# Deep Generative Models

Lecture 11

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## Recap of previous lecture

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

$$q(\mathbf{x}_{\sigma}) = \int \pi(\mathbf{x}) q(\mathbf{x}_{\sigma}|\mathbf{x}) d\mathbf{x}.$$

Then the solution of

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

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

Theorem (denoising score matching)

$$\begin{split} \mathbb{E}_{q(\mathbf{x}_{\sigma})} & \left\| \mathbf{s}_{\boldsymbol{\theta}, \sigma}(\mathbf{x}_{\sigma}) - \nabla_{\mathbf{x}_{\sigma}} \log q(\mathbf{x}_{\sigma}) \right\|_{2}^{2} = \\ & = \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_{\sigma}|\mathbf{x})} & \left\| \mathbf{s}_{\boldsymbol{\theta}, \sigma}(\mathbf{x}_{\sigma}) - \nabla_{\mathbf{x}_{\sigma}} \log q(\mathbf{x}_{\sigma}|\mathbf{x}) \right\|_{2}^{2} + \text{const}(\boldsymbol{\theta}) \end{split}$$

Here  $\nabla_{\mathbf{x}_{\sigma}} \log q(\mathbf{x}_{\sigma}|\mathbf{x}) = -\frac{\mathbf{x}_{\sigma}-\mathbf{x}}{\sigma^2}$ .

- ▶ We do not need to compute  $\nabla_{\mathbf{x}_{\sigma}} \log q(\mathbf{x}_{\sigma})$  at the RHS.
- $ightharpoonup \mathbf{s}_{\theta,\sigma}(\mathbf{x}_{\sigma})$  tries to **denoise** a corrupted sample.
- ▶ Score function  $\mathbf{s}_{\theta,\sigma}(\mathbf{x}_{\sigma})$  parametrized by  $\sigma$ .

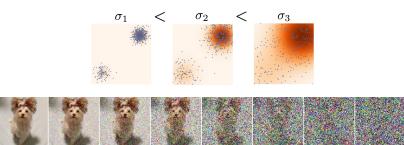
## Recap of previous lecture

#### Noise conditioned score network

- ▶ Define the sequence of noise levels:  $\sigma_1 < \sigma_2 < \cdots < \sigma_T$ .
- ▶ Train denoised score function  $\mathbf{s}_{\theta,\sigma}(\mathbf{x}_{\sigma})$  for each noise level:

$$\sum_{t=1}^{T} \sigma_{t}^{2} \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_{t}|\mathbf{x})} \big\| \mathbf{s}_{\boldsymbol{\theta}, \sigma_{t}}(\mathbf{x}_{t}) - \nabla_{\mathbf{x}_{\sigma}} \log q(\mathbf{x}_{t}|\mathbf{x}) \big\|_{2}^{2} \rightarrow \min_{\boldsymbol{\theta}}$$

▶ Sample from **annealed** Langevin dynamics (for t = 1, ..., T).



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  $t \sim U[1, T]$  and the noise  $\epsilon \sim \mathcal{N}(0, I)$ .
- 3. Get noisy image  $\mathbf{x}_t = \mathbf{x}_0 + \sigma_t \cdot \boldsymbol{\epsilon}$ .
- 4. Compute loss  $\mathcal{L} = \|\mathbf{s}_{\theta,\sigma_t}(\mathbf{x}_t) + \frac{\epsilon}{\sigma_t}\|^2$ .

## NCSN sampling (annealed Langevin dynamics)

- ▶ Sample  $\mathbf{x}_0 \sim \mathcal{N}(0, \sigma_T^2 \cdot \mathbf{I}) \approx q(\mathbf{x}_T)$ .
- ► Apply *L* steps of Langevin dynamic

$$\mathbf{x}_{l} = \mathbf{x}_{l-1} + \frac{\eta_{t}}{2} \cdot \mathbf{s}_{\theta,\sigma_{t}}(\mathbf{x}_{l-1}) + \sqrt{\eta_{t}} \cdot \epsilon_{l}.$$

▶ Update  $\mathbf{x}_0 := \mathbf{x}_L$  and choose the next  $\sigma_t$ .

