Understanding Diffusion Models: A Unified Perspective

Author: Calvin Luo
Presented by : Farzana Yasmin Ahmad
Link: https://arxiv.org/abs/2208.11970

Primary Goal

- Given observed samples x from a distribution of interest.
- Goal: learn to model the true distribution p(x).
- Can generate new samples from the approximate distribution.
- Generative models:
    - Generative Adversarial Network
    - Variational Autoencoder
    - Energy based modeling
    - Score based modeling

Evidence Lower Bound

- Mathematically we can write *p(x,z)*
- In likelihood based generative modeling, maximize the likelihood of *p(x)* for observed data *x*.
- Two ways to manipulate the joint dist to recover *p(x)*.

$$p(\boldsymbol{x}) = \int p(\boldsymbol{x}, \boldsymbol{z}) d\boldsymbol{z}$$

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

Evidence Lower Bound

- Mathematically we can write *p(x,z)*
- In likelihood based generative modeling, maximize the likelihood of *p(x)* for observed data *x*.
- Two ways to manipulate the joint dist to recover *p(x)*.
    -

$$\boxed{p(\boldsymbol{x}) = \int p(\boldsymbol{x}, \boldsymbol{z}) d\boldsymbol{z}}$$

Integrating out all latent variables *z* .
Intractable!

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

Evidence Lower Bound

- Mathematically we can write *p(x,z)*
- In likelihood based generative modeling, maximize the likelihood of *p(x)* for observed data *x*.
- Two ways to manipulate the joint dist to recover *p(x)*.
  - $$p(\boldsymbol{x}) = \int p(\boldsymbol{x}, \boldsymbol{z}) d\boldsymbol{z}$$

$$p(\boldsymbol{x}) = \frac{p(\boldsymbol{x}, \boldsymbol{z})}{\boxed{p(\boldsymbol{z}|\boldsymbol{x})}}$$

Access to the ground truth latent encoder!

Evidence Lower Bound

- Mathematically we can write *p(x,z)*
- In likelihood based generative modeling, maximize the likelihood of *p(x)* for observed data *x*.
- Two ways to manipulate the joint dist to recover *p(x)*.

$$\boxed{p(\boldsymbol{x}) = \int p(\boldsymbol{x}, \boldsymbol{z})d\boldsymbol{z}}$$

$$\boxed{p(\boldsymbol{x}) = \frac{p(\boldsymbol{x}, \boldsymbol{z})}{p(\boldsymbol{z}|\boldsymbol{x})}}$$

Evidence Lower Bound (ELBO)

Evidence and ELBO

- Evidence: *log p(x)*.
- Equation of ELBO is:

$$\mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x},\boldsymbol{z})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\right]$$

- Relationship between them:

$$\log p(\boldsymbol{x}) \geq \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x},\boldsymbol{z})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\right]$$

Evidence and ELBO

$$\log p(\boldsymbol{x}) \geq \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x},\boldsymbol{z})}{\boxed{q_\phi(\boldsymbol{z}|\boldsymbol{x})}}\right]$$

We want to optimize

Evidence and ELBO

$$\log p(\boldsymbol{x}) \geq \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{\boxed{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}}\right] \rightarrow \text{We want to optimize}$$

- In VAE, **increase** lower bound by **tuning** parameters to **maximize** the ELBO.

Evidence and ELBO

$$\begin{aligned}
\log p(\boldsymbol{x}) &= \log \int p(\boldsymbol{x}, \boldsymbol{z}) dz \\
&= \log \int \frac{p(\boldsymbol{x}, \boldsymbol{z}) q_{\phi}(\boldsymbol{z}|\boldsymbol{x})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} dz \\
&= \log \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[\frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \right] \\
&\geq \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \right]
\end{aligned}$$

Evidence and ELBO

$$\begin{aligned}
\log p(\boldsymbol{x}) &= \log \int p(\boldsymbol{x}, \boldsymbol{z}) d\boldsymbol{z} \\
&= \log \int \frac{p(\boldsymbol{x}, \boldsymbol{z}) q_\phi(\boldsymbol{z}|\boldsymbol{x})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})} d\boldsymbol{z} \\
&= \log \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \left[\frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \right] \\
&\geq \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \right]
\end{aligned}$$

- No intuition why ELBO is the lower bound!
- If ELBO is the lower bound then why do we want to maximize this as an objective?

