Deep Generative Models: Diffusion Models

Fall Semester 2025

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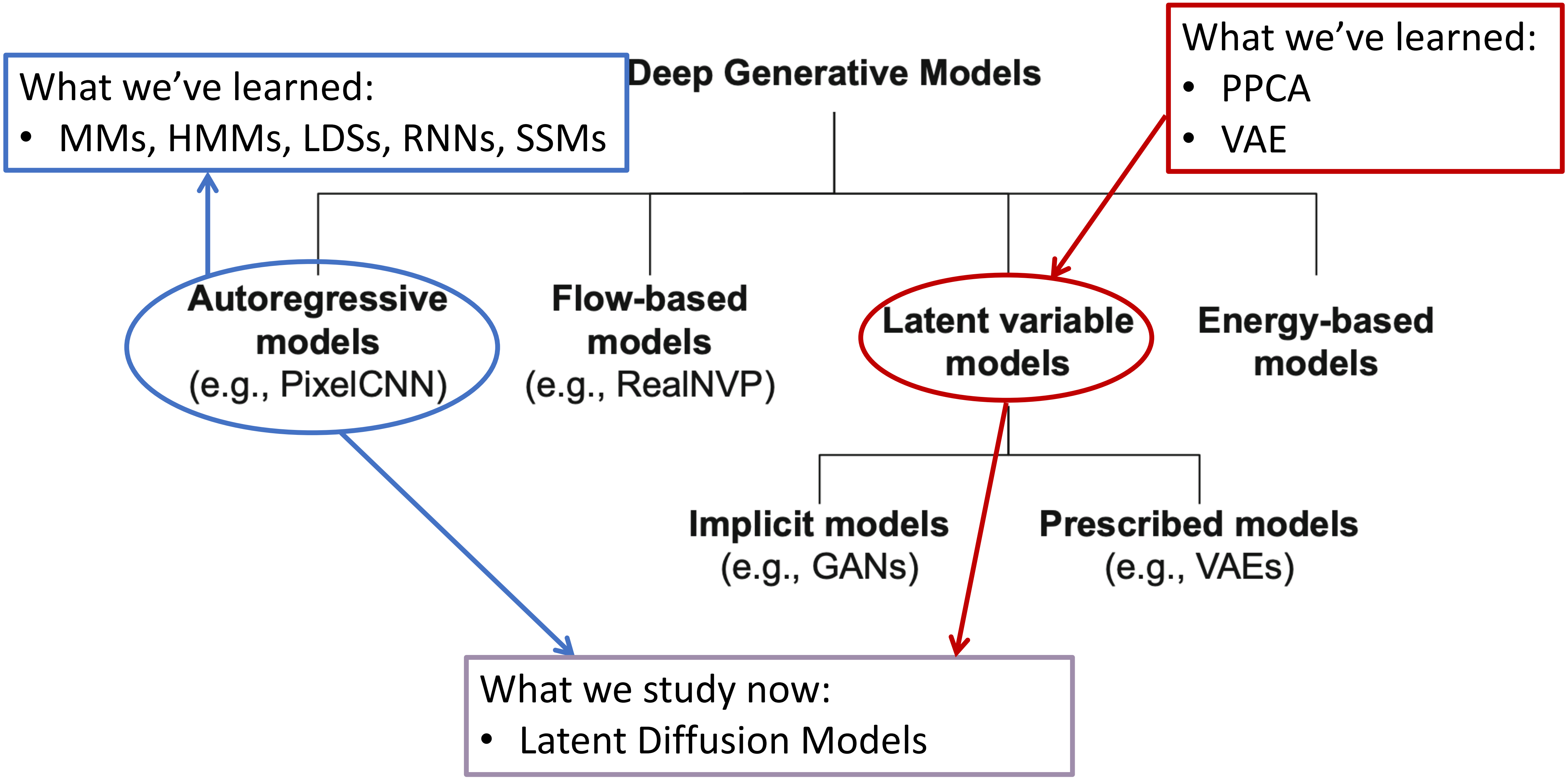
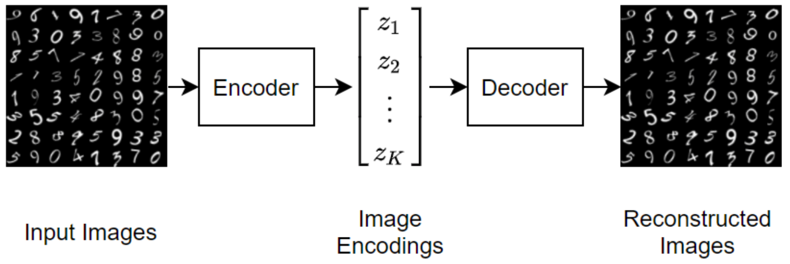
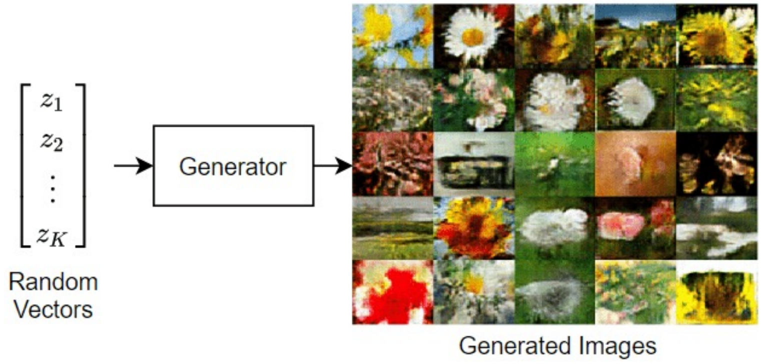
Taxonomy of Generative Models



