Virtual Humans – Winter 24/25

Lecture 13_1 – Diffusion Models Theory

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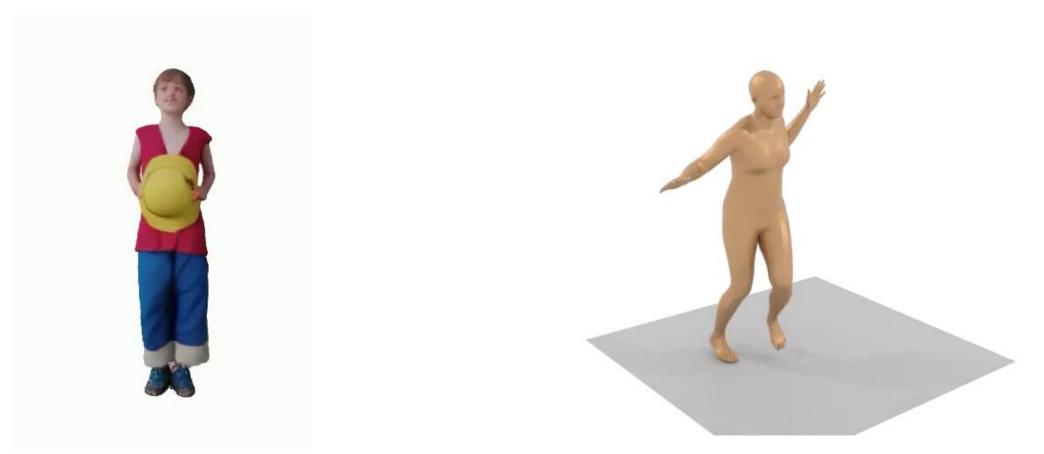
In this lecture...

• Recap of deep generative models

• Introduction of Diffusion Models

• Applications of Diffusion Models

Goal: Generate Virtual Humans



Generate Appearance

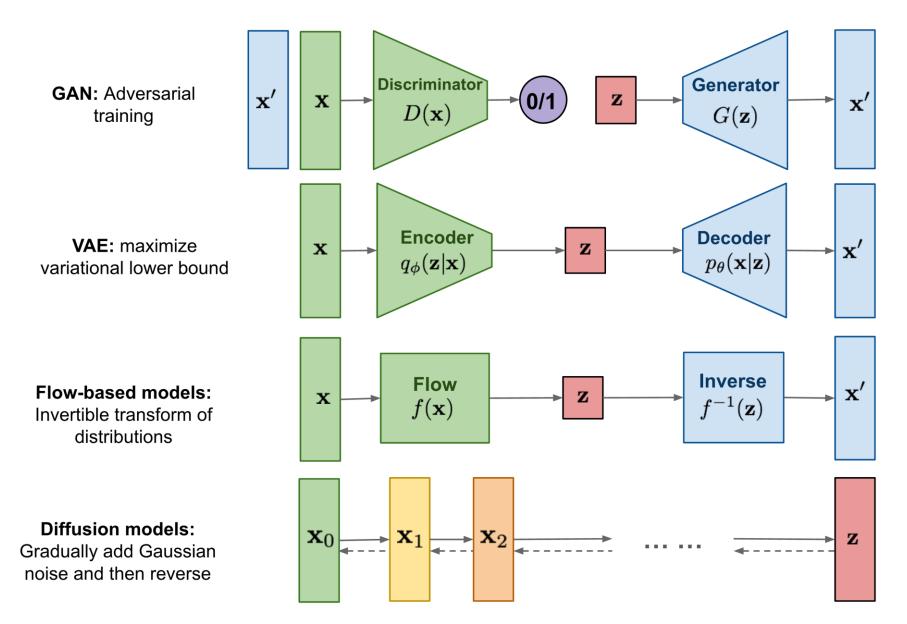
Generate Motion

So far we have seen...

