什么是Diffusion模型

这是一篇关于 What are Diffusion Models的译文。很多地方借鉴了由浅入深了解Diffusion Model

本文主要是介绍什么是DDPM：Denoising Diffusion Probabilistic Models(**DDPM**; Ho et al. 2020).

Basic Knowledge

- Normal Distribution: $\mathcal{N}(x;\mu,\sigma^2)=\frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$
- Conditional Probability: $P(A\mid B)=\frac{P(A\cap B)}{P(B)}$
- Bayes' theorem: $P(A\mid B)=\frac{P(B\mid A)P(A)}{P(B)}$
- KL divergence: $D_{\mathrm{KL}}(q(x)||p(x))=\mathbb{E}_{q(x)}\log[q(x)/p(x)]$

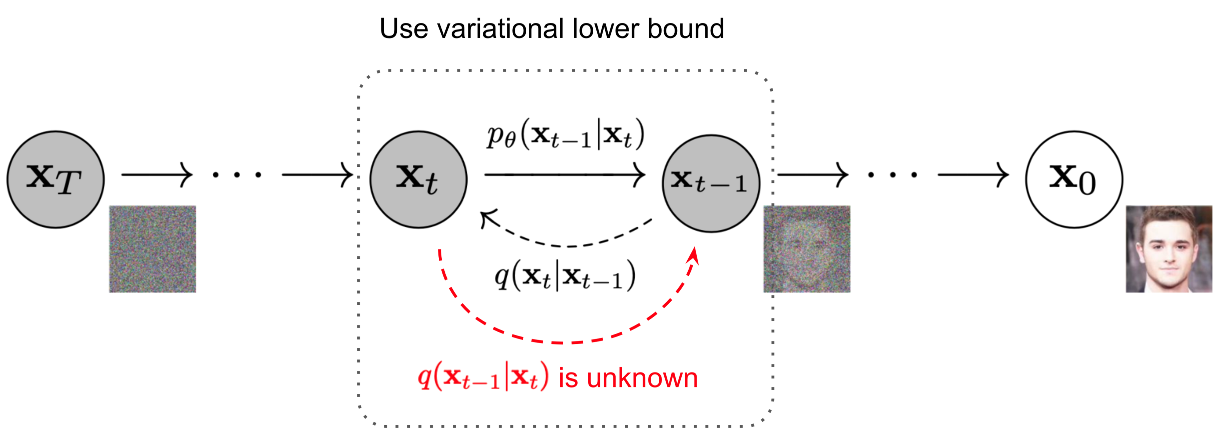
DDPM

Forward diffusion process

从给定的真实数据集中采样一个数据样本：$\mathbf{x}_0\sim q(\mathbf{x})$，我们定义前向扩散过程，在这个过程中，我们逐步向样本中添加少量高斯噪声，产生一系列噪声样本 $\mathbf{x}_1,\dots,\mathbf{x}_T$ 。步长由方差schedule控制$\{\beta_t\in(0,1)\}_{t=1}^T$

$$q(\mathbf{x}_t|\mathbf{x}_{t-1})=\mathcal{N}(\mathbf{x}_t;\sqrt{1-\beta_t}\mathbf{x}_{t-1},\beta_t\mathbf{I})\quad q(\mathbf{x}_{1:T}|\mathbf{x}_0)=\prod_{t=1}^T q(\mathbf{x}_t|\mathbf{x}_{t-1})$$

