forward SDE

$$\begin{cases} dx_t = f(x_t, t)\, dt + g(t)\, dW_t \\ \dfrac{\partial p_t(x)}{\partial t} = -\nabla \cdot [f(x,t)\, p_t(x)] + \frac{1}{2} g(t)^2 \Delta p_t(x) \end{cases}$$

---

let reverse time $\tau = T - t$

reverse SDE

$$\begin{cases} dx_\tau = \tilde{f}(x_\tau, t)\, \overset{-dt}{d\tau} + g(t)\, \overset{\approx\, dW_t}{d\bar{W}_\tau} \\ \dfrac{\partial p_t(x)}{\underset{-\partial t}{\partial \tau}} = -\nabla \cdot [f(x,t)\, p_t(x)] + \frac{1}{2} g(t)^2 \Delta p_t(x) \end{cases}$$

Matching distribution

$$\underbrace{-\nabla \cdot (fp) + \frac{1}{2} g^2 \Delta p}_{\text{forward}} = \underbrace{\nabla \cdot (\tilde{f} p) - \frac{1}{2} g^2 \Delta p}_{\text{reverse}}$$

$$\downarrow$$

$$\nabla \cdot \left((f + \tilde{f})\, p_t(x) \right) = g(t)^2 \Delta p_t(x)$$

$$= \nabla \cdot \left[g(t)^2 p_t(x) \nabla \log p_t(x) \right]$$

for $\tilde{f}(x,t) = -f(x,t) + g(t)^2 \nabla \log p_t(x)$

---

hence,

$$dx_t = \Big[f(x_t, t) - \underbrace{g(t)^2 \nabla \log p_t(x)}_{\text{고밀도 지역}} \Big] dt + g(t)\, d\bar{W}_t$$

$$x_{t-\Delta t} = x_t + \left[-f(x_t, t) + g(t)^2 \nabla \log p_t(x) \right] \Delta t + g(t) \sqrt{\Delta t}\, Z$$

OU Process

① $dX_t = -\beta X_t dt + \sigma dW_t$

② $X_t \mid X_0 \sim N(e^{-\beta t} X_0 , \sigma_t^2 I)$

(i) $\sigma_t^2 = \frac{\sigma^2}{2\beta}(1 - e^{-2\beta t})$

(ii) $X_t \mid X_0 \sim N(0, \frac{\sigma^2}{2\beta} I)$ when $t \to \infty$

③ $d\bar{X_t} = (-\beta X_t - \sigma^2 \nabla_x \log P_t) dt + \sigma d\bar{W_t}$

$$\frac{\partial P}{\partial t} = -\nabla \cdot (fp) + \frac{1}{2} g^2 \nabla^2 p^2$$

$$\begin{cases} p = x^3 + y^2 \\ \nabla p = (3x^2, 2y) \\ \nabla \cdot p = 3x^2 + 2y \\ \nabla^2 p = 6x + 2 \end{cases}$$

$d\bar{X_t} = \left(f(\bar{X_t}, t) - g^2(t) \nabla_x \log P_t(\bar{X_t})\right) dt + g(t) d\bar{W_t}$ (ODE) "품질, 다양성"

$d\bar{X_t} = \left(f(\bar{X_t}, t) - \frac{g^2(t)}{2} \nabla_x \log P_t(\bar{X_t})\right) dt$ (SDE) "속도, 편함"

$\Rightarrow$ same P_t (Fokker - Planck)

$\nabla_x \log_t P \approx S_\theta(x,t)$

$$\mathcal{L}(\theta) = \int_0^T \lambda(t) \mathbb{E}_{x_t\sim p_t}\left[\| S_\theta(x_t,t) - \nabla_{x_t}\log p_t(x_t)\|^2\right] dt$$

$$\begin{cases} \mathcal{L}_{DSM}(\theta) = \int_0^T \lambda(t)\, \mathbb{E}_{x_0} \mathbb{E}_{x_t|x_0}\left[\left\| S_\theta(x_t,t) - \nabla_{x_t}\log p_{t|0}(x_t|x_0)\right\|^2\right] dt \\ \mathcal{L}_{SSM}(\theta) = \int_0^T \lambda(t)\, \mathbb{E}_{x_t}\left[\|S_\theta(x_t,t)\|^2 + 2\,\mathbb{E}_v\left[\frac{d}{du} v^T S_\theta(x_t+hv,t)\Big|_{u=0}\right]\right] dt. \end{cases}$$

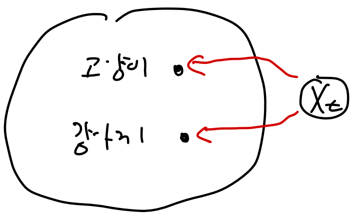
---

① $\nabla_{x_t}\log p_t(x_t) = \dfrac{\nabla_x p_t(x)}{p_t(x)} = \displaystyle\int \nabla_{x_t} p_{t|0}(x_t|x_0)\,\frac{p_0(x_0)}{p_t(x_t)}\, dx_0$

그럴따한 그림

$$= \int \nabla_{x_t} \log p_{t|0}(x_t|x_0)\cdot \underbrace{\frac{p_0(x_0)}{p_t(x_t)}\cdot p_{t|0}(x_t|x_0)}_{= p_{0|t}(x_0|x_t)}\, dx_0$$

