



PATTERN
RECOGNITION

模式识别 Pattern Recognition

李泽桦, 复旦大学 生物医学工程与技术创新学院

课件内容参考MIT 6.S978 Deep Generative Models

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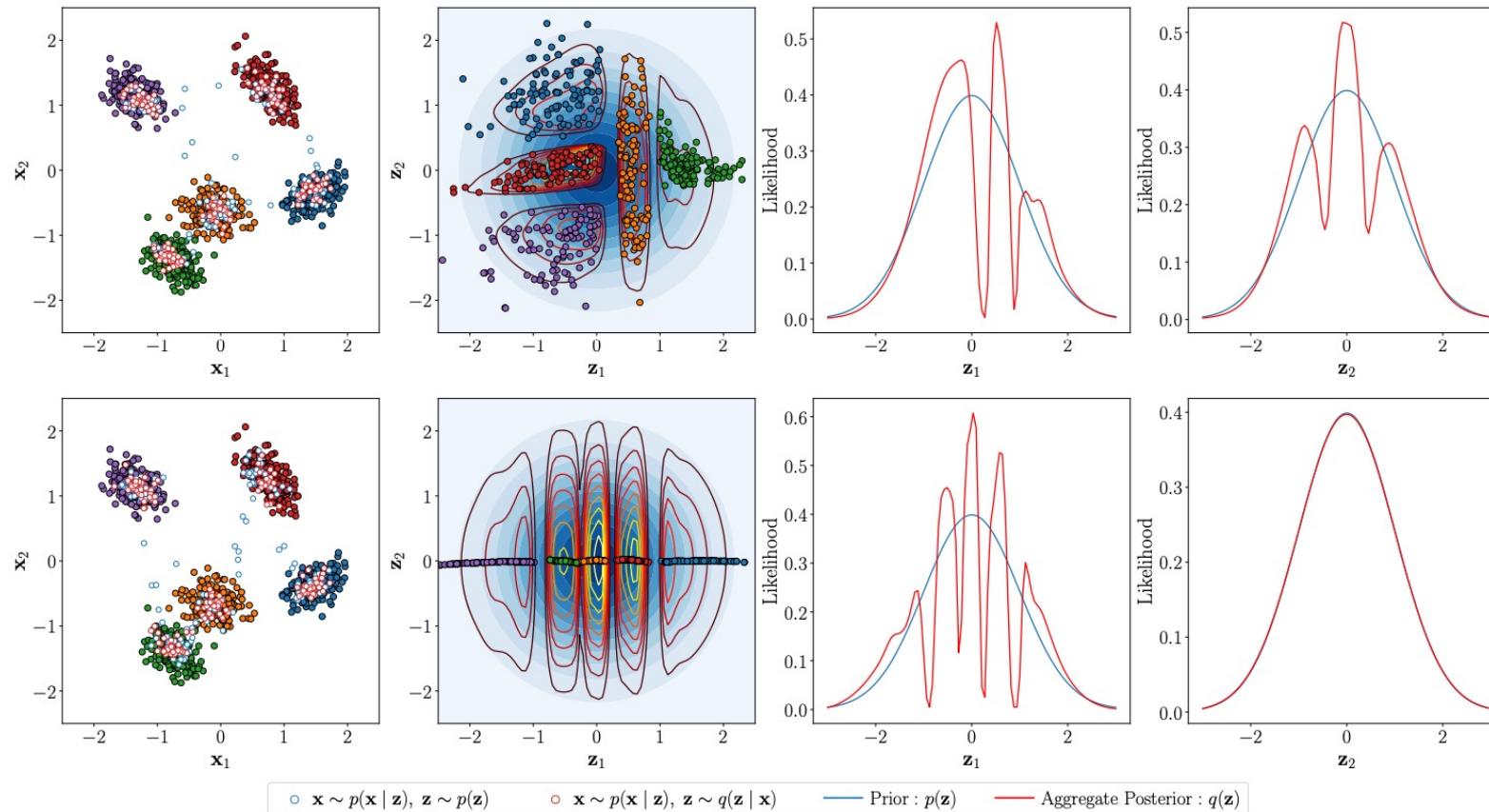
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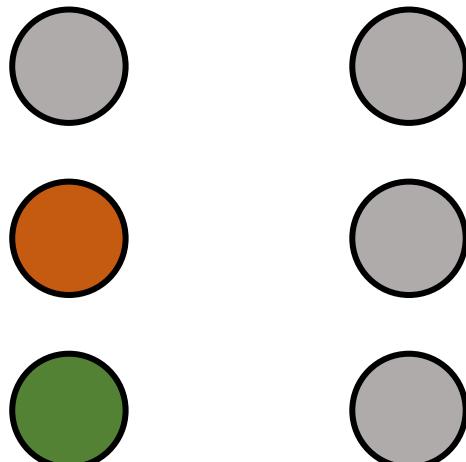
多种参数化形式

