

Deep Generative Models

Lecture 14

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Recap of previous lecture

Continuous-in-time normalizing flows

$$\frac{d\mathbf{z}(t)}{dt} = f(\mathbf{z}(t), t, \theta); \quad \frac{d \log p(\mathbf{z}(t), t)}{dt} = -\text{tr} \left(\frac{\partial f(\mathbf{z}(t), t, \theta)}{\partial \mathbf{z}(t)} \right).$$

Theorem (Picard)

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

Forward transform + log-density

$$\begin{bmatrix} \mathbf{x} \\ \log p(\mathbf{x}|\theta) \end{bmatrix} = \begin{bmatrix} \mathbf{z} \\ \log p(\mathbf{z}) \end{bmatrix} + \int_{t_0}^{t_1} \begin{bmatrix} f(\mathbf{z}(t), t, \theta) \\ -\text{tr} \left(\frac{\partial f(\mathbf{z}(t), t, \theta)}{\partial \mathbf{z}(t)} \right) \end{bmatrix} dt.$$

Hutchinson's trace estimator

$$\log p(\mathbf{z}(t_1)) = \log p(\mathbf{z}(t_0)) - \mathbb{E}_{p(\epsilon)} \int_{t_0}^{t_1} \left[\epsilon^T \frac{\partial f}{\partial \mathbf{z}} \epsilon \right] dt.$$

Recap of previous lecture

SDE basics

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

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

where $\mathbf{w}(t)$ is the standard Wiener process (Brownian motion)

$$\mathbf{w}(t) - \mathbf{w}(s) \sim \mathcal{N}(0, (t-s)\mathbf{I}), \quad d\mathbf{w} = \epsilon \cdot \sqrt{dt}, \text{ where } \epsilon \sim \mathcal{N}(0, \mathbf{I}).$$

Langevin dynamics

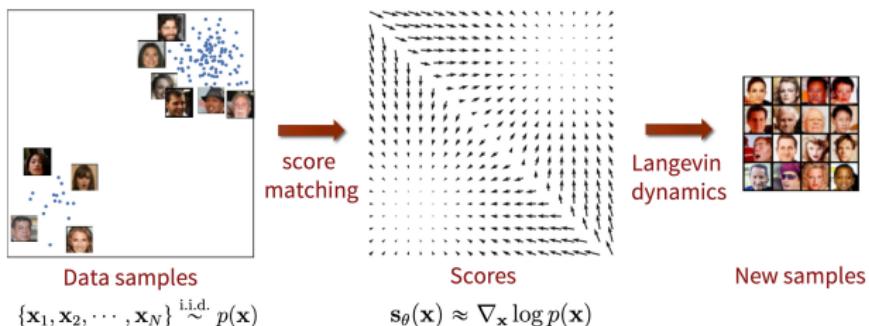
Let \mathbf{x}_0 be a random vector. Then under mild regularity conditions for small enough η samples from the following dynamics

$$\mathbf{x}_{t+1} = \mathbf{x}_t + \eta \frac{1}{2} \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t | \theta) + \sqrt{\eta} \cdot \epsilon, \quad \epsilon \sim \mathcal{N}(0, \mathbf{I}).$$

will come from $p(\mathbf{x} | \theta)$.

The density $p(\mathbf{x} | \theta)$ is a **stationary** distribution for the Langevin SDE.

Recap of previous lecture



Theorem (implicit score matching)

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

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)**.

