Diffusion models

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Laboratory for methods of big data analysis

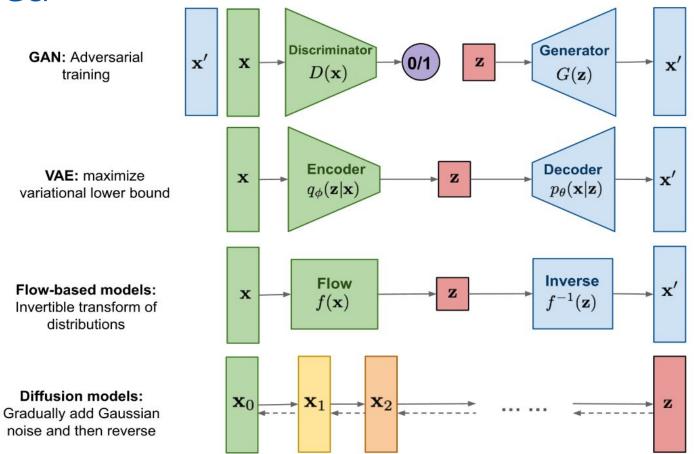




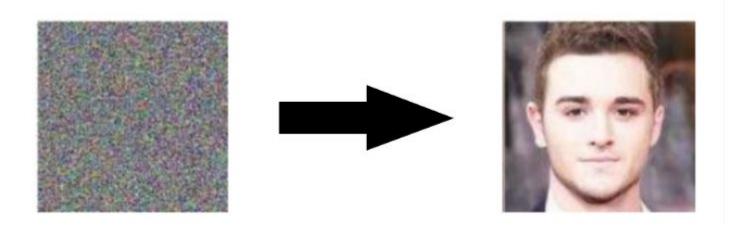
Diffusion process

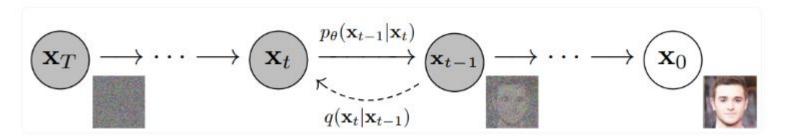


Idea



Idea





Forward process

- $q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t\mathbf{I}) \quad q(\mathbf{x}_{1:T}|\mathbf{x}_0) = \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1})$
- Where β is a variance schedule. If well-behaved, ensures that x_T is nearly an isotropic Gaussian for sufficiently large **T**
- We can sample \mathbf{x}_{t} at any timestamp via reparametrization trick

$$\mathbf{x}_{t} = \sqrt{\alpha_{t}}\mathbf{x}_{t-1} + \sqrt{1 - \alpha_{t}}\boldsymbol{\epsilon}_{t-1} \qquad \text{;where } \boldsymbol{\epsilon}_{t-1}, \boldsymbol{\epsilon}_{t-2}, \dots \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

$$= \sqrt{\alpha_{t}\alpha_{t-1}}\mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t}\alpha_{t-1}}\bar{\boldsymbol{\epsilon}}_{t-2} \qquad \text{;where } \bar{\boldsymbol{\epsilon}}_{t-2} \text{ merges two Gaussians (*)}.$$

$$= \dots \qquad \qquad \boldsymbol{\alpha}_{t} = 1 - \beta_{t} \qquad \bar{\boldsymbol{\alpha}}_{t} = \prod_{i=1}^{t} \alpha_{i}:$$

$$= \sqrt{\bar{\alpha}_{t}}\mathbf{x}_{0} + \sqrt{1 - \bar{\alpha}_{t}}\boldsymbol{\epsilon}$$

$$q(\mathbf{x}_{t}|\mathbf{x}_{0}) = \mathcal{N}(\mathbf{x}_{t}; \sqrt{\bar{\alpha}_{t}}\mathbf{x}_{0}, (1 - \bar{\alpha}_{t})\mathbf{I})$$

