ECE 57000

Introduction to Diffusion models

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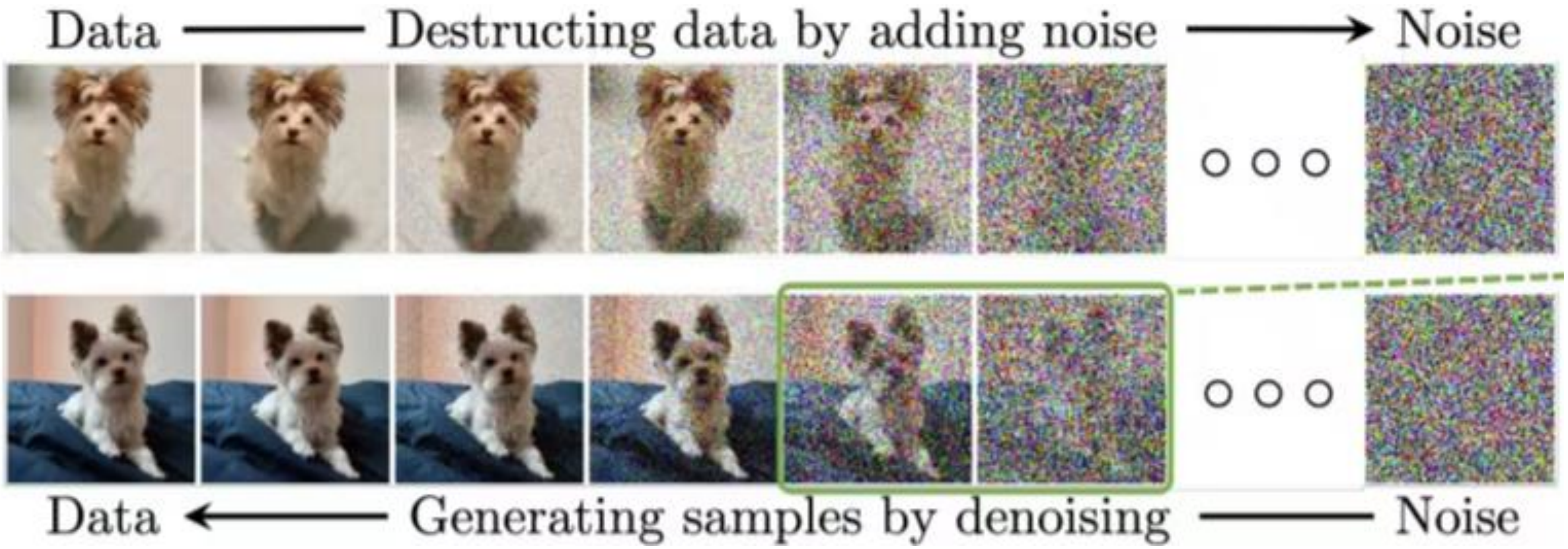
Diffusion model