그럴따한 그림



$$= \mathbb{E}_{x_0|x_t}\left[\nabla_{x_t}\log p_{t|0}(x_t|x_0)\right]$$

고양이 그림.
강아지 그림 .... 끝

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② $\mathcal{L}_{DSM}(\theta) = \int_0^T \lambda(t)\, \mathbb{E}_{x_t}\left[\|S_\theta(x_t,t) - \nabla_{x_t}\log p_t(x_t)\|^2\right] dt$

$$\therefore \quad = \lambda(t)\, \mathbb{E}_{x_t}\left[\|S_\theta\|^2 - 2\langle S_\theta, \nabla_{x_t}\log p_t(x_t)\rangle\right] + \|\nabla \cancel{\log p_t}\|^2$$

$$= \lambda(t)\, \mathbb{E}_{x_t, x_0}\left[\|S_\theta\|^2 - 2\{S_\theta, \nabla_{x_t}\log p(x_t|x_0)\rangle\right]$$

$$= \lambda(t)\, \mathbb{E}_{x_0}\mathbb{E}_{x_t|x_0}\left[\|S_\theta - \nabla_{x_t}\log p(x_t|x_0)\|^2 + \cancel{C}\right]$$

① $\mathcal{L}(\theta) = \int_0^T \lambda(t)\, \mathbb{E}_{X_t}\left[\| S_\theta(X_t, t) - \nabla_{X_t} \log p_t(X_t) \|^2\right] dt$

$$\Downarrow$$

$$\|S_\theta\|^2 - 2\langle S_\theta, \nabla \log p_t \rangle + \cancel{\| \nabla \log p_t \|^2}$$

$\langle S_\theta, \nabla \log p_t \rangle \Uparrow$

를 키워야 하는데, 모든 각도 v에서 줄 수 없다.

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② $\mathbb{E}_{X_t}\left[\langle S_\theta, \nabla \log p_t \rangle\right]$

$$= \int S_\theta(x)^T \cdot \nabla p_t(x)\, dx \qquad \left(\nabla \log p_t = \frac{\nabla p_t}{p_t} \right)$$

$$= -\int (\nabla \cdot S_\theta(x))\, p_t(x)\, dx \qquad \text{(부분적분)}$$

$$= -\mathbb{E}_{X_t}\left[\nabla \cdot S_\theta(x, t) \right] \qquad \text{(Jacobian)}$$

$$= Tr(D_x S_\theta(x, t))$$

Note : 부분적분. (1차원)

$$\cancel{\left[S_\theta(x)\, p(x) \right]_{-\infty}^{\infty}}$$

$$- \int_{-\infty}^{\infty} S_\theta'(x) \cdot p(x)\, dx.$$

---

③ $Tr(D_x S_\theta) = \mathbb{E}_v\left[v^T (D_x S_\theta) v \right]$

when $v \sim N(0, I)$

$$\left(\mathbb{E}_v\left[\sum_{i,j} A_{ij}\, v_i v_j \right] \right)$$

trace만 생존

---

④ $v^T (D_x S_\theta v) = v^T \left(\frac{d}{dh} S_\theta(x + hv, t) \Big|_{h=0} \right)$

---

⑤ $\mathcal{L}_{SSM}(\theta) = \int_0^T \lambda(t)\, \mathbb{E}_{X_t, v}\left[\|S_\theta(X_t, t)\|^2 + 2 \frac{d}{dh} v^T S_\theta(X_t + hv, t) \Big|_{h=0} \right] dt.$

- OU Process : $dX_t = -\beta X_t dt + \sigma dW_t$

- $X_t \mid X_0 \sim N(\mu_t, \Sigma_t)$

$$\boxed{\begin{aligned} \mu_t &= \gamma_t X_0 & \Sigma_t &= \sigma_t^2 I \\ &= e^{-\beta t} X_0 & &= \frac{\sigma^2}{2\beta}(1-e^{-2\beta t}) I \end{aligned}}$$

- $X_t = \gamma_t X_0 + \sigma_t \varepsilon \sim N(0, I)$

Score func

$$\nabla_{X_t} \log p(X_t \mid X_0) = -\frac{X_t - \gamma_t X_0}{\sigma_t^2} = -\frac{\varepsilon}{\sigma_t}$$

$\because$ $$p(x \mid \mu, \Sigma) = \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} \cdot \exp\left(-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)\right)$$

- let $S_\theta = -\dfrac{\varepsilon_\theta(x, t)}{\sigma_t}$

then $$\mathcal{L}(\theta) = \int_0^T \frac{\lambda(t)}{\cancel{\sigma_t^2}} \mathbb{E}_{X_0, \varepsilon}\left[\left\| \varepsilon_\theta(\gamma_t X_0 + \sigma_t \varepsilon, t) - \varepsilon \right\|^2 \right] dt .$$ (DSM)

---

① sample $t \sim \text{Uniform}(0, T)$

② " $x_0 \sim p_{data}$.

③ " $\varepsilon_0 \sim N(0, I)$

④ compute $X_t = \gamma_t X_0 + \sigma_t \varepsilon$

⑤ " $\mathcal{L}_\theta = \| \varepsilon_\theta(X_t, t) - \varepsilon \|^2$

⑥ update θ

Note. Reverse SDE

$$d\bar{X}_t = \left[\frac{\sigma^2}{\sigma_t} \cdot \varepsilon_\theta(\bar{X}_t, t) - \beta \bar{X}_t \right] dt + d\bar{W}_t$$