Reverse process

$$p_{ heta}(\mathbf{x}_{0:T}) = p(\mathbf{x}_T) \prod_{t=1}^T p_{ heta}(\mathbf{x}_{t-1}|\mathbf{x}_t) \quad p_{ heta}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_{ heta}(\mathbf{x}_t, t), \boldsymbol{\Sigma}_{ heta}(\mathbf{x}_t, t))$$

$$t = 0 \qquad t = \frac{T}{2} \qquad t = T$$
The forward trajectory $q(\mathbf{x}_{0:T})$

Reverse process

Problem: However, the inverse process $q(x_{t-1}|x_t)$ is unknown.

$$q(x_{t-1}|x_t) = \frac{q(x_t|x_{t-1}) * q(x_{t-1})}{\int q(x_t|x_{t-1}) * q(x_{t-1}) dx}$$

All we know that $q(x_t)$ and $q(x_t|x_{t-1})$ are Gaussian for all t (these distributions are called by Bayesians conjugate). Hence, $q(x_{t-1}|x_t)$ is also Gaussian!

Let's approximate then our uknown Gaussian denoising process $q(x_{t-1}|x_t)$ with neural network $p_{\theta}(x_{t-1}|x_t) = \mathcal{N}(x_{t-1}|\mu_{\theta}(x_t), \sigma_{\theta}(x_t))$

$$p_{\theta}(\mathbf{x}_{0:T}) = p(\mathbf{x}_T) \prod_{t=1}^{T} p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) \quad p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_{\theta}(\mathbf{x}_t, t), \boldsymbol{\Sigma}_{\theta}(\mathbf{x}_t, t))$$

Reverse process

• How to train p_{θ} ? The same way as VAE

$$-\log p_{\theta}(\mathbf{x}_{0}) \leq -\log p_{\theta}(\mathbf{x}_{0}) + D_{\mathrm{KL}}(q(\mathbf{x}_{1:T}|\mathbf{x}_{0})||p_{\theta}(\mathbf{x}_{1:T}|\mathbf{x}_{0}))$$

$$= -\log p_{\theta}(\mathbf{x}_{0}) + \mathbb{E}_{\mathbf{x}_{1:T} \sim q(\mathbf{x}_{1:T}|\mathbf{x}_{0})} \left[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{0:T})/p_{\theta}(\mathbf{x}_{0})} \right]$$

$$= -\log p_{\theta}(\mathbf{x}_{0}) + \mathbb{E}_{q} \left[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{0:T})} + \log p_{\theta}(\mathbf{x}_{0}) \right]$$

$$= \mathbb{E}_{q} \left[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{0:T})} \right]$$

Let
$$L_{\text{VLB}} = \mathbb{E}_{q(\mathbf{x}_{0:T})} \left[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_{\theta}(\mathbf{x}_{0:T})} \right] \ge -\mathbb{E}_{q(\mathbf{x}_0)} \log p_{\theta}(\mathbf{x}_0)$$