Diffusion model

Markov transition

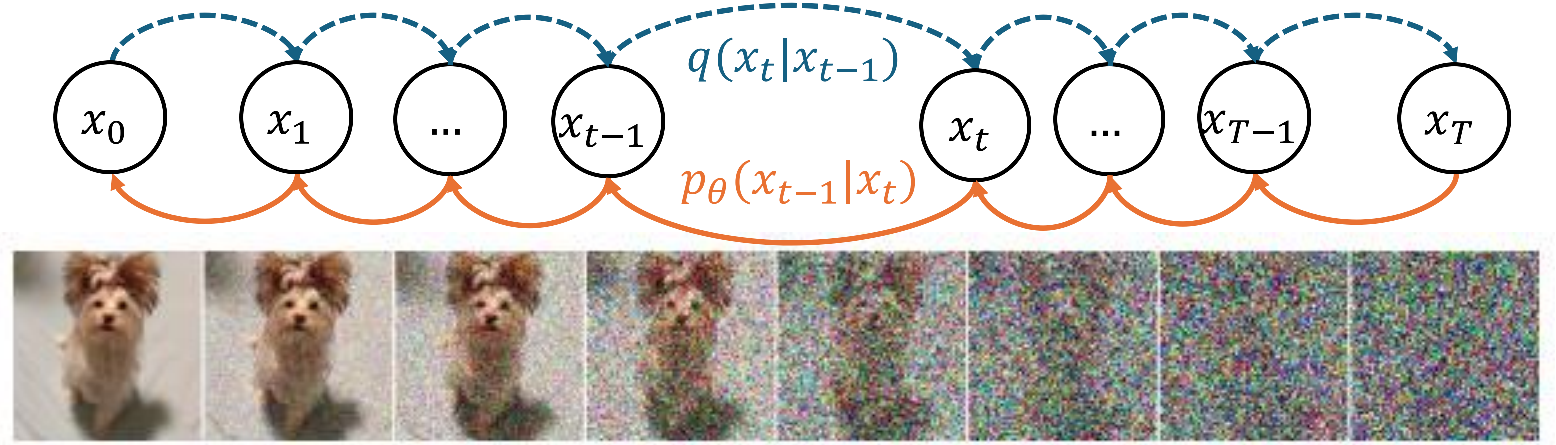
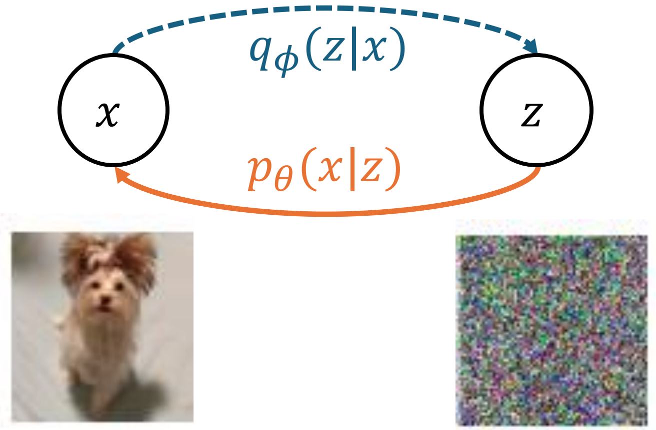


Image from: https://arxiv.org/pdf/2011.13456.pdf

Diffusion models define forward and reverse diffusion processes

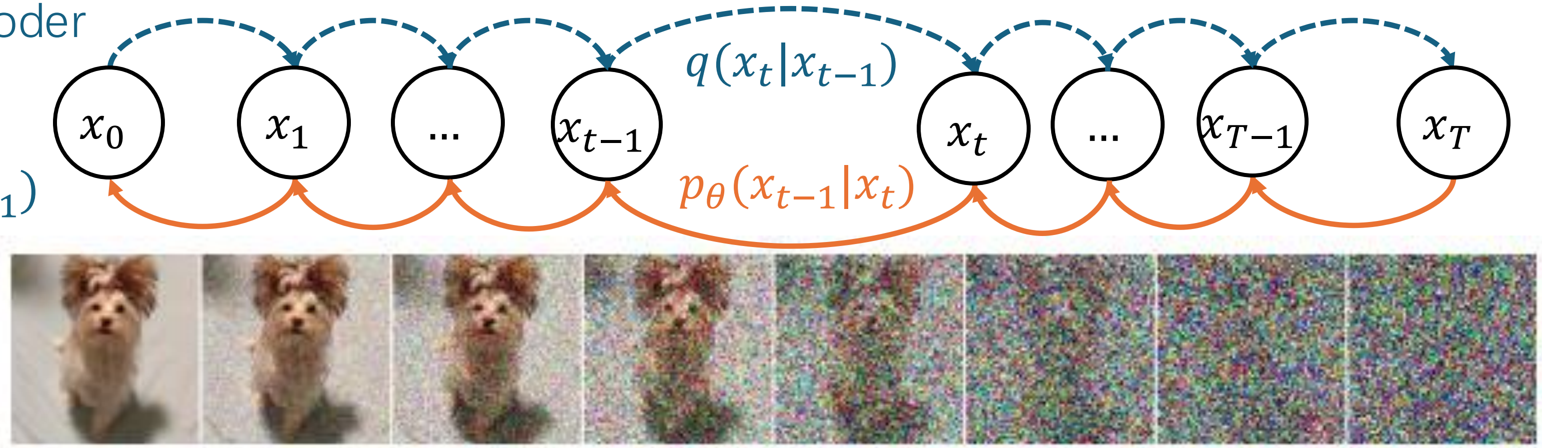
- Diffusion models can be viewed as hierarchical VAEs
  - Forward process = hierarchical **encoder**
  - Reverse process = hierarchical **decoder**
- Several critical differences from VAE
  - Involves **multiple latent representations** rather than one
  - Latent dimension is the **same** as data dimension
  - Hierarchical encoder is **fixed** (i.e., no trainable parameters)
  - **Parameters θ are shared** between decoder steps