- VAE的空洞问题：没采样到的样本很难生成



VAE的空洞问题：

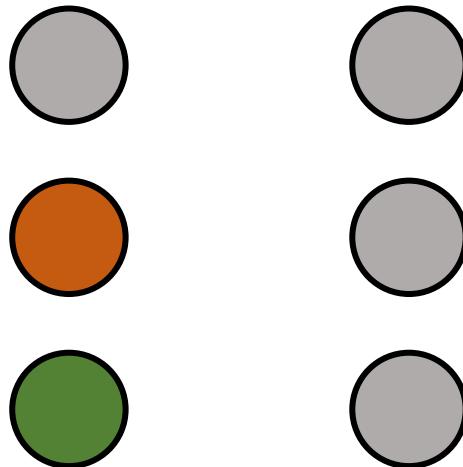
- 表征缺少相关性
- 难以建模没采样到的点



真实 \neq 采样

VAE的空洞问题：

- 表征缺少相关性
- 难以建模没采样到的点



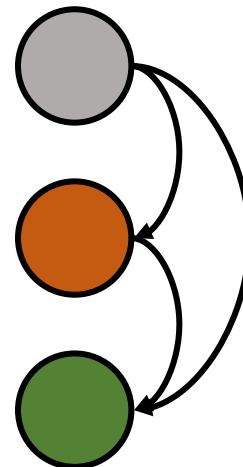
真实



采样