ELBO again

$$\begin{split} L_{\text{VLB}} &= \mathbb{E}_{q(\mathbf{x}_{0:T})} \Big[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{0:T})} \Big] \\ &= \mathbb{E}_{q} \Big[\log \frac{\prod_{t=1}^{T} q(\mathbf{x}_{t}|\mathbf{x}_{t-1})}{p_{\theta}(\mathbf{x}_{T}) \prod_{t=1}^{T} p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_{t})} \Big] \\ &= \mathbb{E}_{q} \Big[-\log p_{\theta}(\mathbf{x}_{T}) + \sum_{t=1}^{T} \log \frac{q(\mathbf{x}_{t}|\mathbf{x}_{t-1})}{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_{t})} \Big] \\ &= \mathbb{E}_{q} \Big[-\log p_{\theta}(\mathbf{x}_{T}) + \sum_{t=2}^{T} \log \frac{q(\mathbf{x}_{t}|\mathbf{x}_{t-1})}{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_{t})} + \log \frac{q(\mathbf{x}_{1}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{0}|\mathbf{x}_{1})} \Big] \\ &= \mathbb{E}_{q} \Big[-\log p_{\theta}(\mathbf{x}_{T}) + \sum_{t=2}^{T} \log \Big(\frac{q(\mathbf{x}_{t-1}|\mathbf{x}_{t},\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_{0})} + \log \frac{q(\mathbf{x}_{1}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{0}|\mathbf{x}_{1})} \Big] \\ &= \mathbb{E}_{q} \Big[-\log p_{\theta}(\mathbf{x}_{T}) + \sum_{t=2}^{T} \log \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_{t},\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_{0})} + \sum_{t=2}^{T} \log \frac{q(\mathbf{x}_{1}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{0}|\mathbf{x}_{1})} \Big] \\ &= \mathbb{E}_{q} \Big[-\log p_{\theta}(\mathbf{x}_{T}) + \sum_{t=2}^{T} \log \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_{t},\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_{0})} + \log \frac{q(\mathbf{x}_{1}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{0}|\mathbf{x}_{1})} \Big] \\ &= \mathbb{E}_{q} \Big[\log \frac{q(\mathbf{x}_{T}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{T})} + \sum_{t=2}^{T} \log \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_{t},\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_{0})} - \log p_{\theta}(\mathbf{x}_{0}|\mathbf{x}_{1}) \Big] \\ &= \mathbb{E}_{q} \Big[\log \frac{q(\mathbf{x}_{T}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{T})} + \sum_{t=2}^{T} \log \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_{t},\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_{0})} - \log p_{\theta}(\mathbf{x}_{0}|\mathbf{x}_{1}) \Big] \\ &= \mathbb{E}_{q} \Big[\log \frac{q(\mathbf{x}_{T}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{T})} + \sum_{t=2}^{T} \log \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_{t},\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_{0})} - \log p_{\theta}(\mathbf{x}_{0}|\mathbf{x}_{1}) \Big] \\ &= \mathbb{E}_{q} \Big[\log \frac{q(\mathbf{x}_{T}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{T})} + \sum_{t=2}^{T} \log \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_{t},\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_{0})} - \log p_{\theta}(\mathbf{x}_{0}|\mathbf{x}_{1}) \Big] \\ &= \mathbb{E}_{q} \Big[\log \frac{q(\mathbf{x}_{T}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{T})} + \sum_{t=2}^{T} \log \frac{q(\mathbf{x}_{T}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_{0})} - \log p_{\theta}(\mathbf{x}_{0}|\mathbf{x}_{1}) \Big] \\ &= \mathbb{E}_{q} \Big[\log \frac{q(\mathbf{x}_{T}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{0})} + \log \frac{q(\mathbf{x}_{T}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{0})} + \log \frac{q(\mathbf{x}_{T}|\mathbf{x}_{0})}{p_{\theta}(\mathbf{x}_{0}|\mathbf{x}_{1})} \Big] \\ &= \mathbb{E}_{q} \Big[\log \frac{q(\mathbf{x}_{$$

ELBO

$$L_{\text{VLB}} = \mathbb{E}_q[\underbrace{D_{\text{KL}}(q(\mathbf{x}_T|\mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_T))}_{L_T} + \sum_{t=2} \underbrace{D_{\text{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t,\mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} \underbrace{-\log p_{\theta}(\mathbf{x}_0|\mathbf{x}_1)}_{L_0}]$$

- L_T is constant w.t. θ , $L_0 = \log \mathcal{N}(\mathbf{x}_0; \mu_{\theta}(\mathbf{x}_1, 1), \Sigma_{\theta}(\mathbf{x}_1, 1))$
- Problem $q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0)$ is unknown. But is it really?