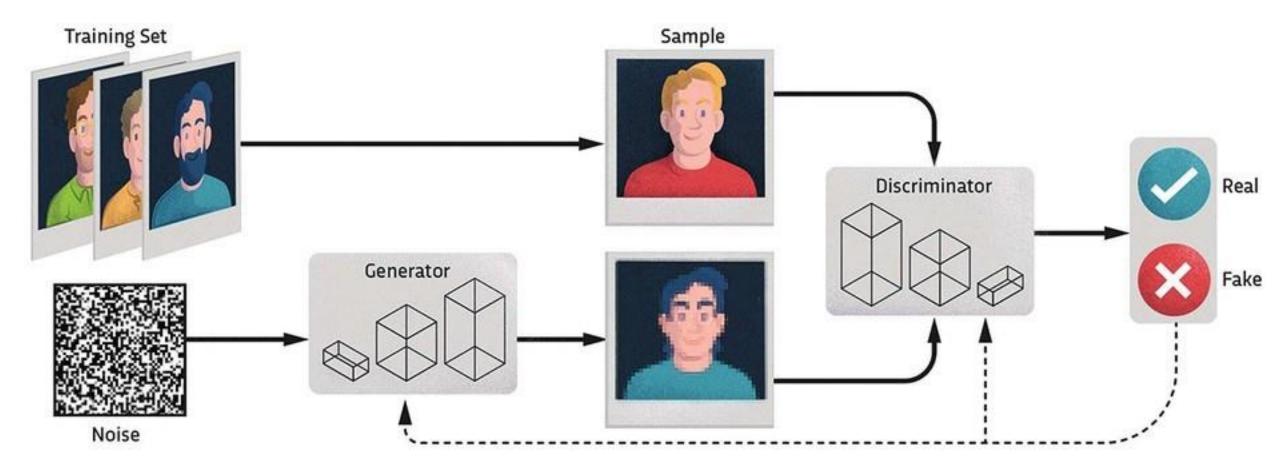
- We can capture human appearance (NeRF, 3DGS)
- We can capture human motion (MoCap, Registration)
- We can capture human-object interaction (Behave, PHOSA, CHORE)

- Can we also generate the appearance and motion of "human"?
- Why is "synthesis" of Virtual Human useful?

