Diffusion Models

Diffusion Models

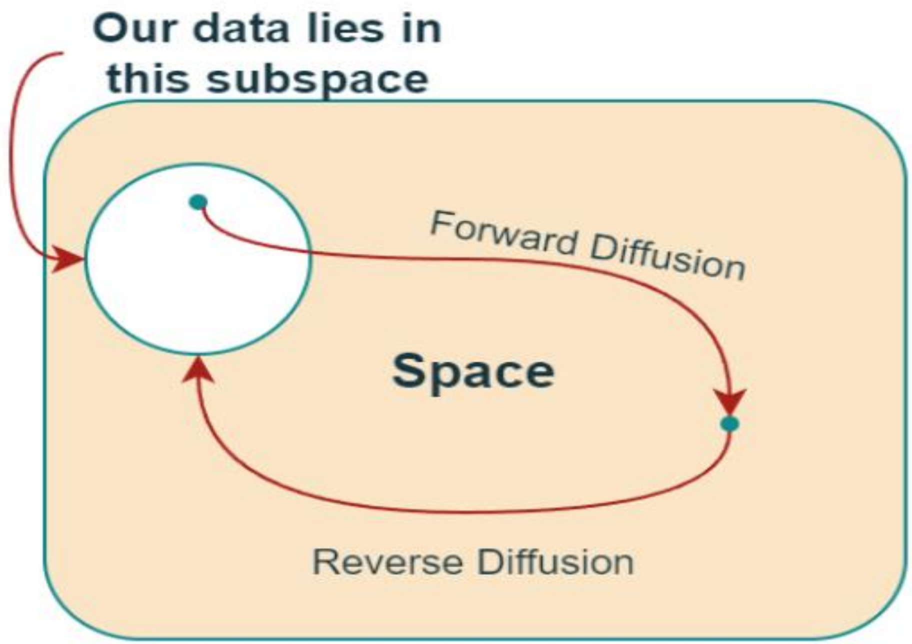
A hedgehog using a calculator.

A corgi wearing a red bowtie and a purple

A transparent sculpture- a duck made out of glas

High-level overview

- Diffusion models are probabilistic models used for image generation
- They involve reversing the process of gradually degrading the data
- Consist of two processes:
  - **The forward process**: data is progressively destroyed by adding noise across multiple time steps
  - **The reverse process**: using a neural network, noise is sequentially removed to obtain the original data



A high-level conceptual overview of the entire image space.

Three Categories

- Denoising Diffusion Probabilistic Models (DDPM)
- Noise Conditioned Score Networks (NCSN)
- Stochastic Differential Equations (SDE)