Diffusion Models

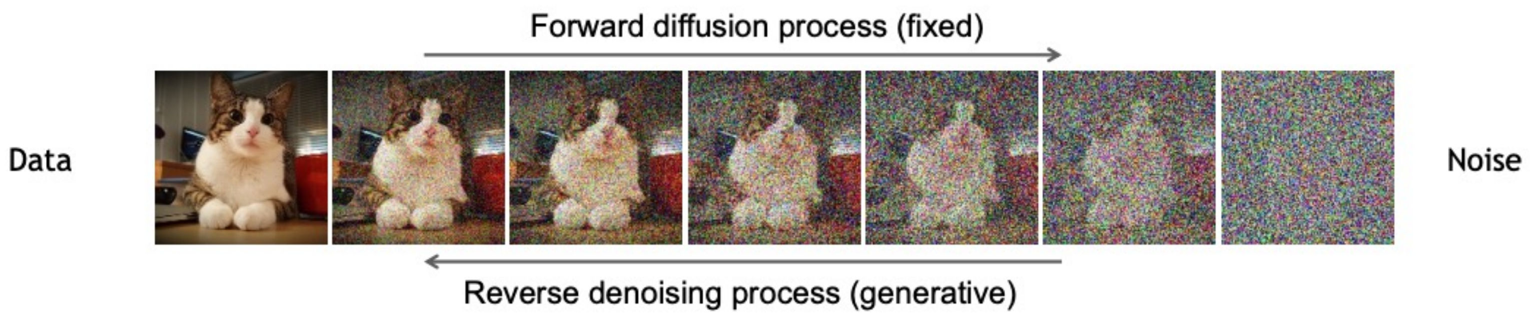
- The journey of generative models has evolved significantly in recent years.
- **Variational Autoencoders (VAEs)** introduce probabilistic modeling for latent representations but struggled with generating high-quality images.
- This led to the rise of **Generative Adversarial Networks (GANs)**, which leverage adversarial learning to produce high-quality, realistic outputs but suffered from issues like mode collapse and unstable training.
- The introduction of **Diffusion Models** achieve state-of-the-art results with superior stability and diversity in generated samples, particularly in multimodal image synthesis.

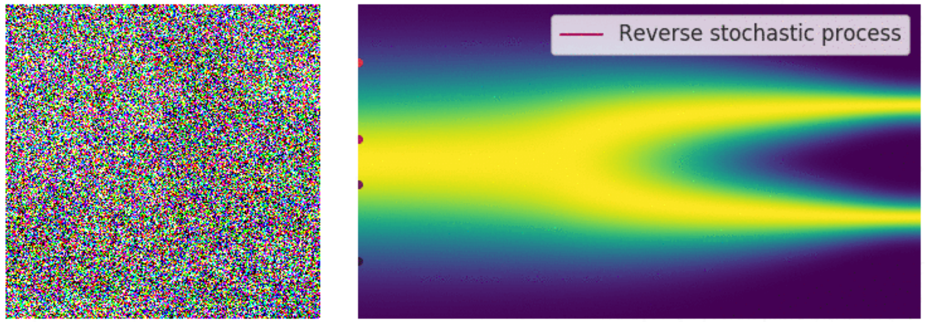




Diffusion Models

- A Latent Diffusion Model is a VAE with an autoregressive latent space.
- The VAE encoder maps data to noise by gradually adding Gaussian noise to the input using a (forward) diffusion process.
- The VAE decoder maps noise to data by learning a transformation that aims to reverse the forward diffusion process.





Outline

- **Markov Hierarchical Variational Auto Encoders (MHVAEs)**
  - Autoregressive Encoder and Autoregressive Decoder of an MHVAE
  - Derivation of the ELBO of an MHVAE

- Diffusion Models as MHVAEs with a Linear Gaussian Autoregressive Latent Space
  - Forward Diffusion Process
  - Reverse Diffusion Process
  - ELBO for Diffusion Models as a particular case of the ELBO for MHVAEs
  - Implementation Details: UNet architecture, Training and Sampling Strategies

- Application of Diffusion Models
  - Stable Diffusion: Text-Conditioned Diffusion Model
  - ControlNet: Multimodal Control for Consistent Synthesis

Recall the Variational Autoencoder (VAE)

Datapoint x

Encoder
$q_\phi(\boldsymbol{z} \mid \boldsymbol{x})$

μ

$\log \sigma^2$

Sampler
$\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{z} \mid \mu_\phi(\boldsymbol{x}), \sigma_\phi^2(\boldsymbol{x}) I)$

Decoder
$p_\theta(\boldsymbol{x} \mid \boldsymbol{z})$

$\mu_\theta(\boldsymbol{z})$

ELBO Objective

$$\mathbb{E}_{\boldsymbol{z} \sim q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log p_\theta(\boldsymbol{x} \mid \boldsymbol{z}) - KL\left(q_\phi(\boldsymbol{z} \mid \boldsymbol{x}) \,||\, p(\boldsymbol{z})\right)\right]$$

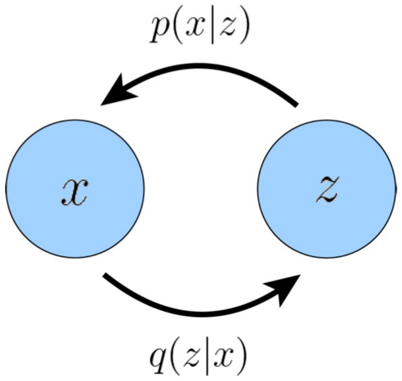
Recall the Evidence Lower Bound (ELBO)

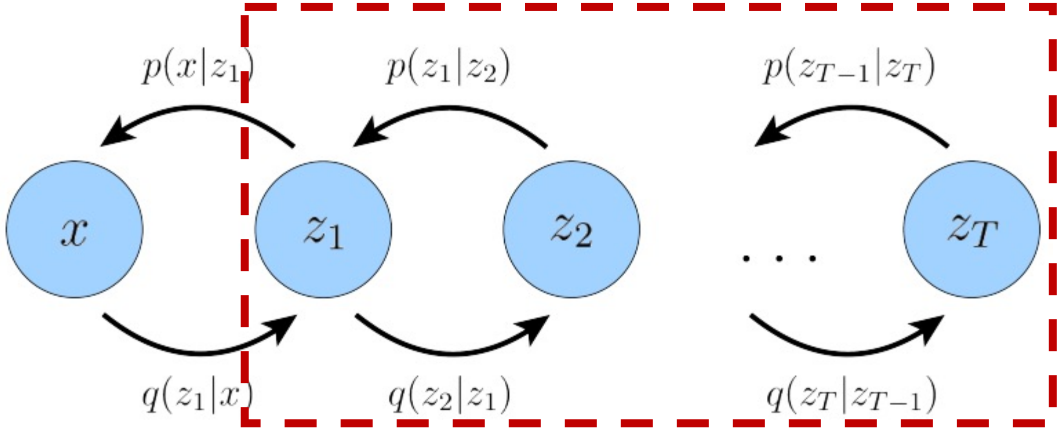
- The ELBO is the sum of a reconstruction term and a prior matching term

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

Latent Diffusion Models as "Autoregressive VAEs"

- A Latent Diffusion Model is as a Markovian Hierarchical Variational Autoencoder (MHVAE) with T hierarchical latents $z = z_{1:T} = \{z_t\}_{t=1}^{T}$ modeled by a Markov chain where each latent z_t is generated only from the previous latent z_{t+1}.