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

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

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

Theorem (denoising score matching)

$$\begin{aligned} \mathbb{E}_{\pi(\mathbf{x}|\sigma)} \| \mathbf{s}(\mathbf{x}, \theta, \sigma) - \nabla_{\mathbf{x}} \log \pi(\mathbf{x}|\sigma) \|_2^2 &= \\ &= \mathbb{E}_{\pi(\mathbf{x}')} \mathbb{E}_{p(\mathbf{x}|\mathbf{x}', \sigma)} \| \mathbf{s}(\mathbf{x}, \theta, \sigma) - \nabla_{\mathbf{x}} \log p(\mathbf{x}|\mathbf{x}', \sigma) \|_2^2 \end{aligned}$$

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 $\nabla_{\mathbf{x}} \log \pi(\mathbf{x})$.
- ▶ $\mathbf{s}(\mathbf{x}, \theta, \sigma)$ tries to **denoise** a corrupted sample.
- ▶ Score function $\mathbf{s}(\mathbf{x}, \theta, \sigma)$ parametrized by σ . How to make it?

Outline

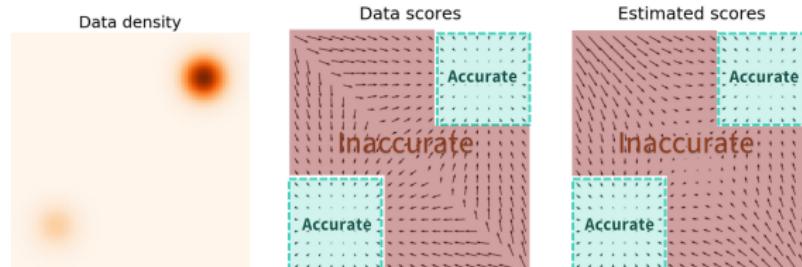
1. Noise conditioned score network
2. Diffusion models
 - Gaussian diffusion process
 - Denoising diffusion probabilistic model (DDPM)

Outline

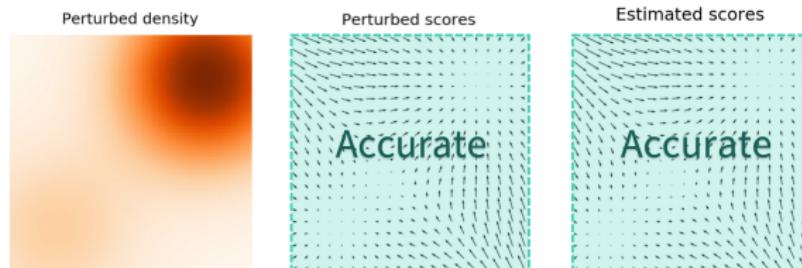
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Denoising score matching

- If σ is **small**, the score function is not accurate and Langevin dynamics will probably fail to jump between modes.



- If σ is **large**, it is good for low-density regions and multimodal distributions, but we will learn too corrupted distribution.

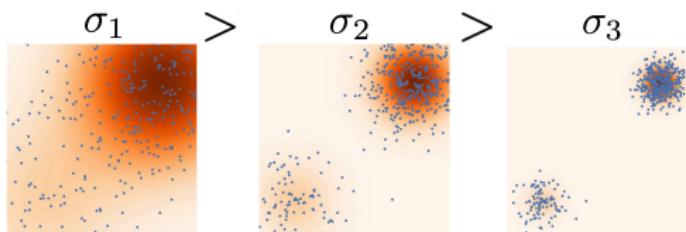


Noise conditioned score network

- ▶ Define the sequence of noise levels: $\sigma_1 > \sigma_2 > \dots > \sigma_L$.
- ▶ Perturb the original data with the different noise level to get $\pi(\mathbf{x}|\sigma_1), \dots, \pi(\mathbf{x}|\sigma_L)$.
- ▶ Train denoised score function $\mathbf{s}(\mathbf{x}, \theta, \sigma)$ for each noise level:

$$\sum_{l=1}^L \sigma_l^2 \mathbb{E}_{\pi(\mathbf{x}')} \mathbb{E}_{p(\mathbf{x}|\mathbf{x}', \sigma_l)} \| \mathbf{s}(\mathbf{x}, \theta, \sigma_l) - \nabla_{\mathbf{x}} \log p(\mathbf{x}|\mathbf{x}', \sigma_l) \|_2^2 \rightarrow \min_{\theta}$$

- ▶ Sample from **annealed** Langevin dynamics (for $l = 1, \dots, L$).