Notations

$p(x_0)$ - data distribution

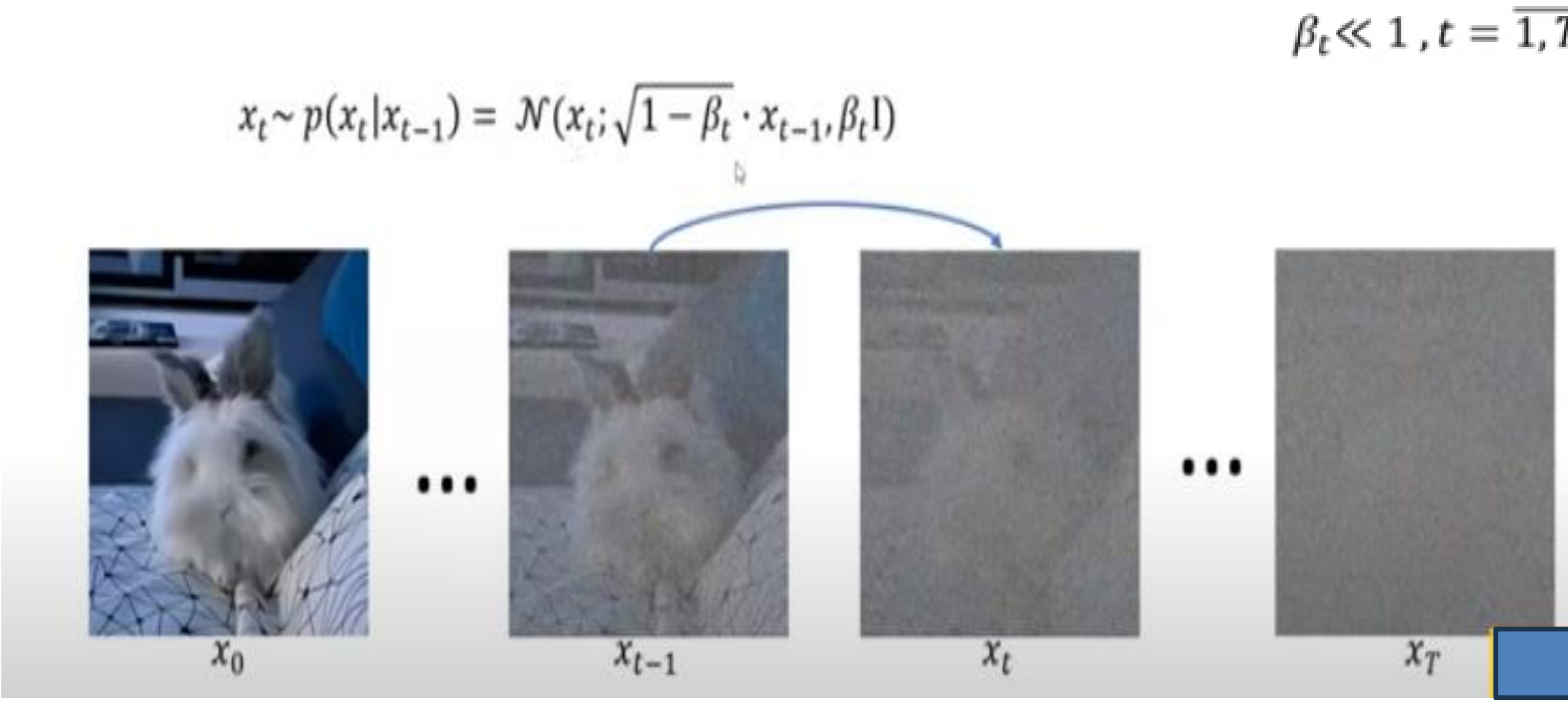
$\mathcal{N}(x; \mu, \sigma \cdot I)$ - Gaussian distribution

Random Variable (image)

