

# Deep Generative Models

## Lecture 7

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## Recap of Previous Lecture

### Frechet Inception Distance (FID)

For normal distributions  $p_{\text{data}}(\mathbf{x}_1) = \mathcal{N}(\boldsymbol{\mu}_{\text{data}}, \boldsymbol{\Sigma}_{\text{data}})$ ,  
 $p(\mathbf{x}_2) = \mathcal{N}(\boldsymbol{\mu}_{\theta}, \boldsymbol{\Sigma}_{\theta})$ :

$$\begin{aligned}\text{FID}(p_{\text{data}}, p_{\theta}) &= W_2^2(p_{\text{data}}, p_{\theta}) = \inf_{\gamma \in \Gamma(p_{\text{data}}, p_{\theta})} \mathbb{E}_{(\mathbf{x}_1, \mathbf{x}_2) \sim \gamma} \|\mathbf{x}_1 - \mathbf{x}_2\|^2 \\ &= \|\boldsymbol{\mu}_{\text{data}} - \boldsymbol{\mu}_{\theta}\|^2 + \text{tr} \left[ \boldsymbol{\Sigma}_{\text{data}} + \boldsymbol{\Sigma}_{\theta} - 2 \left( \boldsymbol{\Sigma}_{\text{data}}^{1/2} \boldsymbol{\Sigma}_{\theta} \boldsymbol{\Sigma}_{\text{data}}^{1/2} \right)^{1/2} \right]\end{aligned}$$

- ▶ Requires a large sample size for evaluation
- ▶ FID computation is relatively slow
- ▶ Results are highly dependent on the chosen pretrained classifier
- ▶ Relies on the normality assumption

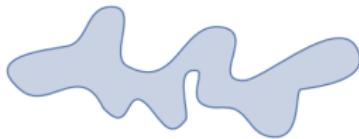
## Recap of Previous Lecture

- ▶  $\mathcal{S}_{\text{data}} = \{\mathbf{x}_i\}_{i=1}^n \sim p_{\text{data}}(\mathbf{x})$ : real samples
- ▶  $\mathcal{S}_{\theta} = \{\mathbf{x}_i\}_{i=1}^n \sim p_{\theta}(\mathbf{x})$ : generated samples

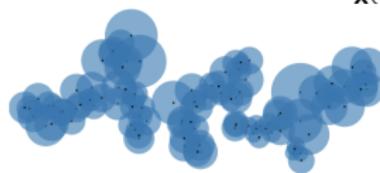
Define a binary indicator function:

$$\mathbb{I}(\mathbf{x}, \mathcal{S}) = \begin{cases} 1, & \text{if } \exists \mathbf{x}' \in \mathcal{S} : \|\mathbf{x} - \mathbf{x}'\|_2 \leq \|\mathbf{x}' - \text{NN}_k(\mathbf{x}', \mathcal{S})\|_2; \\ 0, & \text{otherwise} \end{cases}$$

$$\Pr(\mathcal{S}_{\text{data}}, \mathcal{S}_{\theta}) = \frac{1}{n} \sum_{\mathbf{x} \in \mathcal{S}_{\theta}} \mathbb{I}(\mathbf{x}, \mathcal{S}_{\text{data}}); \quad \text{Rec}(\mathcal{S}_{\text{data}}, \mathcal{S}_{\theta}) = \frac{1}{n} \sum_{\mathbf{x} \in \mathcal{S}_{\text{data}}} \mathbb{I}(\mathbf{x}, \mathcal{S}_{\theta}).$$



(a) True manifold



(b) Approx. manifold

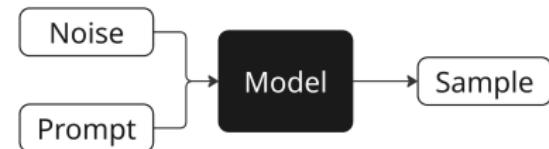
The samples are embedded using a pretrained network, as in FID evaluation.

# Recap of Previous Lecture

## Unconditional Model

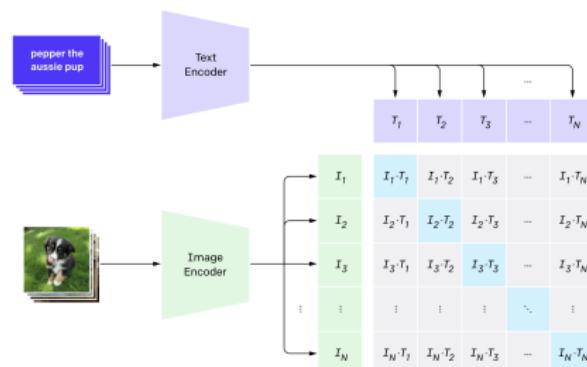


## Conditional Model



We require metrics that evaluate not only the quality of generated images, but also their relevance to the prompt.

## CLIP Score



# Recap of Previous Lecture

- ▶ No perfect automatic evaluation metric exists
- ▶ The most reliable assessment is via human evaluation
- ▶ It's important to evaluate a variety of model aspects

## Human Evaluation

Аспект	Yandex ART 2.0	Mj 6.1	Mj 6	Ideogram	Recraft	Google Imagen3	Dall-E 3	FLUX	SBER Kandi3.1
Релевантность	<b>0,59</b>	<b>0,58</b>	<b>0,63</b>	<b>0,45</b>	<b>0,51</b>	<b>0,50</b>	<b>0,50</b>	<b>0,54</b>	<b>0,75</b>
Эстетика	<b>0,49</b>	<b>0,55</b>	<b>0,55</b>	<b>0,51</b>	<b>0,51</b>	<b>0,61</b>	<b>0,61</b>	<b>0,54</b>	<b>0,59</b>
Комплексность	<b>0,44</b>	<b>0,73</b>	<b>0,70</b>	<b>0,68</b>	<b>0,76</b>	<b>0,75</b>	<b>0,75</b>	<b>0,71</b>	<b>0,74</b>
Дефектность	<b>0,69</b>	<b>0,57</b>	<b>0,68</b>	<b>0,55</b>	<b>0,59</b>	<b>0,63</b>	<b>0,63</b>	<b>0,50</b>	<b>0,75</b>
Предпочтение	<b>0,66</b>	<b>0,60</b>	<b>0,69</b>	<b>0,49</b>	<b>0,54</b>	<b>0,63</b>	<b>0,63</b>	<b>0,51</b>	<b>0,84</b>

# Recap of Previous Lecture

## Langevin Dynamics

Let  $\mathbf{x}_0$  be a random vector. Under mild regularity conditions, samples from the following dynamics will eventually follow  $p_\theta(\mathbf{x})$  (for sufficiently small  $\eta$  and large  $I$ ):

$$\mathbf{x}_{I+1} = \mathbf{x}_I + \frac{\eta}{2} \cdot \nabla_{\mathbf{x}_I} \log p_\theta(\mathbf{x}_I) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}_I, \quad \boldsymbol{\epsilon}_I \sim \mathcal{N}(0, \mathbf{I}).$$

- ▶ The density  $p_\theta(\mathbf{x})$  is the **stationary** distribution of the Markov chain.
- ▶ The gradient is taken with respect to  $\mathbf{x}$ , not  $\theta$ .
- ▶  $\nabla_{\mathbf{x}} \log p_\theta(\mathbf{x})$  defines a vector field.

