DDPM 고홍규

핵심식 2개

GAN : 빠른 생성 + 고품질
VAE : 빠른 생성 + 다양한 그림
Diffusion : 다양한 그림 + 고품질
$\qquad\qquad\qquad \parallel$
Mode Diversity

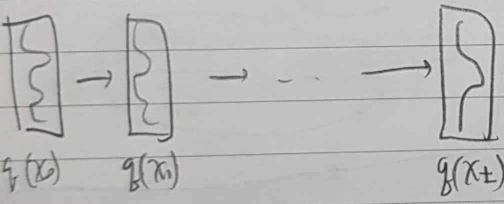
$\left(x_T\right) \rightleftarrows \cdots \underset{q}{\overset{p_\theta}{\rightleftarrows}} \left(x_0\right)$

θ 신경

q = 전파자

Noising

diffusion kernel = 가우시안 분포

- $q(x_t) = \int q(x_0) \cdot \boxed{q(x_t|x_0)}\, dx_0$
- $q(x_t|x_0) = q(x_t|x_{t-1}) \times \cdots \times q(x_2|x_1) \cdot q(x_0)$
  정규분포
- $x_t = \sqrt{1-\beta_t}\, x_{t-1} + \sqrt{\beta_t}\, \varepsilon_t$
- 

pf) $q(x_t|x_{t-1}) = N\big(x_t ; \underbrace{\sqrt{1-\beta_t}\cdot x_{t-1}}_{\mu}, \underbrace{\beta_t}_{\sigma^2}\big)$

$x_t = \sqrt{1-\beta_t}\, x_{t-1} + \sqrt{\beta_t}\, \varepsilon_{t-1}$ start

$\varepsilon_{t-1} \sim N(0,1)$

(Reparameterization trick)

$= \sqrt{\alpha_t}\, x_{t-1} + \sqrt{1-\alpha_t}\cdot\varepsilon_{t-1}$

$= \sqrt{\alpha_t}\left(\sqrt{\alpha_{t-1}}\cdot x_{t-2} + \sqrt{1-\alpha_{t-1}}\cdot\varepsilon_{t-2}\right) + \sqrt{1-\alpha_t}\cdot\varepsilon_{t-1}$

$= \sqrt{\alpha_t}\sqrt{\alpha_{t-1}}\cdot x_{t-2} + \underbrace{\sqrt{\alpha_t}\sqrt{1-\alpha_{t-1}}\,\varepsilon_{t-2} + \sqrt{1-\alpha_t}\cdot\varepsilon_{t-1}}_{\sqrt{1-\alpha_t\alpha_{t-1}}\cdot\varepsilon_{t-2}}$

⋮

$x_t = \sqrt{\alpha_t}\sqrt{\alpha_{t-1}} \times \cdots \sqrt{\alpha_0}\, x_0 + \sqrt{1-\alpha_t\alpha_{t-1}\times\cdots\times\alpha_0}\cdot\varepsilon_t$

$= \sqrt{\bar{\alpha}_t}\cdot x_0 + \sqrt{1-\bar{\alpha}_t}\cdot \underbrace{\bar{\varepsilon}_t}_{\varepsilon_t(t|x_0)}$

$\rightarrow q(x_t|x_0) = N\, x_t ; \big(\underbrace{\sqrt{\bar{\alpha}_t}\, x_0}_{\mu}, \underbrace{1-\bar{\alpha}_t}_{\sigma^2}\big)$

$\rightarrow x_0 = \left(x_t - \sqrt{1-\bar{\alpha}_t}\,\bar{\varepsilon}_t\right)\cdot\dfrac{1}{\sqrt{\bar{\alpha}_t}}$ fin

cf) $\underset{<1}{\alpha_t}\ \overset{0<}{\underset{\approx 0}{\beta_t}}$: Hyper Parameter.

DDPM ⟷ Langevin dynamics

$x_t = \sqrt{1-\beta_t}\cdot x_{t-1} + \sqrt{\beta_t}\cdot\varepsilon_t$ start

$= \left(1 - \frac{1}{2}\beta_t + O(\beta_t)^2\right)\cdot x_{t-1} + \sqrt{\beta_t}\,\varepsilon_t$

$= x_{t-1} \boxed{-} \frac{1}{2}\beta_t \boxed{x_{t-1}} + \sqrt{\beta_t}\cdot\varepsilon_t$

$-x_{t-1} = \nabla_x \log p(x_{t-1}) \quad (\beta_t = \delta)$

$= x_{t-1} + \frac{\delta}{2}\nabla_x \log p(x_{t-1}) + \sqrt{\delta}\cdot\varepsilon_t$ fin.

즉, $(T\to\infty) \rightarrow (\delta\to 0) \rightarrow$ ($x_t \rightarrow$ 정규분포)
$(\sqrt{\beta_t}\to 0)$ $\qquad \parallel$
노이즈 그자체
$N(0, I)$

cf) $0 + \sigma_1\cdot\varepsilon_1 \sim N(0, \sigma_1^2 I)$
$0 + \sigma_2\cdot\varepsilon_2 \sim N(0, \sigma_2^2 I)$
$\rightarrow 0 + \sqrt{\sigma_1^2+\sigma_2^2}\cdot\varepsilon \sim N(0, (\sigma_1^2+\sigma_2^2) I)$

cf) $\bar{\alpha}_1 > \cdots > \bar{\alpha}_T$ = 노이즈
$\beta_1 < \cdots < \beta_T$ = 1 - 노이즈

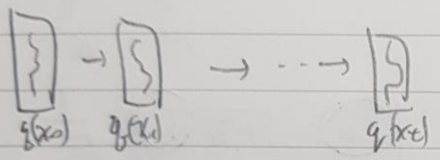
핵심 복기

Denoising

DDPM = Anderson's reverse time SDE

- 그림의 다양성
- 속도 느림
- 각 단계마다 분포변

○ 돌아올때 주사위로 확률성증가



이건 DDIM과 같다.