$$q(\mathbf{x}_{t-1}|\mathbf{x}_{t},\mathbf{x}_{0}) = q(\mathbf{x}_{t}|\mathbf{x}_{t-1},\mathbf{x}_{0}) \frac{q(\mathbf{x}_{t-1}|\mathbf{x}_{0})}{q(\mathbf{x}_{t}|\mathbf{x}_{0})}$$

$$\propto \exp\left(-\frac{1}{2}\left(\frac{(\mathbf{x}_{t}-\sqrt{\alpha_{t}}\mathbf{x}_{t-1})^{2}}{\beta_{t}} + \frac{(\mathbf{x}_{t-1}-\sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_{0})^{2}}{1-\bar{\alpha}_{t-1}} - \frac{(\mathbf{x}_{t}-\sqrt{\bar{\alpha}_{t}}\mathbf{x}_{0})^{2}}{1-\bar{\alpha}_{t}}\right)\right)$$

$$= \exp\left(-\frac{1}{2}\left(\left(\frac{\alpha_{t}}{\beta_{t}} + \frac{1}{1-\bar{\alpha}_{t-1}}\right)\mathbf{x}_{t-1}^{2} - \left(\frac{2\sqrt{\alpha_{t}}}{\beta_{t}}\mathbf{x}_{t} + \frac{2\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}\mathbf{x}_{0}\right)\mathbf{x}_{t-1} + C(\mathbf{x}_{t},\mathbf{x}_{0})\right)\right)$$

$$= \mathcal{N}(x_{t-1}|\tilde{\boldsymbol{\mu}}_{t}(\mathbf{x}_{t},\mathbf{x}_{0}),\tilde{\boldsymbol{\beta}}_{t})$$

ELBO

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

$$\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) = \frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t} \mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1 - \bar{\alpha}_t} \mathbf{x}_0$$

Then,

$$L_{\text{VLB}} = C + \sum_{t=2}^{T} KL(\mathcal{N}(x_t; \frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t} \mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1 - \bar{\alpha}_t} \mathbf{x}_0, \frac{1 - \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t} \cdot \beta_t)||$$

$$N(\mathbf{x}_t; \mu_{\theta}(\mathbf{x}_t), \beta_{\theta}(\mathbf{x}_t))) + \log \mathcal{N}(\mathbf{x}_0; \boldsymbol{\mu}_{\theta}(\mathbf{x}_1, 1), \boldsymbol{\Sigma}_{\theta}(\mathbf{x}_1, 1))$$



Recall that we need to learn a NN to approximate the conditioned probability distributions in the reverse diffusion process $p_{\theta}(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_{\theta}(\mathbf{x}_t, t), \boldsymbol{\Sigma}_{\theta}(\mathbf{x}_t, t))$.

$$\mu_{\theta}(\mathbf{x}_{t}, t) = \frac{1}{\sqrt{\alpha_{t}}} \left(\mathbf{x}_{t} - \frac{1 - \alpha_{t}}{\sqrt{1 - \bar{\alpha}_{t}}} \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, t) \right)$$
Thus $\mathbf{x}_{t-1} = \mathcal{N}(\mathbf{x}_{t-1}; \frac{1}{\sqrt{\alpha_{t}}} \left(\mathbf{x}_{t} - \frac{1 - \alpha_{t}}{\sqrt{1 - \bar{\alpha}_{t}}} \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, t) \right), \boldsymbol{\Sigma}_{\theta}(\mathbf{x}_{t}, t))$

The loss term L_t is parameterized to minimize the difference from $ilde{m{\mu}}$:

$$\begin{split} L_t &= \mathbb{E}_{\mathbf{x}_0, \epsilon} \Big[\frac{1}{2 \|\mathbf{\Sigma}_{\theta}(\mathbf{x}_t, t)\|_2^2} \|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) - \boldsymbol{\mu}_{\theta}(\mathbf{x}_t, t)\|^2 \Big] \\ &= \mathbb{E}_{\mathbf{x}_0, \epsilon} \Big[\frac{1}{2 \|\mathbf{\Sigma}_{\theta}\|_2^2} \|\frac{1}{\sqrt{\alpha_t}} \Big(\mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \boldsymbol{\epsilon}_t \Big) - \frac{1}{\sqrt{\alpha_t}} \Big(\mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t) \Big) \|^2 \Big] \\ &= \mathbb{E}_{\mathbf{x}_0, \epsilon} \Big[\frac{(1 - \alpha_t)^2}{2\alpha_t (1 - \bar{\alpha}_t) \|\mathbf{\Sigma}_{\theta}\|_2^2} \|\boldsymbol{\epsilon}_t - \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t) \|^2 \Big] \\ &= \mathbb{E}_{\mathbf{x}_0, \epsilon} \Big[\frac{(1 - \alpha_t)^2}{2\alpha_t (1 - \bar{\alpha}_t) \|\mathbf{\Sigma}_{\theta}\|_2^2} \|\boldsymbol{\epsilon}_t - \boldsymbol{\epsilon}_{\theta}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}_t, t) \|^2 \Big] \end{split}$$

$$egin{aligned} L_t^{ ext{simple}} &= \mathbb{E}_{t \sim [1,T], \mathbf{x}_0, oldsymbol{\epsilon}_t} \Big[\|oldsymbol{\epsilon}_t - oldsymbol{\epsilon}_{ heta}(\mathbf{x}_t, t)\|^2 \Big] \ &= \mathbb{E}_{t \sim [1,T], \mathbf{x}_0, oldsymbol{\epsilon}_t} \Big[\|oldsymbol{\epsilon}_t - oldsymbol{\epsilon}_{ heta}(\sqrt{ar{lpha}_t}\mathbf{x}_0 + \sqrt{1 - ar{lpha}_t}oldsymbol{\epsilon}_t, t)\|^2 \Big] \end{aligned}$$

Ho et al. (2020)

Algorithm 1 Training

- 1: repeat
- 2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
- 3: $t \sim \text{Uniform}(\{1, \dots, T\})$
- 4: $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
- 5: Take gradient descent step on

$$\nabla_{\theta} \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\theta} (\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}, t) \right\|^2$$

6: until converged

Algorithm 2 Sampling

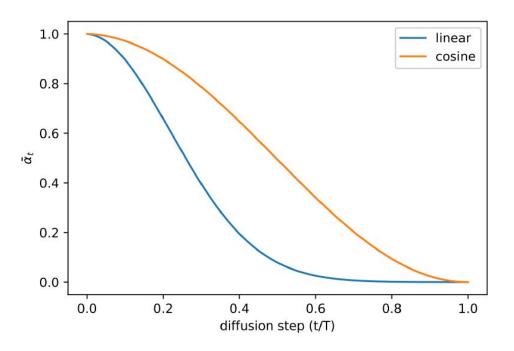
- 1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
- 2: **for** t = T, ..., 1 **do**
- 3: $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if t > 1, else $\mathbf{z} = \mathbf{0}$
- 4: $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}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

Sneak peek forward



Variance scheduling

Set $\beta_t = \text{clip}(1 - \frac{\bar{\alpha}_t}{\bar{\alpha}_{t-1}}, 0.999)$ $\bar{\alpha}_t = \frac{f(t)}{f(0)}$ where $f(t) = \cos\left(\frac{t/T+s}{1+s} \cdot \frac{\pi}{2}\right)^2$ instead of gradually increasing β_t from 10^{-4} to 0.02