## Fisher Divergence

$$D_F(p_{\text{data}}, p_\theta) = \frac{1}{2} \mathbb{E}_\pi \| \nabla_{\mathbf{x}} \log p_\theta(\mathbf{x}) - \nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) \|_2^2 \rightarrow \min_{\theta}$$

# Recap of Previous Lecture

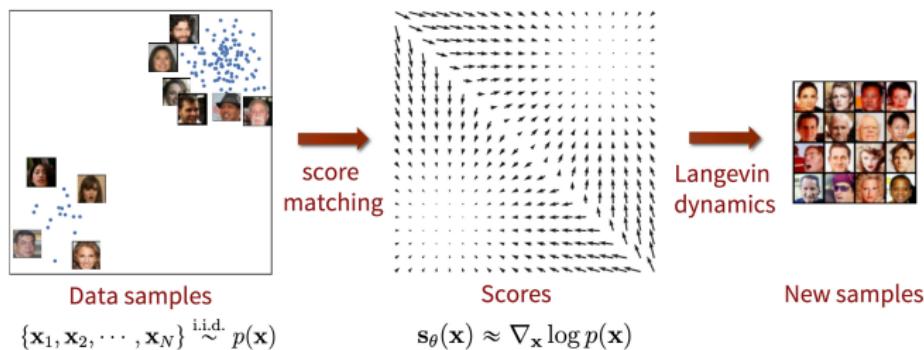
Define **score function**  $\mathbf{s}_\theta(\mathbf{x}) = \nabla_{\mathbf{x}} \log p_\theta(\mathbf{x})$ .

## Training (Score matching)

$$D_F(p_{\text{data}}, p_\theta) = \frac{1}{2} \mathbb{E}_\pi \| \mathbf{s}_\theta(\mathbf{x}) - \nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) \|_2^2 \rightarrow \min_{\theta}$$

## Sampling (Langevin Dynamics)

$$\mathbf{x}_{I+1} = \mathbf{x}_I + \frac{\eta}{2} \cdot \mathbf{s}_\theta(\mathbf{x}) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}_I, \quad \boldsymbol{\epsilon}_I \sim \mathcal{N}(0, \mathbf{I})$$



## Recap of Previous Lecture

Let us perturb the original data with Gaussian noise  
 $q(\mathbf{x}_\sigma | \mathbf{x}) = \mathcal{N}(\mathbf{x}, \sigma^2 \cdot \mathbf{I})$ .

$$q(\mathbf{x}_\sigma) = \int q(\mathbf{x}_\sigma | \mathbf{x}) p_{\text{data}}(\mathbf{x}) d\mathbf{x}.$$

Then the solution of

$$\frac{1}{2} \mathbb{E}_{q(\mathbf{x}_\sigma)} \| \mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma) \|_2^2 \rightarrow \min_{\theta}$$

satisfies  $\mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma) \approx \mathbf{s}_{\theta, 0}(\mathbf{x}_0) = \mathbf{s}_\theta(\mathbf{x})$  if  $\sigma$  is sufficiently small.

**Theorem (Denoising Score Matching)**

$$\begin{aligned} & \mathbb{E}_{q(\mathbf{x}_\sigma)} \| \mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma) \|_2^2 = \\ &= \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma | \mathbf{x})} \| \mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma | \mathbf{x}) \|_2^2 + \text{const}(\theta) \end{aligned}$$

Here,  $\nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma | \mathbf{x}) = -\frac{\mathbf{x}_\sigma - \mathbf{x}}{\sigma^2} = -\frac{\epsilon}{\sigma}$ .  $\mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma)$  attempts to **denoise** a corrupted sample.

# Outline

## 1. Score Matching

Denoising Score Matching (continued)

Noise-Conditioned Score Network

## 2. Forward Gaussian Diffusion Process

## 3. Denoising Score Matching for Diffusion

## 4. Reverse Gaussian Diffusion Process

# Outline

## 1. Score Matching

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## 3. Denoising Score Matching for Diffusion

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# Denoising Score Matching

## Theorem

$$\begin{aligned} & \mathbb{E}_{q(\mathbf{x}_\sigma)} \underbrace{\|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2}_{h(\mathbf{x}_\sigma)} = \\ &= \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})\|_2^2 + \text{const}(\theta) \end{aligned}$$

# Denoising Score Matching

## Theorem

$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_\sigma)} \underbrace{\|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2}_{h(\mathbf{x}_\sigma)} &= \\ &= \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})\|_2^2 + \text{const}(\theta) \end{aligned}$$

## Proof

$$\mathbb{E}_{q(\mathbf{x}_\sigma)} h(\mathbf{x}_\sigma) = \int q(\mathbf{x}_\sigma) h(\mathbf{x}_\sigma) d\mathbf{x}_\sigma$$

# Denoising Score Matching

## Theorem

$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_\sigma)} \underbrace{\|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2}_{h(\mathbf{x}_\sigma)} &= \\ &= \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})\|_2^2 + \text{const}(\theta) \end{aligned}$$

## Proof

$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_\sigma)} h(\mathbf{x}_\sigma) &= \int q(\mathbf{x}_\sigma) h(\mathbf{x}_\sigma) d\mathbf{x}_\sigma = \\ &= \int \left( \int q(\mathbf{x}_\sigma|\mathbf{x}) p_{\text{data}}(\mathbf{x}) d\mathbf{x} \right) h(\mathbf{x}_\sigma) d\mathbf{x}_\sigma = \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} h(\mathbf{x}_\sigma) \end{aligned}$$

# Denoising Score Matching

## Theorem

$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_\sigma)} \underbrace{\|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2}_{h(\mathbf{x}_\sigma)} &= \\ &= \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})\|_2^2 + \text{const}(\theta) \end{aligned}$$

## Proof

$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_\sigma)} h(\mathbf{x}_\sigma) &= \int q(\mathbf{x}_\sigma) h(\mathbf{x}_\sigma) d\mathbf{x}_\sigma = \\ &= \int \left( \int q(\mathbf{x}_\sigma|\mathbf{x}) p_{\text{data}}(\mathbf{x}) d\mathbf{x} \right) h(\mathbf{x}_\sigma) d\mathbf{x}_\sigma = \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} h(\mathbf{x}_\sigma) \\ \mathbb{E}_{q(\mathbf{x}_\sigma)} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2 &= \end{aligned}$$