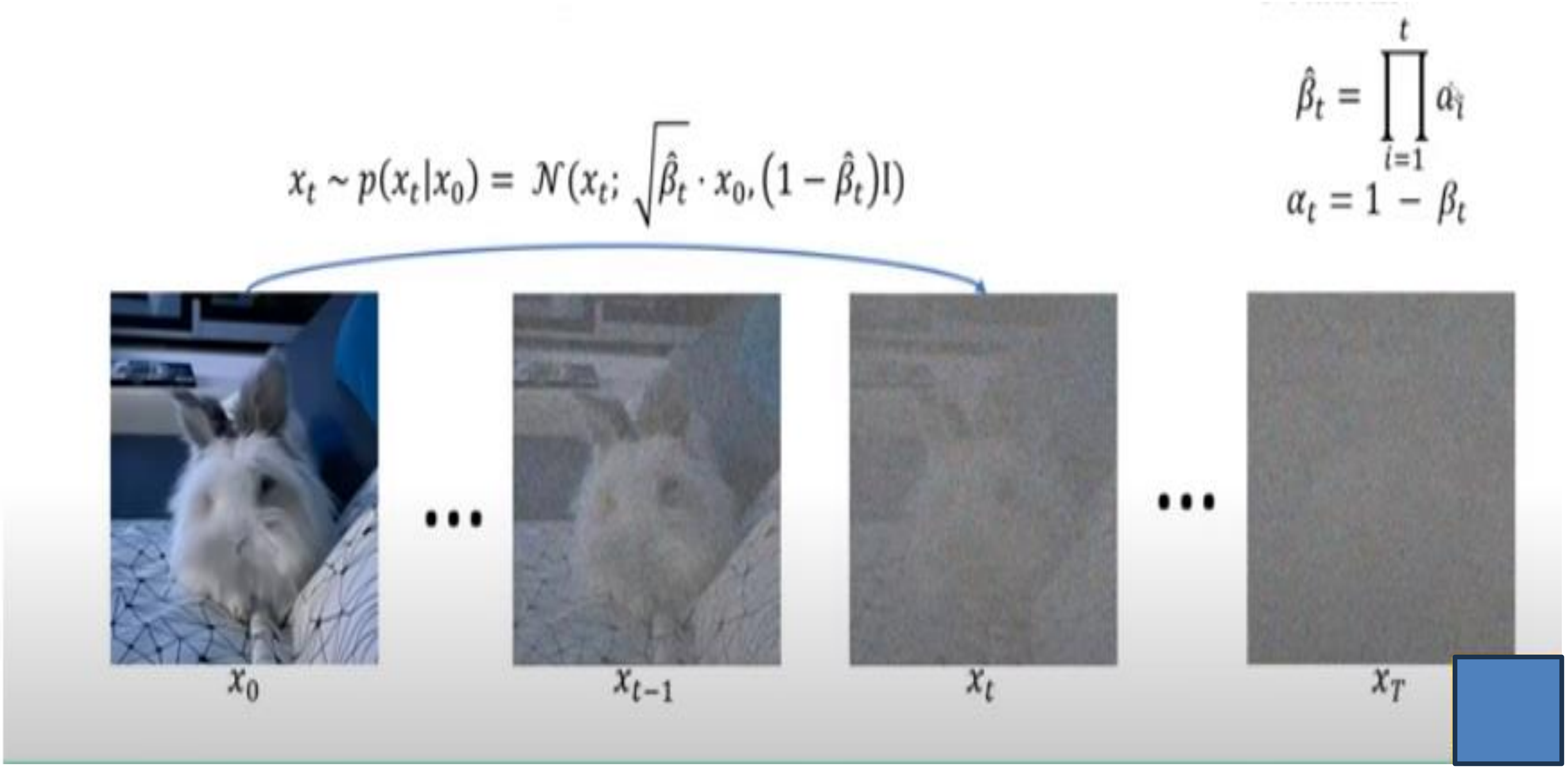
Mean Vector

Covariance matrix. I is the identity matrix

Forward Process (Iterative)



Forward Process (One Shot)

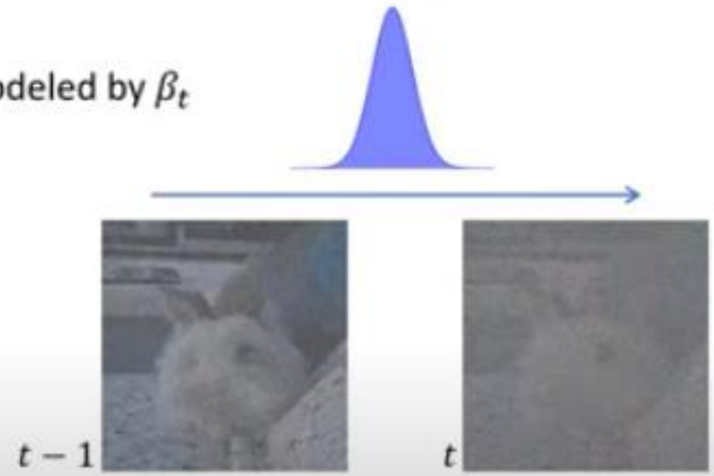


DDPMs. Properties of β_t

✓ 1. $\beta_t \ll 1, t = \overline{1,T}$

$$x_t \sim p(x_t|x_{t-1}) = \mathcal{N}(x_t; \sqrt{1-\beta_t} \cdot x_{t-1}, \beta_t \mathrm{I})$$

