Diffusion models

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Laboratory for methods of big data analysis

LAMBDA • HSE

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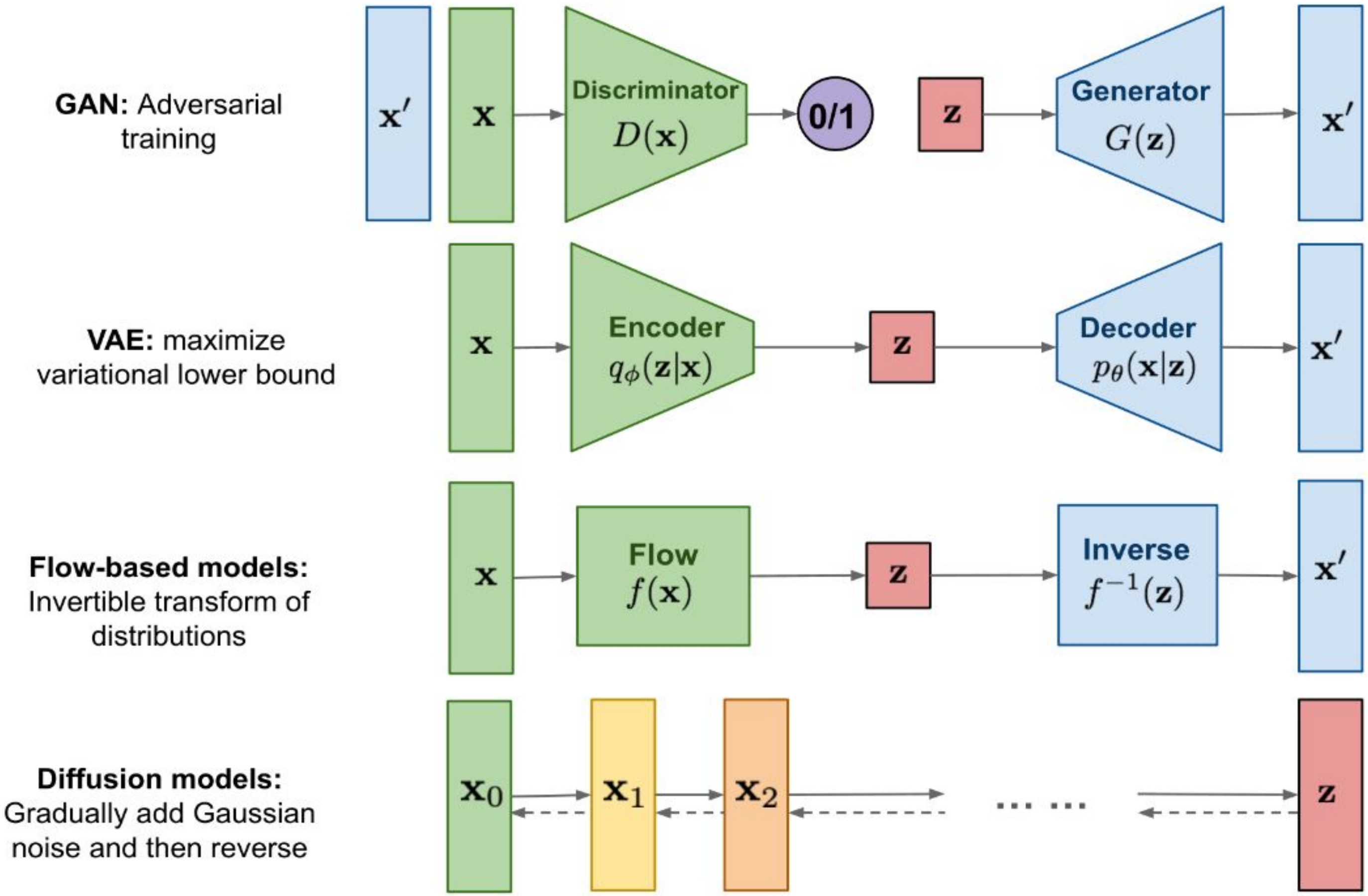
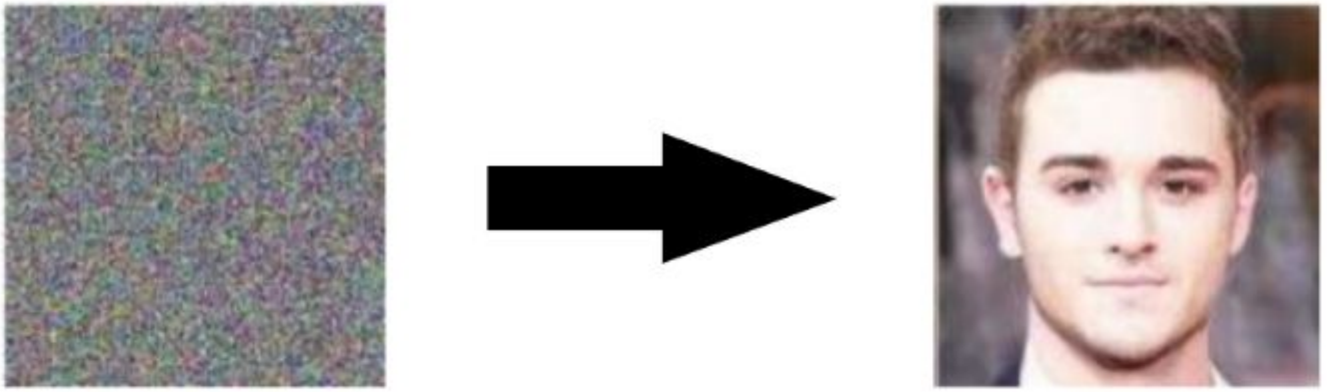
Diffusion process