# Denoising Score Matching

## Theorem

$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_\sigma)} \underbrace{\|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2}_{h(\mathbf{x}_\sigma)} &= \\ &= \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})\|_2^2 + \text{const}(\theta) \end{aligned}$$

## Proof

$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_\sigma)} h(\mathbf{x}_\sigma) &= \int q(\mathbf{x}_\sigma) h(\mathbf{x}_\sigma) d\mathbf{x}_\sigma = \\ &= \int \left( \int q(\mathbf{x}_\sigma|\mathbf{x}) p_{\text{data}}(\mathbf{x}) d\mathbf{x} \right) h(\mathbf{x}_\sigma) d\mathbf{x}_\sigma = \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} h(\mathbf{x}_\sigma) \\ \mathbb{E}_{q(\mathbf{x}_\sigma)} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2 &= \\ &= \mathbb{E}_{q(\mathbf{x}_\sigma)} \left[ \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma)\|^2 + \underbrace{\|\nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2}_{\text{const}(\theta)} - 2\mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma) \right] \end{aligned}$$

# Denoising Score Matching

## Theorem

$$\begin{aligned}\mathbb{E}_{q(\mathbf{x}_\sigma)} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2 &= \\ &= \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})\|_2^2 + \text{const}(\theta)\end{aligned}$$

## Proof (Continued)

$$\mathbb{E}_{q(\mathbf{x}_\sigma)} [\mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)]$$

# Denoising Score Matching

## Theorem

$$\begin{aligned}\mathbb{E}_{q(\mathbf{x}_\sigma)} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2 &= \\ = \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})\|_2^2 + \text{const}(\theta)\end{aligned}$$

## Proof (Continued)

$$\mathbb{E}_{q(\mathbf{x}_\sigma)} [\mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)] = \int q(\mathbf{x}_\sigma) \left[ \mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \frac{\nabla_{\mathbf{x}_\sigma} q(\mathbf{x}_\sigma)}{q(\mathbf{x}_\sigma)} \right] d\mathbf{x}_\sigma$$

# Denoising Score Matching

## Theorem

$$\begin{aligned}\mathbb{E}_{q(\mathbf{x}_\sigma)} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2 &= \\ &= \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})\|_2^2 + \text{const}(\theta)\end{aligned}$$

## Proof (Continued)

$$\begin{aligned}\mathbb{E}_{q(\mathbf{x}_\sigma)} [\mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)] &= \int q(\mathbf{x}_\sigma) \left[ \mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \frac{\nabla_{\mathbf{x}_\sigma} q(\mathbf{x}_\sigma)}{q(\mathbf{x}_\sigma)} \right] d\mathbf{x}_\sigma = \\ &= \int \left[ \mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \left( \int q(\mathbf{x}_\sigma|\mathbf{x}) p_{\text{data}}(\mathbf{x}) d\mathbf{x} \right) \right] d\mathbf{x}_\sigma\end{aligned}$$

# Denoising Score Matching

## Theorem

$$\begin{aligned}\mathbb{E}_{q(\mathbf{x}_\sigma)} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2 &= \\ = \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})\|_2^2 + \text{const}(\theta)\end{aligned}$$

## Proof (Continued)

$$\begin{aligned}\mathbb{E}_{q(\mathbf{x}_\sigma)} [\mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)] &= \int q(\mathbf{x}_\sigma) \left[ \mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \frac{\nabla_{\mathbf{x}_\sigma} q(\mathbf{x}_\sigma)}{q(\mathbf{x}_\sigma)} \right] d\mathbf{x}_\sigma = \\ &= \int \left[ \mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \left( \int q(\mathbf{x}_\sigma|\mathbf{x}) p_{\text{data}}(\mathbf{x}) d\mathbf{x} \right) \right] d\mathbf{x}_\sigma = \\ &= \int \int p_{\text{data}}(\mathbf{x}) [\mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} q(\mathbf{x}_\sigma|\mathbf{x})] d\mathbf{x}_\sigma d\mathbf{x}\end{aligned}$$

# Denoising Score Matching

## Theorem

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## Proof (Continued)

$$\begin{aligned}\mathbb{E}_{q(\mathbf{x}_\sigma)} [\mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)] &= \int q(\mathbf{x}_\sigma) \left[ \mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \frac{\nabla_{\mathbf{x}_\sigma} q(\mathbf{x}_\sigma)}{q(\mathbf{x}_\sigma)} \right] d\mathbf{x}_\sigma = \\ &= \int \left[ \mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \left( \int q(\mathbf{x}_\sigma|\mathbf{x}) p_{\text{data}}(\mathbf{x}) d\mathbf{x} \right) \right] d\mathbf{x}_\sigma = \\ &= \int \int p_{\text{data}}(\mathbf{x}) [\mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} q(\mathbf{x}_\sigma|\mathbf{x})] d\mathbf{x}_\sigma d\mathbf{x} = \\ &= \int \int p_{\text{data}}(\mathbf{x}) q(\mathbf{x}_\sigma|\mathbf{x}) [\mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})] d\mathbf{x}_\sigma d\mathbf{x}\end{aligned}$$

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## Proof (Continued)

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# Denoising Score Matching

## Theorem

$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_\sigma)} \underbrace{\|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2}_{h(\mathbf{x}_\sigma)} &= \\ &= \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})\|_2^2 + \text{const}(\theta) \end{aligned}$$

## Proof (Continued)

$$\mathbb{E}_{q(\mathbf{x}_\sigma)} h(\mathbf{x}_\sigma) = \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} h(\mathbf{x}_\sigma)$$

# Denoising Score Matching

## Theorem

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## Proof (Continued)

$$\mathbb{E}_{q(\mathbf{x}_\sigma)} h(\mathbf{x}_\sigma) = \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} h(\mathbf{x}_\sigma)$$

$$\mathbb{E}_{q(\mathbf{x}_\sigma)} [\mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)] = \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} [\mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})]$$

# Denoising Score Matching

## Theorem

$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_\sigma)} \underbrace{\|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2}_{h(\mathbf{x}_\sigma)} &= \\ &= \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})\|_2^2 + \text{const}(\theta) \end{aligned}$$

## Proof (Continued)

$$\mathbb{E}_{q(\mathbf{x}_\sigma)} h(\mathbf{x}_\sigma) = \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} h(\mathbf{x}_\sigma)$$

$$\mathbb{E}_{q(\mathbf{x}_\sigma)} [\mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)] = \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} [\mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})]$$

$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_\sigma)} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2 &= \\ &= \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} [\|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma)\|^2 - 2\mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})] + \text{const}(\theta) \end{aligned}$$

# Denoising Score Matching

## Theorem

$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_\sigma)} \underbrace{\|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2}_{h(\mathbf{x}_\sigma)} &= \\ &= \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})\|_2^2 + \text{const}(\theta) \end{aligned}$$