随着步长t的变大，数据样本$\mathbf{x}_0$逐渐失去其特征。 最终，当$T\to\infty$, $\mathbf{x}_T$等价于各向同性高斯分布。



上述过程有一个很好的特性，我们可以使用重参数化技巧以封闭形式在任意时间步t采样$\mathbf{x}_t$。

定义 $\alpha_t=1-\beta_t$ and $\bar{\alpha}_t=\prod_{i=1}^t\alpha_i$

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

(*) 合并两个高斯分布

$\mathcal{N}(\mathbf{0}, \sigma_1^2\mathbf{I})$和$\mathcal{N}(\mathbf{0}, \sigma_2^2\mathbf{I})$，得到的新的高斯分布是 $\mathcal{N}(\mathbf{0}, (\sigma_1^2+\sigma_2^2)\mathbf{I})$h合并后的标准差是：$\sqrt{(1-\alpha_t)+\alpha_t(1-\alpha_{t-1})} = \sqrt{1-\alpha_t\alpha_{t-1}}$

Reverse diffusion process

前向过程是扩散（加噪）过程，那么逆向过程就是去噪。如果我们可以反转扩散过程，得到逆转后的分布 $q(\mathbf{x}_{t-1} \vert \mathbf{x}_t)$，就可以从标准高斯分布 $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 中还原出原图分布$\mathbf{x}_0$。

如果β_t足够小的话，$q(\mathbf{x}_{t-1} \vert \mathbf{x}_t)$也是高斯分布。

不过我们无法简单得到$q(\mathbf{x}_{t-1} \vert \mathbf{x}_t)$。因此我们使用深度学习模型$p_\theta$来预测这样一个逆向分布。

$p_\theta(\mathbf{x}_{0:T}) = p(\mathbf{x}_T) \prod^T_{t=1} p_\theta(\mathbf{x}_{t-1} \vert \mathbf{x}_t)$

$p_\theta(\mathbf{x}_{t-1} \vert \mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t))$

我们无法得到逆向后的分布$q(\mathbf{x}_{t-1} \vert \mathbf{x}_t)$，但如果知道$\mathbf{x}_0$，是可以通过贝叶斯公式得到$q(\mathbf{x}_{t-1} \vert \mathbf{x}_t, \mathbf{x}_0)$为：

$$
q(\mathbf{x}_{t-1} \vert \mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}; {\tilde{\boldsymbol{\mu}}}(\mathbf{x}_t, \mathbf{x}_0), {\tilde{\beta}_t \mathbf{I}})
$$

具体的推导如下：

$$
\begin{aligned}
q(\mathbf{x}_{t-1} \vert \mathbf{x}_t, \mathbf{x}_0) &= q(\mathbf{x}_t \vert \mathbf{x}_{t-1}, \mathbf{x}_0) \frac{ q(\mathbf{x}_{t-1} \vert \mathbf{x}_0) }{ q(\mathbf{x}_t \vert \mathbf{x}_0) } \\
&\propto \exp \Big(-\frac{1}{2} \big(\frac{(\mathbf{x}t - \sqrt{\alpha_t} \mathbf{x}_{t-1})^2}{\beta_t} + \frac{(\mathbf{x}_{t-1} - \sqrt{\bar{\alpha}_{t-1}} \mathbf{x}_0)^2}{1-\bar{\alpha}_{t-1}} - \frac{(\mathbf{x}_t - \sqrt{\bar{\alpha}_t} \mathbf{x}_0)^2}{1-\bar{\alpha}_t} \big) \Big) \\
&= \exp \Big(-\frac{1}{2} \big(\frac{\mathbf{x}t^2 - 2\sqrt{\alpha_t} \mathbf{x}_t {\mathbf{x}_{t-1}} {+ \alpha_t} {\mathbf{x}_{t-1}^2} }{\beta_t} + \frac{ {\mathbf{x}_{t-1}^2} {- 2 \sqrt{\bar{\alpha}_{t-1}} \mathbf{x}_0} {\mathbf{x}_{t-1}} {+ \bar{\alpha}_{t-1} \mathbf{x}_0^2} }{1-\bar{\alpha}_{t-1}} - \frac{(\mathbf{x}_t - \sqrt{\bar{\alpha}_t} \mathbf{x}_0)^2}{1-\bar{\alpha}_t} \big) \Big) \\
&= \exp\Big(-\frac{1}{2} \big({(\frac{\alpha_t}{\beta_t} + \frac{1}{1 - \bar{\alpha}_{t-1}})} \mathbf{x}_{t-1}^2 - {(\frac{2\sqrt{\alpha_t}}{\beta_t} \mathbf{x}_t + \frac{2\sqrt{\bar{\alpha}_{t-1}}}{1 - \bar{\alpha}_{t-1}} \mathbf{x}_0)} \mathbf{x}_{t-1} { + C(\mathbf{x}_t, \mathbf{x}_0) \big) \Big)}
\end{aligned}
$$