Evidence and ELBO

$$\log p(\boldsymbol{x}) = \log \int p(\boldsymbol{x}, \boldsymbol{z}) d\boldsymbol{z}$$

$$\geq \mathbb{E}_{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_{\phi}(\boldsymbol{z}|\boldsymbol{x})} \right]$$

- No intuition why ELBO is the lower bound!

Let's see another derivation of ELBO using the chain rule of probability.

Evidence and ELBO

$$
\begin{aligned}
\log p(\boldsymbol{x}) &= \log p(\boldsymbol{x}) \int q_\phi(\boldsymbol{z}|\boldsymbol{x}) dz \\
&= \int q_\phi(\boldsymbol{z}|\boldsymbol{x}) (\log p(\boldsymbol{x})) dz \\
&= \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})} [\log p(\boldsymbol{x})] \\
&= \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{p(\boldsymbol{z}|\boldsymbol{x})} \right] \\
&= \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}) q_\phi(\boldsymbol{z}|\boldsymbol{x})}{p(\boldsymbol{z}|\boldsymbol{x}) q_\phi(\boldsymbol{z}|\boldsymbol{x})} \right] \\
&= \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \right] + \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{q_\phi(\boldsymbol{z}|\boldsymbol{x})}{p(\boldsymbol{z}|\boldsymbol{x})} \right] \\
& \boxed{= \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \right] + D_{\mathrm{KL}}(q_\phi(\boldsymbol{z}|\boldsymbol{x}) \parallel p(\boldsymbol{z}|\boldsymbol{x}))} \\
&\geq \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \right]
\end{aligned}
$$

D_KL ≥ 0

Evidence and ELBO

$$
\begin{aligned}
\boxed{\log p(\boldsymbol{x})} &= \log p(\boldsymbol{x}) \int q_\phi(\boldsymbol{z}|\boldsymbol{x}) dz \\
&= \int q_\phi(\boldsymbol{z}|\boldsymbol{x})(\log p(\boldsymbol{x})) dz \\
&= \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log p(\boldsymbol{x})\right] \\
\text{constant} &= \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{p(\boldsymbol{z}|\boldsymbol{x})}\right] \\
&= \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}) q_\phi(\boldsymbol{z}|\boldsymbol{x})}{p(\boldsymbol{z}|\boldsymbol{x}) q_\phi(\boldsymbol{z}|\boldsymbol{x})}\right] \\
&= \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\right] + \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{q_\phi(\boldsymbol{z}|\boldsymbol{x})}{p(\boldsymbol{z}|\boldsymbol{x})}\right] \\
&= \boxed{\mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\right] + D_{\mathrm{KL}}(q_\phi(\boldsymbol{z}|\boldsymbol{x}) \parallel p(\boldsymbol{z}|\boldsymbol{x}))} \\
&\geq \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\right]
\end{aligned}
$$

Variational AutoEncoder

- In VAE, maximize ELBO.
- Variational: Optimize the best $q_\phi(z|x)$
- Let's dissect ELBO more to understand VAE

Variational AutoEncoder

$$
\begin{aligned}
\mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\right] &= \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\right] \\
&= \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})\right] + \mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{z})}{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\right] \\
&= \underbrace{\mathbb{E}_{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})}\left[\log \boxed{p_{\boldsymbol{\theta}}(\boldsymbol{x}|\boldsymbol{z})}\right]}_{\text{reconstruction term}} - \underbrace{D_{\mathrm{KL}}(\boxed{q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x})} \parallel p(\boldsymbol{z}))}_{\text{prior matching term}}
\end{aligned}
$$

Decoder

Encoder

Variational AutoEncoder

- Defining feature of VAE: ELBO is optimized jointly over θ and ϕ
- Encoder:

$$q_\phi(\boldsymbol{z}|\boldsymbol{x}) = \mathcal{N}(\boldsymbol{z}; \boldsymbol{\mu}_\phi(\boldsymbol{x}), \boldsymbol{\sigma}_\phi^2(\boldsymbol{x})\mathbf{I})$$