## Proof (Continued)

$$\mathbb{E}_{q(\mathbf{x}_\sigma)} h(\mathbf{x}_\sigma) = \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} h(\mathbf{x}_\sigma)$$

$$\mathbb{E}_{q(\mathbf{x}_\sigma)} [\mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)] = \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} [\mathbf{s}_{\theta,\sigma}^\top(\mathbf{x}_\sigma) \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})]$$

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# Denoising Score Matching

Original objective:

$$\mathbb{E}_{p_{\text{data}}(\mathbf{x})} \|\mathbf{s}_\theta(\mathbf{x}) - \nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x})\|_2^2 \rightarrow \min_{\theta}$$

# Denoising Score Matching

Original objective:

$$\mathbb{E}_{p_{\text{data}}(\mathbf{x})} \|\mathbf{s}_\theta(\mathbf{x}) - \nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x})\|_2^2 \rightarrow \min_{\theta}$$

Noisy objective:

$$\mathbb{E}_{q(\mathbf{x}_\sigma)} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}} \log q(\mathbf{x}_\sigma)\|_2^2 \rightarrow \min_{\theta}$$

# Denoising Score Matching

Original objective:

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$$\mathbb{E}_{q(\mathbf{x}_\sigma)} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}} \log q(\mathbf{x}_\sigma)\|_2^2 \rightarrow \min_{\theta}$$

This is equivalent to a denoising task:

$$\mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})\|_2^2 \rightarrow \min_{\theta}$$

# Denoising Score Matching

Original objective:

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$$\mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{\mathcal{N}(0, \mathbf{I})} \left\| \mathbf{s}_{\theta,\sigma}(\mathbf{x} + \sigma\epsilon) + \frac{\epsilon}{\sigma} \right\|_2^2 \rightarrow \min_{\theta}$$

# Denoising Score Matching

Original objective:

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## Langevin Dynamics

$$\mathbf{x}_{l+1} = \mathbf{x}_l + \frac{\eta}{2} \cdot \mathbf{s}_{\theta,\sigma}(\mathbf{x}_l) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}_l, \quad \boldsymbol{\epsilon}_l \sim \mathcal{N}(0, \mathbf{I})$$

# Outline

## 1. Score Matching

Denoising Score Matching (continued)

Noise-Conditioned Score Network

## 2. Forward Gaussian Diffusion Process

## 3. Denoising Score Matching for Diffusion

## 4. Reverse Gaussian Diffusion Process

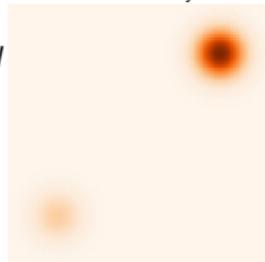
# Denoising Score Matching

$$\mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{\mathcal{N}(0, \mathbf{I})} \left\| \mathbf{s}_{\theta, \sigma}(\mathbf{x} + \sigma \boldsymbol{\epsilon}) + \frac{\boldsymbol{\epsilon}}{\sigma} \right\|_2^2 \rightarrow \min_{\theta}$$

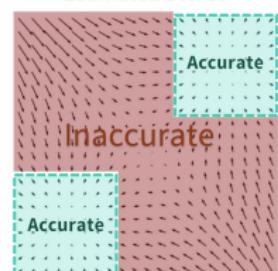
$$\mathbf{x}_{I+1} = \mathbf{x}_I + \frac{\eta}{2} \cdot \mathbf{s}_{\theta, \sigma}(\mathbf{x}_I) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}_I$$

- ▶ For **small**  $\sigma$ ,  $\mathbf{s}_{\theta, \sigma}(\mathbf{x})$  becomes inaccurate and Langevin dynamics fails to traverse modes
- ▶ For **large**  $\sigma$ , robustness in low-density regions is achieved, but the model learns a distribution that is overly corrupted

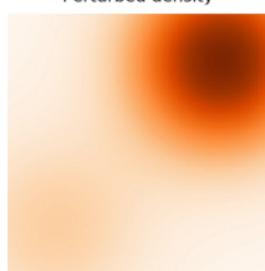
Data density



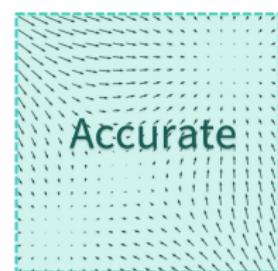
Estimated scores



Perturbed density



Estimated scores



## Noise-Conditioned Score Network (NCSN)

- ▶ Specify a sequence of noise levels:  $\sigma_1 < \sigma_2 < \dots < \sigma_T$
- ▶ Perturb each data point with different noise levels:  
 $\mathbf{x}_t = \mathbf{x} + \sigma_t \boldsymbol{\epsilon}$ , so  $\mathbf{x}_t \sim q(\mathbf{x}_t)$
- ▶ Choose  $\sigma_1, \sigma_T$  such that:

$$q(\mathbf{x}_1) \approx p_{\text{data}}(\mathbf{x}), \quad q(\mathbf{x}_T) \approx \mathcal{N}(0, \sigma_T^2 \mathbf{I})$$

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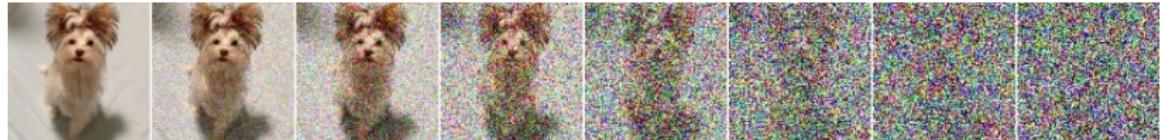
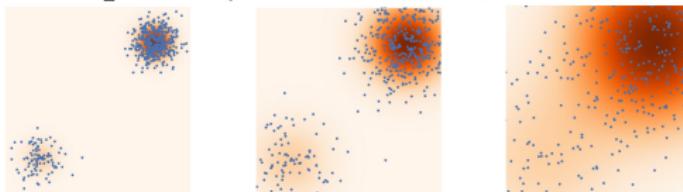
$$\sigma_1$$

$$<$$

$$\sigma_2$$

$$<$$

$$\sigma_3$$



## Noise-Conditioned Score Network (NCSN)

Train the denoising score function  $s_{\theta, \sigma_t}(\mathbf{x}_t)$  for each noise level  $\sigma_t$  using a unified weighted objective:

$$\sum_{t=1}^T \sigma_t^2 \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_t | \mathbf{x})} \|s_{\theta, \sigma_t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x})\|_2^2 \rightarrow \min_{\theta}$$

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Here,  $\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x}) = -\frac{\mathbf{x}_t - \mathbf{x}}{\sigma_t^2} = -\frac{\epsilon}{\sigma_t}$

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Here,  $\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x}) = -\frac{\mathbf{x}_t - \mathbf{x}}{\sigma_t^2} = -\frac{\epsilon}{\sigma_t}$

## Training

1. Sample  $\mathbf{x}_0 \sim p_{\text{data}}(\mathbf{x})$
2. Sample  $t \sim U\{1, T\}$  and  $\epsilon \sim \mathcal{N}(0, \mathbf{I})$
3. Construct noisy image  $\mathbf{x}_t = \mathbf{x}_0 + \sigma_t \epsilon$
4. Evaluate loss  $\mathcal{L} = \sigma_t^2 \left\| \mathbf{s}_{\theta, \sigma_t}(\mathbf{x}_t) + \frac{\epsilon}{\sigma_t} \right\|^2$

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How do we sample from such a model?