其中第一步贝叶斯公式部分：

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

$$
P(A \mid B, C) = \frac{P(B|A,C)\ P(A|C)}{P(B|C)}
$$

▼ Proof:

$$
\begin{aligned}
P(A \mid B, C) &= \frac{P(A, B, C)}{P(B, C)} \\
&= \frac{P(B \mid A, C)\, P(A, C)}{P(B, C)} \\
&= \frac{P(B \mid A, C)\, P(A \mid C)\, P(C)}{P(B, C)} \\
&= \frac{P(B \mid A, C)\, P(A \mid C) P(C)}{P(B \mid C) P(C)} \\
&= \frac{P(B \mid A, C)\, P(A \mid C)}{P(B \mid C)}
\end{aligned}
$$

一般的高斯密度函数的指数部分应该写为：

$$
\exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) = \exp\left(-\frac{1}{2}\left(\frac{1}{\sigma^2}x^2 - \frac{2\mu}{\sigma^2}x + \frac{\mu^2}{\sigma^2}\right)\right)
$$

其中$C(\mathbf{x}_t, \mathbf{x}_0)$是与$\mathbf{x}_{t-1}$无关的常数项。按照标准高斯密度函数，均值和方差可以参数化如下（回想一下$\alpha_t = 1 - \beta_t$ 和 $\bar{\alpha}_t = \prod_{i=1}^{T} \alpha_i$):

$$
\begin{aligned}
\tilde{\beta}t &= 1/\left(\frac{\alpha_t}{\beta_t} + \frac{1}{1 - \bar{\alpha}_{t-1}}\right) = 1/\left(\frac{\alpha_t - \bar{\alpha}_t + \beta_t}{\beta_t(1 - \bar{\alpha}_{t-1})}\right) = {\color{green}\frac{1 - \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t} \cdot \beta_t} \\
\tilde{\boldsymbol{\mu}}_t(\mathbf{x}_t, \mathbf{x}_0) &= \left(\frac{\sqrt{\alpha_t}}{\beta_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}}{1 - \bar{\alpha}_{t-1}}\mathbf{x}0\right)/\left(\frac{\alpha_t}{\beta_t} + \frac{1}{1 - \bar{\alpha}_{t-1}}\right) \\
&= \left(\frac{\sqrt{\alpha_t}}{\beta_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}}{1 - \bar{\alpha}_{t-1}}\mathbf{x}0\right){\color{green}\frac{1 - \bar{\alpha}_{t-1}}{1 - \bar{\alpha}_t} \cdot \beta_t} \\
&= \frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1 - \bar{\alpha}_t}\mathbf{x}_0
\end{aligned}
$$

因为：

$\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}$

可以整理成：

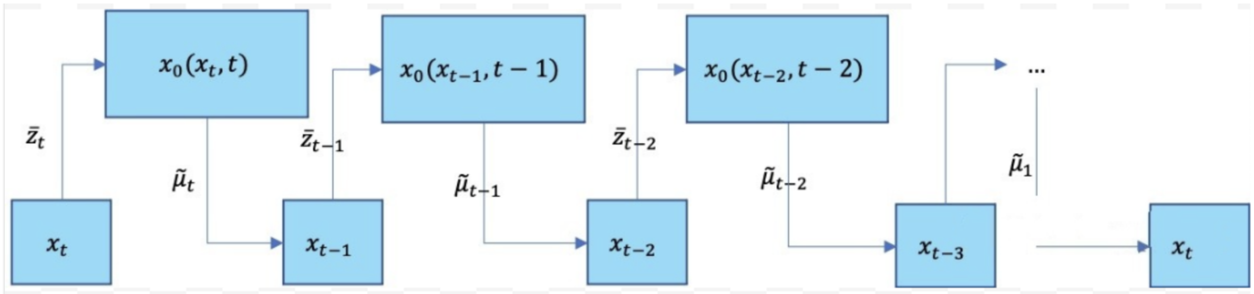
$\mathbf{x}_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}(\mathbf{x}_t - \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}_t)$