Simple VAE
(Same-Dimension)



Hierarchical Encoder

$q(x_{1:T}|x_0) = \prod_{t=1}^{T} q(x_t|x_{t-1})$



Hierarchical Decoder

$\mathrm{p}(x_T)p(x_{0:(T-1)}|x_T) = p(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)$

The forward process is defined by a **fixed** Markov transition distribution $q(x_t|x_{t-1})$

- The forward process starts at the data distribution, i.e.,

$$q(x_0) = p_{data}(x)$$

- Define forward process via Markov transition

$$q(x_t|x_{t-1}) \stackrel{\text{def}}{=} \mathcal{N}\left(x_t; \mu = w_\mu(t) x_{t-1}, \Sigma = w_\sigma(t) I\right)$$

  - where $w_\mu(t)$ and $w_\sigma(t)$ can be functions that vary across time t
  - Notice there are **no trainable parameters**

Forward pass

Assuming Gaussian: $q(x_t|x_{t-1}) = \mathcal{N}(x_t; \sqrt{\alpha_t}x_{t-1}, (1-\alpha_t)I)$

$$x_t = \sqrt{\alpha_t}x_{t-1} + \sqrt{1-\alpha_t}\epsilon_t, \qquad \text{where} \quad \epsilon_t \sim \mathcal{N}(0, I)$$

The need for α_t: preserving variance scale

Independent variables

$$\begin{aligned} Var[x_t] &= Var[\sqrt{\alpha_t}x_{t-1}] + Var[\sqrt{1-\alpha_t}\epsilon_t] \\ &= \alpha_t \cdot Var[x_{t-1}] + (1-\alpha_t) \cdot Var[\epsilon_t] \end{aligned}$$

If these blue factors are absent, variance of x_t builds up towards infinity as t increases

You have the flexibility to choose α_t ($\alpha_t \in (0,1)$), or even train α_t

$$
\begin{aligned}
\boldsymbol{x}_t &= \sqrt{\alpha_t}\boldsymbol{x}_{t-1} + \sqrt{1-\alpha_t}\boldsymbol{\epsilon}^*_{t-1} \\
&= \sqrt{\alpha_t}\left(\sqrt{\alpha_{t-1}}\boldsymbol{x}_{t-2} + \sqrt{1-\alpha_{t-1}}\boldsymbol{\epsilon}^*_{t-2}\right) + \sqrt{1-\alpha_t}\boldsymbol{\epsilon}^*_{t-1} \\
&= \sqrt{\alpha_t\alpha_{t-1}}\boldsymbol{x}_{t-2} + \sqrt{\alpha_t - \alpha_t\alpha_{t-1}}\boldsymbol{\epsilon}^*_{t-2} + \sqrt{1-\alpha_t}\boldsymbol{\epsilon}^*_{t-1} \\
&= \sqrt{\alpha_t\alpha_{t-1}}\boldsymbol{x}_{t-2} + \sqrt{\sqrt{\alpha_t - \alpha_t\alpha_{t-1}}^2 + \sqrt{1-\alpha_t}^2}\boldsymbol{\epsilon}_{t-2} \\
&= \sqrt{\alpha_t\alpha_{t-1}}\boldsymbol{x}_{t-2} + \sqrt{\alpha_t - \alpha_t\alpha_{t-1} + 1 - \alpha_t}\boldsymbol{\epsilon}_{t-2} \\
&= \sqrt{\alpha_t\alpha_{t-1}}\boldsymbol{x}_{t-2} + \sqrt{1 - \alpha_t\alpha_{t-1}}\boldsymbol{\epsilon}_{t-2} \\
&= \ldots \\
&= \sqrt{\prod_{i=1}^{t}\alpha_i}\boldsymbol{x}_0 + \sqrt{1-\prod_{i=1}^{t}\alpha_i}\boldsymbol{\epsilon}_0 \\
&= \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_0 \\
&\sim \mathcal{N}(\boldsymbol{x}_t; \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0, (1-\bar{\alpha}_t)\mathbf{I})
\end{aligned}
$$

