Deep Generative Models: Diffusion Models

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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

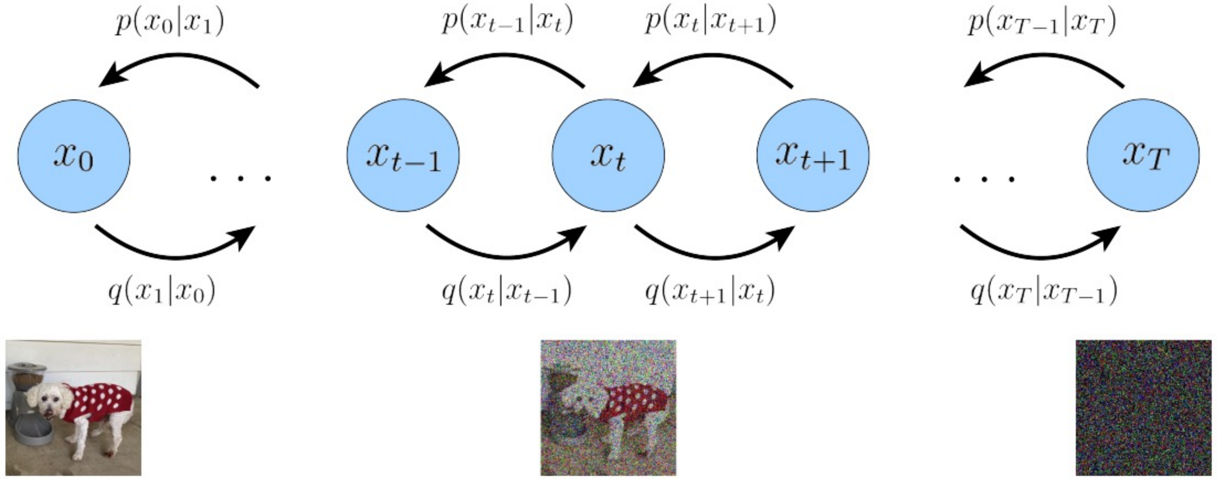
Diffusion Model as MHVAEs with Gaussian Latents

- **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

- Consider the formulation of a single noising step:

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

- Note $x_1 \mid x_0$ and $x_t \mid x_{t-1}$ are Gaussian, hence $x_t \mid x_0 \sim \mathcal{N}(x_t; \mu_q(x_0), \Sigma_q(x_0))$.

- We can compute $\mu_q(x_0) = \mathbb{E}[\, x_t \mid x_0 \,]$, recursively as follows:

$$\begin{aligned}
\mathbb{E}[\, x_t \mid x_0 \,] &= \mathbb{E}\Big[\sqrt{\alpha_t} x_{t-1} + \sqrt{1-\alpha_t}\epsilon_t \mid x_0 \Big] \\
&= \sqrt{\alpha_t}\, \mathbb{E}[\, x_{t-1} \mid x_0 \,] + \sqrt{1-\alpha_t}\underbrace{\mathbb{E}[\epsilon_t]}_{0} \\
&= \sqrt{\alpha_t} \mathbb{E}[\, x_{t-1} \mid x_0 \,] \\
&= \sqrt{\alpha_t}\sqrt{\alpha_{t-1}}\, \mathbb{E}[\, x_{t-2} \mid x_0 \,] \\
&= \sqrt{\alpha_t}\sqrt{\alpha_{t-1}} \cdots \sqrt{\alpha_1}\, x_0 \\
&= \sqrt{\bar{\alpha}_t} x_0
\end{aligned}$$

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

The Forward Process of Diffusion Model

- We can compute $\Sigma_q(x_0) = \mathrm{Var}[\,x_t \mid x_0\,]$, recursively as follows:

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

- That is:

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

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

The Forward Process of Diffusion Model

- We have shown that x_t is a linear Gaussian transformation of x_0 with scheduled randomness (controlled by $\overline{\alpha_t}$) drawn from a standard normal distribution, i.e.,

$$x_t \mid x_0 \sim \mathcal{N}\left(x_t; \sqrt{\overline{\alpha_t}} x_0, (1 - \overline{\alpha_t}) I\right)$$

- Therefore, given x_0, we can sample x_t directly without having to generate all x_t's:

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

- Moreover, we can also generate x_0 from x_t as

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

- This suggests we can reverse the noising process. However, exact reversal requires knowing the exact $\overline{\epsilon_t}$. The reverse diffusion process is designed to predict the noise $\overline{\epsilon_t}$ that needs to be added to x_t to generate x_0.

The Reverse Diffusion Process

- We have designed a forward diffusion process $q_\phi(\, x_t \mid x_{t-1} \,)$ that
  - At each step adds Gaussian noise to the input until it becomes pure noise
  - Allows us to sample $x_t \mid x_0$ without having to compute x_t recursively
  - Allows us to sample $x_0 \mid x_t$ without having to compute x_t recursively

- We now need to design a reverse diffusion process $p_\theta(\, x_{t-1} \mid x_t \,)$ that makes the calculation of the ELBO easy. We do this by
  - Understanding the structure of $q_\phi(\, x_t \mid x_{t-1} \,)$
  - Making $p_\theta(\, x_{t-1} \mid x_t \,)$ match that structure

- Recall the ELBO is given by:

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

ELBO for Diffusion Model: Score Matching Term

- To compute the third term, we need

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

$$\propto \exp\left(-\frac{\| x_t - \sqrt{\alpha_t} x_{t-1} \|^2}{2(1-\alpha_t)}\right) \cdot \exp\left(-\frac{\| x_{t-1} - \sqrt{\overline{\alpha_{t-1}}} x_0 \|^2}{2(1-\overline{\alpha_{t-1}})}\right) \propto \exp\left(-\frac{\alpha_t \| x_{t-1} - \frac{x_t}{\sqrt{\alpha_t}} \|^2}{2(1-\alpha_t)}\right) \cdot \exp\left(-\frac{\| x_{t-1} - \sqrt{\overline{\alpha_{t-1}}} x_0 \|^2}{2(1-\overline{\alpha_{t-1}})}\right)$$