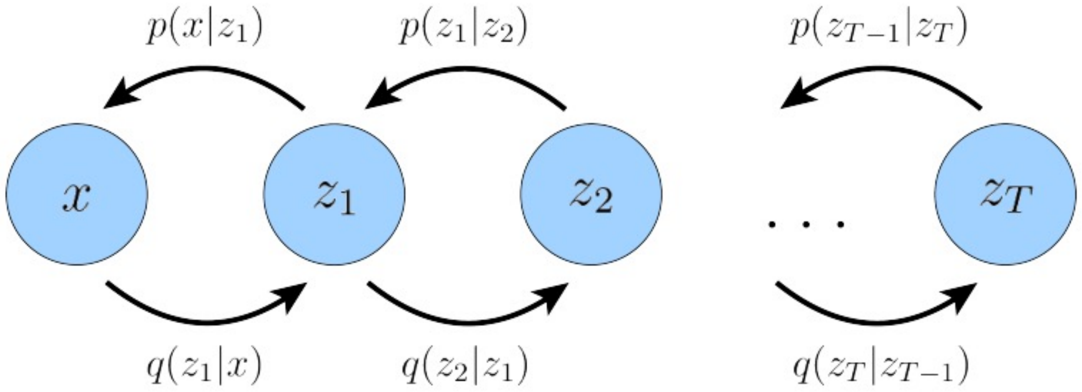


$z = z_{1:T} = \{z_t\}_{t=1}^{T}$

- What is the VAE encoder $q_\phi(z \mid x)$ of a Diffusion Model ?
- What is the VAE decoder $p_\theta(x \mid z)$ of a Diffusion Model ?
- What is the ELBO of a Diffusion Model ?

MHVAE Encoder, Decoder, and ELBO

- A MHVAE is a VAE whose encoder and decoder are autoregressive models:



$$p_\theta(x, z_{1:T}) = p_\theta(z_T) p_\theta(x \mid z_1) \prod_{t=2}^{T} p_\theta(z_{t-1} \mid z_t)$$

$$q_\phi(z_{1:T} \mid x) = q_\phi(z_1 \mid x) \prod_{t=2}^{T} q_\phi(z_t \mid z_{t-1})$$

- Given this joint distribution and posterior, we can rewrite the ELBO for MHVAE as:

$$\mathbb{E}_{q_\phi(z_{1:T}|x)}\left[\log \frac{p_\theta(x, z_{1:T})}{q_\phi(z_{1:T} \mid x)}\right] = \mathbb{E}_{q_\phi(z_{1:T}|x)}\left[\log \frac{p_\theta(z_T) p_\theta(x \mid z_1) \prod_{t=2}^{T} p_\theta(z_{t-1} \mid z_t)}{q_\phi(z_1 \mid x) \prod_{t=2}^{T} q_\phi(z_t \mid z_{t-1})}\right]$$

Decomposition of the ELBO for an MHVAE

- Let us make the change of variables $x \to x_0$ and $z_{1:T} \to x_{1:T}$.
- The ELBO is hard to evaluate because it requires sampling from $q_\phi(x_{1:T} \mid x_0)$.

- **Theorem**: The ELBO for a MHVAE can be written as

$$\mathbb{E}_{q_\phi(x_{1:T}|x_0)}\left[\log \frac{p_\theta(x_T) p_\theta(x_0 \mid x_1) \prod_{t=2}^{T} p_\theta(x_{t-1} \mid x_t)}{q_\phi(x_1 \mid x_0) \prod_{t=2}^{T} q_\phi(x_t \mid x_{t-1})}\right] =$$

$$\underbrace{\mathbb{E}_{q_\phi(x_1|x_0)}[\log p_\theta(x_0 \mid x_1)]}_{\text{reconstruction term}} - \underbrace{D_{\mathrm{KL}}\left(q_\phi(x_T \mid x_0) \,||\, p_\theta(x_T)\right)}_{\text{prior matching term}}$$

$$-\sum_{t=2}^{T} \underbrace{\mathbb{E}_{q_\phi(x_t|x_0)}\left[D_{\mathrm{KL}}\left(q_\phi(x_{t-1} \mid x_t, x_0) \,||\, p_\theta(x_{t-1} \mid x_t)\right)\right]}_{\text{score matching term}}$$

Decomposition of the ELBO for an MHVAE

- **Proof (1/2):** Reversing $q_\phi(x_t \mid x_{t-1})$

$$q_\phi(x_t \mid x_{t-1}) = q_\phi(x_t \mid x_{t-1}, x_0) = \frac{q_\phi(x_{t-1}|x_t, x_0)q_\phi(x_t|x_0)}{q_\phi(x_{t-1}|x_0)}.$$

- Substituting $q_\phi(x_t \mid x_{t-1})$ and using telescopic product to cancel factors

$$\log p(x) \geq \mathbb{E}_{q_\phi(x_{1:T}|x_0)}\left[\log \frac{p_\theta(x_T)p_\theta(x_0 \mid x_1)\prod_{t=2}^{T} p_\theta(x_{t-1} \mid x_t)}{q_\phi(x_1 \mid x_0)\prod_{t=2}^{T} q_\phi(x_t \mid x_{t-1})}\right]$$

$$= \mathbb{E}_{q_\phi(x_{1:T}|x_0)}\left[\log \frac{p_\theta(x_T)p_\theta(x_0 \mid x_1)}{q_\phi(x_1 \mid x_0)}\prod_{t=2}^{T} \frac{p_\theta(x_{t-1} \mid x_t)}{\frac{q_\phi(x_{t-1} \mid x_t, x_0)q_\phi(x_t \mid x_0)}{q_\phi(x_{t-1} \mid x_0)}}\right]$$

$$= \mathbb{E}_{q_\phi(x_{1:T}|x_0)}\left[\log \frac{p_\theta(x_T)p_\theta(x_0 \mid x_1)q_\phi(x_1 \mid x_0)}{q_\phi(x_1 \mid x_0)q_\phi(x_T \mid x_0)}\prod_{t=2}^{T} \frac{p_\theta(x_{t-1} \mid x_t)}{q_\phi(x_{t-1} \mid x_t, x_0)}\right]$$

