# Deep Generative Models

Lecture 10

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Consider Ordinary Differential Equation

$$egin{aligned} rac{d\mathbf{z}(t)}{dt} &= f_{m{ heta}}(\mathbf{z}(t),t); \quad ext{with initial condition } \mathbf{z}(t_0) = \mathbf{z}_0. \ \mathbf{z}(t_1) &= \int_{t_0}^{t_1} f_{m{ heta}}(\mathbf{z}(t),t) dt + \mathbf{z}_0 &= ext{ODESolve}(\mathbf{z}(t_0),f_{m{ heta}},t_0,t_1). \end{aligned}$$

#### Euler update step

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

Residual block

$$\mathbf{z}_{t+1} = \mathbf{z}_t + f_{\boldsymbol{\theta}}(\mathbf{z}_t)$$

It is equivalent to Euler update step for solving ODE with  $\Delta t = 1$ ! In the limit of adding more layers and taking smaller steps we get:

$$\frac{d\mathbf{z}(t)}{dt} = f_{\theta}(\mathbf{z}(t), t); \quad \mathbf{z}(t_0) = \mathbf{x}; \quad \mathbf{z}(t_1) = \mathbf{y}.$$

Forward pass (loss function)

$$L(\mathbf{y}) = L(\mathbf{z}(t_1)) = L\left(\mathbf{z}(t_0) + \int_{t_0}^{t_1} f_{\theta}(\mathbf{z}(t), t) dt\right)$$
  
=  $L(\mathsf{ODESolve}(\mathbf{z}(t_0), f_{\theta}, t_0, t_1))$ 

**Note:** ODESolve could be any method (Euler step, Runge-Kutta methods).

Backward pass (gradients computation)

For fitting parameters we need gradients:

$$\mathbf{a}_{\mathbf{z}}(t) = \frac{\partial L(\mathbf{y})}{\partial \mathbf{z}(t)}; \quad \mathbf{a}_{\boldsymbol{\theta}}(t) = \frac{\partial L(\mathbf{y})}{\partial \boldsymbol{\theta}(t)}.$$

In theory of optimal control these functions called **adjoint** functions. They show how the gradient of the loss depends on the hidden state  $\mathbf{z}(t)$  and parameters  $\boldsymbol{\theta}$ .

$$\mathbf{a_z}(t) = \frac{\partial L(\mathbf{y})}{\partial \mathbf{z}(t)}; \quad \mathbf{a_{\theta}}(t) = \frac{\partial L(\mathbf{y})}{\partial \theta(t)}$$
 - adjoint functions.

## Theorem (Pontryagin)

$$\frac{d\mathbf{a}_{\mathbf{z}}(t)}{dt} = -\mathbf{a}_{\mathbf{z}}(t)^{\mathsf{T}} \cdot \frac{\partial f_{\boldsymbol{\theta}}(\mathbf{z}(t), t)}{\partial \mathbf{z}}; \quad \frac{d\mathbf{a}_{\boldsymbol{\theta}}(t)}{dt} = -\mathbf{a}_{\mathbf{z}}(t)^{\mathsf{T}} \cdot \frac{\partial f_{\boldsymbol{\theta}}(\mathbf{z}(t), t)}{\partial \boldsymbol{\theta}}.$$

## Forward pass

$$\mathbf{z}(t_1) = \int_{t_0}^{t_1} f_{m{ heta}}(\mathbf{z}(t),t) dt + \mathbf{z}_0 \quad \Rightarrow \quad \mathsf{ODE} \; \mathsf{Solver}$$

#### Backward pass

$$\begin{split} &\frac{\partial L}{\partial \boldsymbol{\theta}(t_0)} = \boldsymbol{a}_{\boldsymbol{\theta}}(t_0) = -\int_{t_1}^{t_0} \boldsymbol{a}_{\boldsymbol{z}}(t)^T \frac{\partial f_{\boldsymbol{\theta}}(\boldsymbol{z}(t),t)}{\partial \boldsymbol{\theta}(t)} dt + 0 \\ &\frac{\partial L}{\partial \boldsymbol{z}(t_0)} = \boldsymbol{a}_{\boldsymbol{z}}(t_0) = -\int_{t_1}^{t_0} \boldsymbol{a}_{\boldsymbol{z}}(t)^T \frac{\partial f_{\boldsymbol{\theta}}(\boldsymbol{z}(t),t)}{\partial \boldsymbol{z}(t)} dt + \frac{\partial L}{\partial \boldsymbol{z}(t_1)} \\ &\boldsymbol{z}(t_0) = -\int_{t_1}^{t_0} f_{\boldsymbol{\theta}}(\boldsymbol{z}(t),t) dt + \boldsymbol{z}_1. \end{split} \right\} \Rightarrow \mathsf{ODE} \; \mathsf{Solver}$$

Continuous-in-time normalizing flows

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

## 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

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

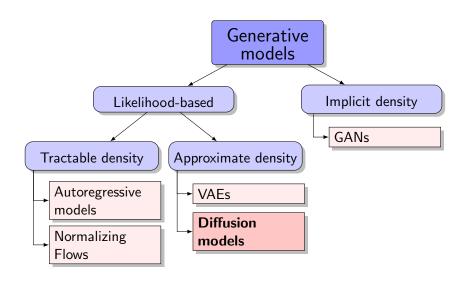
Hutchinson's trace estimator

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

Gaussian diffusion process
 Forward gaussian diffusion process
 Reverse gaussian diffusion process