Gaussian diffusion process
 Forward gaussian diffusion process
 Denoising score matching
 Reverse gaussian diffusion process

Gaussian diffusion process
 Forward gaussian diffusion process
 Denoising score matching
 Reverse gaussian diffusion process

Gaussian diffusion process
 Forward gaussian diffusion process

Denoising score matching Reverse gaussian diffusion process

# Forward gaussian diffusion process

Let 
$$\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$$
,  $\beta_t \in (0,1)$ . Define the Markov chain 
$$\mathbf{x}_t = \sqrt{1-\beta_t} \cdot \mathbf{x}_{t-1} + \sqrt{\beta_t} \cdot \epsilon, \quad \text{where } \epsilon \sim \mathcal{N}(\mathbf{0},\mathbf{I});$$
 
$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\sqrt{1-\beta_t} \cdot \mathbf{x}_{t-1},\beta_t \cdot \mathbf{I}).$$

#### Statement 1

Let denote  $\alpha_t = 1 - \beta_t$  and  $\bar{\alpha}_t = \prod_{s=1}^t \alpha_s$ . Then

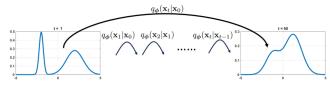
$$q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{lpha}_t}\cdot\mathbf{x}_0, (1-\bar{lpha}_t)\cdot\mathbf{I})$$

We are able to sample from any timestamp using only  $x_0$ !

$$\begin{split} \mathbf{x}_t &= \sqrt{\alpha_t} \cdot \mathbf{x}_{t-1} + \sqrt{1 - \alpha_t} \cdot \boldsymbol{\epsilon}_t = \\ &= \sqrt{\alpha_t} \big( \cdot \sqrt{\alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1}} \cdot \boldsymbol{\epsilon}_{t-1} \big) + \sqrt{1 - \alpha_t} \cdot \boldsymbol{\epsilon}_t = \\ &= \sqrt{\alpha_t} \alpha_{t-1} \cdot \mathbf{x}_{t-2} + \big( \sqrt{\alpha_t} \big( 1 - \alpha_{t-1} \big) \cdot \boldsymbol{\epsilon}_{t-1} + \sqrt{1 - \alpha_t} \cdot \boldsymbol{\epsilon}_t \big) = \\ &= \sqrt{\alpha_t} \alpha_{t-1} \cdot \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1}} \alpha_t \cdot \boldsymbol{\epsilon}_t' = \\ &= \cdots = \sqrt{\overline{\alpha_t}} \cdot \mathbf{x}_0 + \sqrt{1 - \overline{\alpha_t}} \cdot \boldsymbol{\epsilon}, \quad \text{where } \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}). \end{split}$$

# Forward gaussian diffusion process

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}\left(\sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t\mathbf{I}\right); \quad q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}\left(\sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I}\right).$$



#### Statement 2

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

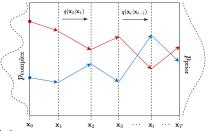
$$p_{\infty}(\mathbf{x}) = \int q(\mathbf{x}|\mathbf{x}')p_{\infty}(\mathbf{x}')d\mathbf{x}'.$$

$$p_{\infty}(\mathbf{x}) = \int q(\mathbf{x}_{\infty}|\mathbf{x}_0)\pi(\mathbf{x}_0)d\mathbf{x}_0 pprox \mathcal{N}(0,\mathbf{I})\int \pi(\mathbf{x}_0)d\mathbf{x}_0 = \mathcal{N}(0,\mathbf{I})$$

Chan S. Tutorial on Diffusion Models for Imaging and Vision, 2024 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.  $x_0 = x \sim \pi(x)$ ;
- 2.  $\mathbf{x}_t = \sqrt{1 \beta_t} \cdot \mathbf{x}_{t-1} + \sqrt{\beta_t} \cdot \epsilon$ , where  $\epsilon \sim \mathcal{N}(0, \mathbf{I})$ ,  $t \geq 1$ ;
- 3.  $\mathbf{x}_T \sim p_{\infty}(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$ , 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  $p_{\infty}(\mathbf{x}) = \mathcal{N}(\mathbf{0}, \mathbf{I})$ . Now our goal is to revert this process.