x_t is created with a small step modeled by β_t



x_{t-1} comes from region close to x_t,
therefore we can model with Gaussian

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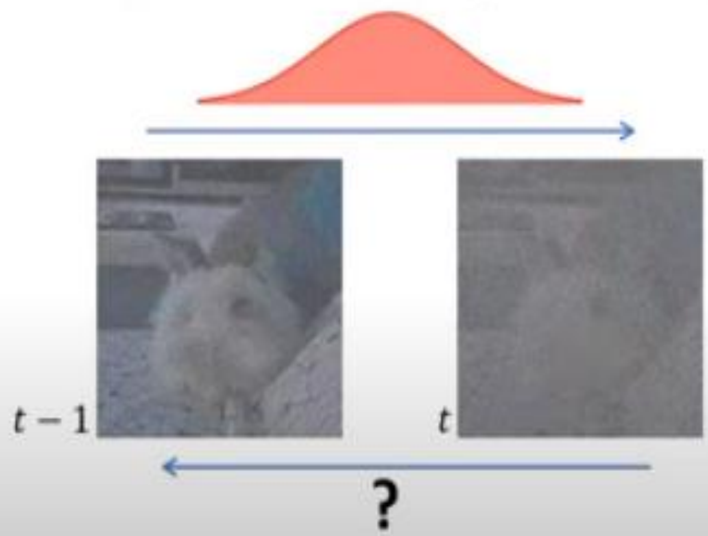
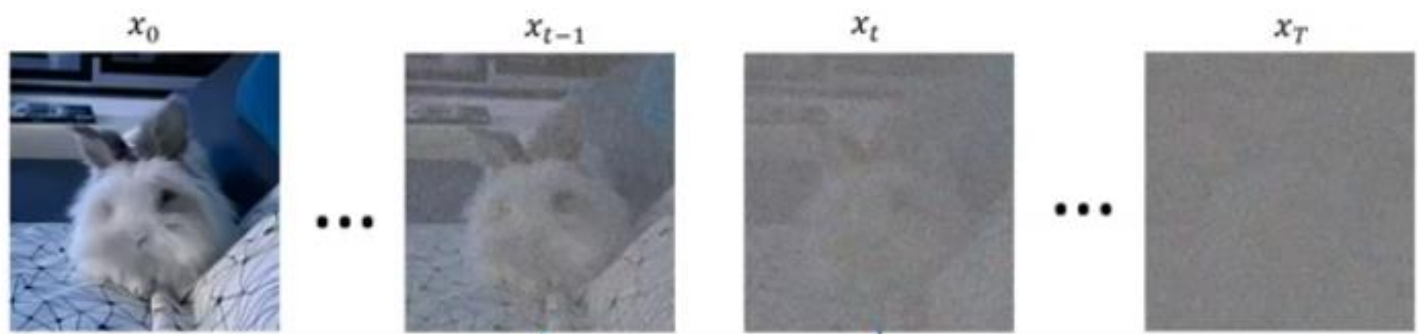


DDPMs. Training objective

Remember that:



$$p(x_{t-1}|x_t) \approx p_\theta(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$$

Reverse process

Neural Network

Cross Entropy and KL (Kullback-Leibler) divergence

- Entropy: $E(P) = - \Sigma_i P(i) \log P(i)$
- Cross Entropy: $C(P) = - \Sigma_i P(i) \log Q(i)$
- KL divergence: $D_{KL}(P \,||\, Q) = \Sigma_i P(i) \log[P(i)/Q(i)] = \Sigma_i P(i)[\log P(i) - \log Q(i)]$

DDPMs. Training Objective

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

$$\min_{\theta} \mathbb{E}_{x_0 \sim p(x_0)} \left[-\log p_\theta(x_0|x_1) + \sum_{t=2}^{T} KL(p(x_{t-1}|x_t,\, x_0)||p_\theta(x_{t-1}|x_t)) \right]$$

Notations:

$$\hat{\beta}_t = \prod_{i=1}^{t} \alpha_i$$

$$\alpha_t = 1 - \beta_t$$

$$p(x_{t-1}|x_t, x_0) = \mathcal{N}\left(x_{t-1};\, \tilde{\mu}(x_t, x_0), \tilde{\beta}_t I\right)$$

$$\tilde{\mu}(x_t, x_0) = \frac{1}{\sqrt{\alpha_t}} \left(x_t - \frac{1 - \alpha_t}{\sqrt{1 - \hat{\beta}_t}} z_t \right), z_t \sim \mathcal{N}(0, I)$$

$$\tilde{\beta}_t = \frac{1 - \hat{\beta}_{t-1}}{1 - \hat{\beta}_t} \cdot \beta_t$$

$$\min_{\theta} \frac{1}{T} \sum_{t=1}^{T} \mathbb{E}_{x_0 \sim p(x_0), z_t \sim \mathcal{N}(0,I)} \| z_t - z_\theta(x_t, t) \|_2^2$$

DDPMs. Training Algorithm

$$\min_{\theta} \underbrace{\frac{1}{T}\sum_{t=1}^{T} \mathbb{E}_{x_0 \sim p(x_0), z_t \sim \mathcal{N}(0,\mathrm{I})} \|z_t - z_\theta(x_t, t)\|_2^2}_{\mathcal{L}_{simple}}$$

Training algorithm:

$$\hat{\beta}_t = \prod_{i=1}^{t} \alpha_i$$

Repeat

$x_0 \sim p(x_0)$

$t \sim \mathcal{U}(\{1, \ldots, T\})$

$z_t \sim \mathcal{N}(0, \mathrm{I})$

$x_t = \sqrt{\hat{\beta}_t} \cdot x_0 + \sqrt{(1 - \hat{\beta}_t)} z_t$

$\theta = \theta - lr \cdot \nabla_\theta \mathcal{L}_{simple}$

Until convergence

Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
  $$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$$
until converged

Algorithm 2 Sampling

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

Thank You