \boldsymbol{\mu})\nabla_{\mathbf{x}_{t-1}} \log p(\mathbf{y}|\mathbf{x}_{t-1}, \phi)|_{\mathbf{x}_{t-1}=\boldsymbol{\mu}} = \\ = (\mathbf{x}_{t-1} - \boldsymbol{\mu}) \cdot \mathbf{g} + \text{const}(\mathbf{x}_{t-1}), \end{aligned}$$

where $\mathbf{g} = \nabla_{\mathbf{x}_{t-1}} \log p(\mathbf{y}|\mathbf{x}_{t-1}, \phi)|_{\mathbf{x}_{t-1}=\boldsymbol{\mu}}$.

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

Classifier guidance

$$\log p(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{y}, \boldsymbol{\theta}, \phi) = \log p(\mathbf{y}|\mathbf{x}_{t-1}, \phi) + \log p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta}) + \text{const}(\mathbf{x}_{t-1})$$

$$\begin{aligned}
\log p(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{y}, \boldsymbol{\theta}, \phi) &= (\mathbf{x}_{t-1} - \boldsymbol{\mu}) \cdot \mathbf{g} - \frac{\|\mathbf{x}_{t-1} - \boldsymbol{\mu}\|^2}{2\boldsymbol{\sigma}^2} + \text{const}(\mathbf{x}_{t-1}) \\
&= -\frac{\|\mathbf{x}_{t-1} - \boldsymbol{\mu} - \boldsymbol{\sigma} \odot \mathbf{g}\|^2}{2\boldsymbol{\sigma}^2} + \text{const}(\mathbf{x}_{t-1}) \\
&= \log \mathcal{N}(\boldsymbol{\mu} + \boldsymbol{\sigma} \odot \mathbf{g}, \boldsymbol{\sigma}^2) + \text{const}(\mathbf{x}_{t-1})
\end{aligned}$$

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

Classifier guidance

Guided sampling

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

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

3. Compute $\mathbf{g} = \nabla_{\mathbf{x}_{t-1}} \log p(\mathbf{y}|\mathbf{x}_{t-1}, \phi)|_{\mathbf{x}_{t-1} = \boldsymbol{\mu}}$
4. Get denoised image $\mathbf{x}_{t-1} = (\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}_t, t) + s \cdot \tilde{\beta}_t \cdot \mathbf{g}) + \sqrt{\tilde{\beta}_t} \cdot \boldsymbol{\epsilon}$, where $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.

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

Outline

1. Classifier guidance

2. The worst course overview

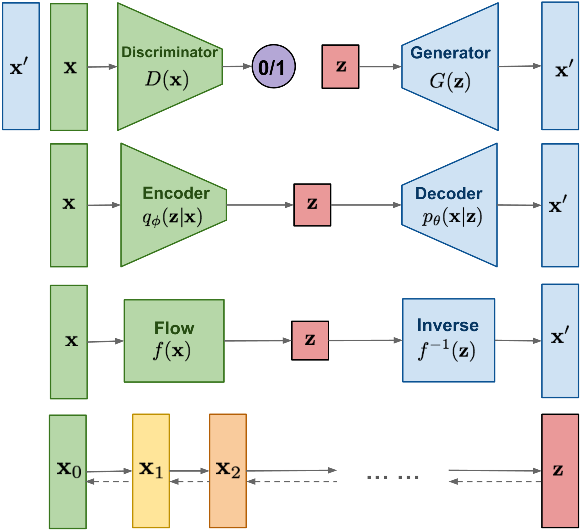
The worst course overview :)

GAN: Adversarial training

VAE: maximize variational lower bound

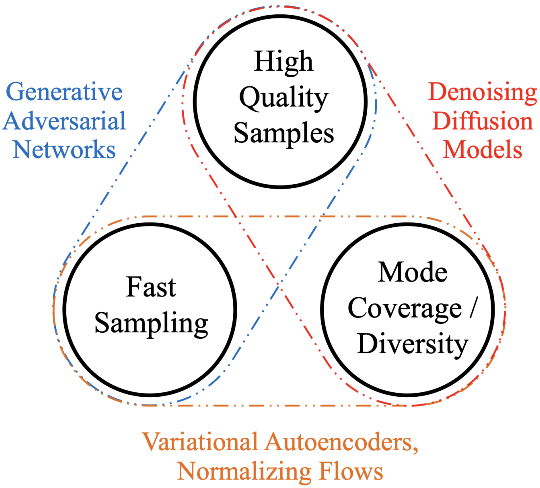
Flow-based models: Invertible transform of distributions

Diffusion models: Gradually add Gaussian noise and then reverse



Weng L. What are Diffusion Models?, blog post, 2021

The worst course overview :)



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

Summary

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