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

1. Gaussian diffusion process

Forward gaussian diffusion proce

Denoising score matching

Reverse gaussian diffusion process

# Denoising score matching

NCSN

$$q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}, \sigma_t^2 \cdot \mathbf{I}), \quad q(\mathbf{x}_1) \approx \pi(\mathbf{x}), \quad q(\mathbf{x}_T) \approx \mathcal{N}(0, \sigma_T^2 \cdot \mathbf{I}).$$

$$abla_{\mathbf{x}_t} \log q(\mathbf{x}_t|\mathbf{x}) = -rac{\mathbf{x}_t - \mathbf{x}}{\sigma_t^2}$$

#### Gaussian diffussion

$$egin{aligned} q(\mathbf{x}_t|\mathbf{x}_0) &= \mathcal{N}(\sqrt{ar{lpha}_t}\cdot\mathbf{x}_0, (1-ar{lpha}_t)\cdot\mathbf{I}), \quad q(\mathbf{x}_1) pprox \pi(\mathbf{x}), \quad q(\mathbf{x}_{\mathcal{T}}) pprox \mathcal{N}(0,\mathbf{I}) \end{aligned}$$
 $abla_{\mathbf{x}_t} \log q(\mathbf{x}_t|\mathbf{x}) &= -rac{\mathbf{x}_t - \sqrt{ar{lpha}_t}\cdot\mathbf{x}_0}{1-ar{lpha}_t}$ 

Theorem (denoising score matching)

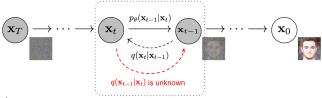
$$\begin{split} \mathbb{E}_{q(\mathbf{x}_t)} & \left\| \mathbf{s}_{\boldsymbol{\theta},t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t) \right\|_2^2 = \\ & = \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_t|\mathbf{x})} & \left\| \mathbf{s}_{\boldsymbol{\theta},t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t|\mathbf{x}) \right\|_2^2 + \text{const}(\boldsymbol{\theta}) \end{split}$$

1. Gaussian diffusion process

Forward gaussian diffusion process Denoising score matching

Reverse gaussian diffusion process

# Reverse gaussian diffusion process



#### Forward process

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

#### Reverse process

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t) = \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1})q(\mathbf{x}_{t-1})}{q(\mathbf{x}_t)} \approx p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta})$$

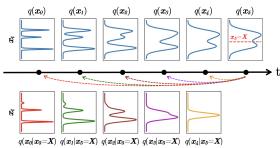
- $ightharpoonup q(\mathbf{x}_{t-1}), \ q(\mathbf{x}_t)$  are intractable.
- ▶ If  $\beta_t$  is small enough,  $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$  will be Gaussian (Feller, 1949).

Feller W. On the theory of stochastic processes, with particular reference to applications, 1949

## Reverse gaussian diffusion process

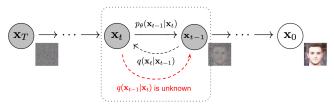
$$\begin{split} q(\mathbf{x}_{t-1}|\mathbf{x}_t) &= \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1})q(\mathbf{x}_{t-1})}{q(\mathbf{x}_t)} \\ q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) &= \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0)q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)} = \mathcal{N}(\tilde{\mu}_t(\mathbf{x}_t,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

- $ightharpoonup q(\mathbf{x}_{t-1}), \ q(\mathbf{x}_t)$  are intractable.
- If  $\beta_t$  is small enough,  $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$  will be Gaussian (Feller, 1949).



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

## Reverse gaussian diffusion process



Let define the reverse process

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

## Forward process

#### Reverse process

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

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

2. 
$$\mathbf{x}_t = \sqrt{1 - \beta_t} \cdot \mathbf{x}_{t-1} + \sqrt{\beta_t} \cdot \epsilon$$
, 2.  $\mathbf{x}_{t-1} =$  where  $\epsilon \sim \mathcal{N}(0, \mathbf{I})$ ,  $t \ge 1$ ;  $\sigma_{\theta}(\mathbf{x}_t, t) \cdot \epsilon + \mu_{\theta}(\mathbf{x}_t, t)$ ;

3. 
$$\mathbf{x}_T \sim p_{\infty}(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$$
. 3.  $\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$ ;