2. Gaussian diffusion model as VAE

#### Generative models zoo



Gaussian diffusion process
 Forward gaussian diffusion process
 Reverse gaussian diffusion process

2. Gaussian diffusion model as VAI

Gaussian diffusion process
 Forward gaussian diffusion process
 Reverse gaussian diffusion process

2. Gaussian diffusion model as VAI

# Forward gaussian diffusion process

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

$$\mathbf{x}_t = \sqrt{1 - eta_t} \cdot \mathbf{x}_{t-1} + \sqrt{eta_t} \cdot \epsilon$$
, where  $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ ;  $q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t | \sqrt{1 - eta_t} \cdot \mathbf{x}_{t-1}, eta_t \cdot \mathbf{I})$ .

#### Statement 1

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

$$\begin{split} \mathbf{x}_t &= \sqrt{\alpha_t} \mathbf{x}_{t-1} + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_t = \\ &= \sqrt{\alpha_t} \big( \sqrt{\alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1}} \boldsymbol{\epsilon}_{t-1} \big) + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_t = \\ &= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \big( \sqrt{\alpha_t (1 - \alpha_{t-1})} \boldsymbol{\epsilon}_{t-1} + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_t \big) = \\ &= \sqrt{\bar{\alpha}_t} \cdot \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \cdot \boldsymbol{\epsilon}, \quad \text{where } \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}). \end{split}$$

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

We could sample from any timestamp using only  $x_0$ !

# Forward gaussian diffusion process

$$\begin{split} q(\mathbf{x}_t|\mathbf{x}_{t-1}) &= \mathcal{N}(\mathbf{x}_t|\sqrt{1-\beta_t}\cdot\mathbf{x}_{t-1},\beta_t\cdot\mathbf{I});\\ q(\mathbf{x}_t|\mathbf{x}_0) &= \mathcal{N}(\mathbf{x}_t|\sqrt{\bar{\alpha}_t}\cdot\mathbf{x}_0,(1-\bar{\alpha}_t)\cdot\mathbf{I}). \end{split}$$

At each step we

- scale magnitude of the signal at rate  $\sqrt{1-\beta_t}$ ;
- ▶ add noise with variance  $\beta_t$ .

#### Statement 2

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

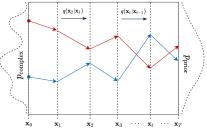
$$ho_{\infty}(\mathbf{x}) = \int q(\mathbf{x}|\mathbf{x}') 
ho_{\infty}(\mathbf{x}') d\mathbf{x}'.$$

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

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.  $\mathbf{x}_t = \sqrt{1 \beta_t} \cdot \mathbf{x}_{t-1} + \sqrt{\beta_t} \cdot \epsilon$ , 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 >> 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

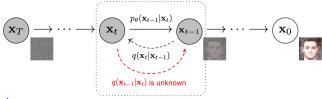
1. Gaussian diffusion process

Forward gaussian diffusion process

Reverse gaussian diffusion process

2. Gaussian diffusion model as VAE

# Reverse gaussian diffusion process



#### Forward process

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

#### Reverse process

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

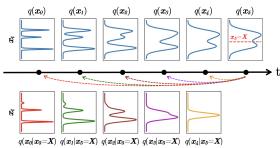
- $ightharpoonup q(\mathbf{x}_{t-1}), \ q(\mathbf{x}_t)$  are intractable.
- If  $\beta_t$  is small enough,  $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$  will be Gaussian (Feller, 1949).

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

## Reverse gaussian diffusion process

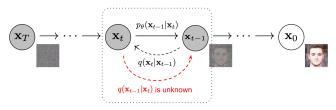
$$\begin{split} q(\mathbf{x}_{t-1}|\mathbf{x}_t) &= \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1})q(\mathbf{x}_{t-1})}{q(\mathbf{x}_t)} \\ q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) &= \frac{q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0)q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)} = \mathcal{N}(\tilde{\mu}_t(\mathbf{x}_t,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

- $ightharpoonup q(\mathbf{x}_{t-1}), \ q(\mathbf{x}_t)$  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

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

## Forward process

## Reverse process

1. 
$$x_0 = x \sim \pi(x)$$
;

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

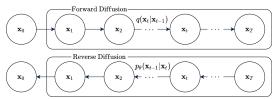
3. 
$$\mathbf{x}_0 = \mathbf{x} \sim \pi(\mathbf{x})$$
;

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

Gaussian diffusion process
 Forward gaussian diffusion process
 Reverse gaussian diffusion process

#### 2. Gaussian diffusion model as VAE

## 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)

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

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

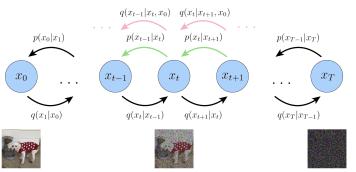
First term is a decoder distribution

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

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.