Noise conditioned score network

Training: loss function

$$\sum_{I=1}^L \sigma_I^2 \mathbb{E}_{\pi(\mathbf{x}')} \mathbb{E}_\epsilon \left\| \mathbf{s}_I + \frac{\epsilon}{\sigma_I} \right\|_2^2,$$

Here

- ▶ $\mathbf{s}_I = \mathbf{s}(\mathbf{x}' + \sigma_I \cdot \epsilon, \theta, \sigma_I)$.
- ▶ $\nabla_{\mathbf{x}} \log p(\mathbf{x} | \mathbf{x}', \sigma) = -\frac{\mathbf{x} - \mathbf{x}'}{\sigma^2} = -\frac{\epsilon}{\sigma_I}$.

Samples



Inference: annealed Langevin dynamic

Algorithm 1 Annealed Langevin dynamics.

Require: $\{\sigma_i\}_{i=1}^L, \epsilon, T$.

```
1: Initialize  $\tilde{\mathbf{x}}_0$ 
2: for  $i \leftarrow 1$  to  $L$  do
3:    $\alpha_i \leftarrow \epsilon \cdot \sigma_i^2 / \sigma_L^2$        $\triangleright \alpha_i$  is the step size.
4:   for  $t \leftarrow 1$  to  $T$  do
5:     Draw  $\mathbf{z}_t \sim \mathcal{N}(0, I)$ 
6:      $\tilde{\mathbf{x}}_t \leftarrow \tilde{\mathbf{x}}_{t-1} + \frac{\alpha_i}{2} \mathbf{s}_\theta(\tilde{\mathbf{x}}_{t-1}, \sigma_i) + \sqrt{\alpha_i} \mathbf{z}_t$ 
7:   end for
8:    $\tilde{\mathbf{x}}_0 \leftarrow \tilde{\mathbf{x}}_T$ 
9: end for
return  $\tilde{\mathbf{x}}_T$ 
```

Outline

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Forward gaussian diffusion process

Let $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$, $\beta \in (0, 1)$. Define the Markov chain

$$\mathbf{x}_t = \sqrt{1 - \beta} \cdot \mathbf{x}_{t-1} + \sqrt{\beta} \cdot \boldsymbol{\epsilon}, \quad \text{where } \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1);$$

$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t | \sqrt{1 - \beta} \cdot \mathbf{x}_{t-1}, \beta \cdot \mathbf{I}).$$

Statement 1

Applying the Markov chain to samples from any $\pi(\mathbf{x})$ we will get $\mathbf{x}_\infty \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, 1)$. Here $p_\infty(\mathbf{x})$ is a **stationary** distribution:

$$p_\infty(\mathbf{x}) = \int q(\mathbf{x} | \mathbf{x}') p_\infty(\mathbf{x}') d\mathbf{x}'.$$

Statement 2

Denote $\bar{\alpha}_t = \prod_{s=1}^t (1 - \beta_s)$. Then

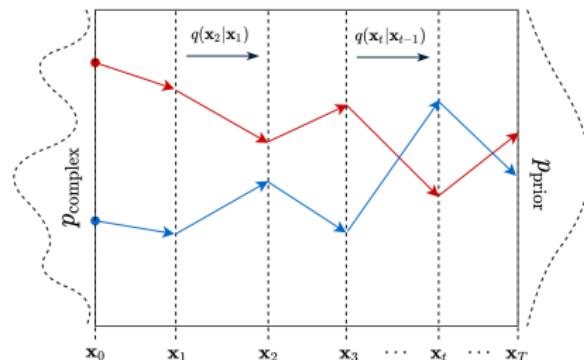
$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}, \quad \text{where } \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1)$$

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

We could sample from any timestamp using only \mathbf{x}_0 !