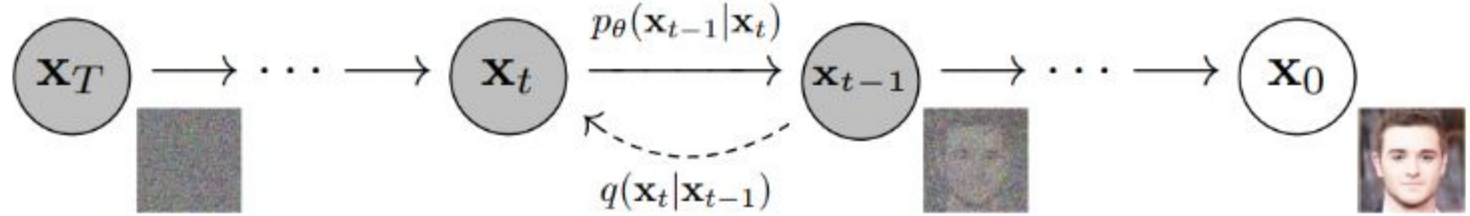
Idea



GAN: Adversarial training
x'
x
Discriminator
D(x)
0/1
z
Generator
G(z)
x'
VAE: maximize variational lower bound
x
Encoder
$q_\phi(\mathbf{z}|\mathbf{x})$
z
Decoder
$p_\theta(\mathbf{x}|\mathbf{z})$
x'
Flow-based models: Invertible transform of distributions
x
Flow
f(x)
z
Inverse
$f^{-1}(\mathbf{z})$
x'
Diffusion models: Gradually add Gaussian noise and then reverse
$\mathbf{x}_0$
$\mathbf{x}_1$
$\mathbf{x}_2$
... ...
z

Idea




$\mathbf{x}_T$
$\mathbf{x}_t$
$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$
$\mathbf{x}_{t-1}$
$q(\mathbf{x}_t|\mathbf{x}_{t-1})$
$\mathbf{x}_0$

