Deep Generative Models

Lecture 10

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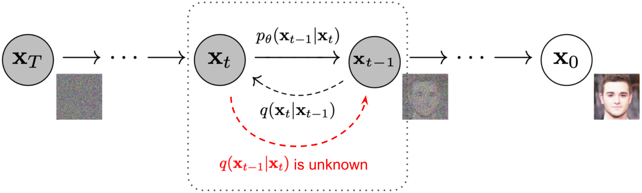
2024, Autumn

Recap of previous lecture



Reverse process

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

Forward process

1. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$;
2. $\mathbf{x}_t = \sqrt{1-\beta_t} \cdot \mathbf{x}_{t-1} + \sqrt{\beta_t} \cdot \boldsymbol{\epsilon}$;
3. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$.

Reverse process

1. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$;
2. $\mathbf{x}_{t-1} = \boldsymbol{\sigma}_{\boldsymbol{\theta},t}(\mathbf{x}_t) \cdot \boldsymbol{\epsilon} + \boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t)$;
3. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$;

Note: The forward process does not have any learnable parameters!

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

Recap of previous lecture

- $\mathbf{z} = (\mathbf{x}_1, \dots, \mathbf{x}_T)$ is a latent variable.
- 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 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

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

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

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

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

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 $\boldsymbol{\epsilon}$ that we used in the forward diffusion process!

Simplified objective

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

Outline

1. Denoising Diffusion Probabilistic Model (DDPM)
   - Reparametrization of Gaussian diffusion model
   - Overview
2. Denosing diffusion as score-based generative model
3. Guidance
   - Classifier guidance
   - Classifier-free guidance
4. Continuous-in-time normalizing flows

Outline

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   Classifier guidance
   Classifier-free guidance
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Reparametrization of DDPM

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

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

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

- There is linear dependence between $\boldsymbol{\epsilon}$, $\mathbf{x}_t$, $\mathbf{x}_0$.
- Let try to rewrite this mean in terms of $\mathbf{x}_t$ and $\boldsymbol{\epsilon}$.

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

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Reparametrization of DDPM

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

Reparametrization

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

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

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

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

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Reparametrization of DDPM

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

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

Let drop the scaling coefficient.

Simplified objective

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

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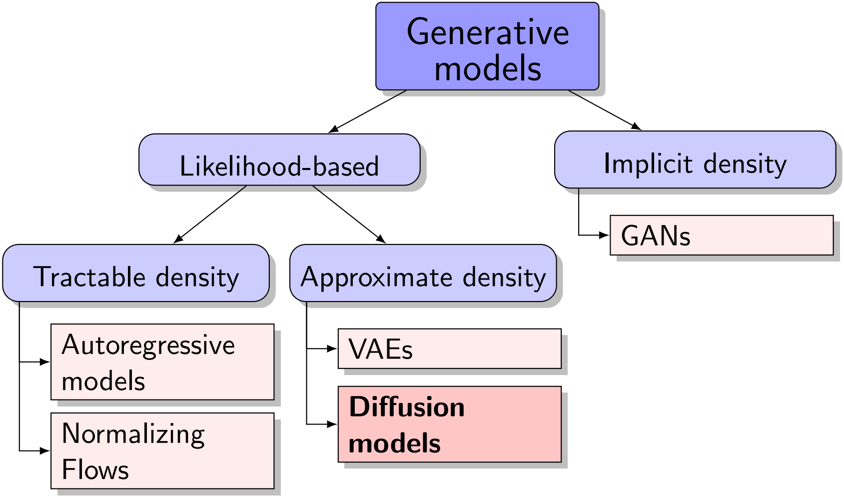
Outline

Generative models zoo



Denoising diffusion probabilistic model (DDPM)

DDPM is a VAE model

- Encoder is a fixed Gaussian Markov chain $q(\mathbf{x}_1, \dots, \mathbf{x}_T | \mathbf{x}_0)$.
- Latent variable is a hierarchical (in each step the dim. of the latent equals to the dim of the input).
- Decoder is a simple Gaussian model $p(\mathbf{x}_0 | \mathbf{x}_1, \boldsymbol{\theta})$.
- Prior distribution is given by parametric Gaussian Makov chain $p(\mathbf{x}_{t-1} | \mathbf{x}_t, \boldsymbol{\theta})$.