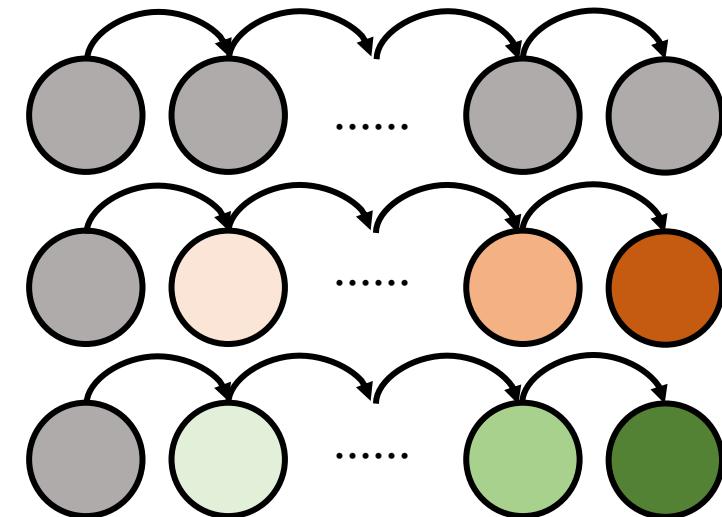
自回归模型：

- 基于时间建模
- 条件依赖，顺序建模

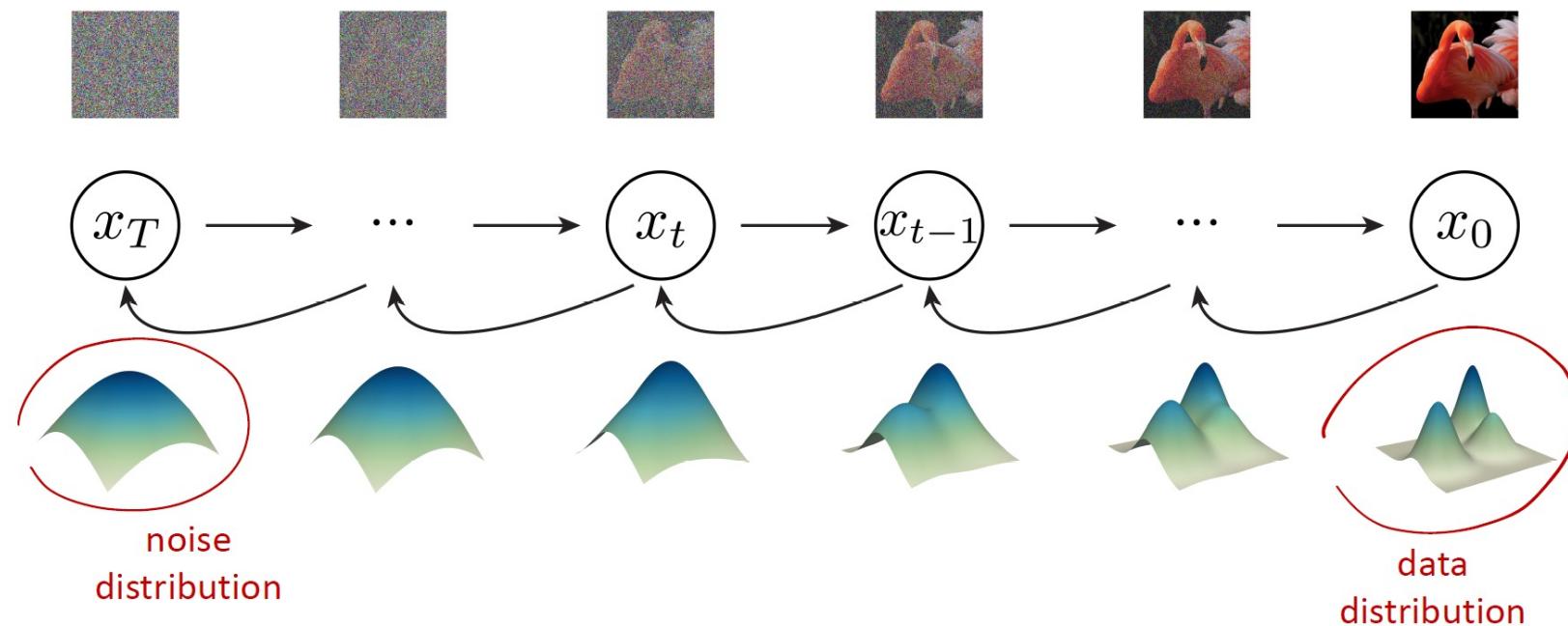


扩散模型：

- 基于空间建模
- 迭代去噪，精炼相关性



- 扩散模型通过构造，将**聚合后验**定义为等于先验来解决空洞问题
- 但因为后验都遵循加噪过程，其牺牲了学习有意义表征的能力