DDIM = Fokker Planck equation

- 돌아올 때 주사위 안던짐
- 미분방정식 씀.

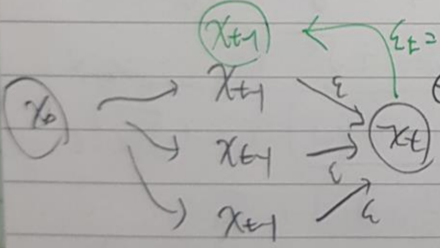
$\nabla_{x_t} \log q_t(x_0)$에 쓰임.

$\epsilon_\theta(x_t, t)$

용표 SS

$\epsilon_t = \epsilon_t(x_t | x_0)$ 쓰임

④ 새로운 ϵ 쓰임.



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

$\tilde{\mu}(x_t, x_0) = \mu$, $\tilde{\beta}_t I = \sigma^2$

④ $q(x_{t-1} | x_t)$: 어렵다.

$$q(x_{t-1} | x_t, x_0) = q(x_t | x_{t-1}, \cancel{x_0}) \cdot \frac{q(x_{t-1} | x_0)}{q(x_t | x_0)}$$

④ $q(x_t | x_{t-1}) = \mathcal{N}(x_t ; \sqrt{1-\beta_t}\, x_{t-1}, \beta_t I)$

$\mathcal{N}(x_t ; \sqrt{\alpha_t}\, x_{t-1}, (1-\alpha_t) I)$

$$q(x_t | x_0) = \mathcal{N}(x_t ; \sqrt{\bar{\alpha}_t} \cdot x_0, (1-\bar{\alpha}_t) \cdot I)$$

$$q(x_{t-1} | x_t, x_0) = q(x_t | x_{t-1}) \cdot \frac{q(x_{t-1} | x_0)}{q(x_t | x_0)}$$

start 1

$$= C_0 \exp\left(-\frac{1}{2} \frac{(x_t - \sqrt{\alpha_t}\, x_{t-1})^2}{\beta_t} + -\frac{1}{2} \frac{(x_{t-1} - \sqrt{\bar{\alpha}_{t-1}} \cdot x_0)^2}{(1-\bar{\alpha}_{t-1})} + \frac{1}{2} \frac{(x_t - \sqrt{\bar{\alpha}_t} \cdot x_0)^2}{1-\bar{\alpha}_t} \right)$$

$$= C_0 \exp -\frac{1}{2} \left(\frac{x_t^2 - 2\sqrt{\alpha_t}\, x_t x_{t-1} + x_{t-1}^2 \alpha_t}{\beta_t} + \frac{x_{t-1}^2 - 2\sqrt{\bar{\alpha}_{t-1}} \cdot x_0 x_{t-1} + x_0^2 \cdot \bar{\alpha}_{t-1}}{1-\bar{\alpha}_{t-1}} - \frac{x_t^2 - 2\sqrt{\bar{\alpha}_t} \cdot x_0 x_t + \bar{\alpha}_t x_0^2}{1-\bar{\alpha}_t} \right)$$

$$= C_0 \exp -\frac{1}{2} \left(\left(\frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}} \right) x_{t-1}^2 + \left(\frac{-2\sqrt{\alpha_t}\, x_t}{\beta_t} + \frac{-2\sqrt{\bar{\alpha}_{t-1}}\, x_0}{1-\bar{\alpha}_{t-1}} \right) x_{t-1} + C \right)$$

식1

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

start 2

$$= C_0 \cdot \exp -\frac{1}{2} \left(\frac{(x_{t-1} - \tilde{\mu}(x_t, x_0))^2}{\tilde{\beta}_t} \right)$$

$$= \frac{x_{t-1}^2 - 2\tilde{\mu}(x_t, x_0) x_{t-1} + (\tilde{\mu}(x_t, x_0))^2}{\tilde{\beta}_t}$$

식2

식1 = 식2

$$\frac{1}{\tilde{\beta}_t} = \frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}}$$

$$\frac{-2\tilde{\mu}(x_t, x_0)}{\tilde{\beta}_t} = \frac{-2\sqrt{\alpha_t}\, x_t}{\beta_t} + \frac{-2\sqrt{\bar{\alpha}_{t-1}} \cdot x_0}{1-\bar{\alpha}_{t-1}}$$

$$\tilde{\beta}_t = \left(\frac{\alpha_t(1-\bar{\alpha}_{t-1}) + \overset{1-\alpha_t}{\beta_t}}{\beta_t(1-\bar{\alpha}_{t-1})}\right)^{-1}$$

$$= \frac{\beta_t(1-\bar{\alpha}_{t-1})}{1-\underbrace{\alpha_t\bar{\alpha}_{t-1}}_{\bar{\alpha}_t}}$$

$$= \left(\frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\right)\cdot\beta_t$$

$$\tilde{\mu}(x_t, x_0) = \frac{\tilde{\beta}_t}{-2}\cdot\left(\frac{-2\sqrt{\alpha_t}\,x_t}{\beta_t} + \frac{-2\sqrt{\bar{\alpha}_{t-1}}\cdot x_0}{1-\bar{\alpha}_{t-1}}\right)$$

$$= \frac{1}{-2}\cdot\frac{\cancel{1-\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_t}\cancel{\beta_t}$$

$$\times\frac{-2x_t\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1}) + \beta_t x_0\sqrt{\bar{\alpha}_{t-1}}(-2)}{\cancel{\beta_t}(\cancel{1-\bar{\alpha}_{t-1}})}$$