Decomposition of the ELBO for an MHVAE

- **Proof (2/2):** expanding into three terms and simplifying expectations

$$\log p(x) \geq \mathbb{E}_{q_\phi(x_{1:T}|x_0)}\left[\log \frac{p_\theta(x_T)p_\theta(x_0 \mid x_1)}{q_\phi(x_T \mid x_0)} \prod_{t=2}^{T} \frac{p_\theta(x_{t-1} \mid x_t)}{q_\phi(x_{t-1} \mid x_t, x_0)}\right]$$

$$= \mathbb{E}_{q_\phi(x_{1:T}|x_0)}\left[\log p_\theta(x_0 \mid x_1)\right] + \mathbb{E}_{q_\phi(x_{1:T}|x_0)}\left[\log \frac{p_\theta(x_T)}{q_\phi(x_T \mid x_0)}\right] + \sum_{t=2}^{T} \mathbb{E}_{q_\phi(x_{1:T}|x_0)}\left[\log \frac{p_\theta(x_{t-1} \mid x_t)}{q_\phi(x_{t-1} \mid x_t, x_0)}\right]$$

$$= \mathbb{E}_{q_\phi(x_1|x_0)}\left[\log p_\theta(x_0 \mid x_1)\right] + \mathbb{E}_{q_\phi(x_T|x_0)}\left[\log \frac{p_\theta(x_T)}{q_\phi(x_T \mid x_0)}\right] + \sum_{t=2}^{T} \mathbb{E}_{q_\phi(x_{t-1}, x_t|x_0)}\left[\log \frac{p_\theta(x_{t-1} \mid x_t)}{q_\phi(x_{t-1} \mid x_t, x_0)}\right]$$

$$= \underbrace{\mathbb{E}_{q_\phi(x_1|x_0)}\left[\log p_\theta(x_0 \mid x_1)\right]}_{\text{reconstruction term}} - \underbrace{D_{\mathrm{KL}}\left(q_\phi(x_T \mid x_0) | p_\theta(x_T)\right)}_{\text{prior matching term}} - \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q_\phi(x_t|x_0)}\left[D_{\mathrm{KL}}\left(q_\phi(x_{t-1} \mid x_t, x_0) \mid\mid p_\theta(x_{t-1} \mid x_t)\right)\right]}_{\text{score matching term}}$$

Why can we Simplify Expectations?

- For the first term:

$$\mathbb{E}_{q_\phi(x_{1:T}|x_0)}[\log(p_\theta(x_0 \mid x_1))] = \int \log(p_\theta(x_0 \mid x_1))\, q_\phi(x_{1:T} \mid x_0) dx_{1:T}$$

$$= \int \log(p_\theta(x_0 \mid x_1))\, q_\phi(x_1, x_{2:T} \mid x_0) dx_{2:T} dx_1$$

$$\boxed{\int q_\phi(x_1, x_{2:T} \mid x_0) dx_{2:T} = q(x_1 \mid x_0)}$$

$$= \int \log p_\theta(x_0 \mid x_1) q_\phi(x_1 \mid x_0) dx_1 = \mathbb{E}_{q_\phi(x_1|x_0)}[\log p_\theta(x_0 \mid x_1)]$$

- For the second term:

$$\mathbb{E}_{q_\phi(x_{1:T}|x_0)}\left[\log \frac{p_\theta(x_T)}{q_\phi(x_T \mid x_0)}\right] = \int \log\left(\frac{p_\theta(x_T)}{q_\phi(x_T \mid x_0)}\right) q_\phi(x_{1:T} \mid x_0) dx_{1:T}$$

$$= \int \log\left(\frac{p_\theta(x_T)}{q_\phi(x_T \mid x_0)}\right) q_\phi(x_{1:T-1}, x_T \mid x_0) dx_{1:T-1} dx_T$$

$$\boxed{\int q_\phi(x_{1:T-1}, x_T \mid x_0) dx_{1:T-1} = q(x_T \mid x_0)}$$

$$= \int \log\left(\frac{p_\theta(x_T)}{q_\phi(x_T \mid x_0)}\right) q_\phi(x_T \mid x_0) dx_T = \mathbb{E}_{q_\phi(x_T|x_0)}\left[\log \frac{p_\theta(x_T)}{q_\phi(x_T \mid x_0)}\right]$$

Why can we Simplify Expectations?

- For the third term:

$$\mathbb{E}_{q_\phi(x_{1:T}|x_0)}\left[\log\left(\frac{p_\theta(x_{t-1} \mid x_t)}{q_\phi(x_{t-1} \mid x_t, x_0)}\right)\right] = \int \log\left(\frac{p_\theta(x_{t-1} \mid x_t)}{q_\phi(x_{t-1} \mid x_t, x_0)}\right) q_\phi(x_{1:T} \mid x_0) dx_{1:T}$$

$$= \int \log\left(\frac{p_\theta(x_{t-1} \mid x_t)}{q_\phi(x_{t-1} \mid x_t, x_0)}\right) q_\phi(x_{1:t-2}, x_{t-1:t}, x_{t+1:T} \mid x_0) dx_{1:t-2} dx_{t+1:T} dx_{t-1} dx_t$$

$$= \int \log\left(\frac{p_\theta(x_{t-1} \mid x_t)}{q_\phi(x_{t-1} \mid x_t, x_0)}\right) q_\phi(x_{t-1}, x_t \mid x_0) dx_{t-1} dx_t$$

$$= \int \log\left(\frac{p_\theta(x_{t-1} \mid x_t)}{q_\phi(x_{t-1} \mid x_t, x_0)}\right) q_\phi(x_{t-1} \mid x_t, x_0) q_\phi(x_t \mid x_0) dx_{t-1} dx_t$$

$$= -\int D_{\mathrm{KL}}\left(q_\phi(x_{t-1} \mid x_t, x_0) \,||\, p_\theta(x_{t-1} \mid x_t)\right) q_\phi(x_t \mid x_0) dx_t$$

$$= -\mathbb{E}_{q_\phi(x_t|x_0)}\left[D_{\mathrm{KL}}\left(q_\phi(x_{t-1} \mid x_t, x_0) \,||\, p_\theta(x_{t-1} \mid x_t)\right)\right]$$

$$\boxed{\int q_\phi(x_{1:t-2}, x_{t-1:t}, x_{t+1:T} \mid x_0) dx_{1:t-2} dx_{t+1:T} = q_\phi(x_{t-1:t} \mid x_0)}$$

Interpretation of the ELBO of an MHVAE

$$= \underbrace{\mathbb{E}_{q_\phi(x_1|x_0)}[\log p_\theta(x_0 \mid x_1)]}_{\text{reconstruction term}} - \underbrace{D_{\text{KL}}\left(q_\phi(x_T \mid x_0)|p_\theta(x_T)\right)}_{\text{prior matching term}} - \sum_{t=2}^{T} \underbrace{\mathbb{E}_{q_\phi(x_t|x_0)}\left[D_{\text{KL}}\left(q_\phi(x_{t-1} \mid x_t, x_0) \,||\, p_\theta(x_{t-1} \mid x_t)\right)\right]}_{\text{score matching term}}$$