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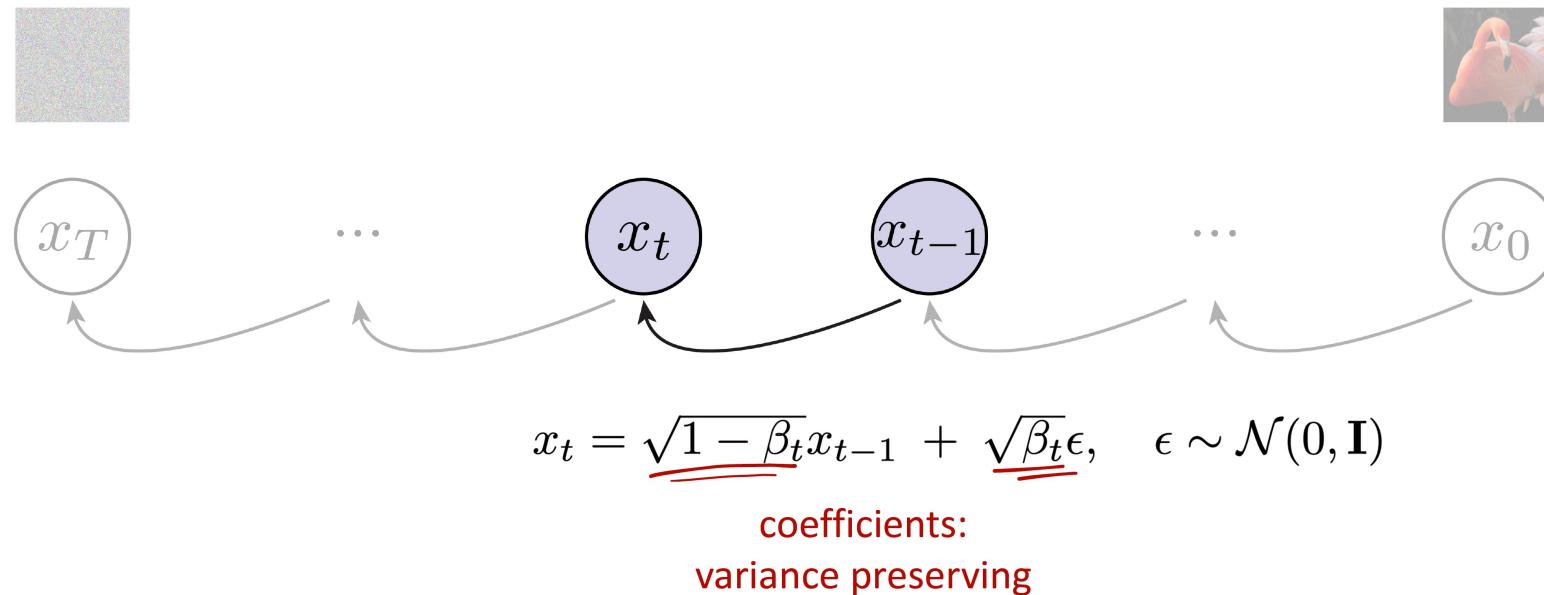
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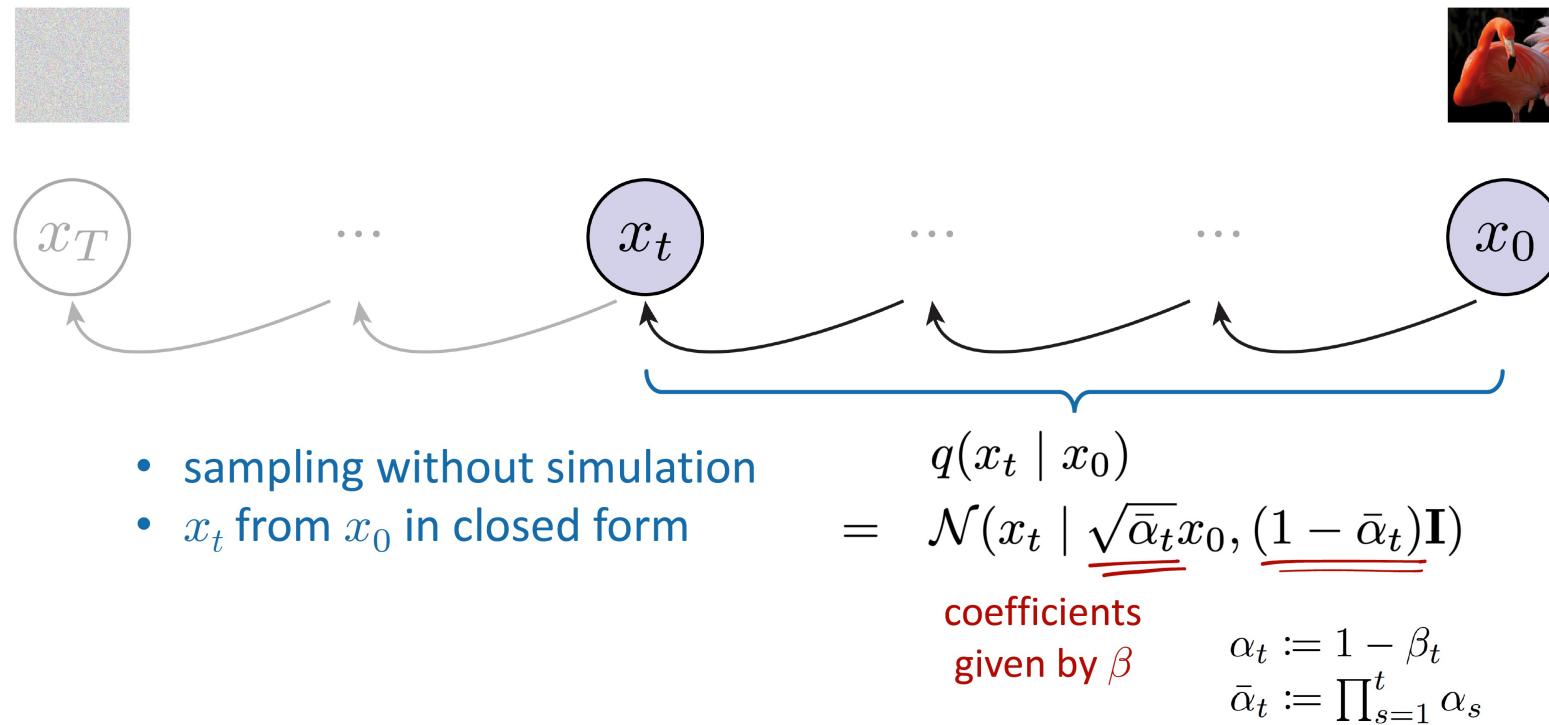
3 训练目标