# Noise-Conditioned Score Network (NCSN)

## Sampling (Annealed Langevin Dynamics)

- ▶ Sample initial point  $\mathbf{x}_0 \sim \mathcal{N}(0, \sigma_T^2 \mathbf{I}) \approx q(\mathbf{x}_T)$
- ▶ At each noise level, apply  $L$  steps of Langevin dynamics:

$$\mathbf{x}_l = \mathbf{x}_{l-1} + \frac{\eta_t}{2} \mathbf{s}_{\theta, \sigma_t}(\mathbf{x}_{l-1}) + \sqrt{\eta_t} \boldsymbol{\epsilon}_l,$$

- ▶ Update  $\mathbf{x}_0 := \mathbf{x}_L$  and reduce to the next lower  $\sigma_t$

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# Outline

## 1. Score Matching

Denoising Score Matching (continued)  
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## 2. Forward Gaussian Diffusion Process

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## Forward Gaussian Diffusion Process

Let  $\mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x})$ ,  $\beta_t \ll 1$ . Define a Markov chain:

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

## Forward Gaussian Diffusion Process

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$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\sqrt{1 - \beta_t} \mathbf{x}_{t-1}, \beta_t \mathbf{I})$$

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## Langevin Dynamics

$$\mathbf{x}_{I+1} = \mathbf{x}_I + \frac{\eta}{2} \cdot \nabla_{\mathbf{x}_I} \log p_{\theta}(\mathbf{x}_I) + \sqrt{\eta} \boldsymbol{\epsilon}_I, \quad \boldsymbol{\epsilon}_I \sim \mathcal{N}(0, \mathbf{I})$$

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$$\begin{aligned} \mathbf{x}_t &= \sqrt{1 - \beta_t} \mathbf{x}_{t-1} + \sqrt{\beta_t} \boldsymbol{\epsilon}_t \approx \left(1 - \frac{\beta_t}{2}\right) \mathbf{x}_{t-1} + \sqrt{\beta_t} \boldsymbol{\epsilon}_t = \\ &= \mathbf{x}_{t-1} + \frac{\beta_t}{2} (-\mathbf{x}_{t-1}) + \sqrt{\beta_t} \boldsymbol{\epsilon}_t \end{aligned}$$

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- ▶  $\beta_t = \eta$
- ▶  $\nabla_{\mathbf{x}_{t-1}} \log p(\mathbf{x}_{t-1} | \theta) = -\mathbf{x}_{t-1} = \nabla_{\mathbf{x}_{t-1}} \log \mathcal{N}(0, \mathbf{I})$

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## Statement 1

Let  $\alpha_t = 1 - \beta_t$  and  $\bar{\alpha}_t = \prod_{s=1}^t \alpha_s = \prod_{s=1}^t (1 - \beta_s)$ . Then

$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0, (1 - \bar{\alpha}_t) \mathbf{I})$$

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Thus, samples at any timestep  $t$  can be generated directly from  $\mathbf{x}_0$

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Thus, samples at any timestep  $t$  can be generated directly from  $\mathbf{x}_0$

$$\begin{aligned}\mathbf{x}_t &= \sqrt{\alpha_t} \mathbf{x}_{t-1} + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_t = \\ &= \sqrt{\alpha_t} (\sqrt{\alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1}} \boldsymbol{\epsilon}_{t-1}) + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_t = \\ &= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + (\sqrt{\alpha_t (1 - \alpha_{t-1})} \boldsymbol{\epsilon}_{t-1} + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_t) = \\ &= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_t \alpha_{t-1}} \boldsymbol{\epsilon}'_t\end{aligned}$$

# Forward Gaussian Diffusion Process

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

$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\sqrt{1 - \beta_t} \mathbf{x}_{t-1}, \beta_t \mathbf{I})$$

## Statement 1

Let  $\alpha_t = 1 - \beta_t$  and  $\bar{\alpha}_t = \prod_{s=1}^t \alpha_s = \prod_{s=1}^t (1 - \beta_s)$ . Then

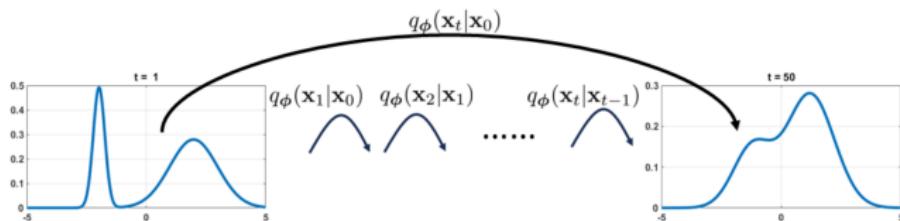
$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0, (1 - \bar{\alpha}_t) \mathbf{I})$$

Thus, samples at any timestep  $t$  can be generated directly from  $\mathbf{x}_0$

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# Forward Gaussian Diffusion Process

$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N} \left( \sqrt{1 - \beta_t} \mathbf{x}_{t-1}, \beta_t \mathbf{I} \right); \quad q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N} \left( \sqrt{\bar{\alpha}_t} \mathbf{x}_0, (1 - \bar{\alpha}_t) \mathbf{I} \right)$$

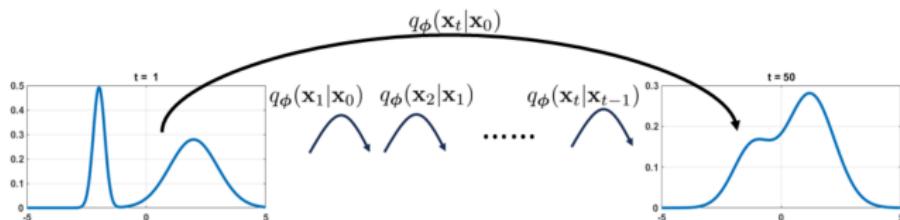


Chan S. Tutorial on Diffusion Models for Imaging and Vision, 2024

Sohl-Dickstein J. Deep Unsupervised Learning using Nonequilibrium Thermodynamics, 2015