Forward process

1. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$;
2. $\mathbf{x}_t = \sqrt{1 - \beta_t} \cdot \mathbf{x}_{t-1} + \sqrt{\beta_t} \cdot \boldsymbol{\epsilon}$;
3. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$.

Reverse process

1. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$;
2. $\mathbf{x}_{t-1} = \boldsymbol{\sigma}_{\boldsymbol{\theta},t}(\mathbf{x}_t) \cdot \boldsymbol{\epsilon} + \boldsymbol{\mu}_{\boldsymbol{\theta},t}(\mathbf{x}_t)$;
3. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$;

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Denoising diffusion probabilistic model (DDPM)

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

Sampling

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

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

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

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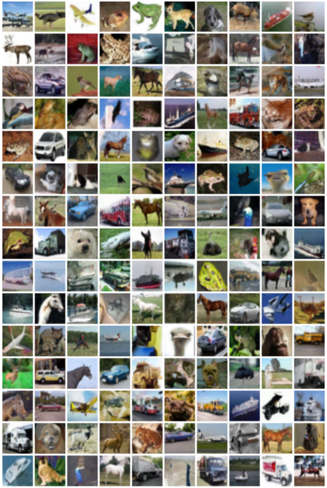
Denoising diffusion probabilistic model (DDPM)

Samples



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Outline

Denosing diffusion as score-based generative model

DDPM objective

$$\mathcal{L}_t = \mathbb{E}_{\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})} \left[\frac{(1-\alpha_t)^2}{2\tilde{\beta}_t \alpha_t (1-\bar{\alpha}_t)} \left\| \boldsymbol{\epsilon}_{\boldsymbol{\theta}, t}\left(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}\right) - \boldsymbol{\epsilon} \right\|_2^2 \right]$$

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

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

Let reparametrize our model:

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

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

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Denosing diffusion as score-based generative model

DDPM objective

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

In practice the coefficient is omitted.

NCSN objective

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

Note: The objective of DDPM and NCSN is almost identical. But the difference in sampling scheme:

- NCSN uses annealed Langevin dynamics;
- DDPM uses ancestral sampling.

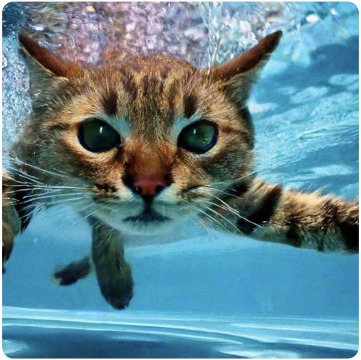
$$\mathbf{s}_{\boldsymbol{\theta},t}(\mathbf{x}_t)=-\frac{\boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t)}{\sqrt{1-\bar{\alpha}_t}}=\nabla_{\mathbf{x}_t}\log p(\mathbf{x}_t|\boldsymbol{\theta})$$

Ho J. Denoising Diffusion Probabilistic Models, 2020

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

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

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

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

Diffusion **unsupervised** guidance

- Assume that we are given the distribution $q(\mathbf{y}|\mathbf{x}_0)$.
- **Forward process:** since we have already defined Markov chain, we have $q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{y}) = q(\mathbf{x}_t|\mathbf{x}_{t-1})$.
- **Reverse process:** let try to find reverse $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{y})$.

Outline

Classifier guidance

DDPM sampling

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

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

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

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

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

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

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

Classifier guidance

Unconditional generation

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

Conditional generation

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

Conditional distribution

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

Here $p(\mathbf{y}|\mathbf{x}_t)$ – classifier on noisy samples (we have to learn it separately).

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

Classifier guidance

Conditional distribution

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

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

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

Guidance scale

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

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

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

Classifier guidance

Classifier-corrected noise prediction

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

Conditional distribution

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

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

Note: Guidance scale γ tries to sharpen the distribution $p(\mathbf{y}|\mathbf{x}_t)$.