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

Variational AutoEncoder

$$\arg\max_{\phi,\theta} \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})} [\log p_\theta(\boldsymbol{x} \mid \boldsymbol{z})] - \mathcal{D}_{\mathrm{KL}}(q_\phi(\boldsymbol{z} \mid \boldsymbol{x}) \,||\, p(\boldsymbol{z}))$$

$$\approx \arg\max_{\phi,\theta} \sum_{l=1}^{L} \log p_\theta(\boldsymbol{x} \mid \boxed{\boldsymbol{z}^{(l)}}) - \mathcal{D}_{\mathrm{KL}}(q_\phi(\boldsymbol{z} \mid \boldsymbol{x}) \,||\, p(\boldsymbol{z}))$$

Stochastic sampling(Non
Differentiable

Variational AutoEncoder

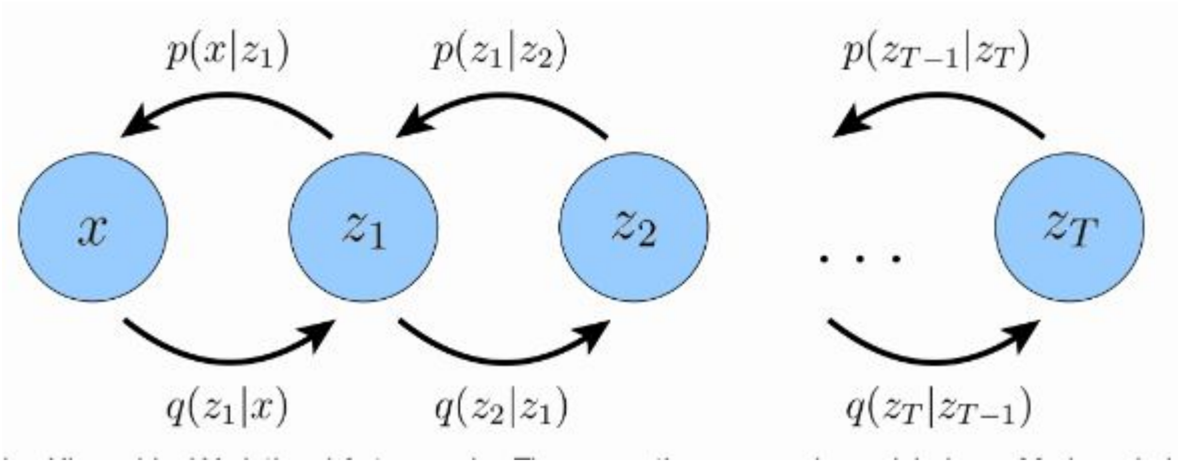
- For example, samples from a normal distribution $x \sim N(x;\mu,\sigma^2)$ with arbitrary mean μ and variance σ^2 can be rewritten as:

$$x = \mu + \sigma\epsilon \quad \text{with } \epsilon \sim \mathcal{N}(\epsilon; 0, \mathrm{I})$$

- In a VAE, each z is thus computed as a deterministic function of input x and auxiliary noise variable ϵ

$$\boldsymbol{z} = \boldsymbol{\mu}_\phi(\boldsymbol{x}) + \boldsymbol{\sigma}_\phi(\boldsymbol{x}) \odot \boldsymbol{\epsilon} \quad \text{with } \boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{\epsilon}; \mathbf{0}, \mathbf{I})$$

Hierarchical VAE



Hierarchical VAE

Joint distribution of Markovian HVAE:

$$p(\boldsymbol{x}, \boldsymbol{z}_{1:T}) = p(\boldsymbol{z}_T)p_\theta(\boldsymbol{x} \mid \boldsymbol{z}_1)\prod_{t=2}^{T} p_\theta(\boldsymbol{z}_{t-1} \mid \boldsymbol{z}_t)$$

And its posterior:

$$q_\phi(\boldsymbol{z}_{1:T} \mid \boldsymbol{x}) = q_\phi(\boldsymbol{z}_1 \mid \boldsymbol{x})\prod_{t=2}^{T} q_\phi(\boldsymbol{z}_t \mid \boldsymbol{z}_{t-1})$$

