

DDPM

Mathematical Foundation

① Markov chain: No memory

Current is only relevant to the last state

e.g. $N \rightarrow N-1 \rightarrow N-2$

$x(t)$ is only dependent on $x(t-1)$ $P(x_t | x_{t-1})$

② Differentiable

$0 \longrightarrow 0$

↑ random sampling: no derivatives

$z \sim N(\mu, \sigma)$ use reparameterization



shift $N(\mu, \sigma)$ to $N(0, 1)$ - throws the randomness outside

Becomes $z := N(z; \mu, \sigma)$

$z = \mu + \overset{\text{dot product}}{\sigma \cdot \epsilon}$, where $\epsilon \sim N(0, 1)$

so z is differentiable, randomness gets thrown

Diffusion: time stamp $(0, 1, \dots, t, \dots, T)$

$\overset{t-1}{0} \xrightarrow{q} \overset{t}{0}$ q : diffuse

Def: $q: x_t \sim N(\underbrace{\sqrt{1-\beta_t} x_{t-1}}_{\mu}, \underbrace{\sqrt{\beta_t}}_{\sigma})$

β_t is a hyperparameter
 $0 < \beta_t < 1$

Use reparameterization.

← unit matrix to keep the shape

$$x_t = N(x_t; \sqrt{1-\beta_t} x_{t-1}, \sqrt{\beta_t} \cdot I)$$

$$= \underbrace{\sqrt{1-\beta_t}}_{0 < \beta_t < 1} x_{t-1} + \sqrt{\beta_t} \cdot \epsilon, \quad \epsilon \sim N(0, I) \quad \text{即, 每一步加 } N \text{ noise}$$

spread out each step, increasing noise

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

$$\boxed{N(0, \sigma_1^2 I) + N(0, \sigma_2^2 I) = N(0, (\sigma_1^2 + \sigma_2^2) I)}$$

$$q(x_{1:T} | x_0) \quad x_0 \rightarrow x_1 \rightarrow x_2 \cdots x_T$$

$$= \prod_{t=1}^T q(x_t | x_{t-1})$$

Properties: ① $x_t \rightarrow x_0, \beta = \langle \beta_1, \beta_2, \dots, \beta_t \rangle$

x_t only relevant to x_0 and β

Proof let $\alpha_t = 1 - \beta_t \quad \bar{\alpha}_t = \prod_{i=1}^t \alpha_i$

$$\begin{cases} x_t = \sqrt{\alpha_t} x_{t-1} + \sqrt{1-\alpha_t} \epsilon_{t-1} \\ x_{t-1} = \sqrt{\alpha_{t-1}} x_{t-2} + \sqrt{1-\alpha_{t-1}} \epsilon_{t-2} \end{cases} \quad \text{substitute}$$

$$\therefore x_t = \sqrt{\alpha_t} (\sqrt{\alpha_{t-1}} x_{t-2}) + \sqrt{\alpha_t} \cdot \sqrt{1-\alpha_{t-1}} \epsilon_{t-2} + \sqrt{1-\alpha_t} \epsilon_{t-1}$$

since $\epsilon \sim N(0, I)$

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

* not correlated

$$= \sqrt{\alpha_t \alpha_{t-1}} x_{t-2} + \sqrt{1-\alpha_t \alpha_{t-1}} \epsilon_{t-2}$$

$$\text{Thus, } \sqrt{\alpha_t \alpha_{t-1} \alpha_{t-2} \cdots \alpha_1} x_0 + \sqrt{1-\alpha_t \alpha_{t-1} \alpha_{t-2} \cdots \alpha_1} \epsilon_0$$

$$x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1-\bar{\alpha}_t} \epsilon, \quad \epsilon \sim N(0, I)$$

Namely, x_t only depends on x_0 and β (indeed Markov chain)

$$\beta \in (0,1)$$

$$\textcircled{2} \lim_{T \rightarrow \infty} x_T = \sqrt{\alpha_T} x_0 + \sqrt{1 - \alpha_T} \varepsilon = 0 + 1 \cdot \varepsilon$$

$$x_T \sim N(0,1) \text{ when } T \rightarrow \infty$$

use random noise to generate an image

Then: differential Markov process

$$x_0 \quad 0 \quad 0 \quad \dots 0 \quad x_T \quad 0 \sim z \sim N(0,1)$$

smaller step
to refine

larger step

$\beta = (0.0001, \dots, 0.02)$ step becomes larger

$$\textcircled{3} \quad 0 \xrightarrow{x_{t-1}} 0 \quad x_t$$

$$q(x_t | x_{t-1})$$

$$\text{reverse: } q(x_{t-1} | x_t)$$

is this also N ?