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

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

$$= \left(\frac{1}{1-\bar{\alpha}_t}\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1}) + \frac{\beta_t\cancel{\sqrt{\bar{\alpha}_{t-1}}}}{(1-\bar{\alpha}_t)\cancel{\sqrt{\bar{\alpha}_t}}\sqrt{\alpha_t}}\right)x_t - \frac{\overset{(1-\alpha_t)}{\beta_t}\cancel{\sqrt{\bar{\alpha}_{t-1}}}}{\sqrt{1-\bar{\alpha}_t}\cancel{\sqrt{\bar{\alpha}_t}}\sqrt{\alpha_t}}\epsilon_t$$

$$= \left(\frac{\cancel{\alpha_t} - \bar{\alpha}_t + 1 - \cancel{\alpha_t}}{(\cancel{1-\bar{\alpha}_t})\cdot\sqrt{\alpha_t}}\right)x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\cdot\frac{1}{\sqrt{\alpha_t}}\cdot\epsilon_t$$

$$= \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_t\right) \quad (1)$$

Date

$$\therefore x_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\underset{\epsilon_t(x_t|x_0)}{\epsilon_t}\right) + \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\cdot\beta_t\,\epsilon$$

의미 ① $x_t \to x_0$ 방향

② $x_t \to x_{t-1}$ 의 평균값

③ x_0 아마 아음.

$$\epsilon_\theta(x_t, t) = \int \epsilon_t(x_t|x_0)\, q(x_0|x_t)\, dx_0$$

목표) $\left|\epsilon_t(x_t|x_0) - \epsilon_\theta(x_t, t)\right|^2 \downarrow$

→ $\epsilon_\theta(x_t, t)$가 다양한 x_0의 영향 골고루 받게 됨.

이제 $\epsilon_t = \epsilon_t(x_t|x_0) = \text{target}$

$\epsilon_\theta(x_t, t)$ 로 하자. $= y$ (예측)

결). $\epsilon_\theta(x_t, t) = \int \epsilon_t(x_t|x_0)\, q(x_0|x_t)\cdot dx_0$

의미
① 다양한 x_0 영향받음 = $\epsilon_t(x_t|x_0)$의 가중값.
② $q(x_0)$의 영향 받음.
③ x_t의 영향 받음.
④. t단계인 x_t의 noise 예측값
⑤ 다양한 x_0분포 고려하여 ϵ_t 예측.

Loss function

$$-\log p_\theta(x_0) \le -\log p_\theta(x_0) + D_{KL}\left(q(x_{1:T}|x_0) \,\|\, p_\theta(x_{1:T}|x_0)\right)$$

$$= E_{x_{1:T} \sim q\, x(1:T|x_0)}\left[\log \frac{q(x_{1:T}|x_0)}{p_\theta(x_{0:T})}\right]$$

$$-E_{q(x_0)} \log p_\theta(x_0) \le E_{q(x_{0:T})}\left[\log \frac{q(x_{1:T}|x_0)}{p_\theta(x_{0:T})}\right]$$

$$= L_{VLB} \downarrow$$

최소화 의미.

$p_\theta \approx q$.

$$L_{VLB} = E_{q(x_0)}\left[D_{KL}\, q(x_t|x_0) \,\|\, p_\theta(x_t)\right] + \sum_{t=2}^{T} E_{q(x_t, x_0)}\left[D_{KL}\, q(x_{t-1}|x_t, x_0) \,\|\, p_\theta(x_{t-1}|x_t)\right] - E_{q(x_0, x_1)}\left[\log p_\theta(x_0|x_1)\right]$$

기본 diffusion

Date

$Q \longrightarrow A$

x_t = 완전노이즈

x_0 = 그림

2) classifier guided Diffusion / guided-free Diffusion

$Q \longrightarrow A$

입력 원하는 거 + x_t = 완전노이즈

x_0 = 원하는 입력에 대한 그림

실은 <학습>에서는

$$Q \longrightarrow y \approx \epsilon_t(x_t|x_0), \quad y = \epsilon(x_t, t), \quad t$$

다양한 x_0 = 이미지

[illegible]) $x_T \underset{q}{\overset{q\,/\,p_\theta}{\rightleftarrows}} x_0$

pf) Loss function)

$$-\log p_\theta(x_0) \le -\log p_\theta(x_0) + D_{KL}\left(q(x_{1:T}|x_0) \,\|\, p_\theta(x_{1:T}|x_0)\right) \quad \cdots \text{①}$$

$$D_{KL}\left(q(x_{1:T}|x_0) \,\|\, p_\theta(x_{1:T}|x_0)\right) = \sum_{x_{1:T}} -q(x_{1:T}|x_0)\cdot\log\frac{p_\theta(x_{1:T}|x_0)}{q(x_{1:T}|x_0)}$$

$$= \sum_{x_{1:T}} + q(x_{1:T}|x_0)\log\frac{q(x_{1:T}|x_0)}{p_\theta(x_{1:T}|x_0)}$$

