Deep Generative Models

Lecture 13

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AI Masters

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Recap of previous lecture

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

Reparametrization

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

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

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

At each step of reverse diffusion process we try to predict the noise $\boldsymbol{\epsilon}$ that we used in the forward diffusion process!

Simplified objective

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

Recap of previous lecture

Training

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 $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}$.
4. Compute loss $\mathcal{L}_{\text{simple}} = \|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\boldsymbol{\theta}}(\mathbf{x}_t, t)\|^2$.

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

Recap of previous lecture

NCSN objective

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

DDPM objective

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

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

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

Let reparametrize our model:

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

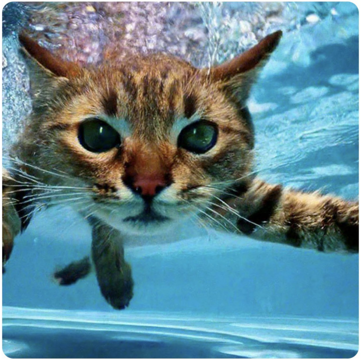
Ho J. Denoising Diffusion Probabilistic Models, 2020

Outline

Outline

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

Guidance

How to make conditional model $p(\mathbf{x}|\mathbf{y}, \boldsymbol{\theta})$?

- If we have **supervised** data $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^m$ we could theat $\mathbf{y}$ as additional model input:
  - $p(x_j|\mathbf{x}_{1:j-1}, \mathbf{y}, \boldsymbol{\theta})$ for AR;
  - Encoder $q(\mathbf{z}|\mathbf{x}, \mathbf{y}, \phi)$ 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 $\{\mathbf{x}_i\}_{i=1}^m$ we need to create the way to convert unconditional model $p(\mathbf{x}|\boldsymbol{\theta})$ to the conditional.

DDPM **unsupervised** 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 $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{y})$.

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

Outline

Classifier guidance

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

Conditional distribution

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

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

- $p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta})$ - our unsupervised diffusion model.
- $p(\mathbf{y}|\mathbf{x}_{t-1}, \phi)$ - classifier for noised samples $\mathbf{x}_{t-1}$

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

Classifier guidance

Conditional distribution

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

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

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

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

Taylor expansion

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

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

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

Guided sampling

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

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

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 $\mathbf{x}_{t-1} = (\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}_t, t) + \sqrt{\tilde{\beta}_t} \cdot \mathbf{g}) + \sqrt{\tilde{\beta}_t} \cdot \boldsymbol{\epsilon}$, where $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.

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

Classifier guidance

Theorem (denoising score matching)

$$\mathbb{E}_{q(\mathbf{x}_t)} \big\| \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}_t, t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t) \big\|_2^2 =$$

$$= \mathbb{E}_{\pi(\mathbf{x}_0)} \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x}_0)} \big\| \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}_t, t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t|\mathbf{x}_0) \big\|_2^2 + \text{const}(\boldsymbol{\theta})$$

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

Conditional distribution

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

Classifier-corrected noise prediction

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

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

Classifier guidance

Classifier-corrected noise prediction

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

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

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

Conditional distribution

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

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

$$p(\mathbf{x}_t|\mathbf{y}, \boldsymbol{\theta}, \boldsymbol{\phi}) = \frac{p(\mathbf{y}|\mathbf{x}_t, \boldsymbol{\phi})^{\gamma} p(\mathbf{x}_t|\boldsymbol{\theta})}{Z}$$

Check that $\nabla_{\mathbf{x}_t} \log Z \neq 0$.

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 "corrected" $\hat{\boldsymbol{\epsilon}}_{\boldsymbol{\theta}}(\mathbf{x}_t, t)$:

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

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

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

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

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

Outline

1. Guidance
   - Classifier guidance
   - Classifier-free guidance
2. SDE basics
3. Diffusion and Score matching SDEs

Classifier-free guidance

Previous methods require training the additional classifier model $p(\mathbf{y}|\mathbf{x}_t, \boldsymbol{\theta})$ on the noisy data. Let try to avoid this requirement.

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

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

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

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

What will we get if $\gamma = 1$?