- $\mathbb{E}_{q(x_1|x_0)}[\log p_\theta(x_0 \mid x_1)]$ can be interpreted as a reconstruction term; like its analogue in the ELBO of a vanilla VAE. This term can be approximated and optimized using a Monte Carlo estimate.
- $D_{\text{KL}}\left(q_\phi(x_T \mid x_0)|p_\theta(x_T)\right)$ represents how close the distribution of the final latent distribution is to the standard Gaussian prior.
- $\mathbb{E}_{q_\phi(x_t|x_0)}\left[D_{\text{KL}}\left(q_\phi(x_{t-1} \mid x_t, x_0) \,||\, p_\theta(x_{t-1} \mid x_t)\right)\right]$ is a score matching term. As we will see, the diffusion model learns the denoising step $p_\theta(x_{t-1} \mid x_t)$ as an approximation to the tractable, ground-truth denoising step $q_\phi(x_{t-1} \mid x_t, x_0)$.

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- Markov Hierarchical Variational Auto Encoders (MHVAEs)
  - Autoregressive Encoder and Autoregressive Decoder of an MHVAE
  - Derivation of the ELBO of an MHVAE

- **Diffusion Models as MHVAEs with a Linear Gaussian Autoregressive Latent Space**
  - Forward Diffusion Process
  - Reverse Diffusion Process
  - ELBO for Diffusion Models as a particular case of the ELBO for MHVAEs
  - Implementation Details: UNet architecture, Training and Sampling Strategies

- Application of Diffusion Models
  - Stable Diffusion: Text-Conditioned Diffusion Model
  - ControlNet: Multimodal Control for Consistent Synthesis

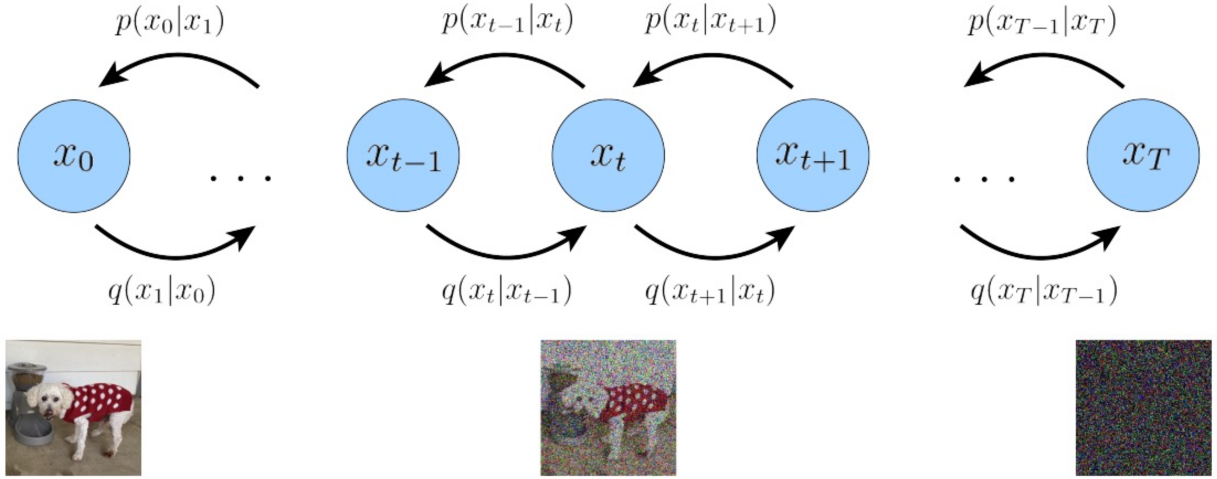
Diffusion Model as MHVAEs with Gaussian Latents

- **A Diffusion Model is an MHVAE** where the latent variables $x_{1:T}$ have the same dimension as the data x_0, and the encoder $q_\phi(x_{1:T} \mid x_0) = \prod_{t=1}^{T} q_\phi(x_t \mid x_{t-1})$ is not learned, but it is pre-specified as a linear Gaussian model

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

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

- The parameter α_t is chosen such that $x_T \sim \mathcal{N}(x_T; 0, I)$ is a standard Gaussian



The Forward Process of Diffusion Model

$$\bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i$$

- Consider the formulation of a single noising step:

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

- we can recursively derive the closed form for arbitrary noising steps:

$$\begin{aligned}
\mathbb{E}[\, x_t \mid x_0 \,] &= \mathbb{E}\left[\, \sqrt{\alpha_t} x_{t-1} + \sqrt{1 - \alpha_t} \varepsilon_t \mid x_0 \,\right] \\
&= \sqrt{\alpha_t}\, \mathbb{E}[\, x_{\mathrm{t}-1} \mid x_0 \,] + \sqrt{1 - \alpha_t} \mathbb{E}[\varepsilon_t] \\
&= \sqrt{\alpha_t} \mathbb{E}[\, x_{\mathrm{t}-1} \mid x_0 \,]
\end{aligned}$$

That is:

$$\begin{aligned}
\mathbb{E}[\, x_t \mid x_0 \,] &= \sqrt{\alpha_t} \sqrt{\alpha_{t-1}}\, \mathbb{E}[\, x_{t-2} \mid x_0 \,] \\
&= \sqrt{\alpha_t} \sqrt{\alpha_{\mathrm{t}-1}} \cdots \sqrt{\alpha_1}\, x_0 \\
&= \sqrt{\bar{\alpha}_t} x_0
\end{aligned}$$

The Forward Process of Diffusion Model

$$\boxed{\bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i}$$

The variance is given by

$$
\begin{aligned}
\mathrm{Var}(\, x_t \mid x_0 \,) &= \mathrm{Var}\left(\sqrt{\alpha_t} x_{t-1} + \sqrt{1-\alpha_t} \varepsilon_t \mid x_0 \right) \\
&= \alpha_t \mathrm{Var}(\, x_{t-1} \mid x_0 \,) + (1-\alpha_t) \, \mathrm{Var}(\varepsilon_t) \\
&= \alpha_t \mathrm{Var}(\, x_{t-1} \mid x_0 \,) + (1-\alpha_t) \, I
\end{aligned}
$$