Forward process

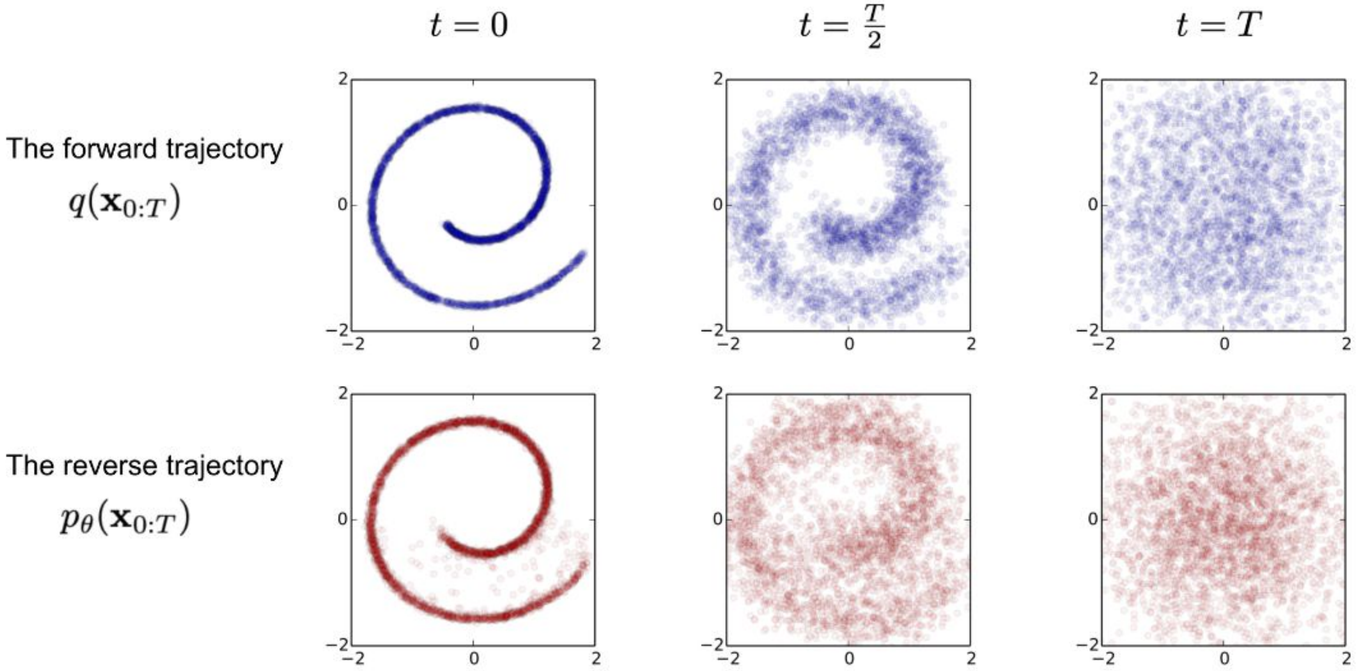
- $$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t\mathbf{I}) \quad q(\mathbf{x}_{1:T}|\mathbf{x}_0) = \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1})$$
- Where β is a variance schedule. If well-behaved, ensures that x_T is nearly an isotropic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

$$\begin{aligned}
\mathbf{x}_t &= \sqrt{\alpha_t}\mathbf{x}_{t-1} + \sqrt{1-\alpha_t}\boldsymbol{\epsilon}_{t-1} && ;\text{where } \boldsymbol{\epsilon}_{t-1}, \boldsymbol{\epsilon}_{t-2}, \dots \sim \mathcal{N}(\mathbf{0}, \mathbf{I}) \\
&= \sqrt{\alpha_t \alpha_{t-1}}\mathbf{x}_{t-2} + \sqrt{1-\alpha_t \alpha_{t-1}}\bar{\boldsymbol{\epsilon}}_{t-2} && ;\text{where } \bar{\boldsymbol{\epsilon}}_{t-2} \text{ merges two Gaussians (*).} \\
&= \dots && \alpha_t = 1-\beta_t \qquad \bar{\alpha}_t = \textstyle\prod_{i=1}^{t}\alpha_i; \\
&= \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}
\end{aligned}$$

$$q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I})$$

Reverse process

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



Langevin dynamics

- We can sample from $p(x)$ using only the gradients $\nabla_x \log p(x)$ in a Markov chain of updates:

$$\mathbf{x}_t = \mathbf{x}_{t-1} + \frac{\delta}{2}\nabla_{\mathbf{x}} \log p(\mathbf{x}_{t-1}) + \sqrt{\delta}\boldsymbol{\epsilon}_t, \quad \text{where } \boldsymbol{\epsilon}_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