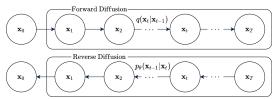
3. 
$$\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$$
;

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

#### 1. Gaussian diffusion process

Forward gaussian diffusion process Denoising score matching Reverse gaussian diffusion process

## 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

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = p(\mathbf{x}_0|\mathbf{x}_1, \boldsymbol{\theta}); \quad p(\mathbf{z}|\boldsymbol{\theta}) = \prod_{t=2}^{r} p(\mathbf{x}_{t-1}|\mathbf{x}_t, \boldsymbol{\theta}) \cdot p(\mathbf{x}_T)$$

#### Standard ELBO

$$\log p(\mathbf{x}|oldsymbol{ heta}) \geq \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log rac{p(\mathbf{x},\mathbf{z}|oldsymbol{ heta})}{q(\mathbf{z}|\mathbf{x})} = \mathcal{L}(q,oldsymbol{ heta}) 
ightarrow \max_{q,oldsymbol{ heta}}$$

#### Derivation

$$\begin{split} \mathcal{L}(q, \theta) &= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \log \frac{\rho(\mathbf{x}_0, \mathbf{x}_{1:T}|\theta)}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \\ &= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \log \frac{\rho(\mathbf{x}_T) \prod_{t=1}^T \rho(\mathbf{x}_{t-1}|\mathbf{x}_t, \theta)}{\prod_{t=1}^T q(\mathbf{x}_t|\mathbf{x}_{t-1})} \\ &= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \log \frac{\rho(\mathbf{x}_T) \rho(\mathbf{x}_0|\mathbf{x}_1, \theta) \prod_{t=2}^T \rho(\mathbf{x}_{t-1}|\mathbf{x}_t, \theta)}{q(\mathbf{x}_1|\mathbf{x}_0) \prod_{t=2}^T q(\mathbf{x}_t|\mathbf{x}_{t-1})} \\ &= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \log \frac{\rho(\mathbf{x}_T) \rho(\mathbf{x}_0|\mathbf{x}_1, \theta) \prod_{t=2}^T \rho(\mathbf{x}_{t-1}|\mathbf{x}_t, \theta)}{q(\mathbf{x}_1|\mathbf{x}_0) \prod_{t=2}^T \rho(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0)} \end{split}$$

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

#### Derivation (continued)

$$\begin{split} \mathcal{L}(q, \boldsymbol{\theta}) &= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_{0})} \log \frac{p(\mathbf{x}_{T})p(\mathbf{x}_{0}|\mathbf{x}_{1}, \boldsymbol{\theta}) \prod_{t=2}^{T} p(\mathbf{x}_{t-1}|\mathbf{x}_{t}, \boldsymbol{\theta})}{q(\mathbf{x}_{1}|\mathbf{x}_{0}) \prod_{t=2}^{T} q(\mathbf{x}_{t}|\mathbf{x}_{t-1}, \mathbf{x}_{0})} = \\ &= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_{0})} \log \frac{p(\mathbf{x}_{T})p(\mathbf{x}_{0}|\mathbf{x}_{1}, \boldsymbol{\theta}) \prod_{t=2}^{T} p(\mathbf{x}_{t-1}|\mathbf{x}_{t}, \boldsymbol{\theta})}{q(\mathbf{x}_{1}|\mathbf{x}_{0}) \prod_{t=2}^{T} \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_{t}, \mathbf{x}_{0})q(\mathbf{x}_{t}|\mathbf{x}_{0})}{q(\mathbf{x}_{t-1}|\mathbf{x}_{0})}} = \\ &= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_{0})} \log \frac{p(\mathbf{x}_{T})p(\mathbf{x}_{0}|\mathbf{x}_{1}, \boldsymbol{\theta}) \prod_{t=2}^{T} p(\mathbf{x}_{t-1}|\mathbf{x}_{t}, \boldsymbol{\theta})}{q(\mathbf{x}_{T}|\mathbf{x}_{0}) \prod_{t=2}^{T} q(\mathbf{x}_{t-1}|\mathbf{x}_{t}, \mathbf{x}_{0})} = \\ &= \mathbb{E}_{q(\mathbf{x}_{1:T}|\mathbf{x}_{0})} \left[ \log p(\mathbf{x}_{0}|\mathbf{x}_{1}, \boldsymbol{\theta}) + \log \frac{p(\mathbf{x}_{T})}{q(\mathbf{x}_{T}|\mathbf{x}_{0})} + \sum_{t=2}^{T} \log \left( \frac{p(\mathbf{x}_{t-1}|\mathbf{x}_{t}, \boldsymbol{\theta})}{q(\mathbf{x}_{t-1}|\mathbf{x}_{t}, \mathbf{x}_{0})} \right) \right] = \\ &= \mathbb{E}_{q(\mathbf{x}_{1}|\mathbf{x}_{0})} \log p(\mathbf{x}_{0}|\mathbf{x}_{1}, \boldsymbol{\theta}) + \mathbb{E}_{q(\mathbf{x}_{T}|\mathbf{x}_{0})} \log \frac{p(\mathbf{x}_{T})}{q(\mathbf{x}_{T}|\mathbf{x}_{0})} + \\ &+ \sum_{t=2}^{T} \mathbb{E}_{q(\mathbf{x}_{t-1}, \mathbf{x}_{t}|\mathbf{x}_{0})} \log \left( \frac{p(\mathbf{x}_{t-1}|\mathbf{x}_{t}, \boldsymbol{\theta})}{q(\mathbf{x}_{t-1}|\mathbf{x}_{t}, \boldsymbol{x}_{0})} \right) \end{split}$$