# Forward Gaussian Diffusion Process

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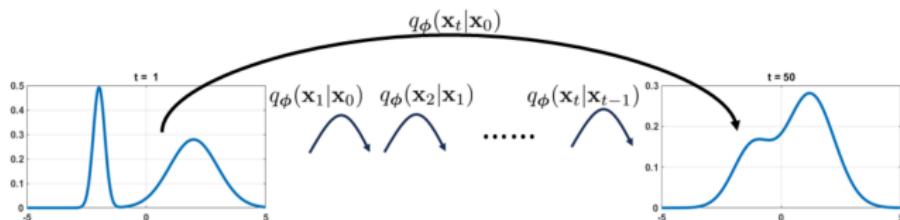
## Statement 2

Applying the Markov chain to any distribution  $p_{\text{data}}(\mathbf{x})$  yields  $\mathbf{x}_\infty \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$ , the **stationary** (limiting) distribution:

$$p_\infty(\mathbf{x}) = \int q(\mathbf{x} | \mathbf{x}') p_\infty(\mathbf{x}') d\mathbf{x}'$$

# Forward Gaussian Diffusion Process

$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N} \left( \sqrt{1 - \beta_t} \mathbf{x}_{t-1}, \beta_t \mathbf{I} \right); \quad q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N} \left( \sqrt{\bar{\alpha}_t} \mathbf{x}_0, (1 - \bar{\alpha}_t) \mathbf{I} \right)$$



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$$p_\infty(\mathbf{x}) = \int q(\mathbf{x}_\infty | \mathbf{x}_0) p_{\text{data}}(\mathbf{x}_0) d\mathbf{x}_0 \approx \mathcal{N}(0, \mathbf{I}) \int p_{\text{data}}(\mathbf{x}_0) d\mathbf{x}_0 = \mathcal{N}(0, \mathbf{I})$$

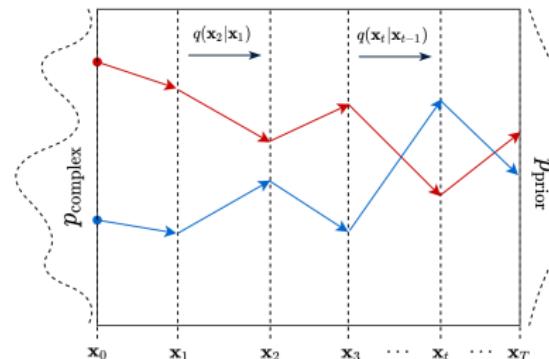
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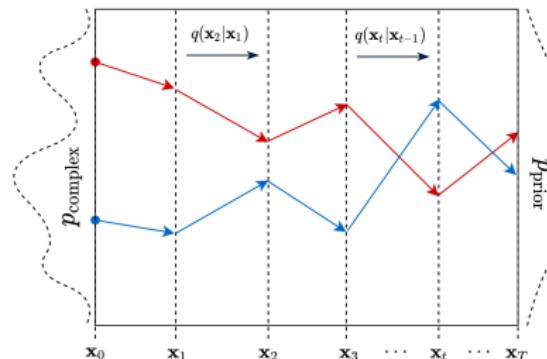
# Forward Gaussian Diffusion Process

**Diffusion** describes the migration of particles from regions of high density to those of low density.



# Forward Gaussian Diffusion Process

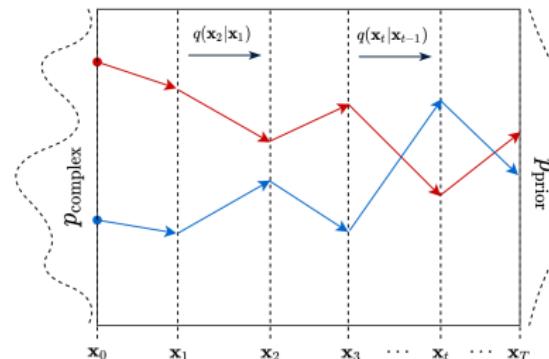
**Diffusion** describes the migration of particles from regions of high density to those of low density.



1.  $x_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x})$
2.  $\mathbf{x}_t = \sqrt{1 - \beta_t} \mathbf{x}_{t-1} + \sqrt{\beta_t} \boldsymbol{\epsilon}, \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}), t \geq 1$
3. After  $T \gg 1$  steps:  $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$

# Forward Gaussian Diffusion Process

**Diffusion** describes the migration of particles from regions of high density to those of low density.



1.  $\mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x})$
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3. After  $T \gg 1$  steps:  $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$

If this process can be reversed, we can sample from  $p_{\text{data}}(\mathbf{x})$  by starting from noise  $p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$ .

Our goal now becomes inverting this diffusion.

# Outline

## 1. Score Matching

- Denoising Score Matching (continued)
- Noise-Conditioned Score Network

## 2. Forward Gaussian Diffusion Process

## 3. Denoising Score Matching for Diffusion

## 4. Reverse Gaussian Diffusion Process

# Denoising Score Matching

## NCSN

$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_0, \sigma_t^2 \mathbf{I}), \quad q(\mathbf{x}_1) \approx p_{\text{data}}(\mathbf{x}), \quad q(\mathbf{x}_T) \approx \mathcal{N}(0, \sigma_T^2 \mathbf{I})$$

$$\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x}) = -\frac{\mathbf{x}_t - \mathbf{x}}{\sigma_t^2}$$

# Denoising Score Matching

## NCSN

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## Gaussian Diffusion

$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0, (1 - \bar{\alpha}_t) \mathbf{I}), \quad q(\mathbf{x}_1) \approx p_{\text{data}}(\mathbf{x}), \quad q(\mathbf{x}_T) \approx \mathcal{N}(0, \mathbf{I})$$

$$\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x}_0) = -\frac{\mathbf{x}_t - \sqrt{\bar{\alpha}_t} \mathbf{x}_0}{1 - \bar{\alpha}_t}$$

# Denoising Score Matching

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$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_0, \sigma_t^2 \mathbf{I}), \quad q(\mathbf{x}_1) \approx p_{\text{data}}(\mathbf{x}), \quad q(\mathbf{x}_T) \approx \mathcal{N}(0, \sigma_T^2 \mathbf{I})$$

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## Theorem (Denoising Score Matching)

$$\begin{aligned} \mathbb{E}_{q(\mathbf{x}_t)} \|\mathbf{s}_{\theta,t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t)\|_2^2 &= \\ &= \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_t | \mathbf{x})} \|\mathbf{s}_{\theta,t}(\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t | \mathbf{x})\|_2^2 + \text{const}(\theta) \end{aligned}$$

# Denoising Score Matching

## NCSN

$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_0, \sigma_t^2 \mathbf{I}), \quad q(\mathbf{x}_1) \approx p_{\text{data}}(\mathbf{x}), \quad q(\mathbf{x}_T) \approx \mathcal{N}(0, \sigma_T^2 \mathbf{I})$$

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## Gaussian Diffusion

$$q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0, (1 - \bar{\alpha}_t) \mathbf{I}), \quad q(\mathbf{x}_1) \approx p_{\text{data}}(\mathbf{x}), \quad q(\mathbf{x}_T) \approx \mathcal{N}(0, \mathbf{I})$$

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**Note:** This enables applying the NCSN approach with annealed Langevin dynamics to diffusion-based denoising models.