Hierarchical VAE

Now ELBO can be defined as

$$
\begin{aligned}
\log p(\boldsymbol{x}) &= \log \int p(\boldsymbol{x}, \boldsymbol{z}_{1:T}) d\boldsymbol{z}_{1:T} \\
&= \log \int \frac{p(\boldsymbol{x}, \boldsymbol{z}_{1:T}) q_\phi(\boldsymbol{z}_{1:T} \mid \boldsymbol{x})}{q_\phi(\boldsymbol{z}_{1:T} \mid \boldsymbol{x})} d\boldsymbol{z}_{1:T} \\
&= \log \mathbb{E}_{q_\phi(\boldsymbol{z}_{1:T}|\boldsymbol{x})} \left[\frac{p(\boldsymbol{x}, \boldsymbol{z}_{1:T})}{q_\phi(\boldsymbol{z}_{1:T} \mid \boldsymbol{x})} \right] \\
&\geq \mathbb{E}_{q_\phi(\boldsymbol{z}_{1:T}|\boldsymbol{x})} \left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}_{1:T})}{q_\phi(\boldsymbol{z}_{1:T} \mid \boldsymbol{x})} \right]
\end{aligned}
$$

Hierarchical VAE

Now ELBO can be defined as

$$\mathbb{E}_{q_\phi(\boldsymbol{z}_{1:T}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{x}, \boldsymbol{z}_{1:T})}{q_\phi(\boldsymbol{z}_{1:T} \mid \boldsymbol{x})}\right] = \mathbb{E}_{q_\phi(\boldsymbol{z}_{1:T}|\boldsymbol{x})}\left[\log \frac{p(\boldsymbol{z}_T)p_\theta(\boldsymbol{x} \mid \boldsymbol{z}_1)\prod_{t=2}^{T} p_\theta(\boldsymbol{z}_{t-1} \mid \boldsymbol{z}_t)}{q_\phi(\boldsymbol{z}_1 \mid \boldsymbol{x})\prod_{t=2}^{T} q_\phi(\boldsymbol{z}_t \mid \boldsymbol{z}_{t-1})}\right]$$

Variational Diffusion Models

Simply a Markovian Hierarchical Variational Autoencoder with three key restrictions:

1. The latent dimension is exactly equal to the data dimension
2. The structure of the latent encoder at each timestep is not learned; it is pre-defined as a linear Gaussian model.
3. The Gaussian parameters of the latent encoders vary over time in such a way that the distribution of the latent at final timestep T is a standard Gaussian.

Variational Diffusion Models

Simply a Markovian Hierarchical Variational Autoencoder with three key restrictions:

1. The latent dimension is exactly equal to the data dimension. Now VDM posterior:

$$q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0) = \prod_{t=1}^{T} q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1})$$

Variational Diffusion Models

Simply a Markovian Hierarchical Variational Autoencoder with three key restrictions:

2. The structure of the latent encoder at each timestep is not learned; it is pre-defined as a linear Gaussian model. Encoder transitions are denoted as:

$$q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}) = \mathcal{N}(\boldsymbol{x}_t; \sqrt{\alpha_t}\boldsymbol{x}_{t-1}, (1-\alpha_t)\mathbf{I})$$

Variational Diffusion Models

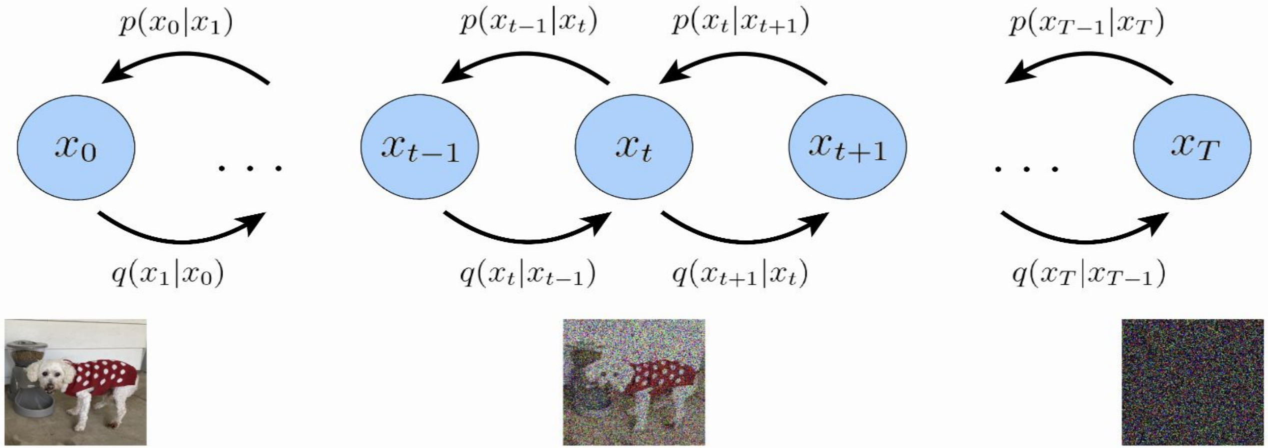
3. The Gaussian parameters of the latent encoders vary over time in such a way that the distribution of the latent at final timestep T is a standard Gaussian.