That is:

$$
\begin{aligned}
\mathrm{Var}(\, x_t \mid x_0 \,) &= \alpha_t \left[\alpha_{t-1} \mathrm{Var}(\, x_{t-2} \mid x_0 \,) + (1-\alpha_{t-1}) \, I\right] + (1-\alpha_t) \, I \\
&= \alpha_t \alpha_{t-1} \mathrm{Var}(\, x_{t-2} \mid x_0 \,) + (1-\alpha_t \alpha_{t-1}) I \\
&= \cdots \\
&= \alpha_t \alpha_{t-1} \ldots \alpha_1 \, \cancelto{0}{\mathrm{Var}(\, x_0 \mid x_0 \,)} + \left(1 - \prod_{i=1}^{t} \alpha_i \right) I \\
&= \left(1 - \textstyle\prod_{i=1}^{t} \alpha_i \right) I = (1 - \overline{\alpha_t}) I
\end{aligned}
$$

The Forward Process of Diffusion Model

To summarize:

$$x_t = \sqrt{\overline{\alpha_t}} x_0 + \sqrt{1 - \overline{\alpha_t}}\, \epsilon, \epsilon \sim \mathcal{N}(\epsilon; 0, I)$$

That is: $x_0 = \frac{x_t - \sqrt{1-\overline{\alpha_t}}\epsilon_0}{\sqrt{\overline{\alpha_t}}}$

The forward diffusion process can be seen as a paradigm where x_t is a linear Gaussian transformation of x_0 with scheduled randomness from a standard normal distribution.

We will use this for the reparameterization trick later.

ELBO for Diffusion Model: Score Matching Term

$$\bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i$$

- To compute the third term, we need

$$q(x_t \mid x_{t-1}) = \mathcal{N}(x_t; \sqrt{\alpha_t} x_{t-1}, (1-\alpha_t) I)$$
$$q(x_t \mid x_0) = \mathcal{N}\left(x_t; \sqrt{\bar{\alpha}_t} x_0, (1-\bar{\alpha}_t) I\right)$$

$$q(x_{t-1} \mid x_t, x_0) = \frac{q(x_t \mid x_{t-1}, x_0)\, q(x_{t-1} \mid x_0)}{q(x_t \mid x_0)}$$
$$= \frac{\mathcal{N}\left(x_t; \sqrt{\alpha_t} x_{t-1}, (1-\alpha_t) I\right) \mathcal{N}\left(x_{t-1}; \sqrt{\bar{\alpha}_{t-1}} x_0, (1-\bar{\alpha}_{t-1}) I\right)}{\mathcal{N}\left(x_t; \sqrt{\bar{\alpha}_t} x_0, (1-\bar{\alpha}_t) I\right)}$$

Applying the product rule for normal distributions, we get

$$\mathcal{N}(x; \mu_1, \Sigma_1)\, \mathcal{N}(x; \mu_2, \Sigma_2) \propto \mathcal{N}(x; \bar{\mu}, \bar{\Sigma})$$
$$\bar{\mu} = \bar{\Sigma}\, (\Sigma_1^{-1}\mu_1 + \Sigma_2^{-1}\mu_2), \bar{\Sigma} = (\Sigma_1^{-1} + \Sigma_2^{-1})^{-1}$$

$$\Sigma_q(t) = \left(\frac{1}{1-\alpha_t} I + \frac{1}{1-\bar{\alpha}_{t-1}} I\right)^{-1} = \frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t} I$$

$$\mu_q(x_t, x_0) = \Sigma_q \left(\frac{1}{1-\alpha_t} \sqrt{\alpha_t} x_{t-1} + \frac{1}{1-\bar{\alpha}_{t-1}} \sqrt{\bar{\alpha}_{t-1}} x_0\right) = \frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t} \left(\frac{1}{1-\alpha_t} \sqrt{\alpha_t} x_{t-1} + \frac{1}{1-\bar{\alpha}_{t-1}} \sqrt{\bar{\alpha}_{t-1}} x_0\right) =$$
$$\frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1}) x_t + \bar{\alpha}_{t-1}(1-\alpha_t) x_0}{1-\bar{\alpha}_t}$$

Thus, it holds

$$q(x_{t-1} \mid x_t, x_0) \propto \mathcal{N}(x_{t-1}; \mu_q, \Sigma_q)$$

ELBO for Diffusion Model: Matching the Mean

$$\Sigma_q(t) \to \sigma_q^2(t) = \frac{(1-\alpha_t)(1-\overline{\alpha_{t-1}})}{1-\overline{\alpha_t}}$$

- Recall KL divergence for Gaussians

$$D_{\mathrm{KL}}\left(\mathcal{N}(x;\mu_x,\Sigma_x)\,||\,\mathcal{N}(y;\mu_y,\Sigma_y)\right) = \frac{1}{2}\left[\cancel{log\frac{|\Sigma_y|}{|\Sigma_x|}} - \mathrm{d} + \cancel{\mathrm{tr}(\Sigma_y^{-1}\Sigma_x)} + (\mu_y-\mu_x)^{\mathrm{T}}\Sigma_y^{-1}(\mu_y-\mu_x)\right]$$

- Choose variance of p to match exactly variance of q

$$D_{\mathrm{KL}}(q(x_{t-1} \mid x_t, x_0)\,||\,p_\theta(x_{t-1} \mid x_t))$$
$$= D_{\mathrm{KL}}\left(\mathcal{N}\left(x_{t-1};\mu_q,\Sigma_q(t)\right)||\,\mathcal{N}\left(x_{t-1};\mu_\theta,\Sigma_q(t)\right)\right)$$
$$= \frac{1}{2\sigma_q^2(t)}\left[||\,\mu_\theta - \mu_q\,||_2^2\right]$$

- Choose mean of p to match form of mean of q

$$\mu_\theta(x_t,t) = \frac{\sqrt{\alpha_t}(1-\overline{\alpha_{t-1}})x_t + \sqrt{\overline{\alpha_{t-1}}}(1-\alpha_t)\widehat{x_\theta}(x_t,t)}{1-\overline{\alpha_t}},$$
$$\mu_q(x_t,x_0) = \frac{\sqrt{\alpha_t}(1-\overline{\alpha_{t-1}})x_t + \sqrt{\overline{\alpha_{t-1}}}(1-\alpha_t)x_0}{1-\overline{\alpha_t}}$$

$$D_{\mathrm{KL}}(q(x_{t-1} \mid x_t, x_0)\,||\,p_\theta(x_{t-1} \mid x_t)) = \frac{1}{2\sigma_q^2(t)}\frac{\overline{\alpha_{t-1}}(1-\alpha_t)^2}{(1-\overline{\alpha_t})^2}\left[||\widehat{x_\theta}(x_t,t) - x_0||_2^2\right]$$