✓ $\left(p_\theta(x_{1:T}|x_0) = \dfrac{p_\theta(x_{0:T})}{p_\theta(x_0)} \quad \because p(A|B) = \dfrac{p(A,B)}{p(B)} \right)$

$$= \sum_{x_{1:T}} q(x_{1:T}|x_0)\cdot\log\frac{q(x_{1:T}|x_0)}{p_\theta(x_{0:T}|x_0)/p_\theta(x_0)}$$

$$= E_{x_{1:T}\sim q(x_{1:T}|x_0)}\left[\log\frac{q(x_{1:T}|x_0)}{p_\theta(x_{0:T}|x_0)} + \log p_\theta(x_0)\right]$$

by ①,

$$-\log p_\theta(x_0) \le \cancel{-\log p_\theta(x_0)} + E_{x_{1:T}\sim q(x_{1:T}|x_0)}\left[\log\frac{q(x_{1:T}|x_0)}{p_\theta(x_{0:T}|x_0)}\right] + \cancel{\log p_\theta(x_0)}$$

$$-E_{q(x_0)}\left[\log p_\theta(x_0)\right] \le E_{q(x_0)}\left[E_{x_{1:T}\sim q(x_{1:T}|x_0)}\left[\log\frac{q(x_{1:T}|x_0)}{p_\theta(x_{0:T}|x_0)}\right]\right]$$

$$\| $$

$\sum q(x_0)\cdot\sum_{x_{1:T}} q(x_{1:T}|x_0)$ 식.

$$\|$$

✓ $\sum \cancel{q(x_0)}\cdot\dfrac{q(x_{0:T})}{\cancel{q(x_0)}}\cdot$ 식

$$\|$$

$E_{q(x_{0:T})}[$식$]$

$$\|$$

$$L_{VLB} = E_{q(x_{0:T})}\left[\log\frac{q(x_{1:T}|x_0)}{p_\theta(x_{0:T})}\right]$$

$L_{VLB}\downarrow \;\rightarrow\; p_\theta \approx q$

$$L_{VLB} = E_{q(x_{0:T})}\left[\log\frac{q(x_{1:T}|x_0)}{p_\theta(x_{0:T})}\right]$$

$$q(x_{1:T}|x_0) = q(x_1, x_2, \cdots x_t) = q(x_t|x_{t-1})\times\cdots\times q(x_1|x_0) = \prod_1^T q(x_t|x_{t-1})$$

$$p_\theta(x_{0:T}) = p_\theta(x_0, x_1, \cdots, x_T) = p(x_T)\cdot p_\theta(x_0|x_1)\cdot p_\theta(x_1|x_2)\times\cdots\times p_\theta(x_{t-1}|x_t) = p(x_T)\cdot\prod_1^T p_\theta(x_{t-1}|x_t)$$

✓ $$L_{VLB} = E_{q(x_{0:T})}\left[\log\frac{\prod_1^T q(x_t|x_{t-1})}{p_\theta(x_T)\cdot\prod_1^T p_\theta(x_{t-1}|x_t)}\right]$$

$$q(x_t|x_{t-1}) = \frac{q(x_{t-1}|x_t)\cdot q(x_t)}{q(x_{t-1})} = \frac{q(x_{t-1}|x_t)\, q(x_t|x_0)}{q(x_{t-1}|x_0)}$$

✓ $$L_{VLB} = E_{q(x_{0:T})}\left[-\log p(x_T) + \sum_1^T \log\frac{q(x_{t-1}|x_t)\cdot q(x_t|x_0)}{p_\theta(x_{t-1}|x_t)\, q(x_{t-1}|x_0)}\right]$$

✓ $$= E_{q(x_{0:T})}\left[-\log p(x_T) + \sum_2^T \log\frac{q(x_{t-1}|x_t)\cdot q(x_t|x_0)}{p_\theta(x_{t-1}|x_t)\cdot q(x_{t-1}|x_0)} + \log\frac{\cancel{q(x_0|x_1)}\, q(x_1|x_0)}{p_\theta(x_0|x_1)\cdot \cancel{q(x_0|x_0)}}\right]$$

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$$L_{VLB} = \mathbb{E}_{q(x_{0:T})}\left[-\log p_\theta(x_T) + \sum_{t=2}^{T} \log \frac{q(x_{t-1}|x_t,x_0)}{p_\theta(x_{t-1}|x_t)} + \sum_{t=2}^{T} \log \frac{q(x_t|x_0)}{q(x_{t-1}|x_0)} + \log \frac{q(x_1|x_0)}{p_\theta(x_0|x_1)} \right]$$

$$\sum_{t=2}^{T} \log \frac{q(x_t|x_0)}{q(x_{t-1}|x_0)} = \log \frac{\cancel{q(x_2|x_0)}}{q(x_1|x_0)} \frac{\cancel{q(x_3|x_0)}}{\cancel{q(x_2|x_0)}} \cdots \frac{q(x_T|x_0)}{\cancel{}} = \log \frac{q(x_T|x_0)}{q(x_1|x_0)}$$

$$= \mathbb{E}_{q(x_{0:T})}\left[-\log p_\theta(x_T) + \log q(x_T|x_0) + \sum_{t=2}^{T} \log \frac{q(x_{t-1}|x_t,x_0)}{p_\theta(x_{t-1}|x_t)} + \cancel{\log q(x_1|x_0)} - \cancel{\log q(x_1|x_0)} - \log p_\theta(x_0|x_1) \right]$$