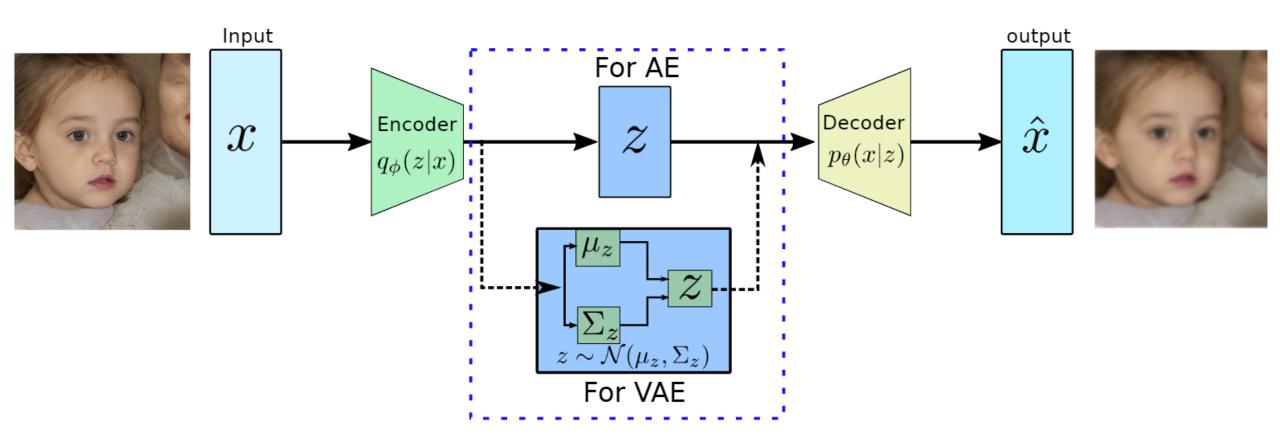
Generative Models



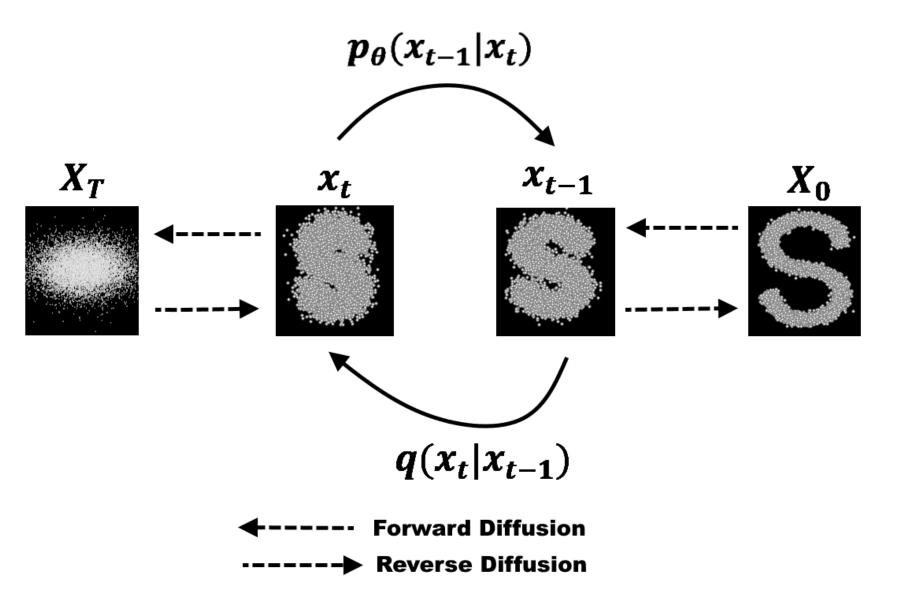
GAN



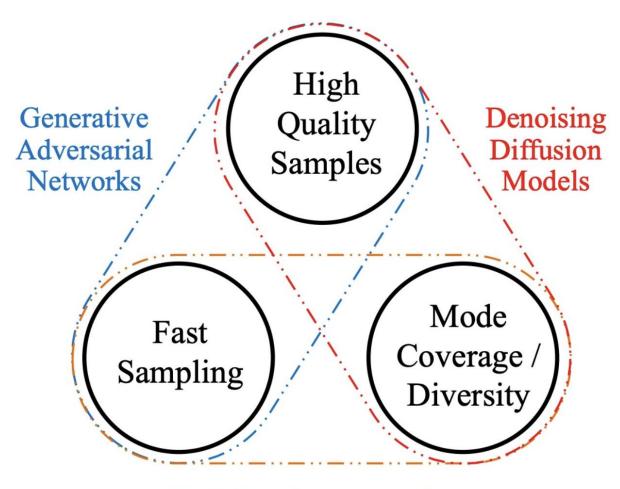
VAE



Diffusion Models



Trilemma: Quality, Diversity Speed



Variational Autoencoders, Normalizing Flows

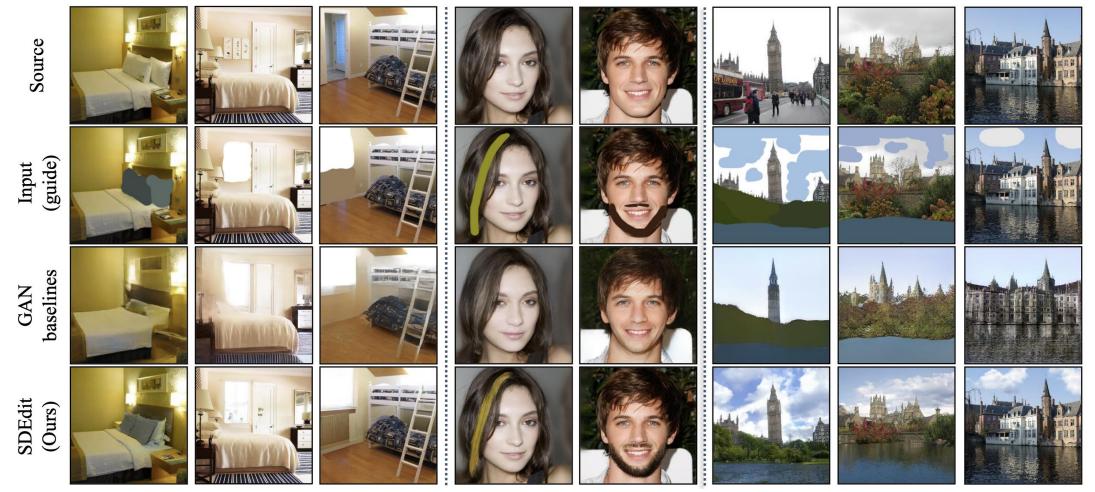
• Diffusion model is SOTA on image generation



- Stable Diffusion
- Mid-Journey
- Flux

• •••

• Diffusion model is useful for image editing



• Diffusion model is useful for image editing



"zebras roaming in the field"

"a girl hugging a corgi on a pedestal"