Reparameterization as an Alternative Form for ELBO

- Plugging our previous finding $x_0 = \frac{x_t - \sqrt{1-\bar{\alpha}_t}\epsilon_0}{\sqrt{\bar{\alpha}_t}}$ into the denoising transition mean $\mu_q(x_t, x_0)$, we have:

$$\mu_q(x_t, x_0) = \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})x_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)x_0}{1-\bar{\alpha}_t}$$

$$= \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})x_t + \sqrt{\bar{\alpha}_{t-1}}(1-\alpha_t)\frac{x_t - \sqrt{1-\bar{\alpha}_t}\epsilon_0}{\sqrt{\bar{\alpha}_t}}}{1-\bar{\alpha}_t}$$

$$= \frac{1-\bar{\alpha}_t}{(1-\bar{\alpha}_t)\sqrt{\alpha_t}}x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}\sqrt{\alpha_t}}\epsilon_0$$

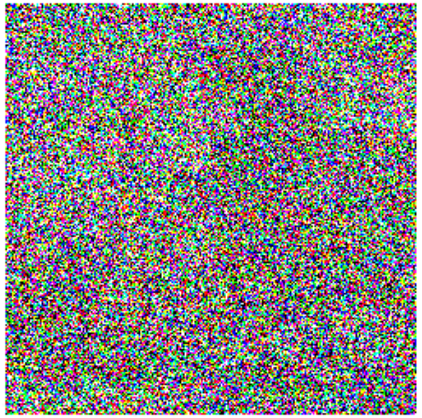
$$= \frac{1}{\sqrt{\alpha_t}}x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}\sqrt{\alpha_t}}\epsilon_0$$

- This inspires us to approximate the denoising transition mean as choosing the mean of p to match q: $\mu_\theta(x_t, t) = \frac{1}{\sqrt{\alpha_t}}x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}\sqrt{\alpha_t}}\hat{\epsilon}_\theta(x_t, t)$

Progressive Denoising or Direct Reconstruction?

- The model predicts the noise to be removed in each step (i.e., denoising) by optimizing score matching term. This reduces to minimizing the difference between the predicted noise and the ground-truth schedule noise:

$$
\begin{aligned}
&\underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, D_{\mathrm{KL}}\left(q(x_{t-1} \mid x_t, x_0) \parallel p_\theta(x_{t-1} \mid x_t)\right) \\
&= \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, D_{\mathrm{KL}}\left(\mathcal{N}\left(x_{t-1}; \mu_q, \Sigma_q(t)\right) \parallel \mathcal{N}\left(x_{t-1}; \mu_\theta, \Sigma_q(t)\right)\right) \\
&= \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, \frac{1}{2\sigma_q^2(t)} \left[\left\| \frac{1}{\sqrt{\alpha_t}} x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}\sqrt{\alpha_t}} \hat{\epsilon}_\theta(x_t, t) - \frac{1}{\sqrt{\alpha_t}} x_t + \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}\sqrt{\alpha_t}} \epsilon_0 \right\|_2^2\right] \\
&= \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, \frac{1}{2\sigma_q^2(t)} \frac{(1-\alpha_t)^2}{(1-\bar{\alpha}_t)\alpha_t} \left[\left\| \epsilon_0 - \hat{\epsilon}_\theta(x_t, t) \right\|_2^2\right]
\end{aligned}
$$



- Predicting x_0 from a highly noisy x_t in one step is complex because the signal is buried under significant noise, especially at large t.
- By predicting the noise at each step, the model progressively refines x_t towards x_0, which makes the learning task more manageable (e.g., converges better or requires smaller network capacity).

Training and Sampling from Diffusion Model

- [Ho et al., 2020] (DDPM) chooses to build the training procedure by performing SGD on the set of training images over timesteps.
- The sampling procedure iteratively executes the denoising process from a Gaussian initialization x_T.

Algorithm 1 Training

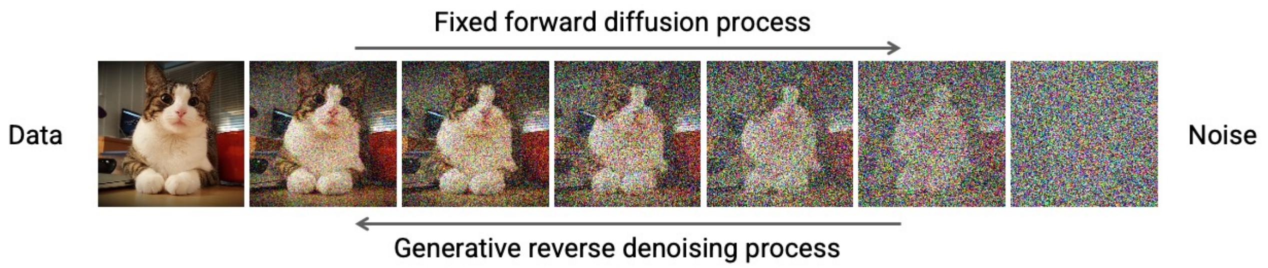
1: **repeat**
2: $\quad \mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $\quad t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
4: $\quad \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
5: $\quad$ Take gradient descent step on

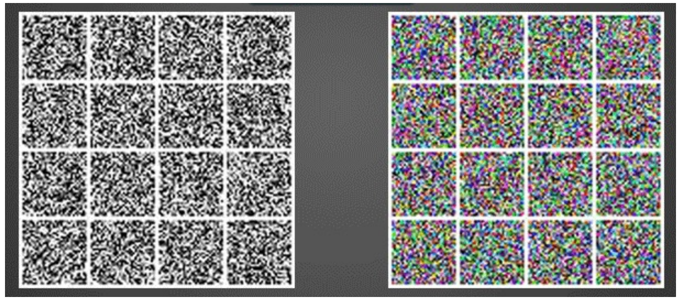
$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta\left(\underbrace{\boxed{\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}}}_{\sqrt{\alpha_t}\, x_t}, t\right) \right\|^2$$

6: **until** converged

Algorithm 2 Sampling

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \ldots, 1$ **do**
3: $\quad \mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
4: $\quad \mathbf{x}_{t-1} = \underbrace{\boxed{\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right)}}_{\mu_\theta(x_t, t)} + \sigma_t \mathbf{z}$
5: **end for**
6: **return** $\mathbf{x}_0$