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

$$
\begin{aligned}
-\log p_\theta(\mathbf{x}_0) &\le -\log p_\theta(\mathbf{x}_0) + D_{\mathrm{KL}}(q(\mathbf{x}_{1:T}|\mathbf{x}_0)\|p_\theta(\mathbf{x}_{1:T}|\mathbf{x}_0)) \\
&= -\log p_\theta(\mathbf{x}_0) + \mathbb{E}_{\mathbf{x}_{1:T}\sim q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\Big[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})/p_\theta(\mathbf{x}_0)}\Big] \\
&= -\log p_\theta(\mathbf{x}_0) + \mathbb{E}_q\Big[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})} + \log p_\theta(\mathbf{x}_0)\Big] \\
&= \mathbb{E}_q\Big[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})}\Big]
\end{aligned}
$$

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

ELBO again

Sohl-Dickstein et al., 2015
(appendix B)

$$
\begin{aligned}
L_{\mathrm{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}_t)}\cdot\frac{q(\mathbf{x}_t|\mathbf{x}_0)}{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}\Big) + \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}_t)} + \sum_{t=2}^T \log\frac{q(\mathbf{x}_t|\mathbf{x}_0)}{q(\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}_t)} + \log\frac{q(\mathbf{x}_T|\mathbf{x}_0)}{q(\mathbf{x}_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}_t)} - \log p_\theta(\mathbf{x}_0|\mathbf{x}_1)\Big] \\
&= \mathbb{E}_q[\underbrace{D_{\mathrm{KL}}(q(\mathbf{x}_T|\mathbf{x}_0)\parallel p_\theta(\mathbf{x}_T))}_{L_T} + \sum_{t=2}^T \underbrace{D_{\mathrm{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}]
\end{aligned}
$$

ELBO

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

- L_T is constant w.t. θ, $L_0 = \log \mathcal{N}(x_0; \mu_\theta(x_1, 1), \Sigma_\theta(x_1, 1))$
- Problem $q(x_{t-1} \mid x_t, x_0)$ is unknown. But is it really?

$$\begin{aligned}
q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) &= q(\mathbf{x}_t|\mathbf{x}_{t-1}, \mathbf{x}_0)\frac{q(\mathbf{x}_{t-1}|\mathbf{x}_0)}{q(\mathbf{x}_t|\mathbf{x}_0)} \\
&\propto \exp\Big(-\frac{1}{2}\big(\frac{(\mathbf{x}_t - \sqrt{\alpha_t}\mathbf{x}_{t-1})^2}{\beta_t} + \frac{(\mathbf{x}_{t-1} - \sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0)^2}{1-\bar{\alpha}_{t-1}} - \frac{(\mathbf{x}_t - \sqrt{\bar{\alpha}_t}\mathbf{x}_0)^2}{1-\bar{\alpha}_t}\big)\Big) \\
&= \exp\Big(-\frac{1}{2}\big((\frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}})\mathbf{x}_{t-1}^2 - (\frac{2\sqrt{\alpha_t}}{\beta_t}\mathbf{x}_t + \frac{2\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}\mathbf{x}_0)\mathbf{x}_{t-1} + C(\mathbf{x}_t, \mathbf{x}_0)\big)\Big) \\
&= \mathcal{N}(x_{t-1}|\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t)
\end{aligned}$$