(math problem)

(it is)

when β is small \sim Normal

want to find $P_\theta(x_{t-1} | x_t)$ just a predict though

note that P_θ is based on x_0

$$P_\theta(x_{t-1} | (x_t, x_0))$$

only
backward

determined by x_0 though?

$$= N(x_{t-1} ; \hat{\mu}(x_t, x_0), \tilde{\beta}_t I) \quad \text{use Bayesian estimate}$$

reverse

$$q(x_{t-1} | (x_t, x_0)) \stackrel{4)}{=} \frac{q(x_t, x_0, x_{t-1})}{q(x_t, x_0)}$$

$$1) P(A|B) = \frac{P(A)P(B|A)}{P(B)}$$

$$2) P(AB) = P(A)P(B|A)$$

$$3) P(ABC) = \frac{P(A)P(B|A)P(C|AB)}{P(C|AB)}$$

$$\begin{aligned} & \frac{q(x_t) q(x_{t-1}|x_0) q(x_t|x_{t-1}, x_0)}{q(x_0) q(x_t|x_0)} \Rightarrow P(A|B) = \frac{P(AB)}{P(B)} \end{aligned}$$

$$= q(x_t|x_{t-1}, x_0) \frac{q_0(x_{t-1}|x_0)}{q_0(x_t|x_0)} \rightarrow \text{reverse so contains } \theta$$

based on property B, x_t only relevant to x_{t-1}

$$= q(x_t|x_{t-1}) \frac{q_0(x_{t-1}|x_0)}{q_0(x_t|x_0)}$$

$$\begin{aligned} & \left[x_t \sim N(\mu, \sigma^2) \propto e^{-\frac{(x-\mu)^2}{2\sigma^2}} = \exp\left(-\frac{1}{2}\left(\frac{x^2}{\sigma^2} - \frac{2\mu x}{\sigma^2} + \frac{\mu^2}{\sigma^2}\right)\right) \right] \\ & = \exp\left(-\frac{1}{2}\left(\frac{(x_t - \sqrt{\alpha_t} x_{t-1})^2}{\beta_t} + \frac{(x_{t-1} - \sqrt{\alpha_{t-1}} x_0)^2}{1 - \alpha_{t-1}} - \frac{(x_t - \sqrt{\alpha_t} x_0)^2}{1 - \alpha_t}\right)\right) \\ & = \exp\left(-\frac{1}{2}\left(\frac{\alpha_t}{\beta_t} + \frac{1}{1 - \alpha_{t-1}} x_{t-1}^2\right) - \left(\frac{2\sqrt{\alpha_t}}{\beta_t} x_t + \frac{2\sqrt{\alpha_{t-1}}}{1 - \alpha_{t-1}} x_0\right) x_{t-1} \right. \\ & \quad \left. + \text{constant } x_{t-1}^0\right) \end{aligned}$$

then, align the power term

$$\tilde{\beta}_t = \frac{1 - \alpha_{t-1}}{1 - \alpha_t} \beta_t \quad \tilde{\mu}_t(x_t, x_0) = \frac{\sqrt{\alpha_t} (1 - \alpha_{t-1})}{1 - \alpha_t} x_t + \frac{\sqrt{\alpha_{t-1}} \beta_t}{1 - \alpha_t} x_0$$

Because $x_t = \sqrt{\alpha_t} x_0 + \sqrt{1 - \alpha_t} \varepsilon$ \nearrow Substitute... long... $x_0 = ? x_t$

$$\tilde{\mu}_t(x_t, x_0) = \frac{1}{\sqrt{\alpha_t}} \left(x_t - \frac{1 - \alpha_t}{\sqrt{1 - \alpha_t}} \varepsilon_t \right) \quad \text{estimation} \quad (\text{solvable})$$

$P_\theta(\cdot|q)$

Then, $x_t = N(x_{t-1}; \mu_t, \sigma_t^2) = N(x_{t-1}; \frac{1}{\sqrt{\alpha_t}} (x_t - \frac{1-\alpha_t}{\sqrt{1-\alpha_t}} \epsilon_t))$

$T \rightarrow \infty, \beta_t \ll 1$, and $\beta_t \in (0, 1)$

Backward solvable

$$P(x_{t-1} | (G, x_0)) \sim N\left(\frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t} x_t + \frac{\sqrt{\bar{\alpha}_{t-1}}(1-\beta_t)}{1-\bar{\alpha}_t} x_0,\right.$$

$$\left.\left(\frac{\sqrt{1-\alpha_t} \sqrt{1-\bar{\alpha}_{t-1}}}{\sqrt{1-\bar{\alpha}_t}}\right)^2\right).$$

*

no beta

Namely, $\mu_{t-1} = \frac{x_t}{\sqrt{\alpha_t}} - \frac{1-\alpha_t}{\sqrt{\alpha_t}\sqrt{1-\bar{\alpha}_t}} \cdot \epsilon$

$$\sigma^2 = \left(\frac{(1-\alpha_t)(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\right) = \frac{\beta_t(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}$$