The forward process can be **collapsed** into a single step

Forward pass

We need the sequence $\alpha_1, \alpha_2, \cdots, \alpha_T$ vary over time in such a way that the distribution of the latent x_T at final step T is a standard Gaussian

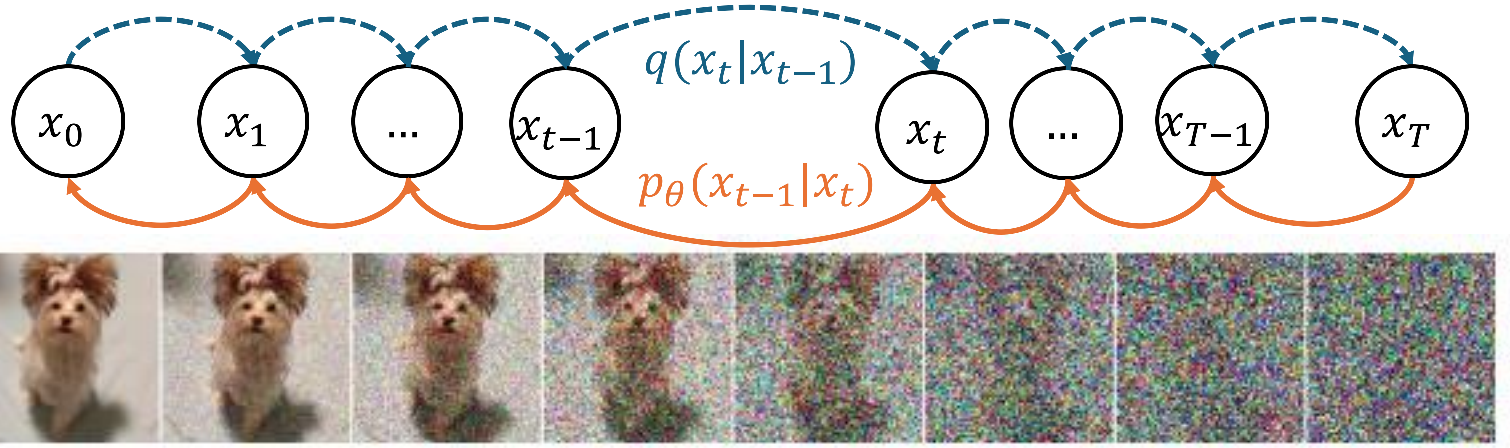
$$x_t \sim \mathcal{N}(x_t; \sqrt{\bar{\alpha}_t} x_0, (1 - \bar{\alpha}_t) I)$$