Forward gaussian diffusion process

Diffusion refers to the flow of particles from high-density regions towards low-density regions.

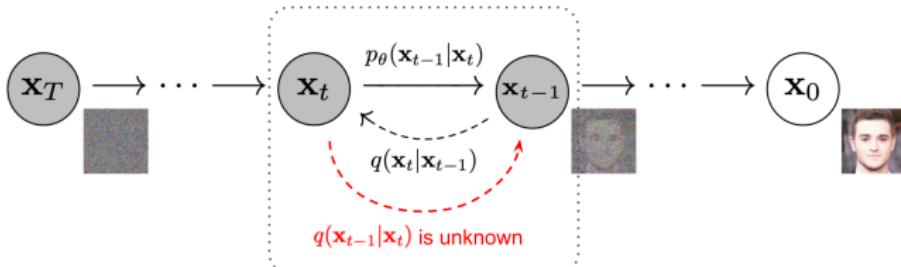


1. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x});$
2. $\mathbf{x}_t = \sqrt{1 - \beta} \cdot \mathbf{x}_{t-1} + \sqrt{\beta} \cdot \epsilon,$ where $\epsilon \sim \mathcal{N}(0, 1), t \geq 1;$
3. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, 1),$ where $T \gg 1.$

If we are able to invert this process, we will get the way to sample $\mathbf{x} \sim \pi(\mathbf{x})$ using noise samples $p_\infty(\mathbf{x}) = \mathcal{N}(0, 1).$

Now our goal is to revert this process.

Reverse gaussian diffusion process



Let define the reverse process

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

Forward process

1. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x});$

2. $\mathbf{x}_t = \sqrt{1 - \beta} \cdot \mathbf{x}_{t-1} + \sqrt{\beta} \cdot \boldsymbol{\epsilon},$ where $\boldsymbol{\epsilon} \sim \mathcal{N}(0, 1), t \geq 1;$

3. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, 1).$

Reverse process

1. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, 1);$

2. $\mathbf{x}_{t-1} = \sigma(\mathbf{x}_t, \theta, t) \cdot \boldsymbol{\epsilon} + \mu(\mathbf{x}_t, \theta, t);$

3. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x});$

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

Outline

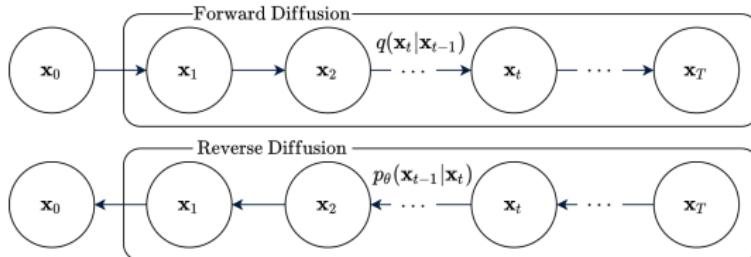
1. Noise conditioned score network

2. Diffusion models

Gaussian diffusion process

Denoising diffusion probabilistic model (DDPM)

Gaussian diffusion model as VAE



- ▶ Let treat $\mathbf{z} = (x_1, \dots, x_T)$ as a latent variable (**note**: each x_t has the same size).
- ▶ Variational posterior distribution (**note**: there is no learnable parameters)

$$q(\mathbf{z}|\mathbf{x}) = q(x_1, \dots, x_T | x_0) = \prod_{t=1}^T q(x_t | x_{t-1}).$$

- ▶ Probabilistic model

$$p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) = p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})p(\mathbf{z}|\boldsymbol{\theta})$$

- ▶ Generative distribution and prior

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = p(x_0|x_1, \boldsymbol{\theta}); \quad p(\mathbf{z}|\boldsymbol{\theta}) = \prod_{t=2}^T p(x_{t-1}|x_t, \boldsymbol{\theta})$$