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

where,

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

Variational Diffusion Models



Visual representation of a Variational Diffusion Model. An input is steadily noised over time until it becomes identical to Gaussian noise; a diffusion model learns to reverse this process.

ELBO for Variational Diffusion Models

$$
\begin{aligned}
\log p(\boldsymbol{x}) &\geq \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0)}\right] \\
&= \boxed{\underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_\theta(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)\right]}_{\text{reconstruction term}}} - \underbrace{\mathbb{E}_{q(\boldsymbol{x}_{T-1}|\boldsymbol{x}_0)}\left[\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_T \mid \boldsymbol{x}_{T-1}) \,\|\, p(\boldsymbol{x}_T))\right]}_{\text{prior matching term}} \\
&\quad - \sum_{t=1}^{T-1} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_{t-1},\boldsymbol{x}_{t+1}|\boldsymbol{x}_0)}\left[\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}) \,\|\, p_\theta(\boldsymbol{x}_t \mid \boldsymbol{x}_{t+1}))\right]}_{\text{consistency term}}
\end{aligned}
$$

ELBO for Variational Diffusion Models

$$\log p(\boldsymbol{x}) \geq \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0)}\right]$$

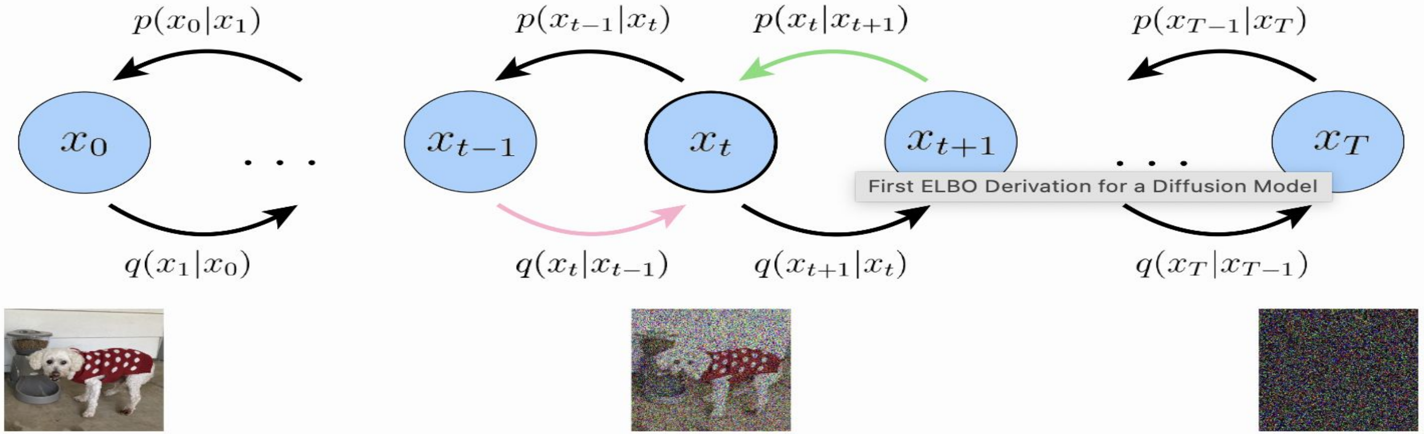
$$= \underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_\theta(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)\right]}_{\text{reconstruction term}} - \boxed{\underbrace{\mathbb{E}_{q(\boldsymbol{x}_{T-1}|\boldsymbol{x}_0)}\left[\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_T \mid \boldsymbol{x}_{T-1})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

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

ELBO for Variational Diffusion Models

$$\begin{aligned}\log p(\boldsymbol{x}) &\geq \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0)}\right] \\ &= \underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_\theta(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)\right]}_{\text{reconstruction term}} - \underbrace{\mathbb{E}_{q(\boldsymbol{x}_{T-1}|\boldsymbol{x}_0)}\left[\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_T \mid \boldsymbol{x}_{T-1}) \,||\, p(\boldsymbol{x}_T))\right]}_{\text{prior matching term}} \\ &\quad - \boxed{\sum_{t=1}^{T-1} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_{t-1},\boldsymbol{x}_{t+1}|\boldsymbol{x}_0)}\left[\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}) \,||\, p_\theta(\boldsymbol{x}_t \mid \boldsymbol{x}_{t+1}))\right]}_{\text{consistency term}}}\end{aligned}$$

ELBO for Variational Diffusion Models



A VDM can be optimized by ensuring that for every intermediate latent, the posterior from the latent above it matches the Gaussian corruption of the latent before it. In this figure, for each intermediate latent, we minimize the difference between the distributions represented by the pink and green arrows.