- Applying the product rule, we get $q(x_{t-1} \mid x_t, x_0) = \mathcal{N}(x_{t-1}; \mu_q(x_0), \Sigma_q)$, where

$$\Sigma_q := \mathrm{Cov}(x_{t-1} \mid x_t, x_0) = \left(\frac{\alpha_t}{1-\alpha_t} I + \frac{1}{1-\overline{\alpha_{t-1}}} I\right)^{-1} = \frac{(1-\alpha_t)(1-\overline{\alpha_{t-1}})}{1-\overline{\alpha_t}} I$$

$$\mu_q(x_t, x_0) := \mathbb{E}(x_{t-1} \mid x_t, x_0) = \Sigma_q \left(\frac{\alpha_t}{1-\alpha_t} I \frac{x_t}{\sqrt{\alpha_t}} + \frac{1}{1-\overline{\alpha_{t-1}}} I \sqrt{\overline{\alpha_{t-1}}} x_0\right)$$

$$= \frac{(1-\alpha_t)(1-\overline{\alpha_{t-1}})}{1-\overline{\alpha_t}} I \left(\frac{\sqrt{\alpha_t}}{1-\alpha_t} x_t + \frac{\sqrt{\overline{\alpha_{t-1}}}}{1-\overline{\alpha_{t-1}}} x_0\right) = \frac{\sqrt{\alpha_t}(1-\overline{\alpha_{t-1}}) x_t + \overline{\alpha_{t-1}}(1-\alpha_t) x_0}{1-\overline{\alpha_t}}$$

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

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

$$\mu_1 = \frac{x_t}{\sqrt{\alpha_t}}, \Sigma_1 = \frac{1-\alpha_t}{\alpha_t} I,$$
$$\mu_2 = \sqrt{\overline{\alpha_{t-1}}} x_0,\ \Sigma_2 = (1-\overline{\alpha_{t-1}}) I$$

ELBO for Diffusion Model: Decoder Matches Encoder

- Recall KL divergence for Gaussians

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

- Choosing mean of $p_\theta(\,x_{t-1}\mid x_t\,)$ to match form of mean of $q(\,x_{t-1}\mid x_t, x_0\,)$

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

- Choosing variance of $p_\theta(\,x_{t-1}\mid x_t\,)$ to match exactly variance of $q(\,x_{t-1}\mid x_t, x_0\,)$

$$\Sigma_q = \frac{(1-\alpha_t)(1-\overline{\alpha_{t-1}})}{1-\overline{\alpha_t}}I \quad\Rightarrow\quad \Sigma_\theta = \frac{(1-\alpha_t)(1-\overline{\alpha_{t-1}})}{1-\overline{\alpha_t}}I$$

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

- The ELBO reduces to:

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

$$= \frac{1}{2\sigma_q^2(t)}\left[||\,\mu_\theta - \mu_q\,||_2^2\right] = \frac{1}{2\sigma_q^2(t)}\frac{\overline{\alpha_{t-1}}(1-\alpha_t)^2}{(1-\overline{\alpha_t})^2}\left[||\widehat{x_\theta}(x_t,t) - x_0||_2^2\right]$$

Reparameterization as an Alternative Form for ELBO

- Plugging $x_0 = \frac{x_t - \sqrt{1-\bar{\alpha}_t}\,\bar{\epsilon}_t}{\sqrt{\bar{\alpha}_t}}$ into the denoising transition mean $\mu_q(x_t, x_0)$, we obtain:

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

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

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

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

- Choosing the mean and variance of p to match the mean and variance of q:

$$\mu_\theta(x_t, t) = \frac{1}{\sqrt{\alpha_t}}x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}\sqrt{\alpha_t}}\bar{\epsilon}_t, \qquad \Sigma_\theta(t) = \frac{(1-\alpha_t)(1-\overline{\alpha_{t-1}})}{1-\overline{\alpha_t}}I$$

The Reverse Diffusion Process for DDPM

- Finally, putting it all together, the reverse diffusion process is given by:

$$p_\theta(x_{t-1} \mid x_t) \sim \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(t))$$

- Therefore, we generate an image via the reverse diffusion process

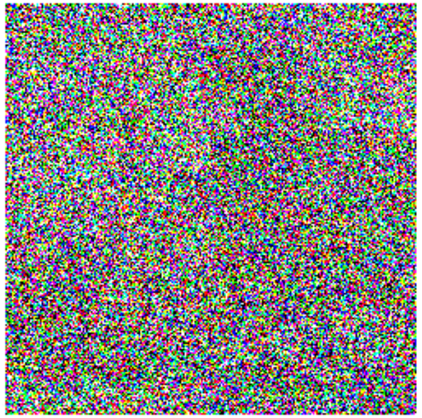
$$x_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\hat{\epsilon}_\theta(x_t, t)\right) + \sqrt{\beta_t}\,\epsilon_t$$

- Where $x_T \sim \mathcal{N}(x_T; 0, I)$, $\epsilon_t \sim \mathcal{N}(\epsilon_t; 0, I)$.

Progressive Denoising or Direct Reconstruction?

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

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



- Predicting x_0 from a highly noisy x_t in one step is complex, as the signal is dominated by significant noise for large t.
- Predicting the noise at each step and refining x_t towards x_0 makes learning more manageable (e.g., it converges faster or it requires a smaller network capacity).