把它带入上述方程得到：

$$
\begin{aligned}
\tilde{\boldsymbol{\mu}}_t &= \frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1 - \bar{\alpha}_t}\frac{1}{\sqrt{\bar{\alpha}_t}}(\mathbf{x}_t - \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}_t) \\
&= {\color{cyan}\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}}\boldsymbol{\epsilon}_t\right)}
\end{aligned}
$$

如此DDPM的每一步推断可以总结为：

1. 每个时间步通过$\mathbf{x}_t$和t来预测高斯噪声ϵ_t，然后根据 $\tilde{\boldsymbol{\mu}}_t = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}}\boldsymbol{\epsilon}_t\right)$得到$\mu_t$
2. DDPM中方差部分$\Sigma_\theta(x_t, t)$与$\tilde{\beta}_t$相关
3. 根据$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}; \tilde{\mu}(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t\mathbf{I})$，利用重参数得到$x_{t-1}$：



Diffusion训练

如上文所描述的diffusion逆向过程，我们需要训练diffusion模型得到可用的 $\mu_\theta(x_t,t)$。

Diffusion的设置设置与 VAE 非常相似，因此我们可以使用变分下限来优化负对数似然：

$$\begin{aligned}
\log p_\theta(\mathbf{x}_0) &\leq -\log p_\theta(\mathbf{x}_0) + DKL(q(\mathbf{x}_{1:T}|\mathbf{x}_0)\|p_\theta(\mathbf{x}_{1:T}|\mathbf{x}_0)) \\
&= -\log p_\theta(\mathbf{x}_0) + \mathbb{E}\mathbf{x}_{1:T} \sim q(\mathbf{x}_{1:T}|\mathbf{x}_0)\Big[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})/p_\theta(\mathbf{x}_0)}\Big] \\
&= -\log p\theta(\mathbf{x}_0) + \mathbb{E}q\Big[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})} + \log p_\theta(\mathbf{x}_0)\Big] \\
&= \mathbb{E}q\Big[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})}\Big] \\
\text{Let } L_{\mathrm{VLB}} &= \mathbb{E}q(\mathbf{x}_{0:T})\Big[\log \frac{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})}\Big] \geq -\mathbb{E}_{q(\mathbf{x}_0)}\log p_\theta(\mathbf{x}_0)
\end{aligned}$$