Gaussian diffusion model as VAE

ELBO

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

Statement

$$\begin{aligned}\mathcal{L}(q, \theta) &= \mathbb{E}_{q(\mathbf{x}_1, \dots, \mathbf{x}_T | \mathbf{x}_0)} \frac{p(\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_T | \theta)}{q(\mathbf{x}_1, \dots, \mathbf{x}_T | \mathbf{x}_0)} = \\ &= \mathbb{E}_q \left[\cancel{KL(q(\mathbf{x}_T | \mathbf{x}_0) || p(\mathbf{x}_T))} + \sum_{t=2}^T \underbrace{KL(q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) || p(\mathbf{x}_{t-1} | \mathbf{x}_t, \theta))}_{\mathcal{L}_t} - \right. \\ &\quad \left. - \log p(\mathbf{x}_0 | \mathbf{x}_1, \theta) \right]\end{aligned}$$

- ▶ First term is constant (KL between two standard normals).
- ▶ Third term is a decoder distribution (could be AR model or discretized distribution (like mixture of logistics)).

Gaussian diffusion model as VAE

$$\mathcal{L}_t = KL(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) || p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta})).$$

Here

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

$\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0)$ and $\tilde{\beta}_t$ have analytical formulas (we omit it) and both dependent on β_t .

- ▶ **Note:** We do not have an analytical expression for $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$.
- ▶ Assume $\sigma^2(\mathbf{x}_t, \boldsymbol{\theta}, t) = \tilde{\beta}_t \mathbf{I}$ (reminder:
 $p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}_{t-1} | \mu(\mathbf{x}_t, \boldsymbol{\theta}, t), \sigma^2(\mathbf{x}_t, \boldsymbol{\theta}, t))$).
- ▶ Use KL formula between two normal distributions:

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

Gaussian diffusion model as VAE

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

Here we used the analytic expression for $\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0)$.

Reparametrization

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

KL term

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

$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t} \cdot \epsilon, \quad \text{where } \epsilon \sim \mathcal{N}(0, 1)$$

Gaussian diffusion model vs Score matching

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

- ▶ Result from Statement 2

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

- ▶ Score of noised distribution

$$\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x}_0) = -\frac{\epsilon}{\sqrt{1-\bar{\alpha}_t}}, \quad \text{where } \epsilon \sim \mathcal{N}(0, 1).$$

- ▶ Let reparametrize our model:

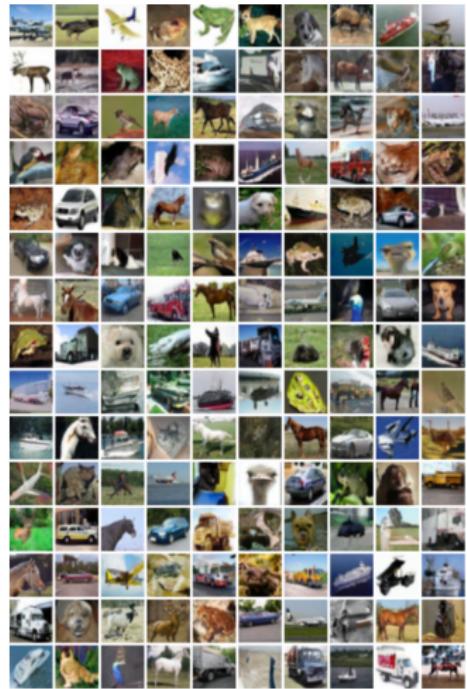
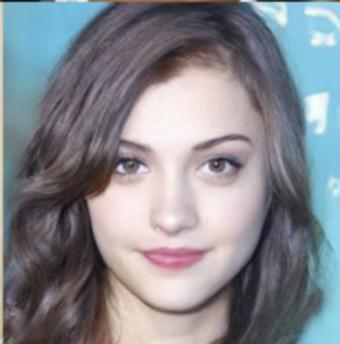
$$\mathbf{s}(\mathbf{x}_t, \theta, t) = \frac{\epsilon(\mathbf{x}_t, \theta, t)}{\sqrt{1-\bar{\alpha}_t}}.$$