$$x_T \sim \mathcal{N}(x_T; 0, I)$$

Example: let $\alpha_t = \alpha = 1 - \delta$, and $T \rightarrow \infty$

then $\bar{\alpha}_T = (1 - \delta)^T \rightarrow 0, as\ t \rightarrow \infty$

backward pass: denoising



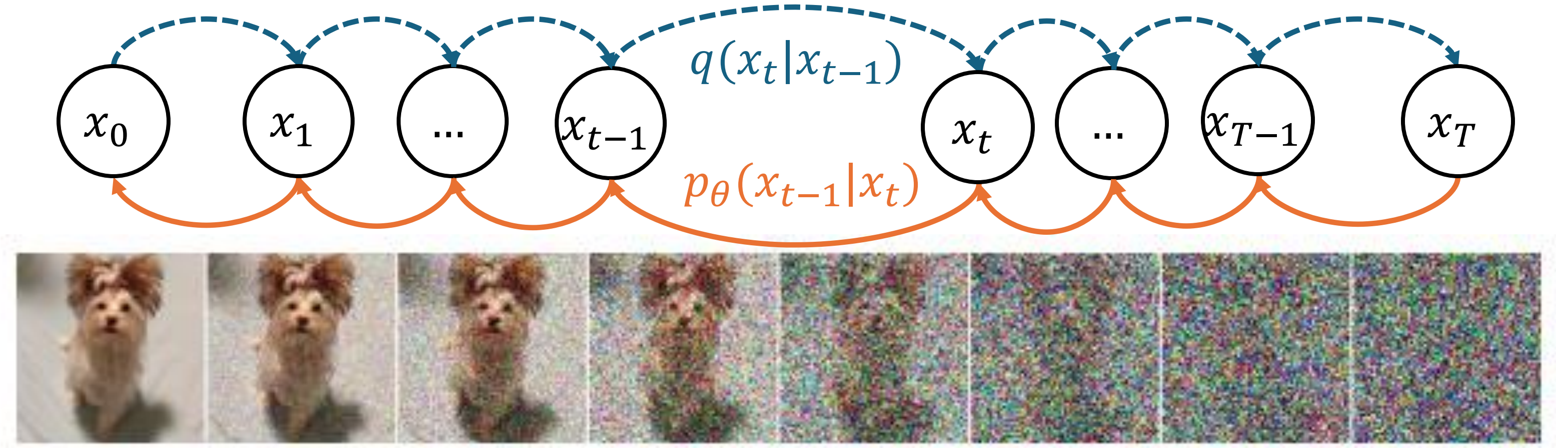
Find (train) model parameters θ to reconstruct data x_0 from "noise" x_T

$$p(\boldsymbol{x}_{0:T}) = p(\boldsymbol{x}_T)\prod_{t=1}^{T} p_\theta(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)$$

where,

$$p(\boldsymbol{x}_T) = \mathcal{N}(\boldsymbol{x}_T; \mathbf{0}, \mathbf{I})$$

backward pass: denoising



Objective function: ELBO

$$\underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)\right]}_{\text{reconstruction term}} - \underbrace{\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_T \mid \boldsymbol{x}_0) \,||\, p(\boldsymbol{x}_T))}_{\text{prior matching term}}$$

$$- \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}\left[\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) \,||\, p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t))\right]}_{\text{denoising matching term}}$$

Objective function

$$\underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)\right]}_{\text{reconstruction term}} - \underbrace{\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_T \mid \boldsymbol{x}_0) \parallel p(\boldsymbol{x}_T))}_{\text{prior matching term}}$$
$$- \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}\left[\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) \parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t))\right]}_{\text{denoising matching term}}$$

- *Reconstruction term*: analogous to the VAE reconstruction term
- *Prior matching term*: no trainable parameters, effectively zero by our requirement
- *Denoising matching term*: we learn desired denoising transition step $p_\theta(x_{t-1}|x_t)$ as an approximation to the ground-truth denoising transition step $q(x_{t-1}|x_t, x_0)$

The denoising matching term

$$D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t, x_0))$$

$\mathcal{N}(x_t; \sqrt{\alpha_t}x_{t-1}, (1 - \alpha_t I)$

Bayes rule:

$$q(x_{t-1}|x_t, x_0) = \frac{q(x_t|x_{t-1}, x_0)q(x_{t-1}|x_0)}{q(x_t|x_0)}$$

$\mathcal{N}(x_{t-1}; \sqrt{\bar{\alpha}_{t-1}}x_{t-1}, (1 - \bar{\alpha}_{t-1} I)$