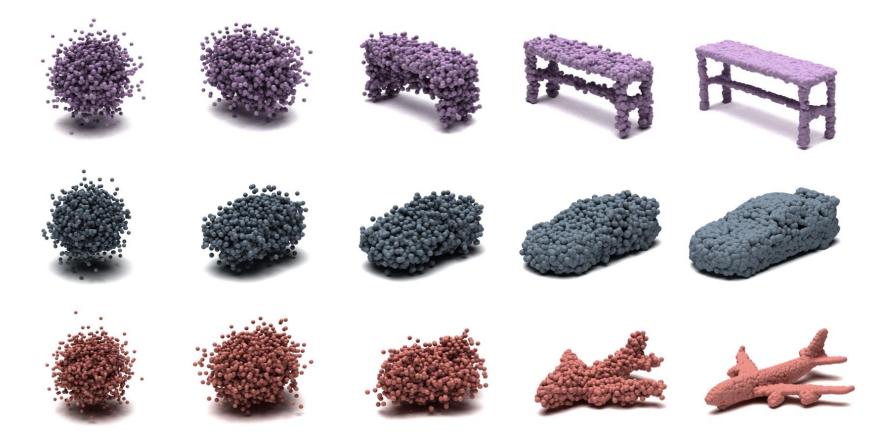




- Diffusion model is applicable for other non-visual domains
 - Generate motion from text

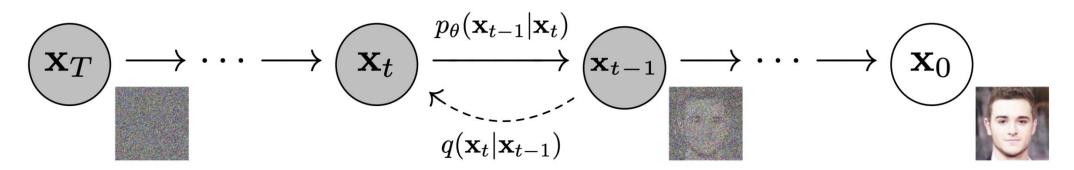


- Diffusion model is applicable for other non-visual domains
 - Generate 3D point cloud



- Diffusion model aims to learn the **reverse** of noise generation procedure
 - Forward step: (Iteratively) Add noise to the original sample
 - \rightarrow The sample x! converges to the complete noise x_T (e.g., $\sim \mathcal{N}(0, I)$)
 - **Reverse step**: Recover the original sample from the noise
 - \rightarrow Note that it is the "generation" procedure

Reverse process



Forward (diffusion) process

- Diffusion model aims to learn the **reverse** of noise generation procedure
 - Forward step: (Iteratively) Add noise to the original sample
 - \rightarrow Technically, it is a product of conditional noise distributions $q(\mathbf{x}_{t} | \mathbf{x}_{t-1})$
 - Usually, the parameters β_t are fixed (one can jointly learn, but not beneficial)
 - • Noise annealing (i.e., reducing noise scale $\beta_t < \beta_{t-1}$) is crucial to the performance

$$q(\mathbf{x}_{1:T}|\mathbf{x}_0) \coloneqq \prod_{t=1}^T q(\mathbf{x}_t|\mathbf{x}_{t-1}), \qquad q(\mathbf{x}_t|\mathbf{x}_{t-1}) \coloneqq \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t \mathbf{I})$$

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- **Reverse step**: Recover the original sample from the noise
 - \rightarrow It is also a product of conditional (de)noise distributions $p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_{t})$
 - Use the learned parameters: denoiser $oldsymbol{\mu}_{ heta}$ (main part) and randomness $oldsymbol{\Sigma}_{ heta}$

$$p_{\theta}(\mathbf{x}_{0:T}) \coloneqq p(\mathbf{x}_{T}) \prod_{t=1}^{T} p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_{t}), \qquad p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_{t}) \coloneqq \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_{\theta}(\mathbf{x}_{t}, t), \boldsymbol{\Sigma}_{\theta}(\mathbf{x}_{t}, t))$$

- Diffusion model aims to learn the **reverse** of noise generation procedure
 - Forward step: (Iteratively) Add noise to the original sample
 - **Reverse step**: Recover the original sample from the noise

$$q(\mathbf{x}_{1:T}|\mathbf{x}_0) \coloneqq \prod_{t=1}^T q(\mathbf{x}_t|\mathbf{x}_{t-1}), \qquad p_{\theta}(\mathbf{x}_{0:T}) \coloneqq p(\mathbf{x}_T) \prod_{t=1}^T p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t),$$

• Training: Minimize variational lower bound of the model $p_{\theta}(\mathbf{x}_0)$

$$\mathbb{E}\left[-\log p_{\theta}(\mathbf{x}_{0})\right] \leq \mathbb{E}_{q}\left[-\log \frac{p_{\theta}(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_{0})}\right]$$