Classifier-free-corrected noise prediction

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

In practice we could train the single model $\boldsymbol{\epsilon}_{\boldsymbol{\theta}}(\mathbf{x}_t, \mathbf{y}, t)$ on **supervised** data alternating with real conditioning $\mathbf{y}$ and empty conditioning $\mathbf{y} = \emptyset$.

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

Outline

1. Guidance
   - Classifier guidance
   - Classifier-free guidance

2. SDE basics

3. Diffusion and Score matching SDEs

Stochastic differential equation (SDE)

Let define stochastic process $\mathbf{x}(t)$ with initial condition $\mathbf{x}(0) \sim p_0(\mathbf{x})$:

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$$

- $\mathbf{f}(\mathbf{x}, t)$ is the **drift** function of $\mathbf{x}(t)$.
- $g(t)$ is the **diffusion** coefficient of $\mathbf{x}(t)$.
- If $g(t) = 0$ we get standard ODE.
- $\mathbf{w}(t)$ is the standard Wiener process (Brownian motion):
  1. $\mathbf{w}(0) = 0$ (almost surely);
  2. $\mathbf{w}(t)$ has independent increments;
  3. $\mathbf{w}(t) - \mathbf{w}(s) \sim \mathcal{N}(0, (t-s)\mathbf{I})$.
- $d\mathbf{w} = \mathbf{w}(t + dt) - \mathbf{w}(t) = \mathcal{N}(0, \mathbf{I} \cdot dt) = \boldsymbol{\epsilon} \cdot \sqrt{dt}$, where $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$.

Note: In contrast to ODE, initial condition $\mathbf{x}(0)$ does not uniquely determine the process trajectory.

Stochastic differential equation (SDE)

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}, \quad d\mathbf{w} = \boldsymbol{\epsilon} \cdot \sqrt{dt}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}).$$

- At each moment t we have the density $p(\mathbf{x}(t), t)$.
- How to get distribution $p(\mathbf{x}, t)$ for $\mathbf{x}(t)$?

Theorem (Kolmogorov-Fokker-Planck)

Evolution of the distribution $p(\mathbf{x}, t)$ is given by the following ODE:

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = \mathrm{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\big[\mathbf{f}(\mathbf{x}, t)p(\mathbf{x}, t)\big] + \frac{1}{2}g^2(t)\frac{\partial^2 p(\mathbf{x}, t)}{\partial \mathbf{x}^2}\right)$$

Note: This is the generalization of KFP theorem that we used in continuous-in-time NF.

Langevin SDE (special case)

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$$

$$d\mathbf{x} = \frac{1}{2}\frac{\partial}{\partial \mathbf{x}}\log p(\mathbf{x}, t)dt + 1 \cdot d\mathbf{w}$$

Langevin SDE (special case)

$$d\mathbf{x} = \frac{1}{2}\frac{\partial}{\partial \mathbf{x}} \log p(\mathbf{x}, t) dt + 1 \cdot d\mathbf{w}$$

Let apply KFP theorem.

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} = \mathrm{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[p(\mathbf{x}, t)\frac{1}{2}\frac{\partial}{\partial \mathbf{x}} \log p(\mathbf{x}, t)\right] + \frac{1}{2}\frac{\partial^2 p(\mathbf{x}, t)}{\partial \mathbf{x}^2}\right) =$$

$$= \mathrm{tr}\left(-\frac{\partial}{\partial \mathbf{x}}\left[\frac{1}{2}\frac{\partial}{\partial \mathbf{x}} p(\mathbf{x}, t)\right] + \frac{1}{2}\frac{\partial^2 p(\mathbf{x}, t)}{\partial \mathbf{x}^2}\right) = 0$$

The density $p(\mathbf{x}, t) = \mathrm{const}(t)$!