进一步对L_{VLB}推导，可以得到熵与多个KL散度的累加，推导过程

$$
\begin{aligned}
L_\text{VLB} &= \mathbb{E}_{q(\mathbf{x}_{0:T})} \Big[\log\frac{q(\mathbf{x}_{1:T}\vert\mathbf{x}_0)}{p_\theta(\mathbf{x}_{0:T})} \Big] \\
&= \mathbb{E}_q \Big[\log\frac{\prod_{t=1}^T q(\mathbf{x}_t\vert\mathbf{x}_{t-1})}{ p_\theta(\mathbf{x}_T) \prod_{t=1}^T p_\theta(\mathbf{x}_{t-1} \vert\mathbf{x}_t) } \Big] \\
&= \mathbb{E}_q \Big[-\log p_\theta(\mathbf{x}_T) + \sum_{t=1}^T \log \frac{q(\mathbf{x}_t\vert\mathbf{x}_{t-1})}{p_\theta(\mathbf{x}_{t-1} \vert\mathbf{x}_t)} \Big] \\
&= \mathbb{E}_q \Big[-\log p_\theta(\mathbf{x}_T) + \sum_{t=2}^T \log \frac{q(\mathbf{x}_t\vert\mathbf{x}_{t-1})}{p_\theta(\mathbf{x}_{t-1} \vert\mathbf{x}_t)} + \log\frac{q(\mathbf{x}_1 \vert \mathbf{x}_0)}{p_\theta(\mathbf{x}_0 \vert \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} \vert \mathbf{x}_t, \mathbf{x}_0)}{p_\theta(\mathbf{x}_{t-1} \vert\mathbf{x}_t)}\cdot \frac{q(\mathbf{x}_t \vert \mathbf{x}_0)}{q(\mathbf{x}_{t-1}\vert\mathbf{x}_0)} \Big) + \log \frac{q(\mathbf{x}_1 \vert \mathbf{x}_0)}{p_\theta(\mathbf{x}_0 \vert \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} \vert \mathbf{x}_t, \mathbf{x}_0)}{p_\theta(\mathbf{x}_{t-1} \vert\mathbf{x}_t)} + \sum_{t=2}^T \log \frac{q(\mathbf{x}_t \vert \mathbf{x}_0)}{q(\mathbf{x}_{t-1} \vert \mathbf{x}_0)} + \log\frac{q(\mathbf{x}_1 \vert \mathbf{x}_0)}{p_\theta(\mathbf{x}_0 \vert \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} \vert \mathbf{x}_t, \mathbf{x}_0)}{p_\theta(\mathbf{x}_{t-1} \vert\mathbf{x}_t)} + \log\frac{q(\mathbf{x}_T \vert \mathbf{x}_0)}{q(\mathbf{x}_1 \vert \mathbf{x}_0)} + \log \frac{q(\mathbf{x}_1 \vert \mathbf{x}_0)}{p_\theta(\mathbf{x}_0 \vert \mathbf{x}_1)} \Big]\\
&= \mathbb{E}_q \Big[\log\frac{q(\mathbf{x}_T \vert \mathbf{x}_0)}{p_\theta(\mathbf{x}_T)} + \sum_{t=2}^T \log \frac{q(\mathbf{x}_{t-1} \vert \mathbf{x}_t, \mathbf{x}_0)}{p_\theta(\mathbf{x}_{t-1} \vert\mathbf{x}_t)} - \log p_\theta(\mathbf{x}_0 \vert \mathbf{x}_1) \Big] \\
&= \mathbb{E}_q [\underbrace{D_\text{KL}(q(\mathbf{x}_T \vert \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_T))}_{L_T} + \sum_{t=2}^T \underbrace{D_\text{KL}(q(\mathbf{x}_{t-1} \vert \mathbf{x}_t, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_{t-1} \vert\mathbf{x}_t))}_{L_{t-1}} \underbrace{- \log p_\theta(\mathbf{x}_0 \vert \mathbf{x}_1)}_{L_0}]
\end{aligned}
$$

▼ Notes:

- basic knowledge about logarithms:

$$
\begin{aligned}
logA + logB &= logAB \\
logA - logB &= logA/B \\
logA^n &= nlogA
\end{aligned}
$$

- line 4 → line 5: Markov property of the forward process, and the Bayes' rule

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

也可以写作：

$$
\begin{aligned}
L_\text{VLB} &= L_T + L_{T-1} + \dots + L_0 \\
\text{where } L_T &= D_\text{KL}(q(\mathbf{x}_T \vert \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_T)) \\
L_t &= D_\text{KL}(q(\mathbf{x}_t \vert \mathbf{x}_{t+1}, \mathbf{x}_0) \parallel p_\theta(\mathbf{x}_t \vert\mathbf{x}_{t+1})) \text{ for }1 \leq t \leq T-1 \\
L_0 &= - \log p_\theta(\mathbf{x}_0 \vert \mathbf{x}_1)
\end{aligned}
$$