$$\sum_{x_0,x_1\cdots x_T} q(x_0,x_1\cdots x_T)\cdot 식$$
$$\sum_{x_0,x_T} q(x_0,x_T)\ 식$$
$$\sum_{x_0,x_T} q(x_0)\cdot q(x_T|x_0)\cdot 식$$
$$\sum_{x_0} q(x_0)\cdot \sum_{x_T} q(x_T|x_0)\ 식$$
$$\mathbb{E}_{q(x_0)}\left[\mathbb{E}_{q(x_T|x_0)}[식]\right]$$

$$\sum_{x_0,\cdots x_T} q(x_0,\cdots x_T)\ 식$$
$$\sum_{x_0,x_t,x_{t-1}} q(x_0,x_{t-1},x_t)\cdot 식$$
$$\sum_{x_0,x_t,x_{t-1}} q(x_t,x_0)\, q(x_{t-1}|x_t,x_0)\cdot 식$$
$$\sum_{x_t,x_0} q(x_t,x_0) \sum_{x_{t-1}} q(x_{t-1}|x_t,x_0)\cdot 식$$
$$\mathbb{E}_{q(x_t,x_0)}\left[\mathbb{E}_{q(x_{t-1}|x_t,x_0)}[식]\right]$$

$$= \Bigg(\mathbb{E}_{q(x_{0:T})}\left[\log \frac{q(x_T|x_0)}{p_\theta(x_T)}\right] = \mathbb{E}_{q(x_0)}\left[\mathbb{E}_{q(x_T|x_0)} \log \frac{q(x_T|x_0)}{p_\theta(x_T)}\right] = \mathbb{E}_{q(x_0)}\left[D_{KL}\left(q(x_T|x_0)\,\|\,p_\theta(x_T)\right)\right]$$

$$+ \sum_{t=2}^{T} \mathbb{E}_{q(x_{0:T})}\left[\log \frac{q(x_{t-1}|x_t,x_0)}{p_\theta(x_{t-1}|x_t)}\right] = \mathbb{E}_{q(x_t,x_0)}\left[\mathbb{E}_{q(x_{t-1}|x_t,x_0)} \log \frac{q(x_{t-1}|x_t,x_0)}{p_\theta(x_{t-1}|x_t)}\right] = \mathbb{E}_{q(x_t,x_0)}\left[D_{KL}\left(q(x_{t-1}|x_t,x_0)\,\|\,p_\theta(x_{t-1}|x_t)\right)\right]$$

$$- \mathbb{E}_{q(x_{0:T})}\left[\log p_\theta(x_0|x_1)\right] = -\mathbb{E}_{q(x_0,x_1)}\left[\log p_\theta(x_0|x_1)\right] \Bigg)$$

$$= \underbrace{\mathbb{E}_{q(x_0)}\left[D_{KL}\left(q(x_T|x_0)\,\|\,p_\theta(x_T)\right)\right]}_{\approx\, 0} + \sum_{t=2}^{T} \mathbb{E}_{q(x_t,x_0)}\left[D_{KL}\left(q(x_{t-1}|x_t,x_0)\,\|\,p_\theta(x_{t-1}|x_t)\right)\right] - \underbrace{\mathbb{E}_{q(x_0,x_1)}\left[\log p_\theta(x_0|x_1)\right]}_{\approx\, \beta\ \approx\, 0}$$

$\because q(x_T|x_0) \approx p_\theta(x_T) \approx N(0,I)$ = 노이즈.

β = Control 가능

Date

μ_q

f). $q(x_{t-1} \mid x_t, x_0) = \mathcal{N}\left(\boxed{\frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\,\varepsilon_t(x_t \mid x_0)\right)},\ \beta_t I\right)$

$p_\theta(x_{t-1} \mid x_t) = \mathcal{N}\left(\underbrace{\boxed{\frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\,\varepsilon_\theta(x_t, t)\right)}}_{\mu_p},\ \Sigma_\theta(x_t, t)\right)$

$$D_{KL}(p \| q) = \frac{1}{2}\left[\log\frac{|\Sigma_q|}{|\Sigma_p|} - k + (\mu_p - \mu_q)^t \cdot \Sigma_q^{-1} \cdot (\mu_p - \mu_q) + tr(\Sigma_q^{-1}\Sigma_p)\right]$$

C.

$$\sum_{t=2}^{T} E_{q(x_t, x_0)}\left[D_{KL}\left(q(x_{t-1} \mid x_t, x_0) \,\|\, p_\theta(x_{t-1} \mid x_t)\right)\right]$$

$$= \sum_{t=2}^{T} E_{q(x_t, x_0)}\left[\frac{1}{2} \cdot \frac{1}{|\Sigma_\theta(x_t, t)|_2^2}(\mu_q - \mu_p)^2 + C\right]$$

$$= \sum_{t=2}^{T} E_{x_0, \varepsilon}\left[\frac{1}{2}\frac{1}{|\Sigma_\theta|_2^2} \cdot \left(\cancel{\frac{1}{\sqrt{\alpha_t}} x_t} - \frac{1-\alpha_t}{\sqrt{\alpha_t}\sqrt{1-\bar{\alpha}_t}}\varepsilon_t(x_t \mid x_0) - \cancel{\frac{1}{\sqrt{\alpha_t}} x_t} + \frac{1-\alpha_t}{\sqrt{\alpha_t}\sqrt{1-\bar{\alpha}_t}}\varepsilon_\theta(x_t, t)\right)^2 + C\right]$$

$$= \sum_{t=2}^{T} E_{x_0, \varepsilon}\left[\cancel{\frac{1}{2|\Sigma_\theta|_2^2}\frac{(1-\alpha_t)^2}{\alpha_t(1-\bar{\alpha}_t)}}\left(\varepsilon_t(x_t \mid x_0) - \varepsilon_\theta(x_t, t)\right)^2 \cancel{+ C}\right]$$

그냥 무시. 그냥 무시.

