Diffusion

To know the distribution of data

↳ manifold

$z \xrightarrow{f(z)} x$

High Entropy
Low information

'loss'

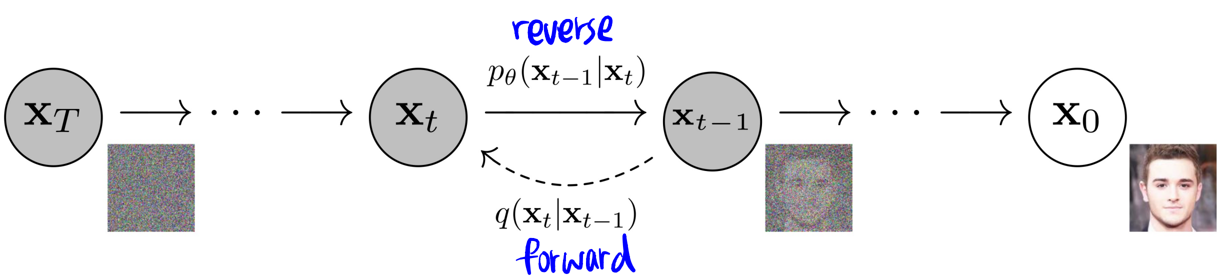
Low Entropy
High Information

⟨Diffusion Models⟩

$x \longrightarrow z \longrightarrow \hat{x}$

fixed encoder

only train decoder!



$$q(x_{1:T}|x_0) := \prod_{t=1}^{T} q(x_t|x_{t-1}) \qquad q(x_t|x_{t-1}) := \mathcal{N}(x_t; \sqrt{1-\beta_t}\,x_{t-1}, \beta_t I)$$

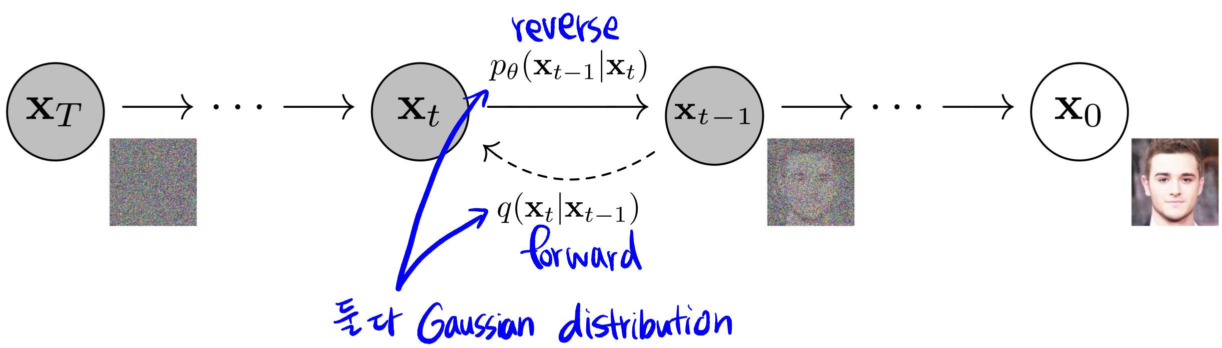
$$p_\theta(x_{0:T}) = p(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1}|x_t) \qquad p_\theta(x_{t-1}|x_t) := \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$$

x_t를 보고
x_{t-1}의 평균을 예측

cf. VAE Loss : $\underbrace{D_{KL}(q_\phi(z|x)\|p_\theta(z))}_{\text{Regularization Loss}} + \underbrace{\mathbb{E}_{q_\phi(z|x)}\{\log p_\theta(x|z)\}}_{\text{Reconstruction Loss}}$

Regularization Loss
(= Make approximate posterior distribution close to prior)

Reconstruction Loss
(= Reconstruct the input data)



Diffusion Loss

denoise

$x_t \xrightarrow[\text{add noise}]{} x_{t-1}$

Learning β_t

$$\mathbb{E}_q\Big[\underbrace{D_{KL}(q(x_T|x_0)\|p(x_T))}_{L_T} + \sum_{t>1}\underbrace{D_{KL}(q(x_{t-1}|x_t,x_0)\|p_\theta(x_{t-1}|x_t))}_{L_{t-1}}\underbrace{-\log p_\theta(x_0|x_1)}_{L_0}\Big]$$

Regularization

x_0가 주어진 상황에서 diffusion의 역 process

Reconstruction Loss

x_t에서 x_{t-1}을 예측

▨ Residual estimation : residual을 예측하자!

x를 통해 μ를 한꺼번에 예측하는 것이 아니라 residual ϵ을 활용하자

$$\mu_\theta(x_t,t) = \tilde{\mu}_t\left(x_t, \frac{1}{\sqrt{\bar{\alpha}_t}}\left(x_t - \sqrt{1-\bar{\alpha}_t}\,\epsilon_\theta(x_t)\right)\right)$$

$$= \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(x_t, t)\right)$$

$$\underset{\text{Noise}}{x_T} \underset{\text{add noise } q}{\overset{p_\theta \text{ denoise}}{\rightleftarrows}} \underset{\text{img}}{x_0} \qquad x_t \xrightarrow{\text{denoise}} x_{t-1}$$

▨ Loss Simplification #1

$$\mathbb{E}_q\Big[\underbrace{\boxed{D_{KL}(q(x_T|x_0)\,\|\,p(x_T))}}_{L_T} + \sum_{t>1}\underbrace{D_{KL}(q(x_{t-1}|x_t,x_0)\,\|\,p_\theta(x_{t-1}|x_t))}_{L_{t-1}} \underbrace{-\log p_\theta(x_0|x_1)}_{L_0}\Big]$$

$$\Downarrow$$

$$L_{simple}(\theta) = \mathbb{E}_{t,x_0,\epsilon}\left[\|\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\,\epsilon, t)\|^2\right]$$

← MSE Loss → Denoising

*ϵ : residual

β_t를 같이 학습하려고

(→ But fixed)

(inductive bias (β_t)를 늘리는 방향)

인간의 사전지식 넣음

▨ Loss Simplification #2 - Not to learn variance

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

$$\Sigma_\theta(x_t,t) = \sigma^2 I$$

$$\sigma_t^2 = \tilde{\beta}_t = \left(\frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\right)\beta_t \quad \text{or} \quad \sigma_t^2 = \beta_t$$

Loss Simplification

$$\mathbb{E}_q\left[\cancel{D_{KL}(q(x_T|x_0)\|p(x_T))} + \sum_{t>1} \underbrace{D_{KL}(q(x_{t-1}|x_t, x_0)\| p_\theta(x_{t-1}|x_t))}_{L_{t-1}} \underbrace{- \log p_\theta(x_0|x_1)}_{L_0}\right]$$

$$\mathcal{L}_{t-1} = \mathbb{E}_q\left[\frac{1}{2\sigma_t^2}\|\tilde{\mu}_t(x_t, x_0) - \mu_\theta(x_t, t)\|^2\right] + C$$

$$\mu_\theta(x_t, t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(x_t, t)\right)$$

$$\mathbb{E}_{x_0, \epsilon}\left[\underbrace{\frac{\beta_t^2}{2\sigma_t^2 \alpha_t (1-\bar{\alpha}_t)}}_{\text{상수}} \|\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}\, x_0 + \sqrt{1-\bar{\alpha}_t}\, \epsilon, t)\|^2\right]$$

$$\Downarrow$$

$$\mathbb{E}_{x_0, \epsilon}\left[\|\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}\, x_0 + \sqrt{1-\bar{\alpha}_t}\, \epsilon, t)\|^2\right]$$