$$\begin{split} \mathcal{L}(q, \theta) &= \mathbb{E}_{q(\mathbf{x}_{1}|\mathbf{x}_{0})} \log p(\mathbf{x}_{0}|\mathbf{x}_{1}, \theta) + \mathbb{E}_{q(\mathbf{x}_{T}|\mathbf{x}_{0})} \log \frac{p(\mathbf{x}_{T})}{q(\mathbf{x}_{T}|\mathbf{x}_{0})} + \\ &+ \sum_{t=2}^{T} \mathbb{E}_{q(\mathbf{x}_{t-1},\mathbf{x}_{t}|\mathbf{x}_{0})} \log \left( \frac{p(\mathbf{x}_{t-1}|\mathbf{x}_{t}, \theta)}{q(\mathbf{x}_{t-1}|\mathbf{x}_{t}, \mathbf{x}_{0})} \right) = \\ &= \mathbb{E}_{q(\mathbf{x}_{1}|\mathbf{x}_{0})} \log p(\mathbf{x}_{0}|\mathbf{x}_{1}, \theta) - \mathcal{K}L(q(\mathbf{x}_{T}|\mathbf{x}_{0})||p(\mathbf{x}_{T})) - \\ &- \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\mathbf{x}_{t}|\mathbf{x}_{0})} \mathcal{K}L(q(\mathbf{x}_{t-1}|\mathbf{x}_{t}, \mathbf{x}_{0})||p(\mathbf{x}_{t-1}|\mathbf{x}_{t}, \theta))}_{\mathcal{L}_{t}} \end{split}$$

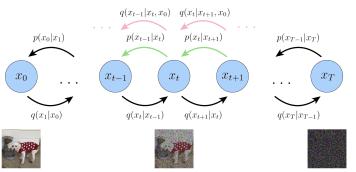
First term is a decoder distribution

$$\log p(\mathbf{x}_0|\mathbf{x}_1, \boldsymbol{\theta}) = \log \mathcal{N}(\mathbf{x}_0|\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}_1, t), \boldsymbol{\sigma}_{\boldsymbol{\theta}}^2(\mathbf{x}_1, t)).$$

Second term is constant  $(p(\mathbf{x}_T))$  is a standard Normal,  $q(\mathbf{x}_T|\mathbf{x}_0)$  is a non-parametrical Normal).

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

 $q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0)$  defines how to denoise a noisy image  $\mathbf{x}_t$  with access to what the final, completely denoised image  $\mathbf{x}_0$  should be.



Luo C. Understanding Diffusion Models: A Unified Perspective, 2022

# Summary

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.
- ► ELBO of DDPM could be represented as a sum of KL terms.