(∵ 이렇게 하는것이 경험적으로 잘 되서)

$$= E_{t \sim [1, T], x_0, \varepsilon_t}\left[\left\| \varepsilon_t(x_t \mid x_0) - \varepsilon_\theta(x_t, t) \right\|^2\right]$$

$$= E_{t \sim [1, T], x_0, \varepsilon_t}\left[\left\| \varepsilon_t(x_t \mid x_0) - \varepsilon_\theta\left(\sqrt{\bar{\alpha}_t} x_0 + \sqrt{1-\bar{\alpha}_t}\cdot\varepsilon, t\right) \right\|^2\right]$$ 최소화하자.

이후

supervised learning.

$Q \to y \approx t$

$\varepsilon_\theta(x_t, t) \quad \varepsilon_t(x_t \mid x_0)$

step 1. 학습

$x_0 \sim q(x_0)$, $\varepsilon \sim \mathcal{N}(0, I)$

$\nabla_\theta \left\| \varepsilon_t(x_t \mid x_0) - \varepsilon_\theta\left(\sqrt{\bar{\alpha}_t}\cdot x_0 + \sqrt{1-\bar{\alpha}_t}\cdot\varepsilon, t\right) \right\|^2$

$\hookrightarrow \varepsilon_\theta(x_t, t) = \int_{S(x_0)} \varepsilon_t(x_t \mid x_0) \cdot q(x_0 \mid x_t)\, dx_0$

코 나옴.

step 2. 이미지 생성

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

$x_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \sqrt{\frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}}\,\varepsilon_\theta(x_t, t)\right) + \sigma_t z$

$Q \to A$.

x_t (= 노이즈) $\quad x_0$.

ibis

학습 생성 쉽게 쉽게 loss function (푸리에)

ELBO

Date

c) p_θ 에서 분산은?

$$\| \quad \Sigma_\theta(x_t, t) \quad \| \quad \beta_t^{v} \cdot \tilde{\beta}_t^{1-v}$$

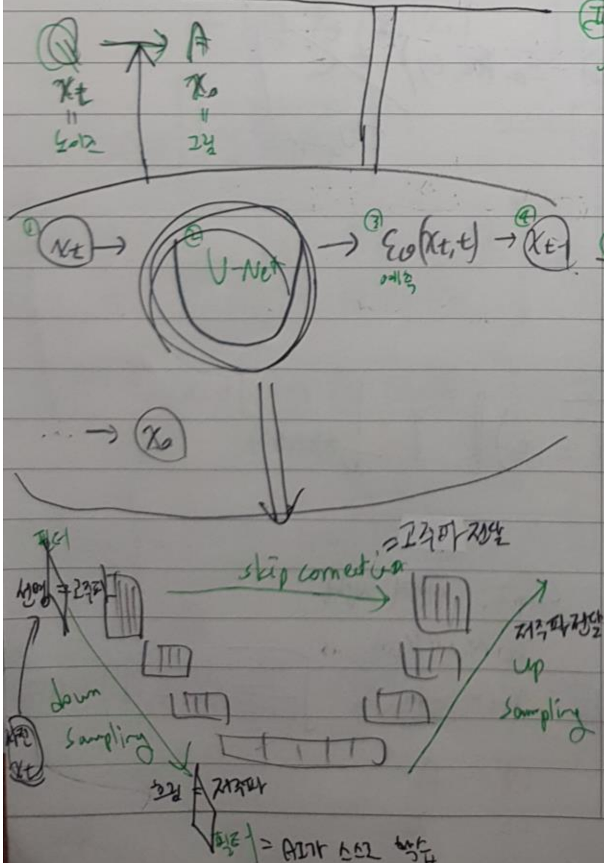
즉 [β_t (x_0 앎) / $\tilde{\beta}_t$ (x_0 모름)] 섞어서 쓰자는 의미

step 2. 이미지 생성

에서 U-Net / 푸리에 series 쓰임.

$x_t \sim N(0, I)$

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



푸리에 series

- 저주파 : 함수의 큰 틀 설명
- 고주파 : 함수의 미세 부분 설명
- 미분가능성 L_2-norm 의 $(a_n^2 + b_n^2)$ ↓ 빠르게 작아져야 미분이 잘된다.
  ≃ 매끄러워진다.
- 내적하면 0이 되는 성분있다.

