Deep Generative Models

Lecture 14

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AI Masters

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Recap of previous lecture

Continuous-in-time normalizing flows

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

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

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

Hutchinson's trace estimator

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

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

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)

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

Langevin dynamics

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

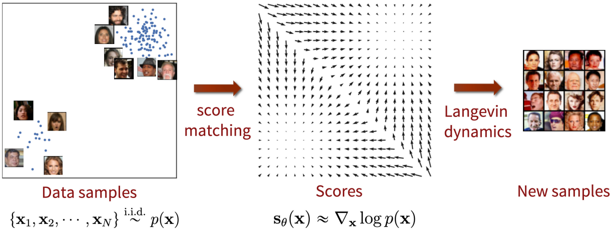
$$\mathbf{x}_{t+1} = \mathbf{x}_t + \eta \frac{1}{2} \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\boldsymbol{\theta}) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}).$$

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

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

Welling M. Bayesian Learning via Stochastic Gradient Langevin Dynamics, 2011

Recap of previous lecture



Theorem (implicit score matching)

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

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

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

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

Theorem (denoising score matching)

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

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

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

Outline

1. Noise conditioned score network

2. Diffusion models
   - Gaussian diffusion process
   - Denoising diffusion probabilistic model (DDPM)

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1. Noise conditioned score network

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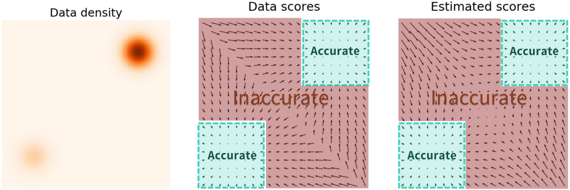
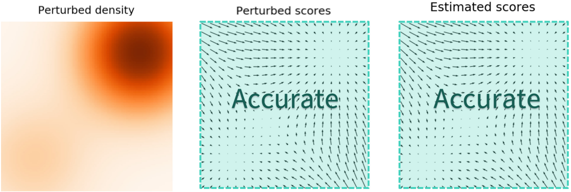
Denoising score matching

- 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.



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

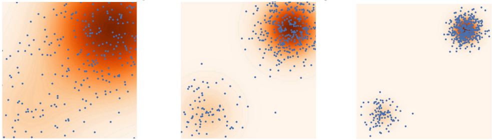
Noise conditioned score network

- 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 $\mathbf{s}(\mathbf{x}, \boldsymbol{\theta}, \sigma)$ for each noise level:

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

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

$\sigma_1 > \sigma_2 > \sigma_3$



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

Noise conditioned score network

Training: loss function

$$\sum_{i=1}^{L} \sigma_l^2 \mathbb{E}_{\pi(\mathbf{x}')} \mathbb{E}_{\boldsymbol{\epsilon}} \left\| \mathbf{s}_l - \boldsymbol{\epsilon} \right\|_2^2,$$

where $\mathbf{s}_l = \mathbf{s}(\mathbf{x}' + \sigma_l \cdot \boldsymbol{\epsilon}, \boldsymbol{\theta}, \sigma_l)$.

Inference: annealed Langevin dynamic

Algorithm 1 Annealed Langevin dynamics.

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

Initialize $\tilde{\mathbf{x}}_0$
for $i \leftarrow 1$ to L **do**
  $\alpha_i \leftarrow \epsilon \cdot \sigma_i^2 / \sigma_L^2$ ▷ α_i is the step size.
  for $t \leftarrow 1$ to T **do**
    Draw $\mathbf{z}_t \sim \mathcal{N}(0, I)$
    $\tilde{\mathbf{x}}_t \leftarrow \tilde{\mathbf{x}}_{t-1} + \frac{\alpha_i}{2} \mathbf{s}_{\boldsymbol{\theta}}(\tilde{\mathbf{x}}_{t-1}, \sigma_i) + \sqrt{\alpha_i}\, \mathbf{z}_t$
  end for
  $\tilde{\mathbf{x}}_0 \leftarrow \tilde{\mathbf{x}}_T$
end for
return $\tilde{\mathbf{x}}_T$

Samples

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

Outline

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Outline

Forward gaussian diffusion process

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

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

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

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

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

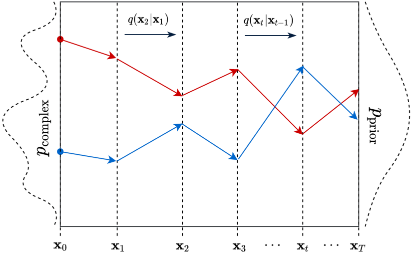
$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t | \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1 - \bar{\alpha}_t)\mathbf{I}).$$

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

Sohl-Dickstein J. Deep Unsupervised Learning using Nonequilibrium Thermodynamics, 2015

Forward gaussian diffusion process

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

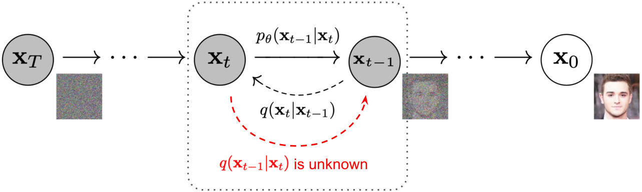


1. $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$;
2. $\mathbf{x}_t = \sqrt{1-\beta} \cdot \mathbf{x}_{t-1} + \sqrt{\beta} \cdot \boldsymbol{\epsilon}$, where $\boldsymbol{\epsilon} \sim \mathcal{N}(0, 1)$, $t \geq 1$;
3. $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, 1)$, where $T >> 1$.