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• \rightarrow It can be decomposed to the step-wise losses (for each step t)

$$\mathbb{E}_{q}\left[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{T}|\mathbf{x}_{0}) \parallel p(\mathbf{x}_{T}))}_{L_{T}} + \sum_{t>1}\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_{t},\mathbf{x}_{0}) \parallel p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_{t}))}_{L_{t-1}} \underbrace{-\log p_{\theta}(\mathbf{x}_{0}|\mathbf{x}_{1})}_{L_{0}}\right]$$

- Diffusion model aims to learn the **reverse** of noise generation procedure
 - Training: Minimize variational lower bound of the model $p_{\theta}(\mathbf{x}_0)$
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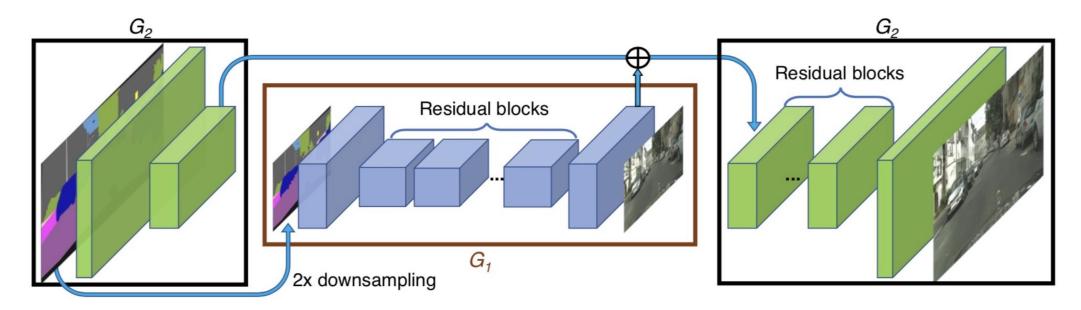
$$\mathbb{E}_{q}\left[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{T}|\mathbf{x}_{0}) \parallel p(\mathbf{x}_{T}))}_{L_{T}} + \sum_{t>1}\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_{t},\mathbf{x}_{0}) \parallel p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_{t}))}_{L_{t-1}} \underbrace{-\log p_{\theta}(\mathbf{x}_{0}|\mathbf{x}_{1})}_{L_{0}}\right]$$

- Here, the true reverse step $q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0)$ can be computed as a closed form of β_t
- Note that we only define the true forward step $q(\mathbf{x}_{t} | \mathbf{x}_{t-1})$

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}; \tilde{\mu_t}(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t^3 \mathbf{I})$$

where
$$ilde{oldsymbol{\mu}}_t(\mathbf{x}_t,\mathbf{x}_0):= ilde{eta}_t^1\mathbf{x}_0+ ilde{eta}_t^2\mathbf{x}_t$$

- Diffusion model aims to learn the **reverse** of noise generation procedure
 - Network: Use the image-to-image translation (e.g., U-Net) architectures
 - Recall that input is **x**t and output is **x**t-1, both are images
 - • It is expensive since both input and output are high-dimensional
 - • Note that the denoiser $\mu_{\theta}(\mathbf{x}_{t}, t)$ conditioned by step t



- Diffusion model aims to learn the **reverse** of noise generation procedure
 - Sampling: Draw a random noise x_T then apply the reverse step $p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_t)$
 - It often requires the 1000 reverse steps (very slow)



- Diffusion model aims to learn the **reverse** of noise generation procedure
 - Sampling: Draw a random noise x_{T} then apply the reverse step $p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_{t})$
 - Early and late steps change the high- and low-level attributes, respectively



Share x₁₀₀₀

Share x750

Share x₅₀₀

Share x₂₅₀

Share x₀

Denoising Diffusion Probabilistic Models

- DDPM reparametrizes the reverse distributions of diffusion models
 - Key idea: The original reverse step fully creates the denoiser $\mu_{\theta}(\mathbf{x}_{t}, t)$
 - However, $\boldsymbol{x}_{t\text{-}1}$ and \boldsymbol{x}_{t} share most information, and thus it is redundant
 - \rightarrow Instead, create the **residual** $\epsilon_{\theta}(\mathbf{x}_{t}, t)$ and add to the original \mathbf{x}_{t}
 - Formally, DDPM reparametrizes the learned reverse distribution as

$$\boldsymbol{\mu}_{\theta}(\mathbf{x}_{t}, t) = \frac{1}{\sqrt{\alpha_{t}}} \left(\mathbf{x}_{t} - \frac{\beta_{t}}{\sqrt{1 - \bar{\alpha}_{t}}} \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, t) \right)$$