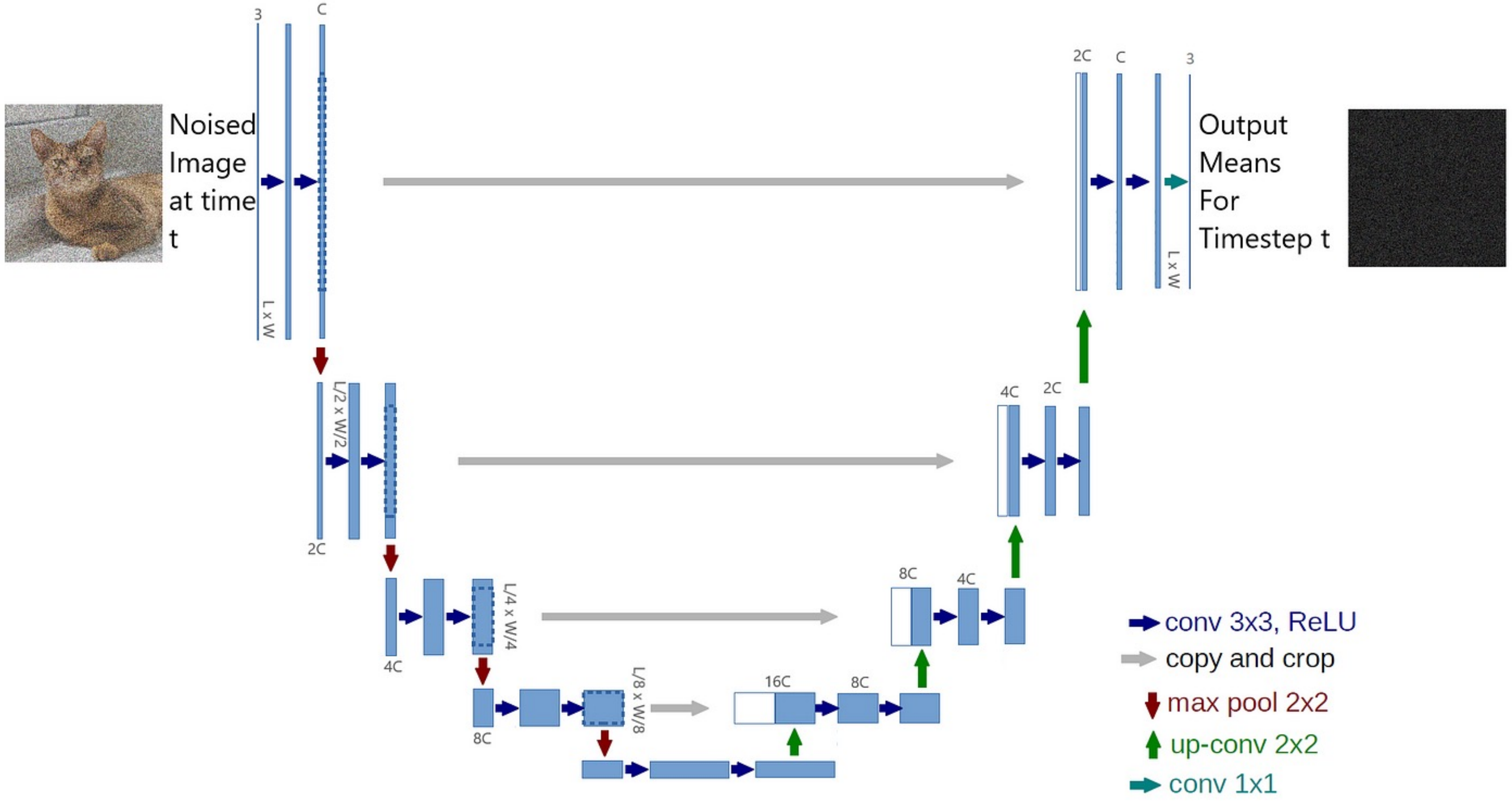




Implementation (DDPM)

DDPM uses U-Net with residual connection and self-attention layers to represent $\epsilon_\theta(x_t, t)$.

The time representation is conditioned in the U-Net as sinusoidal positional embeddings or Fourier features.



Implementation (DDPM)

Scheduler for beta (β_t) indicates a predefined sequence of noise variances for each timestep t.

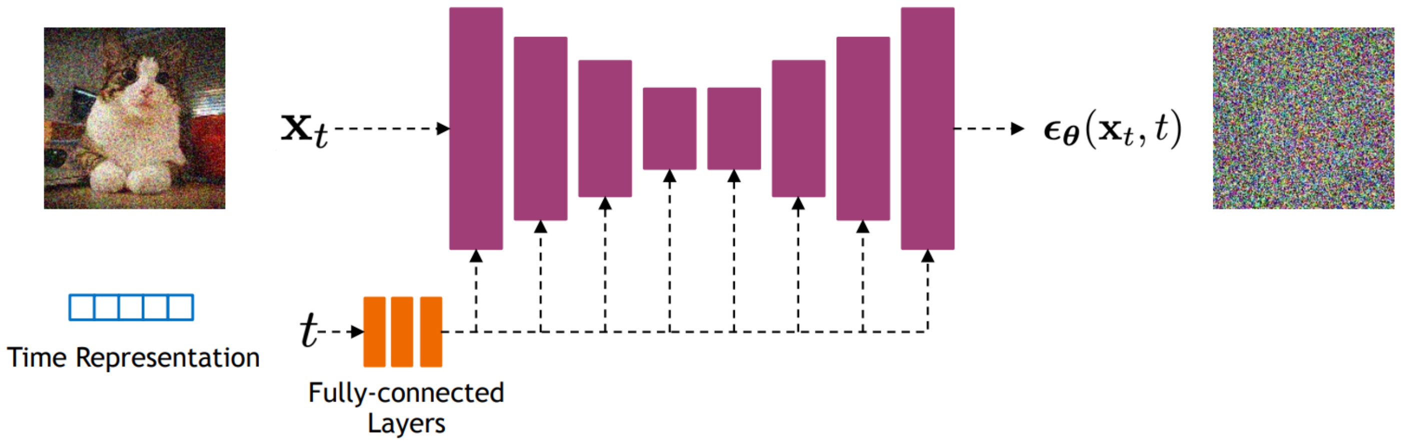
- Linear Schedule: β_t increases linearly from a small initial value to a maximum value.
- Cosine Schedule: Uses a cosine function to define β_t for smoother transitions.

Alpha Terms (α_t and $\bar{\alpha}_t$) are then derived from the beta terms:

- $\alpha_t = 1 - \beta_t$
- $\bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$

Creating Training Data as the forward diffusion (noising) process is simulated by adding Gaussian noise to images according to the noise schedule. For each training image x_0 and timestep t, we generate a noisy image x_t using the closed-form equation:

$$x_t = \sqrt{\overline{\alpha_t}} x_0 + \sqrt{1 - \overline{\alpha_t}}\, \epsilon, \epsilon \sim \mathcal{N}(\epsilon; 0, I)$$



Implementation

- Samples of DDPM