증명하기

Ⅰ $\epsilon_\theta(x, t) = \int \epsilon_t(x_t|x_0) \cdot q(x_0|x_t)\, dx_0$

Ⅱ $\nabla_{x_t} \log q(x_t|x_0) = \frac{-1}{\sqrt{1-\bar{\alpha}_t}} \cdot \epsilon_t(x_t|x_0)$

Ⅲ $\nabla_{x_t} \log q(x_t) = \frac{-1}{\sqrt{1-\bar{\alpha}_t}} \cdot \epsilon_\theta(x_t, t)$

pf) Ⅱ)

$$x_t = \sqrt{\bar{\alpha}_t} \cdot x_0 + \sqrt{1-\bar{\alpha}_t} \cdot \epsilon_t(x_t|x_0)$$

$$\epsilon_t(x_t|x_0) = (x_t - \sqrt{\bar{\alpha}_t} \cdot x_0) \cdot \frac{1}{\sqrt{1-\bar{\alpha}_t}}$$

$$q(x_t|x_0) = N(x_t ; \sqrt{\bar{\alpha}_t} x_0, 1-\bar{\alpha}_t)$$

$$= C \cdot \exp\left(\frac{-1}{2} \cdot \frac{1}{(1-\bar{\alpha}_t)} \cdot (x_t - \sqrt{\bar{\alpha}_t} \cdot x_0)^2\right)$$

$$\nabla_{x_t} \log q(x_t|x_0)$$

$$= \frac{-1}{2} \cdot 2 \cdot \boxed{\frac{x_t - \sqrt{\bar{\alpha}_t} \cdot x_0}{(1-\bar{\alpha}_t)}}$$

$$= -\frac{1}{\sqrt{1-\bar{\alpha}_t}} \cdot \epsilon_t(x_t|x_0)$$

☑

pf) (I))

$\epsilon_\theta(x_t,t) = f_*(x_t)$

$$\epsilon_\theta(x_t,t) = \arg\min_{f(\cdot)} \mathop{E}_{x_0\sim q(x_0)}\left[\mathop{E}_{x_t\sim q(x_t|x_0)}\left[\|\epsilon_t(x_t|x_0) - f(x_t)\|^2\right]\right]$$

$h(\cdot)$를 임의적으로 설정.

$(f_* + sh)(x_t) = f_*(x_t) + sh(x_t)$

$$F_h(s) = \mathop{E}_{x_0\sim q(x_0)}\left[\mathop{E}_{x_t\sim q(x_t|x_0)}\left[\|\epsilon_t(x_t|x_0) - (f_*+sh)(x_t)\|^2\right]\right]$$

$s=0$ 일때

$F_h(s)$ 가 최소가 됨

$\rightarrow (F_h)'(0) = 0.$

$$(F_h)'(0) = 0 = \mathop{E}_{x_0\sim q(x_0)}\left[\mathop{E}_{x_t\sim q(x_t|x_0)} 2\|\epsilon_t(x_t|x_0) - (f_*)(x_t)\| \cdot (-h(x_t))\right]$$

$$0 = \mathop{E}_{x_0\sim q(x_0)}\left[\mathop{E}_{x_t\sim q(x_t|x_0)}\left[\|\epsilon_t(x_t|x_0) - f_*(x_t)\| \cdot h(x_t)\right]\right]$$

$$0 = \int_{\Omega(x_0)}\int_{\Omega(x_t)} \left(\epsilon_t(x_t|x_0) - f_*(x_t)\right)\cdot \boxed{h(x_t)}\, q(x_t|x_0)\, \boxed{d(x_t)}\ \underline{q(x_0)\,dx_0}$$

$$= \int_{\Omega(x_t)} \underbrace{\left(\int_{\Omega(x_0)} \left(\epsilon_t(x_t|x_0) - f_*(x_t)\right)\cdot q(x_t|x_0)\cdot q(x_0)\, dx_0\right)}_{= g(x_t)} \cdot h(x_t)\, d(x_t) \quad \checkmark$$

$\Rightarrow h(x_t)$는 아무거나 상관X

$\rightarrow h(x_t) = g(x_t)$ 라 가정.

$$0 = \int_{\Omega(x_t)} (g(x_t))^2\, dx_t$$

$$\rightarrow g(x_t) = 0 = \int_{\Omega(x_0)} \left(\epsilon_t(x_t|x_0) - f_*(x_t)\right)\cdot q(x_t|x_0)\cdot q(x_0)\, dx_0$$

$$= \int_{\Omega(x_0)} \left(\epsilon_t(x_t|x_0) - f_*(x_t)\right)\cdot q(x_t, x_0)\, dx_0 \quad \checkmark$$

$$\rightarrow \int_{\Omega(x_0)} \epsilon_t(x_t|x_0)\cdot q(x_t,x_0)\, dx_0 = f_*(x_t)\cdot q(x_t) \text{ (Marginalization)} \quad \checkmark$$

$$\rightarrow f_*(x_t) = \underline{\epsilon_\theta(x_t,t) = \int \epsilon_t(x_t|x_0)\cdot q(x_0|x_t)\, dx_0}$$

+) (Ⅳ))

$$f_*(x_t)\cdot q(x_t) = \int \underbrace{\boxed{\varepsilon_t(x_t|x_0)}}_{(\text{by Ⅱ})} \cdot q(x_t, x_0)\, dx_0$$

$$= \int \left(-\sqrt{1-\bar{\alpha}_t}\right) \cdot \nabla_{x_t} \log q(x_t|x_0) \cdot q(x_t, x_0)\, dx_0$$

$$= -\sqrt{1-\bar{\alpha}_t} \cdot \int \frac{\nabla_{x_t} q(x_t|x_0)}{\cancel{q(x_t|x_0)}}\, \cancel{q(x_t|x_0)} \cdot q(x_0)\, dx_0$$

$$= -\sqrt{1-\bar{\alpha}_t} \int \nabla_{x_t} q(x_t|x_0) \cdot q(x_0)\, dx_0$$

$$= -\sqrt{1-\bar{\alpha}_t} \cdot \nabla_{x_t} \underbrace{\int q(x_t, x_0)\, dx_0}_{\text{marginalization}}$$

$$= -\sqrt{1-\bar{\alpha}_t} \cdot \nabla_{x_t} \cdot q(x_t)$$

$$\rightarrow f_*(x_t) = -\sqrt{1-\bar{\alpha}_t} \cdot \frac{\nabla_{x_t} \cdot q(x_t)}{q(x_t)}$$

$$\varepsilon_\theta(x_t, t) = -\sqrt{1-\bar{\alpha}_t} \cdot \nabla_{x_t} \log q(x_t)$$

$$\rightarrow \nabla_{x_t} \log q(x_t) = \frac{-1}{\sqrt{1-\bar{\alpha}_t}}\, \varepsilon_\theta(x_t, t) \quad \boxed{Ⅳ} \quad Ⅳ$$