# Outline

## 1. Score Matching

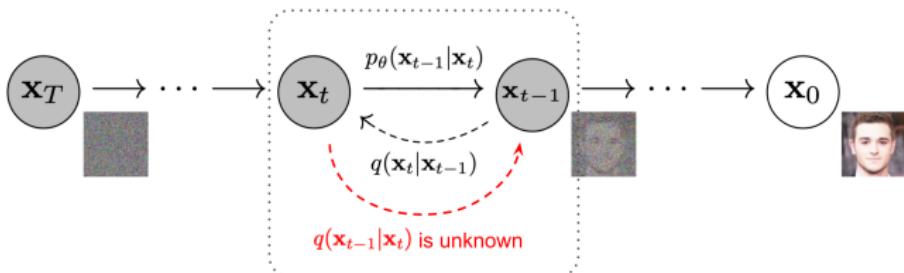
- Denoising Score Matching (continued)
- Noise-Conditioned Score Network

## 2. Forward Gaussian Diffusion Process

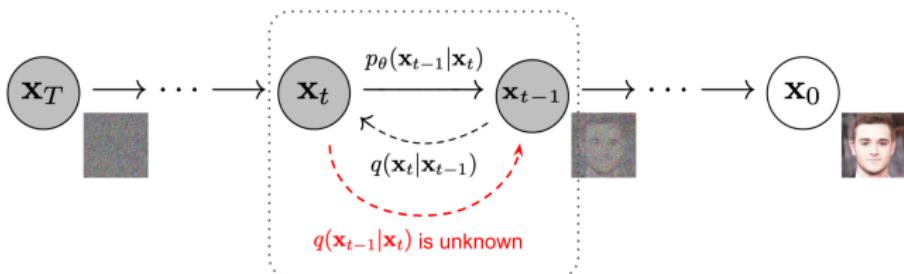
## 3. Denoising Score Matching for Diffusion

## 4. Reverse Gaussian Diffusion Process

# Reverse Gaussian Diffusion Process



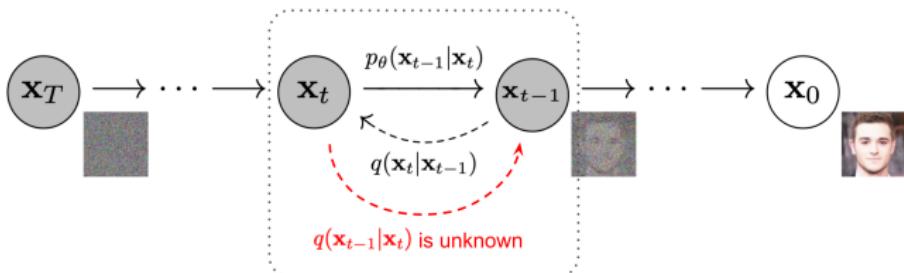
# Reverse Gaussian Diffusion Process



Forward Process

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}\left(\sqrt{1 - \beta_t}\mathbf{x}_{t-1}, \beta_t\mathbf{I}\right)$$

# Reverse Gaussian Diffusion Process



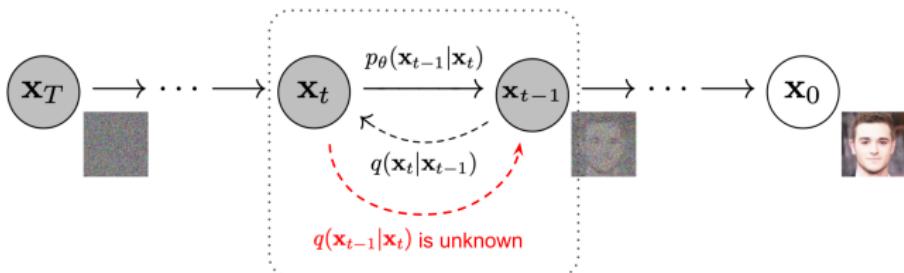
Forward Process

$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N} \left( \sqrt{1 - \beta_t} \mathbf{x}_{t-1}, \beta_t \mathbf{I} \right)$$

Reverse Process

$$q(\mathbf{x}_{t-1} | \mathbf{x}_t) = \frac{q(\mathbf{x}_t | \mathbf{x}_{t-1}) q(\mathbf{x}_{t-1})}{q(\mathbf{x}_t)} \approx p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)$$

# Reverse Gaussian Diffusion Process



Forward Process

$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}\left(\sqrt{1 - \beta_t} \mathbf{x}_{t-1}, \beta_t \mathbf{I}\right)$$

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$q(\mathbf{x}_{t-1})$  and  $q(\mathbf{x}_t)$  are intractable:

$$q(\mathbf{x}_t) = \int q(\mathbf{x}_t | \mathbf{x}_0) p_{\text{data}}(\mathbf{x}_0) d\mathbf{x}_0$$

## Reverse Gaussian Diffusion Process

$$q(\mathbf{x}_{t-1} | \mathbf{x}_t) = \frac{q(\mathbf{x}_t | \mathbf{x}_{t-1}) q(\mathbf{x}_{t-1})}{q(\mathbf{x}_t)}$$

Theorem (Feller, 1949)

If  $\beta_t$  is sufficiently small,  $q(\mathbf{x}_{t-1} | \mathbf{x}_t)$  is Gaussian (thus, diffusion requires  $T \approx 1000$  steps for convergence)

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Feller W. *On the theory of stochastic processes, with particular reference to applications*, 1949

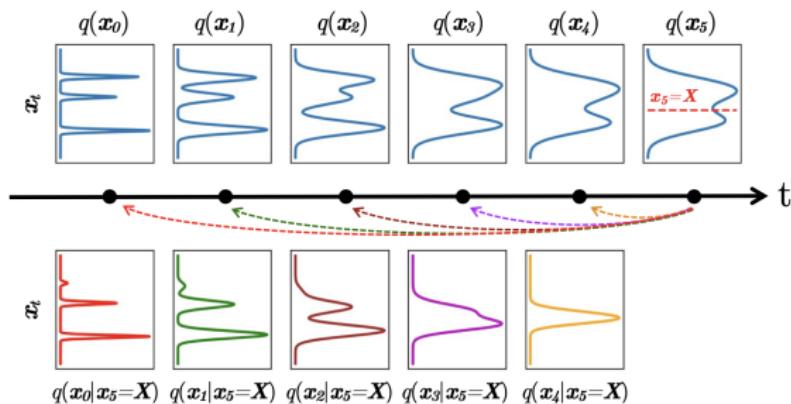
Xiao Z., Kreis K., Vahdat A. *Tackling the generative learning trilemma with denoising diffusion GANs*, 2021