4 多种参数化形式

- 基于马尔可夫链的加入高斯噪声
- 为了保证图像可控，一般噪声会遵循Variance Preserving (VP)



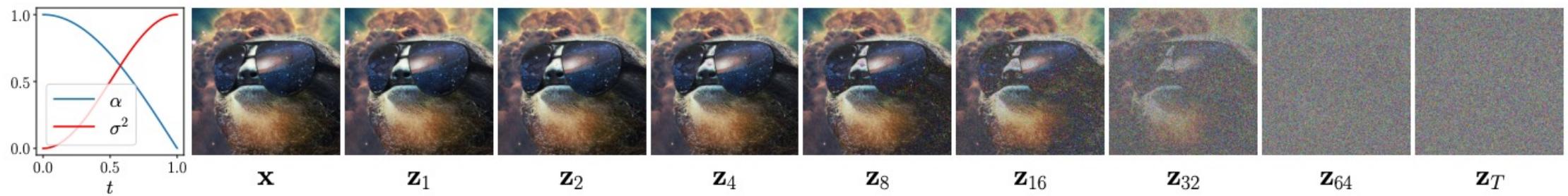
- 高斯分布再生性：多个独立高斯随机变量的和仍然是高斯分布
- 所以可以训练的时候随机取一步



前向过程



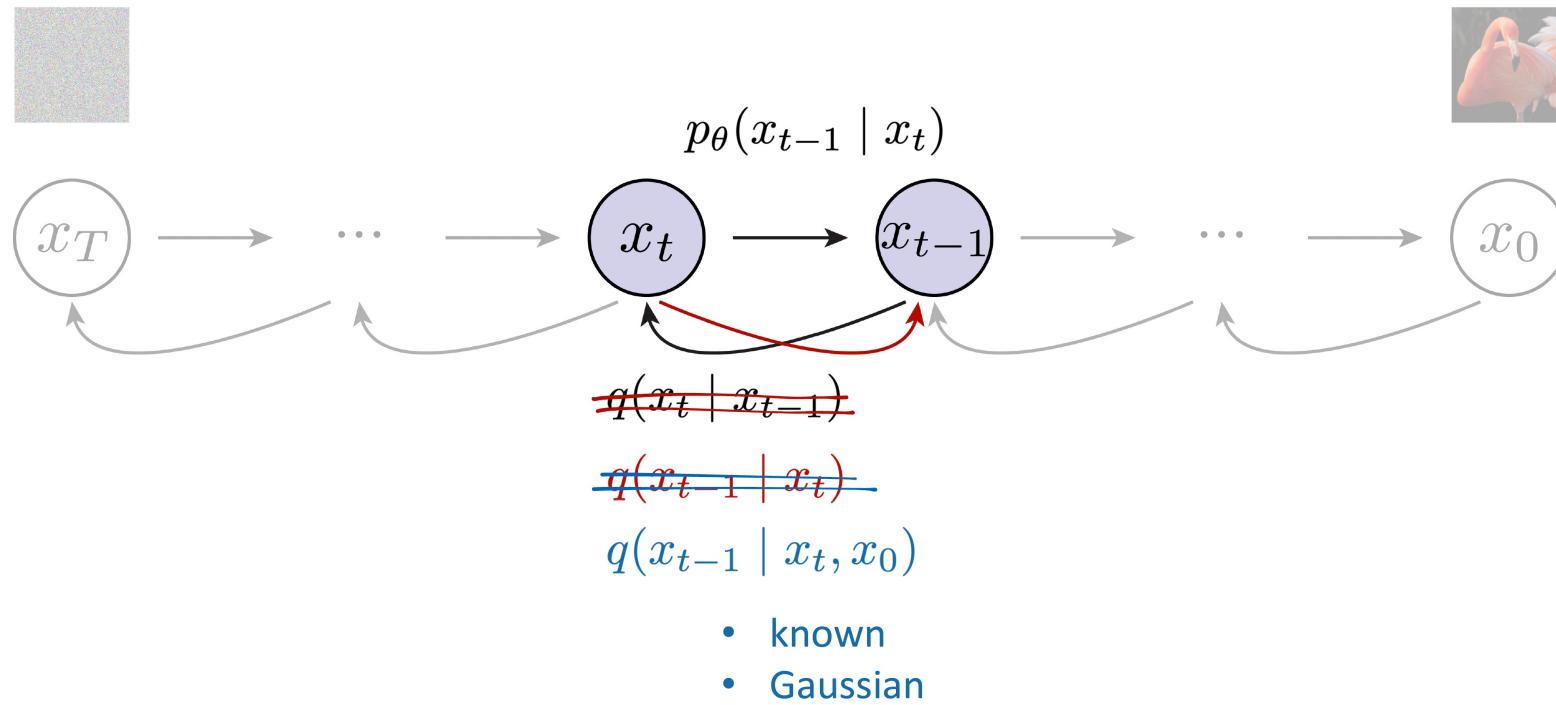
- 噪声在干净步骤均值最接近1，方差最小
- 噪声在噪声步骤均值最接近0，方差最大