ELBO for Variational Diffusion Models

$$\log p(\boldsymbol{x}) \geq \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0)}\right]$$

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

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

ELBO for Variational Diffusion Models

$$q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{x}_0) = \frac{q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) q(\boldsymbol{x}_t \mid \boldsymbol{x}_0)}{q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_0)}$$

$$\begin{aligned} \log p(\boldsymbol{x}) &\geq \mathbb{E}_{q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0)}\right] \\ &= \boxed{\underbrace{\mathbb{E}_{q(\boldsymbol{x}_1 \mid \boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)\right]}_{\text{reconstruction term}}} - \underbrace{\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_T \mid \boldsymbol{x}_0) \,\|\, p(\boldsymbol{x}_T))}_{\text{prior matching term}} \\ &\quad - \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_t \mid \boldsymbol{x}_0)}\left[\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) \,\|\, p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t))\right]}_{\text{denoising matching term}} \end{aligned}$$

ELBO for Variational Diffusion Models

$$q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{x}_0) = \frac{q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0)q(\boldsymbol{x}_t \mid \boldsymbol{x}_0)}{q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_0)}$$

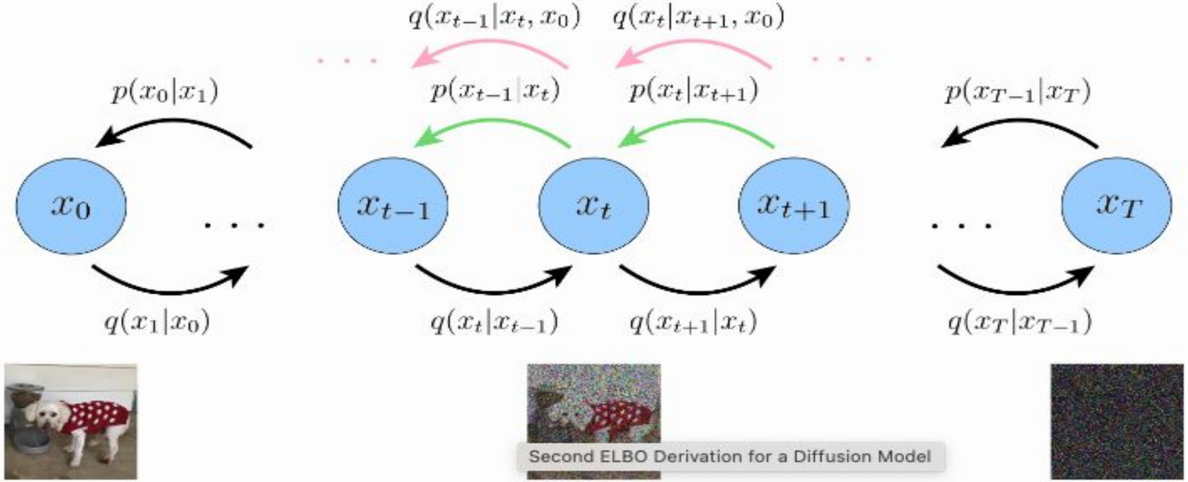
$$\begin{aligned}
\log p(\boldsymbol{x}) &\geq \mathbb{E}_{q(\boldsymbol{x}_{1:T}|\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0)}\right] \\
&= \underbrace{\mathbb{E}_{q(\boldsymbol{x}_1|\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)\right]}_{\text{reconstruction term}} - \boxed{\underbrace{\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_T \mid \boldsymbol{x}_0) \parallel p(\boldsymbol{x}_T))}_{\text{prior matching term}}} \\
&\quad - \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_t|\boldsymbol{x}_0)}\left[\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) \parallel p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t))\right]}_{\text{denoising matching term}}
\end{aligned}$$