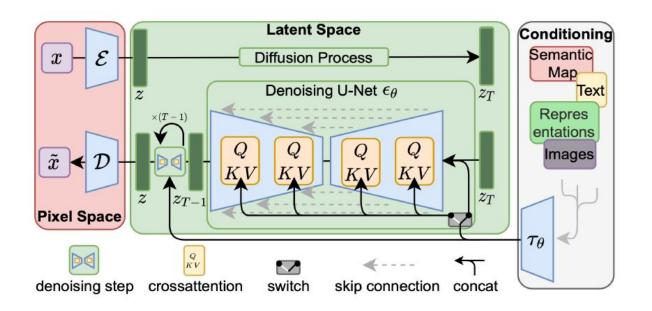


Performance trick

- Learn the variance. Set $\Sigma_{\theta}(\mathbf{x}_t, t) = \exp(\mathbf{v} \log \beta_t + (1 \mathbf{v}) \log \tilde{\beta}_t)$ instead of $\Sigma_{\theta}(\mathbf{x}_t, t) = \sigma_t^2 \mathbf{I}$ in DDPM
- Sample every S steps (strided sampling) $q_{\sigma,\tau}(\mathbf{x}_{\tau_{i-1}}|\mathbf{x}_{\tau_t},\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{\tau_{i-1}};\sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_{t-1}}-\sigma_t^2\frac{\mathbf{x}_{\tau_i}-\sqrt{\bar{\alpha}_t}\mathbf{x}_0}{\sqrt{1-\bar{\alpha}_t}},\sigma_t^2\mathbf{I})$

Latent Diffusion

Attention(
$$\mathbf{Q}, \mathbf{K}, \mathbf{V}$$
) = softmax $\left(\frac{\mathbf{Q}\mathbf{K}^{\top}}{\sqrt{d}}\right) \cdot \mathbf{V}$
where $\mathbf{Q} = \mathbf{W}_{Q}^{(i)} \cdot \varphi_{i}(\mathbf{z}_{i}), \ \mathbf{K} = \mathbf{W}_{K}^{(i)} \cdot \tau_{\theta}(y), \ \mathbf{V} = \mathbf{W}_{V}^{(i)} \cdot \tau_{\theta}(y)$
and $\mathbf{W}_{Q}^{(i)} \in \mathbb{R}^{d \times d_{\epsilon}^{i}}, \ \mathbf{W}_{K}^{(i)}, \mathbf{W}_{V}^{(i)} \in \mathbb{R}^{d \times d_{\tau}}, \ \varphi_{i}(\mathbf{z}_{i}) \in \mathbb{R}^{N \times d_{\epsilon}^{i}}, \ \tau_{\theta}(y) \in \mathbb{R}^{M \times d}$



Classifier guidance

$$\nabla_{\mathbf{x}_{t}} \log q(\mathbf{x}_{t}, y) = \nabla_{\mathbf{x}_{t}} \log q(\mathbf{x}_{t}) + \nabla_{\mathbf{x}_{t}} \log q(y|\mathbf{x}_{t})$$

$$\approx -\frac{1}{\sqrt{1 - \bar{\alpha}_{t}}} \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, t) + \nabla_{\mathbf{x}_{t}} \log f_{\phi}(y|\mathbf{x}_{t})$$

$$= -\frac{1}{\sqrt{1 - \bar{\alpha}_{t}}} (\boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, t) - \sqrt{1 - \bar{\alpha}_{t}} \nabla_{\mathbf{x}_{t}} \log f_{\phi}(y|\mathbf{x}_{t}))$$

Classifier-Free Guidance

$$\nabla_{\mathbf{x}_{t}} \log p(y|\mathbf{x}_{t}) = \nabla_{\mathbf{x}_{t}} \log p(\mathbf{x}_{t}|y) - \nabla_{\mathbf{x}_{t}} \log p(\mathbf{x}_{t})$$

$$= -\frac{1}{\sqrt{1 - \bar{\alpha}_{t}}} \left(\boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, t, y) - \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, t) \right)$$

$$\bar{\boldsymbol{\epsilon}}_{\theta}(\mathbf{x}_{t}, t, y) = \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, t, y) - \sqrt{1 - \bar{\alpha}_{t}} \ w \nabla_{\mathbf{x}_{t}} \log p(y|\mathbf{x}_{t})$$

$$= \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, t, y) + w \left(\boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, t, y) - \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, t) \right)$$

$$= (w + 1) \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, t, y) - w \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_{t}, t)$$

Cascaded diffusion