ELBO

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

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

Then,

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

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

DDPM

DDPM

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

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

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

DDPM

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

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

$$
\begin{aligned}
L_t^{\text{simple}} &= \mathbb{E}_{t\sim[1,T],\mathbf{x}_0,\boldsymbol{\epsilon}_t}\Big[\|\boldsymbol{\epsilon}_t - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t,t)\|^2\Big] \\
&= \mathbb{E}_{t\sim[1,T],\mathbf{x}_0,\boldsymbol{\epsilon}_t}\Big[\|\boldsymbol{\epsilon}_t - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_t, t)\|^2\Big]
\end{aligned}
$$

Ho et al. (2020)

DDPM

Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
    $\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$
until converged

Algorithm 2 Sampling

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

- Where ε_θ is a noise component which we predicts with a NN.
- Though diffusion models is **highly flexible,** it is restricted to have an output of the same dimensions as input. Thus, it is very optimal to use U-Net-like architectures

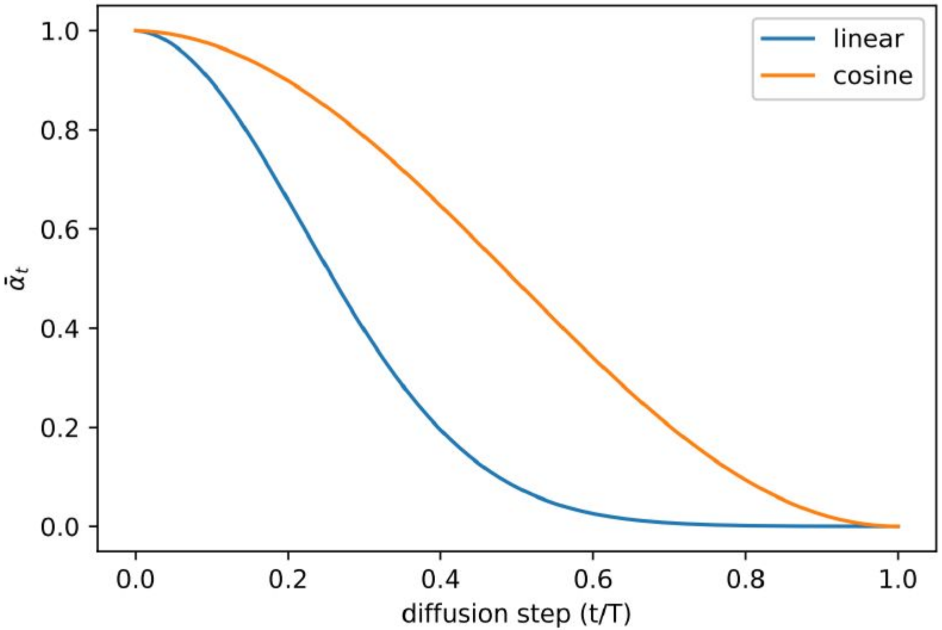
Summary

- Our Diffusion Model is parameterized as a Markov chain, meaning that our latent variables $x_1, \dots, x_T$ depend only on the previous timestamp
- The transition distributions in the Markov chain are Gaussian, where the forward process requires a variance schedule, and the reverse process parameters are learned.
- The diffusion process ensures that x_T is asymptotically distributed as an isotropic Gaussian for sufficiently large T.
- Diffusion Models are highly flexible and allow for *any* architecture whose input and output dimensionality are the same to be used. Many implementations use U-Net-like architectures.
- Using a simplified training objective to train a function which predicts the noise component of a given latent variable yields the best and most stable results.