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

Classifier guidance

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

Guided sampling

1. Sample $\mathbf{x}_T \sim \mathcal{N}(0, \mathbf{I})$.
2. Compute "corrected" $\boldsymbol{\epsilon}_{\boldsymbol{\theta},t}(\mathbf{x}_t, \mathbf{y})$:

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

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

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

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

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

Outline

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

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

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

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.

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

Outline

Continuous-in-time normalizing flows

Discrete-in-time NF

Previously we assume that the time axis is discrete:

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

Let assume the more general case of continuous time. It means that we will have the dynamic function $\mathbf{z}(t)$.

Continuous-in-time dynamics

Consider Ordinary Differential Equation (ODE)

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

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

Here we need to define the computational procedure $\text{ODESolve}(\mathbf{z}(t_0), \mathbf{f}_{\boldsymbol{\theta}}, t_0, t_1)$.

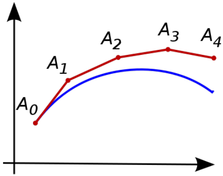
Grathwohl W. et al. FFJORD: Free-form Continuous Dynamics for Scalable Reversible Generative Models, 2018

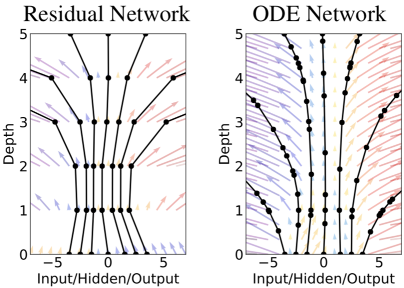
Continuous-in-time normalizing flows

Euler update step

$$\frac{\mathbf{z}(t+\Delta t) - \mathbf{z}(t)}{\Delta t} = \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z}(t), t) \;\Rightarrow\; \mathbf{z}(t+\Delta t) = \mathbf{z}(t) + \Delta t \cdot \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z}(t), t)$$

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





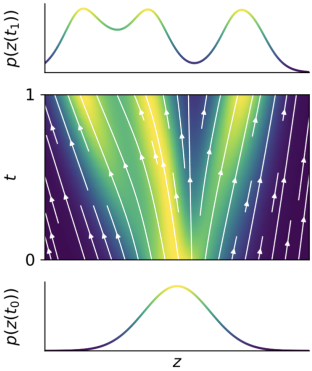
Chen R. T. Q. et al. Neural Ordinary Differential Equations, 2018

Continuous-in-time Normalizing Flows

Neural ODE

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

- $\mathbf{z}(t_0)$ is a random variable with the density function $p(\mathbf{z}(t_0))$.
- $\mathbf{z}(t_1)$ is a random variable with the density function $p(\mathbf{z}(t_1))$.
- $p_t(\mathbf{z}) = p(\mathbf{z}, t)$ is the joint density function (probability path).
  What is the difference between $p_t(\mathbf{z}(t))$ and $p_t(\mathbf{z})$?
- Let consider time interval $[t_0, t_1] = [0, 1]$ without loss of generality.



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

Continuous-in-time Normalizing Flows

Let say that $p_0(\mathbf{z})$ is the base distribution ($\mathcal{N}(0, \mathbf{I})$) and $p_1(\mathbf{z})$ is the desired model distribution $p(\mathbf{x}|\boldsymbol{\theta})$.

Theorem (Picard)

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

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

Forward and inverse transforms

$$\mathbf{x} = \mathbf{z}(1) = \mathbf{z}(0) + \int_0^1 \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z}(t), t) dt$$
$$\mathbf{z} = \mathbf{z}(0) = \mathbf{z}(1) + \int_1^0 \mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z}(t), t) dt$$

Note: Unlike discrete-in-time NF, $\mathbf{f}$ does not need to be bijective (uniqueness guarantees bijectivity).

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

Summary

- At each step DDPM predicts the noise that was used in the forward diffusion process. This noise is used in the reverse process.
- DDPM is a VAE model that tries to invert forward diffusion process using variational inference. DDPM is really slow, because we have to apply the model T times.
- Objective of DDPM is closely related to the noise conditioned score network and score matching.
- 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.
- Continuous-in-time NF uses neural ODE to define continuous dynamic $\mathbf{z}(t)$. It has less functional restrictions.