前向q没有可学习参数，x_T是纯噪声，L_T可以当作是常数项忽略。而L_t则可以看做拉近两个高斯分布 $q(\mathbf{x}_{t-1} \vert \mathbf{x}_t, \mathbf{x}_0)$和 $p_\theta(\mathbf{x}_{t-1} \vert\mathbf{x}_t)$, 根据多元高斯分布的KL散度求解：

参数化L_t

我们需要学习一个神经网络来逼近反向扩散过程中的条件概率分布：$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)=\mathcal{N}(\mathbf{x}_{t-1};\mu_\theta(\mathbf{x}_t,t),\Sigma_\theta(\mathbf{x}_t,t))$。我们需要训练一个$\boldsymbol{\mu}_\theta$来预测$\tilde{\boldsymbol{\mu}}_t=\frac{1}{\sqrt{\alpha_t}}\Big(\mathbf{x}_t-\frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_t\Big)$。因为$\mathbf{x}_t$在训练时是当作输入参数，我们可以重新参数化高斯噪声项，以使其根据 timestep t的输入x_t来预测ϵ_t：

$$\mu_\theta(\mathbf{x}_t,t)=\frac{1}{\sqrt{\alpha_t}}\Big(\mathbf{x}_t-\frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(\mathbf{x}_t,t)\Big)$$

$$\text{Thus }\mathbf{x}_{t-1}=\mathcal{N}(\mathbf{x}_{t-1};\frac{1}{\sqrt{\alpha_t}}\Big(\mathbf{x}_t-\frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}t}}\epsilon_\theta(\mathbf{x}_t,t)\Big),\Sigma_\theta(\mathbf{x}_t,t))$$

The loss term L_t

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

💡 diffusion训练的核心就是取学习高斯噪声 ϵt 和 $\epsilon\theta$ 之间的MSE

简化 L_t

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

最后的目标函数是：

$$L_{\text{simple}}=L_t^{\text{simple}}+C$$

训练过程可以归纳为：

1. 从真实数据分布中随机sample一个 x_0, 从$1\ldots T$随机采样一个t.
2. 从标准高斯分布采样一个噪声 $\epsilon_t\sim\mathcal{N}(0,I)$
3. 最小化 $[\|\epsilon_t-\epsilon_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0+\sqrt{1-\bar{\alpha}_t}\epsilon_t,t)\|$

Algorithm 1 Training

1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $t \sim \text{Uniform}(\{1, \dots, T\})$
4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
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** $t = T, \dots, 1$ **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** $\mathbf{x}_0$

小结

💡 综上所述，理解DDPM可以分成3个部分：

1. Forward diffusion process: 前向扩散过程，这部分主要是通过重参数化，得到

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

2. Reverse diffusion process：反向扩散处理（去噪），这部分主要通过利用贝叶斯公式，利用x_t, x_0得到x_{t-1}

$$q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}t-1; \tilde{\mu}(\mathbf{x}_t, \mathbf{x}_0), \tilde{\beta}_t\mathbf{I})$$
$$\tilde{\mu}_t = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_t\right) \text{;where } \epsilon_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

3. Diffusion训练，这部分首先利用变分下限来优化负对数似然来得到：

$$L_{\text{VLB}} = L_T + L_{T-1} + \cdots + L_0$$
$$\text{where } L_t = D_{\text{KL}}(q(\mathbf{x}_t|\mathbf{x}_{t+1}, \mathbf{x}0) \parallel p_\theta(\mathbf{x}_t|\mathbf{x}_{t+1})) \text{ for } 1 \leq t \leq T-1$$