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.

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

Reverse gaussian diffusion process



Let define the reverse process

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

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

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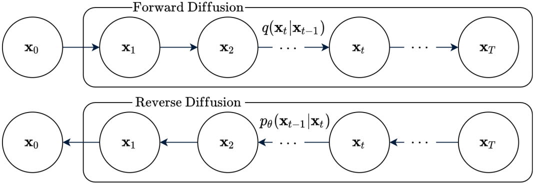
Gaussian diffusion model as VAE



- Let treat $\mathbf{z} = (\mathbf{x}_1, \dots, \mathbf{x}_T)$ as a latent variable (**note:** each $\mathbf{x}_t$ has the same size).
- Variational posterior distribution (**note:** there is no learnable parameters)
$$q(\mathbf{z}|\mathbf{x}) = q(\mathbf{x}_1, \dots, \mathbf{x}_T|\mathbf{x}_0) = \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1}).$$
- 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
$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = p(\mathbf{x}_0|\mathbf{x}_1, \boldsymbol{\theta}); \quad p(\mathbf{z}|\boldsymbol{\theta}) = \prod_{t=2}^{T} p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta})$$

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

Gaussian diffusion model as VAE

ELBO

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

Statement

$$\mathcal{L}(q, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{x}_1, \dots, \mathbf{x}_T|\mathbf{x}_0)} \frac{p(\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_T|\boldsymbol{\theta})}{q(\mathbf{x}_1, \dots, \mathbf{x}_T|\mathbf{x}_0)} =$$

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

$$- \log p(\mathbf{x}_0|\mathbf{x}_1, \boldsymbol{\theta}) \Big]$$

- 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)).

Ho J. Denoising Diffusion Probabilistic Models, 2020

Gaussian diffusion model as VAE

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

Here

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

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

- Assume $\boldsymbol{\sigma}^2(\mathbf{x}_t, \boldsymbol{\theta}, t) = \tilde{\beta}_t \mathbf{I}$ (reminder: $p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}_{t-1}|\boldsymbol{\mu}(\mathbf{x}_t, \boldsymbol{\theta}, t), \boldsymbol{\sigma}^2(\mathbf{x}_t, \boldsymbol{\theta}, t))$).
- Use KL formula for normal distributions.
- Use the fact $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}$

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

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

Gaussian diffusion model as VAE

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

Reparametrization

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

KL term

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

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

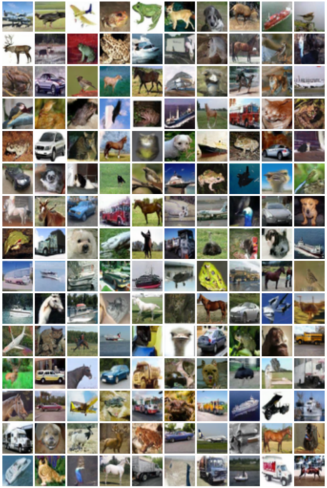
Noise conditioned score network

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

Ho J. Denoising Diffusion Probabilistic Models, 2020

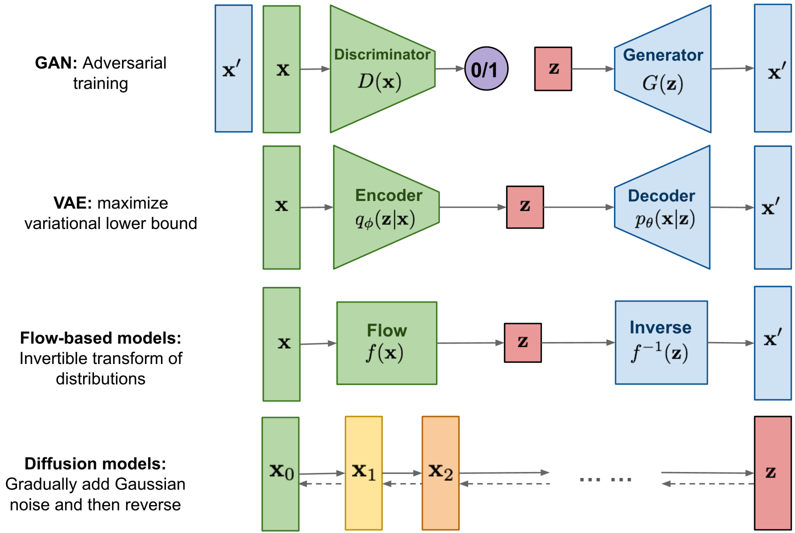
Denoising diffusion probabilistic model (DDPM)

Samples



Ho J. Denoising Diffusion Probabilistic Models, 2020

The poorest course overview :)



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

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.