ELBO for Variational Diffusion Models

$$q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{x}_0) = \frac{q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0)q(\boldsymbol{x}_t \mid \boldsymbol{x}_0)}{q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_0)}$$

$$\begin{aligned}
\log p(\boldsymbol{x}) &\geq \mathbb{E}_{q(\boldsymbol{x}_{1:T}\mid\boldsymbol{x}_0)}\left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0)}\right] \\
&= \underbrace{\mathbb{E}_{q(\boldsymbol{x}_1\mid\boldsymbol{x}_0)}\left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1)\right]}_{\text{reconstruction term}} - \underbrace{\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_T \mid \boldsymbol{x}_0) \,||\, p(\boldsymbol{x}_T))}_{\text{prior matching term}} \\
&\quad \boxed{- \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_t\mid\boldsymbol{x}_0)}\left[\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) \,||\, p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t))\right]}_{\text{denoising matching term}}}
\end{aligned}$$

ELBO for Variational Diffusion Models



A VDM can also be optimized by learning the denoising step for each individual latent by matching it with a tractably computed ground-truth denoising step. This is once again denoted visually by matching the distributions represented by the green arrows with those of the pink arrows. Artistic liberty is at play here; in the full picture, each pink arrow must also stem from the ground-truth image, as it is also a conditioning term.

ELBO for Variational Diffusion Models

$$q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{x}_0) = \frac{q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) q(\boldsymbol{x}_t \mid \boldsymbol{x}_0)}{q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_0)}$$

$$\begin{aligned}
\log p(\boldsymbol{x}) &\geq \mathbb{E}_{q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0)} \left[\log \frac{p(\boldsymbol{x}_{0:T})}{q(\boldsymbol{x}_{1:T} \mid \boldsymbol{x}_0)} \right] \\
&= \underbrace{\mathbb{E}_{q(\boldsymbol{x}_1 \mid \boldsymbol{x}_0)} \left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_0 \mid \boldsymbol{x}_1) \right]}_{\text{reconstruction term}} - \underbrace{\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_T \mid \boldsymbol{x}_0) \mid\mid p(\boldsymbol{x}_T))}_{\text{prior matching term}} \\
&\quad \boxed{- \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q(\boldsymbol{x}_t \mid \boldsymbol{x}_0)} \left[\mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) \mid\mid p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)) \right]}_{\text{denoising matching term}}}
\end{aligned}$$

ELBO for Variational Diffusion Models

$$q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) = \frac{q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{x}_0)q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_0)}{q(\boldsymbol{x}_t \mid \boldsymbol{x}_0)}$$

ELBO for Variational Diffusion Models

$$q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) = \frac{q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{x}_0) q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_0)}{q(\boldsymbol{x}_t \mid \boldsymbol{x}_0)}$$

From our assumption we know that,

$$q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{x}_0) = q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}) = \mathcal{N}(\boldsymbol{x}_t; \sqrt{\alpha_t}\boldsymbol{x}_{t-1}, (1 - \alpha_t)\mathbf{I})$$

ELBO for Variational Diffusion Models

$$q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) = \frac{q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{x}_0)\boxed{q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_0)}}{\boxed{q(\boldsymbol{x}_t \mid \boldsymbol{x}_0)}}$$

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

$$\boldsymbol{x}_{t-1} = \sqrt{\alpha_{t-1}}\boldsymbol{x}_{t-2} + \sqrt{1-\alpha_{t-1}}\boldsymbol{\epsilon} \quad \text{with } \boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{\epsilon}; \mathbf{0}, \mathbf{I})$$

Reparam trick

$$x_t \sim \mathcal{N}(\boldsymbol{x}_t; \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0, (1-\bar{\alpha}_t)\mathbf{I})$$

ELBO for Variational Diffusion Models

$$
\begin{aligned}
q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) &= \frac{q(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{x}_0)q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_0)}{q(\boldsymbol{x}_t \mid \boldsymbol{x}_0)} \\
&= \frac{\mathcal{N}(\boldsymbol{x}_t; \sqrt{\alpha_t}\boldsymbol{x}_{t-1}, (1-\alpha_t)\mathbf{I})\mathcal{N}(\boldsymbol{x}_{t-1}; \sqrt{\bar{\alpha}_{t-1}}\boldsymbol{x}_0, (1-\bar{\alpha}_{t-1})\mathbf{I})}{\mathcal{N}(\boldsymbol{x}_t; \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0, (1-\bar{\alpha}_t)\mathbf{I})} \\
&\propto \mathcal{N}(\boldsymbol{x}_{t-1}; \underbrace{\frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\boldsymbol{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar{\alpha}_t}}_{\mu_q(\boldsymbol{x}_t, \boldsymbol{x}_0)}, \underbrace{\frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{I}}_{\boldsymbol{\Sigma}_q(t)})
\end{aligned}
$$