# Reverse Gaussian Diffusion Process

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Theorem (Feller, 1949)

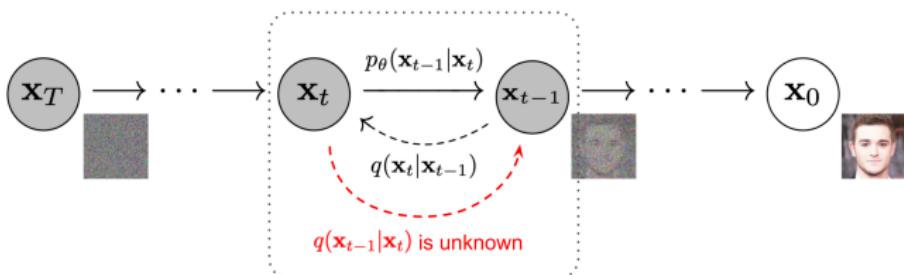
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# Reverse Gaussian Diffusion Process (Ancestral Sampling)

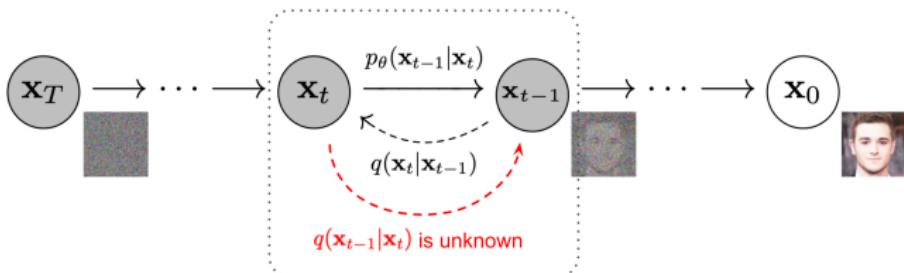


Define the reverse process as:

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t) \approx p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\boldsymbol{\mu}_{\theta,t}(\mathbf{x}_t), \sigma_{\theta,t}^2(\mathbf{x}_t))$$

Feller's theorem justifies this Gaussian assumption.

# Reverse Gaussian Diffusion Process (Ancestral Sampling)



Define the reverse process as:

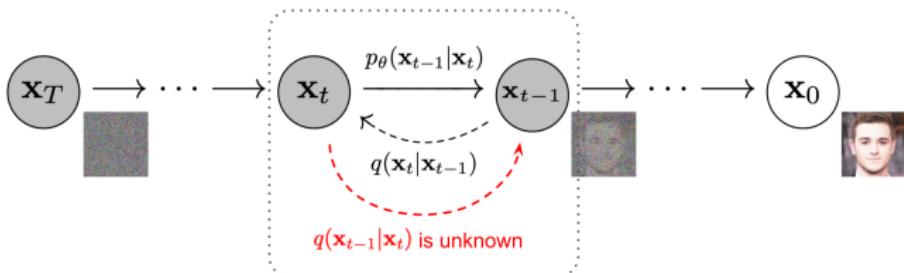
$$q(\mathbf{x}_{t-1}|\mathbf{x}_t) \approx p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\boldsymbol{\mu}_{\theta,t}(\mathbf{x}_t), \sigma_{\theta,t}^2(\mathbf{x}_t))$$

Feller's theorem justifies this Gaussian assumption.

## Forward Process

1.  $\mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x})$
2.  $\mathbf{x}_t = \sqrt{1 - \beta_t} \mathbf{x}_{t-1} + \sqrt{\beta_t} \boldsymbol{\epsilon}$
3.  $\mathbf{x}_T \sim p_{\infty}(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$

# Reverse Gaussian Diffusion Process (Ancestral Sampling)



Define the reverse process as:

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t) \approx p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mu_{\theta,t}(\mathbf{x}_t), \sigma_{\theta,t}^2(\mathbf{x}_t))$$

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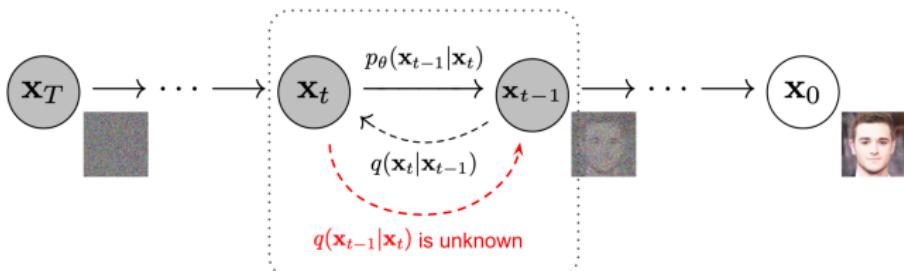
Forward Process

1.  $\mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x})$
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3.  $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$

Reverse Process

1.  $\mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$
2.  $\mathbf{x}_{t-1} = \sigma_{\theta,t}(\mathbf{x}_t) \boldsymbol{\epsilon} + \mu_{\theta,t}(\mathbf{x}_t)$
3.  $\mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x})$

# Reverse Gaussian Diffusion Process (Ancestral Sampling)



Define the reverse process as:

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t) \approx p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mu_{\theta,t}(\mathbf{x}_t), \sigma_{\theta,t}^2(\mathbf{x}_t))$$

Feller's theorem justifies this Gaussian assumption.

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$$1. \quad \mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x})$$

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## Reverse Process

$$1. \quad \mathbf{x}_T \sim p_\infty(\mathbf{x}) = \mathcal{N}(0, \mathbf{I})$$

$$2. \quad \mathbf{x}_{t-1} = \sigma_{\theta,t}(\mathbf{x}_t) \boldsymbol{\epsilon} + \mu_{\theta,t}(\mathbf{x}_t)$$

$$3. \quad \mathbf{x}_0 = \mathbf{x} \sim p_{\text{data}}(\mathbf{x})$$

**Note:** The forward process is non-learnable, i.e., it does not involve trainable parameters

## Summary

- ▶ Denoising score matching minimizes the Fisher divergence on corrupted samples, making the divergence estimable via sampling
- ▶ The noise-conditioned score network leverages a range of noise levels and annealed Langevin dynamics to learn the score function and enable sampling
- ▶ The Gaussian diffusion process is a Markov chain that incrementally corrupts data with carefully structured Gaussian noise
- ▶ Denoising score matching, together with Langevin dynamics, can be applied to the Gaussian diffusion process
- ▶ The reverse process reconstructs data from noise samples, although its precise form is intractable