• and the step-wise objective L_{t-1} can be reformulated as

$$\mathbb{E}_{t,\mathbf{x}_{0},\boldsymbol{\epsilon}}\left[\left\|\boldsymbol{\epsilon}-\boldsymbol{\epsilon}_{\theta}(\sqrt{\bar{\alpha}_{t}}\mathbf{x}_{0}+\sqrt{1-\bar{\alpha}_{t}}\boldsymbol{\epsilon},t)\right\|^{2}\right]$$

- DDIM roughly sketches the final sample, then refine it with the reverse process
 - Motivation:
 - Diffusion model is slow due to the iterative procedure
 - GAN/VAE creates the sample by one-shot forward operation
 - ⇒ Can we combine the advantages for **fast sampling** of diffusion models?

• Technical spoiler:

- Instead of naïvely applying diffusion model upon GAN/VAE,
- DDIM proposes a principled approach of rough sketch + refinement

- DDIM roughly sketches the final sample, then refine it with the reverse process
 - Key Idea:
 - Given \mathbf{x}_{t} , generate the rough sketch \mathbf{x}_{0} and refine $p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_{t})$
 - Unlike original diffusion model, it is not a Markovian structure



Original Diffusion

Non-Markovian

- DDIM roughly sketches the final sample, then refine it with the reverse process
 - Key Idea: Given \mathbf{x}_{t} , generate the rough sketch \mathbf{x}_{0} and refine $p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_{t})$



• Formulation: Define the forward distribution $q(\mathbf{x}_{t-1}|\mathbf{x}_{t}, \mathbf{x}_{0})$ as

$$q_{\sigma}(\boldsymbol{x}_{t-1}|\boldsymbol{x}_{t},\boldsymbol{x}_{0}) = \mathcal{N}\left(\sqrt{\alpha_{t-1}}\boldsymbol{x}_{0} + \sqrt{1 - \alpha_{t-1} - \sigma_{t}^{2}} \cdot \frac{\boldsymbol{x}_{t} - \sqrt{\alpha_{t}}\boldsymbol{x}_{0}}{\sqrt{1 - \alpha_{t}}}, \sigma_{t}^{2}\boldsymbol{I}\right)$$

then, the forward process is derived from Bayes' rule

$$q_{\sigma}(m{x}_t | m{x}_{t-1}, m{x}_0) = rac{q_{\sigma}(m{x}_{t-1} | m{x}_t, m{x}_0) q_{\sigma}(m{x}_t | m{x}_0)}{q_{\sigma}(m{x}_{t-1} | m{x}_0)}$$

- DDIM roughly sketches the final sample, then refine it with the reverse process
 - Key Idea: Given \mathbf{x}_{t} , generate the rough sketch \mathbf{x}_{0} and refine $p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_{t})$



• Formulation: Forward process is
$$q_{\sigma}(\boldsymbol{x}_t | \boldsymbol{x}_{t-1}, \boldsymbol{x}_0) = rac{q_{\sigma}(\boldsymbol{x}_{t-1} | \boldsymbol{x}_t, \boldsymbol{x}_0) q_{\sigma}(\boldsymbol{x}_t | \boldsymbol{x}_0)}{q_{\sigma}(\boldsymbol{x}_{t-1} | \boldsymbol{x}_0)}$$

and reverse process is

$$\boldsymbol{x}_{t-1} = \sqrt{\alpha_{t-1}} \underbrace{\left(\frac{\boldsymbol{x}_t - \sqrt{1 - \alpha_t} \epsilon_{\theta}^{(t)}(\boldsymbol{x}_t)}{\sqrt{\alpha_t}} \right)}_{\text{"predicted } \boldsymbol{x}_0\text{"}} + \underbrace{\sqrt{1 - \alpha_{t-1} - \sigma_t^2} \cdot \epsilon_{\theta}^{(t)}(\boldsymbol{x}_t)}_{\text{"direction pointing to } \boldsymbol{x}_t\text{"}} + \underbrace{\sigma_t \epsilon_t}_{\text{random noise}}$$

- DDIM significantly reduces the sampling steps of diffusion model
 - Creates the outline of the sample after only 100 steps (DDPM needs thousands)



Takeaways

- New golden era of generative models
- Competition of various approaches: GAN, VAE, flow, diffusion model
- Diffusion model seems to be a nice option for high-quality generation