ELBO for Variational Diffusion Models

$$\boldsymbol{\mu}_q(\boldsymbol{x}_t, \boldsymbol{x}_0) = \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\boldsymbol{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar{\alpha}_t}$$

$$\boldsymbol{\mu}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) = \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\boldsymbol{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\hat{\boldsymbol{x}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t)}{1-\bar{\alpha}_t}$$

ELBO for Variational Diffusion Models

$$
\begin{aligned}
&\arg\min_{\boldsymbol{\theta}} D_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) \mid\mid p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)) \\
&= \arg\min_{\boldsymbol{\theta}} D_{\mathrm{KL}}\left(\mathcal{N}\left(\boldsymbol{x}_{t-1}; \boldsymbol{\mu}_q, \boldsymbol{\Sigma}_q\left(t\right)\right) \mid\mid \mathcal{N}\left(\boldsymbol{x}_{t-1}; \boldsymbol{\mu}_{\boldsymbol{\theta}}, \boldsymbol{\Sigma}_q\left(t\right)\right)\right) \\
&= \arg\min_{\boldsymbol{\theta}} \frac{1}{2\sigma_q^2(t)} \frac{\bar{\alpha}_{t-1}(1-\alpha_t)^2}{(1-\bar{\alpha}_t)^2}\left[\left\|\hat{\boldsymbol{x}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) - \boldsymbol{x}_0\right\|_2^2\right]
\end{aligned}
$$

ELBO for Variational Diffusion Models

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

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

ELBO for Variational Diffusion Models

$$x_t \sim \mathcal{N}(\boldsymbol{x}_t; \sqrt{\bar{\alpha}_t}\boldsymbol{x}_0, (1-\bar{\alpha}_t)\mathbf{I})$$

$$\boldsymbol{x}_0 = \frac{\boldsymbol{x}_t - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_0}{\sqrt{\bar{\alpha}_t}}$$

ELBO for Variational Diffusion Models

$$\boldsymbol{\mu}_q(\boldsymbol{x}_t, \boldsymbol{x}_0) = \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})\boldsymbol{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\boldsymbol{x}_0}{1-\bar{\alpha}_t}$$

$$= \frac{1}{\sqrt{\alpha_t}}\boldsymbol{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}\sqrt{\alpha_t}}\boldsymbol{\epsilon}_0$$

$$\boldsymbol{\mu}_\theta(\boldsymbol{x}_t, t) = \frac{1}{\sqrt{\alpha_t}}\boldsymbol{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}\sqrt{\alpha_t}}\hat{\boldsymbol{\epsilon}}_\theta(\boldsymbol{x}_t, t)$$

ELBO for Variational Diffusion Models

ELBO for Variational Diffusion Models

$$
\begin{aligned}
&\arg\min_{\boldsymbol{\theta}} \mathcal{D}_{\mathrm{KL}}(q(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t, \boldsymbol{x}_0) \,||\, p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t-1} \mid \boldsymbol{x}_t)) \\
&= \arg\min_{\boldsymbol{\theta}} \mathcal{D}_{\mathrm{KL}} \left(\mathcal{N}\left(\boldsymbol{x}_{t-1}; \boldsymbol{\mu}_q, \boldsymbol{\Sigma}_q\left(t\right)\right) \,||\, \mathcal{N}\left(\boldsymbol{x}_{t-1}; \boldsymbol{\mu}_{\boldsymbol{\theta}}, \boldsymbol{\Sigma}_q\left(t\right)\right)\right) \\
&= \arg\min_{\boldsymbol{\theta}} \frac{1}{2\sigma_q^2(t)} \frac{(1-\alpha_t)^2}{(1-\bar{\alpha}_t)\alpha_t} \left[\left\|\boldsymbol{\epsilon}_0 - \hat{\boldsymbol{\epsilon}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t)\right\|_2^2\right]
\end{aligned}
$$