Classifier guided Diffusion

(단점) $T=1000$ 이라서 1000개의 classifier 가 필요

→나중에 guided free diffusion 나옴

$$\nabla_{x_t} \log P(x_t|y) = \nabla_{x_t} \log \frac{P(y|x_t)\cdot P(x_t)}{P(y)}$$

$$= \nabla_{x_t} \log\left(P(y|x_t)\cdot P(x_t)\right) - \cancel{\nabla_{x_t} P(y)}$$

$$= \nabla_{x_t} \log P(x_t) + \nabla_{x_t} \log P(y|x_t)$$

$$= \frac{-1}{\sqrt{1-\bar{\alpha}_t}}\, \varepsilon_\theta(x_t, t) + \nabla_{x_t} \log P(y|x_t)$$

원래는 $P(x_t|y)$ 여서 [illegible] y 일때 x_t에 대한 확률

이제는 노이즈 x_t 보고 그 x_t가 뭔지에 대한 classifier 로 바뀜!

$$\underbrace{-\sqrt{1-\bar{\alpha}_t}\cdot \nabla_{x_t} \log P(x_t|y)}_{\parallel} = \boxed{\varepsilon_\theta(x_t, t) - \sqrt{1-\bar{\alpha}_t}\cdot \nabla_{x_t} \log P(y|x_t)}$$

① $\varepsilon_\theta(x_t|y)$ 만듦

② $\boxed{x_{t-1}} = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\, \varepsilon_\theta(x_t|y)\right) + \sigma_t \cdot z$

이렇게 $\boxed{x_0}$ 생성.

ELBO

$$P(y^*|x^*, D) = \int P(y^*|x^*, w)\, \boxed{P(w|D)}\, dw$$

목표 $\quad \| \quad q_\theta(w)$

$$0 \le \underbrace{KL\left(q_\theta(w) \,\|\, P(w|D)\right)}_{\text{목표}} \downarrow = \int q_\theta(w) \cdot \log \frac{q_\theta(w)}{P(w|D)}\, dw$$

Q1.

$$= \int q_\theta(w) \left[\log q_\theta(w) - \log P(w|D)\right] dw$$

$$= \int q_\theta(w) \left[\log q_\theta(w) - \log \frac{P(D|w) \cdot P(w)}{P(D)}\right] dw \quad \checkmark$$

$$= \int q_\theta(w) \log \frac{q_\theta(w)}{P(w)}\, dw - \int q_\theta(w) \cdot \log P(D|w)\, dw + \int q_\theta(w) \cdot \log P(D)\, dw \quad \checkmark$$

$$= KL\left(q_\theta(w) \,\|\, P(w)\right) - \int q_\theta(w) \cdot \log P(D|w)\, dw + \log P(D)$$

$$\rightarrow KL\left(q_\theta(w) \,\|\, P(w|D)\right) \boxed{- KL\left(q_\theta(w) \,\|\, P(w)\right) + \int q_\theta(w) \cdot \log P(D|w)\, dw} = \log P(D)$$

$$\rightarrow \quad 0 \quad + \quad \underset{\text{ELBO}}{\|} \quad \le \quad \underset{\text{evidence.}}{\Downarrow}$$

(∵ 만약 $q_\theta(w) \approx P(w|D)$ 라면)

ELBO = Evidence Lower Bound

Q2.

ELBO $\uparrow$ → $\log P(D)$에 가까워짐.

→ $KL\left(q_\theta(w) \,\|\, p(w|D)\right) \downarrow$

→ $q_\theta(w) \approx P(w|D)$ 목표

Date

$$ELBO = -\int q_{\theta}(w) \log P(D|w)\, dw - KL(q_{\theta}(w) \| P(w)) \leq \log P(D)$$

$$= \underset{w \sim q_{\theta}(w)}{E}[\log P(D|w)] \uparrow - KL(q_{\theta}(w) \| P(w)) \downarrow \leq \log P(D)$$

증가 감소

Q3.

$$= -\left(\underbrace{\underset{w \sim q_{\theta}(w)}{E}[-\log P(D|w)]}_{} \downarrow + \underbrace{KL(q_{\theta}(w) \| P(w))}_{} \uparrow\right) \leq \log P(D)$$

① MLE

③

$$① \sum_{i=1}^{N} \| f(x_i | w) - y_i \|^2 + \lambda \|w\|^2$$

② 이게 튀어나옴.

③. 즉 $KL(q_{\theta}(w) \| P(w)) \approx \lambda \|w\|^2$

Regularization

단순화해라

Occam's razor.

Q3. Data fitting term

$$\underset{w \sim q_{\theta}(w)}{E}[+\log P(D|w)]$$

Q3. KL Regulariser term / Occam's razor term

$$KL(q_{\theta}(w) \| P(w))$$

Q3. 이유?