然后利用1，2中的结论代入到L_t:

$$\begin{aligned}
L_t &= \mathbb{E}_{\mathbf{x}_0,\epsilon}\left[\frac{1}{2\|\Sigma\theta(\mathbf{x}_t, t)\|_2^2}\|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu\theta(\mathbf{x}_t, t)\|^2\right] \\
&= \mathbb{E}\mathbf{x}0, \epsilon\left[\frac{1}{2\|\Sigma\theta\|_2^2}\|\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_t\right) - \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}t}}\epsilon\theta(\mathbf{x}_t, t)\right)\|^2\right] \\
&= \mathbb{E}\mathbf{x}_0, \epsilon\left[\frac{(1-\alpha_t)^2}{2\alpha_t(1-\bar{\alpha}_t)\|\Sigma\theta\|_2^2}\|\epsilon_t - \epsilon_\theta(\mathbf{x}_t, t)\|^2\right] \\
&= \mathbb{E}\mathbf{x}_0, \epsilon\left[\frac{(1-\alpha_t)^2}{2\alpha_t(1-\bar{\alpha}_t)\|\Sigma\theta\|_2^2}\|\epsilon_t - \epsilon_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\epsilon_t, t)\|^2\right]
\end{aligned}$$

在训练的时候loss为：

$\|\epsilon_t - \epsilon_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\epsilon_t, t)\|$da

代码部分

Training

```
def forward(self, x_0):
        """
```

```
        Algorithm 1.
        """
        t = torch.randint(self.T, size=(x_0.shape[0],), device=x_0.device)
        noise = torch.randn_like(x_0)
        x_t = (
            extract(self.sqrt_alphas_bar, t, x_0.shape) * x_0
            + extract(self.sqrt_one_minus_alphas_bar, t, x_0.shape) * noise
        )
        loss = F.mse_loss(self.model(x_t, t), noise, reduction="none")
        return loss
```

Sampling

```
class GaussianDiffusionSampler(nn.Module):
    def __init__(self, model, beta_1, beta_T, T):
        super().__init__()

        self.model = model
        self.T = T

        self.register_buffer("betas", torch.linspace(beta_1, beta_T, T).double())
        alphas = 1.0 - self.betas
        alphas_bar = torch.cumprod(alphas, dim=0)
        alphas_bar_prev = F.pad(alphas_bar, [1, 0], value=1)[:T]

        self.register_buffer("coeff1", torch.sqrt(1.0 / alphas))
        self.register_buffer(
            "coeff2", self.coeff1 * (1.0 - alphas) / torch.sqrt(1.0 - alphas_bar)
        )

        self.register_buffer(
            "posterior_var", self.betas * (1.0 - alphas_bar_prev) / (1.0 - alphas_bar)
        )

    def predict_xt_prev_mean_from_eps(self, x_t, t, eps):
        assert x_t.shape == eps.shape
        return (
            extract(self.coeff1, t, x_t.shape) * x_t
            - extract(self.coeff2, t, x_t.shape) * eps
        )

    def p_mean_variance(self, x_t, t):
        # below: only log_variance is used in the KL computations
        var = torch.cat([self.posterior_var[1:2], self.betas[1:]])
        var = extract(var, t, x_t.shape)

        eps = self.model(x_t, t)
        xt_prev_mean = self.predict_xt_prev_mean_from_eps(x_t, t, eps=eps)

        return xt_prev_mean, var

    def forward(self, x_T):
        """
        Algorithm 2.
        """
        x_t = x_T
        for time_step in reversed(range(self.T)):
            print(time_step)
            t = (
                x_t.new_ones(
                    [
                        x_T.shape[0],
                    ],
                    dtype=torch.long,
                )
                * time_step
            )
            mean, var = self.p_mean_variance(x_t=x_t, t=t)
            # no noise when t == 0
            if time_step > 0:
                noise = torch.randn_like(x_t)
            else:
                noise = 0
            x_t = mean + torch.sqrt(var) * noise
```

```
            assert torch.isnan(x_t).int().sum() == 0, "nan in tensor."
        x_0 = x_t
        return torch.clip(x_0, -1, 1)
```