Discretized Langevin SDE

$$\mathbf{x}_{t+1} - \mathbf{x}_t = \frac{\eta}{2} \cdot \frac{\partial}{\partial \mathbf{x}} \log p(\mathbf{x}, t) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}, \quad \eta \approx dt.$$

Langevin dynamic

$$\mathbf{x}_{t+1} = \mathbf{x}_t + \frac{\eta}{2} \cdot \nabla_{\mathbf{x}} \log p(\mathbf{x}|\boldsymbol{\theta}) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}, \quad \eta \approx dt.$$

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Score matching SDE

Denoising score matching

$$\mathbf{x}_l = \mathbf{x} + \sigma_l \cdot \boldsymbol{\epsilon}_l, \quad p(\mathbf{x}_l|\mathbf{x}, \sigma_l) = \mathcal{N}(\mathbf{x}, \sigma_l^2 \mathbf{I})$$
$$\mathbf{x}_{l-1} = \mathbf{x} + \sigma_{l-1} \cdot \boldsymbol{\epsilon}_{l-1}, \quad p(\mathbf{x}_{l-1}|\mathbf{x}, \sigma_{l-1}) = \mathcal{N}(\mathbf{x}, \sigma_{l-1}^2 \mathbf{I})$$

$$\mathbf{x}_l = \mathbf{x}_{l-1} + \sqrt{\sigma_l^2 - \sigma_{l-1}^2} \cdot \boldsymbol{\epsilon}, \quad p(\mathbf{x}_l|\mathbf{x}_{l-1}, \sigma_l) = \mathcal{N}(\mathbf{x}_{l-1}, (\sigma_l^2 - \sigma_{l-1}^2) \cdot \mathbf{I})$$

Let turn this Markov chain to the continuous stochastic process $\mathbf{x}(t)$ taking $L \to \infty$:

$$\mathbf{x}(t + dt) = \mathbf{x}(t) + \sqrt{\frac{\sigma^2(t + dt) - \sigma^2(t)}{dt}} dt \cdot \boldsymbol{\epsilon} = \mathbf{x}(t) + \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}$$

Variance Exploding SDE

$$d\mathbf{x} = \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}$$

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

Diffusion SDE

Denoising Diffusion

$$\mathbf{x}_t = \sqrt{1-\beta_t}\cdot\mathbf{x}_{t-1} + \sqrt{\beta_t}\cdot\boldsymbol{\epsilon}, \quad q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\sqrt{1-\beta_t}\cdot\mathbf{x}_{t-1}, \beta_t\cdot\mathbf{I})$$

Let turn this Markov chain to the continuous stochastic process taking $T \to \infty$ and taking $\beta(\frac{t}{T}) = \beta_t \cdot T$

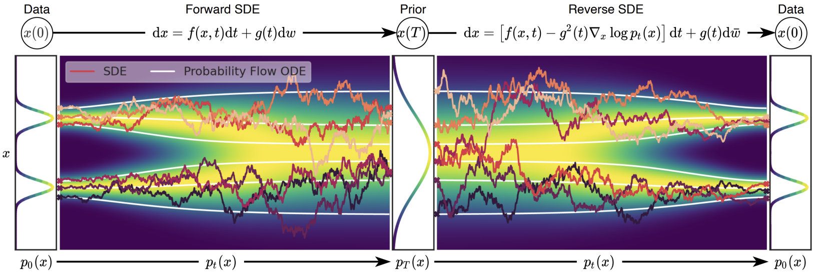
$$\begin{aligned}
\mathbf{x}(t) &= \sqrt{1-\beta(t)dt}\cdot\mathbf{x}(t-dt) + \sqrt{\beta(t)dt}\cdot\boldsymbol{\epsilon} \approx \\
&\approx (1 - \frac{1}{2}\beta(t)dt)\cdot\mathbf{x}(t-dt) + \sqrt{\beta(t)dt}\cdot\boldsymbol{\epsilon} = \\
&= \mathbf{x}(t-dt) - \frac{1}{2}\beta(t)\mathbf{x}(t-dt)dt + \sqrt{\beta(t)}\cdot d\mathbf{w}
\end{aligned}$$

Variance Preserving SDE

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}(t)dt + \sqrt{\beta(t)}\cdot d\mathbf{w}$$

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

Diffusion SDE



Variance Exploding SDE (NCSN)

$$d\mathbf{x} = \sqrt{\frac{d[\sigma^2(t)]}{dt}} \cdot d\mathbf{w}$$

Variance Preserving SDE (DDPM)

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}(t)dt + \sqrt{\beta(t)} \cdot d\mathbf{w}$$

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

Summary

- Score matching (NCSN) and diffusion models (DDPM) are the discretizations of the SDEs (variance exploding and variance preserving).
- Conditional models use labels $\mathbf{y}$ as the additional input. Majority of the modern generative models are conditional.
- 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.