Sneak peek forward

Variance scheduling

Set $\beta_t = \text{clip}(1 - \frac{\bar{\alpha}_t}{\bar{\alpha}_{t-1}}, 0.999)$ $\quad \bar{\alpha}_t = \frac{f(t)}{f(0)}$ $\quad$ 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

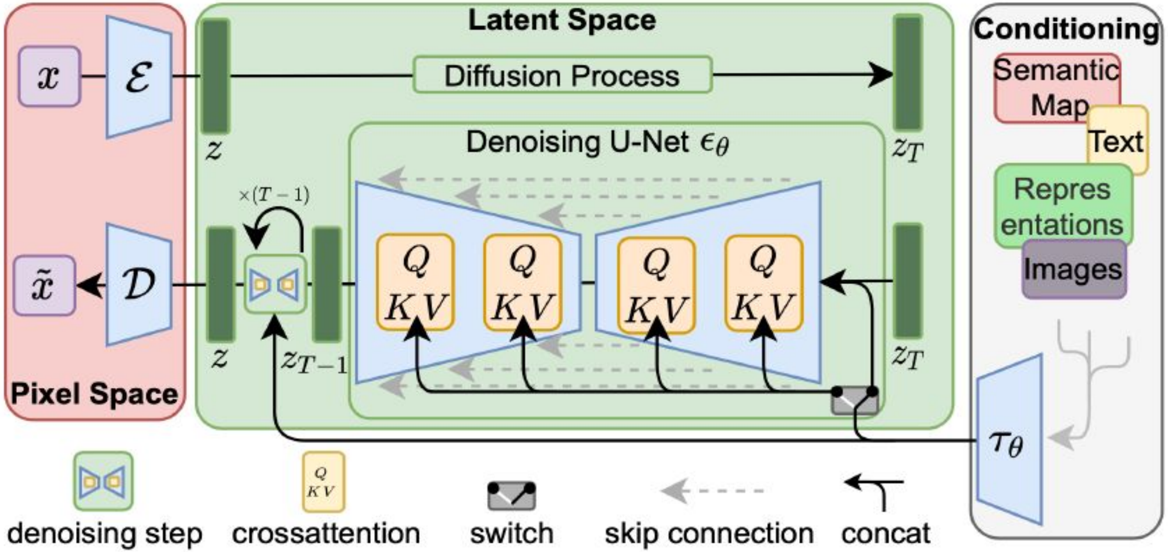
- Learn the variance. Set $\mathbf{\Sigma}_\theta(\mathbf{x}_t, t) = \exp(\mathbf{v}\log\beta_t + (1-\mathbf{v})\log\tilde{\beta}_t)$ instead of $\mathbf{\Sigma}_\theta(\mathbf{x}_t, t) = \sigma_t^2\mathbf{I}$ in DDPM
- Sample every S steps (strided sampling)
  $q_{\sigma,\tau}(\mathbf{x}_{\tau_{i-1}}|\mathbf{x}_{\tau_t},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

Latent Diffusion

$$\text{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{softmax}\left(\frac{\mathbf{Q}\mathbf{K}^\top}{\sqrt{d}}\right) \cdot \mathbf{V}$$

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

$$
\begin{aligned}
\nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t, y) &= \nabla_{\mathbf{x}_t} \log q(\mathbf{x}_t) + \nabla_{\mathbf{x}_t} \log q(y|\mathbf{x}_t) \\
&\approx -\frac{1}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) + \nabla_{\mathbf{x}_t} \log f_\phi(y|\mathbf{x}_t) \\
&= -\frac{1}{\sqrt{1-\bar{\alpha}_t}} \left(\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) - \sqrt{1-\bar{\alpha}_t} \nabla_{\mathbf{x}_t} \log f_\phi(y|\mathbf{x}_t)\right)
\end{aligned}
$$

Classifier-Free Guidance

$$
\begin{aligned}
\nabla_{\mathbf{x}_t} \log p(y|\mathbf{x}_t) &= \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|y) - \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t) \\
&= -\frac{1}{\sqrt{1-\bar{\alpha}_t}} \Big(\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t, y) - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \Big) \\
\bar{\boldsymbol{\epsilon}}_\theta(\mathbf{x}_t, t, y) &= \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t, y) - \sqrt{1-\bar{\alpha}_t}\; w \nabla_{\mathbf{x}_t} \log p(y|\mathbf{x}_t) \\
&= \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t, y) + w \big(\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t, y) - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \big) \\
&= (w+1) \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t, y) - w \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)
\end{aligned}
$$

Cascaded diffusion