Gaussian

$\mathcal{N}(x_{t-1}; \sqrt{\bar{\alpha}_t}x_{t-1}, (1 - \bar{\alpha}_t I)$

$$\arg\min_{\boldsymbol{\theta}} \sum_{t=2}^{T} \mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)} \left[\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) \mid\mid p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t))\right]$$

$$= \arg\min_{\boldsymbol{\theta}} \mathbb{E}_{t\sim U\{2,T\}} \left[\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)} \left[\frac{1}{2\sigma_q^2(t)} \frac{\bar{\alpha}_{t-1}(1-\alpha_t)^2}{(1-\bar{\alpha}_t)^2} \left[\left\|\hat{\boldsymbol{x}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) - \boldsymbol{x}_0\right\|_2^2\right]\right]\right]$$

https://calvinyluo.com/2022/08/26/diffusion-tutorial.html

Derivation [time-permitting]

$$
\begin{aligned}
\log p(\boldsymbol{x}) &= \log \int p(\boldsymbol{x}_{0:T}) d\boldsymbol{x}_{1:T} \\
&= \log \int \frac{p(\boldsymbol{x}_{0:T}) q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0)}{q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0)} d\boldsymbol{x}_{1:T} \\
&= \log \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0)} \right] \\
&\geq \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0)} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T) \prod_{t=1}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)}{\prod_{t=1}^{T} q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1})} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T) p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1) \prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)}{q(\boldsymbol{x}_1 \mid \boldsymbol{x}_0) \prod_{t=2}^{T} q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1})} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T) p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1) \prod_{t=2}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)}{q(\boldsymbol{x}_1 \mid \boldsymbol{x}_0) \prod_{t=2}^{T} q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{x}_0)} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_T) p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)}{q(\boldsymbol{x}_1 \mid \boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)}{q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{x}_0)} \right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_T) p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)}{q(\boldsymbol{x}_1 \mid \boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)}{\frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t, \boldsymbol{x}_0) q(\boldsymbol{x}_t|\boldsymbol{x}_0)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}} \right]
\end{aligned}
$$

log is concave

$$p(\boldsymbol{x}_{0:T}) = p(\boldsymbol{x}_T) \prod_{t=1}^{T} p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)$$

where,

$$p(\boldsymbol{x}_T) = \mathcal{N}(\boldsymbol{x}_T; \mathbf{0}, \mathbf{I})$$

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$$
\begin{aligned}
\log p(\boldsymbol{x}) &\geq \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)}{q(\boldsymbol{x}_1 \mid \boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)}{\frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)q(\boldsymbol{x}_t|\boldsymbol{x}_0)}{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)}{q(\boldsymbol{x}_1 \mid \boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)}{\frac{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_t,\boldsymbol{x}_0)\cancel{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}}{\cancel{q(\boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}}}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)}{\cancel{q(\boldsymbol{x}_1 \mid \boldsymbol{x}_0)}} + \log \frac{\cancel{q(\boldsymbol{x}_1 \mid \boldsymbol{x}_0)}}{q(\boldsymbol{x}_T \mid \boldsymbol{x}_0)} + \log \prod_{t=2}^{T} \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)}{q(\boldsymbol{x}_T \mid \boldsymbol{x}_0)} + \sum_{t=2}^{T} \log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)] + \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)}{q(\boldsymbol{x}_T \mid \boldsymbol{x}_0)}\right] + \sum_{t=2}^{T} \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0)}\right] \\
&= \mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)] + \mathbb{E}_{q(\boldsymbol{x}_T|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_T)}{q(\boldsymbol{x}_T \mid \boldsymbol{x}_0)}\right] + \sum_{t=2}^{T} \mathbb{E}_{q(\boldsymbol{x}_t, \boldsymbol{x}_{t-1}|\boldsymbol{x}_0)}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)}{q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0)}\right] \\
&= \underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)]}_{\text{reconstruction term}} - \underbrace{\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_T \mid \boldsymbol{x}_0) \parallel p(\boldsymbol{x}_T))}_{\text{prior matching term}} - \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}[\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) \parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t))]}_{\text{denoising matching term}}
\end{aligned}
$$

$\boxed{\text{From last slide}}$

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