Noise conditioned score network

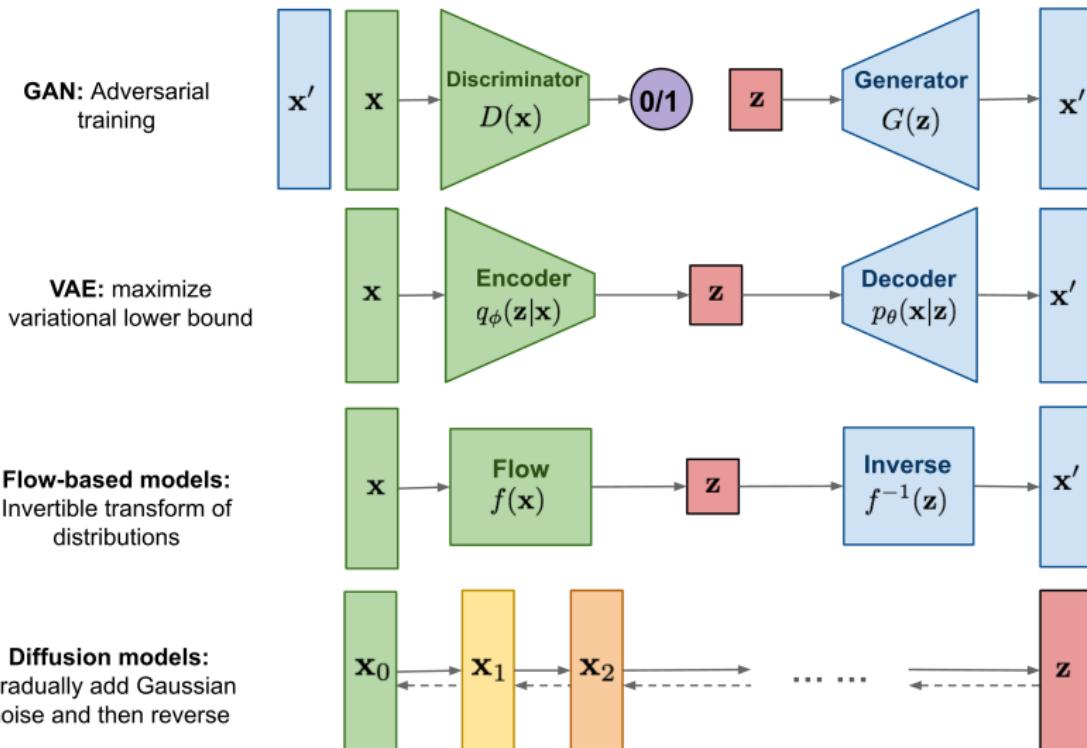
$$\mathbb{E}_{p(\mathbf{x}|\mathbf{x}', \sigma_I)} \left\| \mathbf{s}(\mathbf{x}, \theta, \sigma_I) - \nabla_{\mathbf{x}} \log p(\mathbf{x}|\mathbf{x}', \sigma_I) \right\|_2^2 \rightarrow \min_{\theta}$$

Denoising diffusion probabilistic model (DDPM)

Samples



The poorest course overview :)



Summary

- ▶ Noise conditioned score network uses multiple noise levels and annealed Langevin dynamics to fit score function.
- ▶ Gaussian diffusion process is a Markov chain that injects special form of Gaussian noise to the samples.
- ▶ Reverse process allows to sample from the real distribution $\pi(\mathbf{x})$ using samples from noise.
- ▶ Diffusion model is a VAE model which reverts gaussian diffusion process using variational inference.
- ▶ Objective of diffusion model is closely related to the noise conditioned score network and score matching.