反向过程



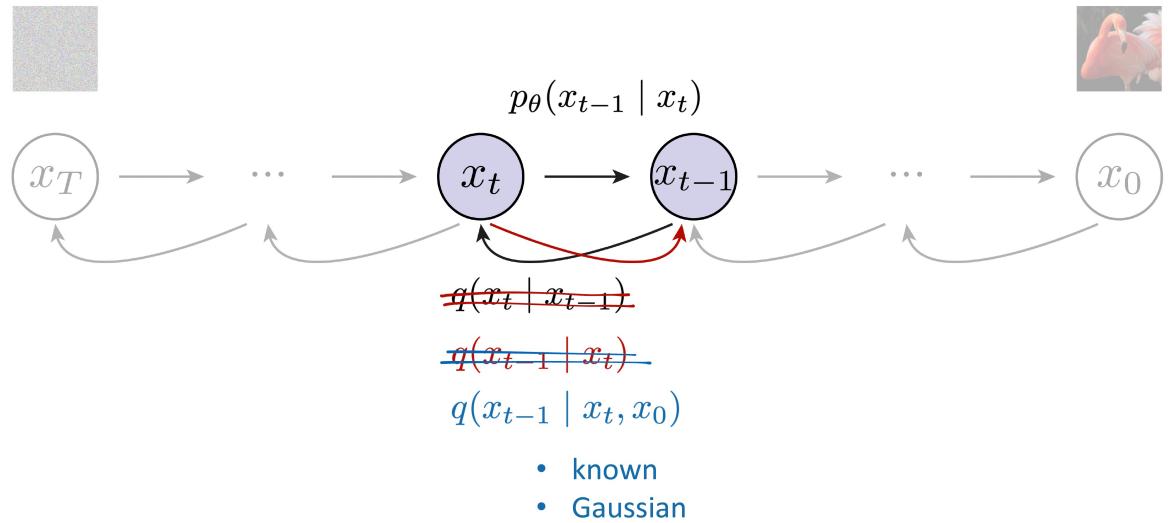
- 在同时观察到 x_t 和知道 x_0 的情况下, 对 x_{t-1} 的估计



反向过程



- 在同时观察到 x_t 和知道 x_0 的情况下，对 x_{t-1} 的估计



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

马尔可夫性 \Rightarrow

$$q(x_{t-1} | x_t, x_0) = \mathbf{q}(\mathbf{x}_t | \mathbf{x}_{t-1}) \frac{\mathbf{q}(\mathbf{x}_{t-1} | \mathbf{x}_0)}{q(x_t | x_0)}$$

代入高斯分布，忽略与 x_{t-1} 无关常数 \Rightarrow

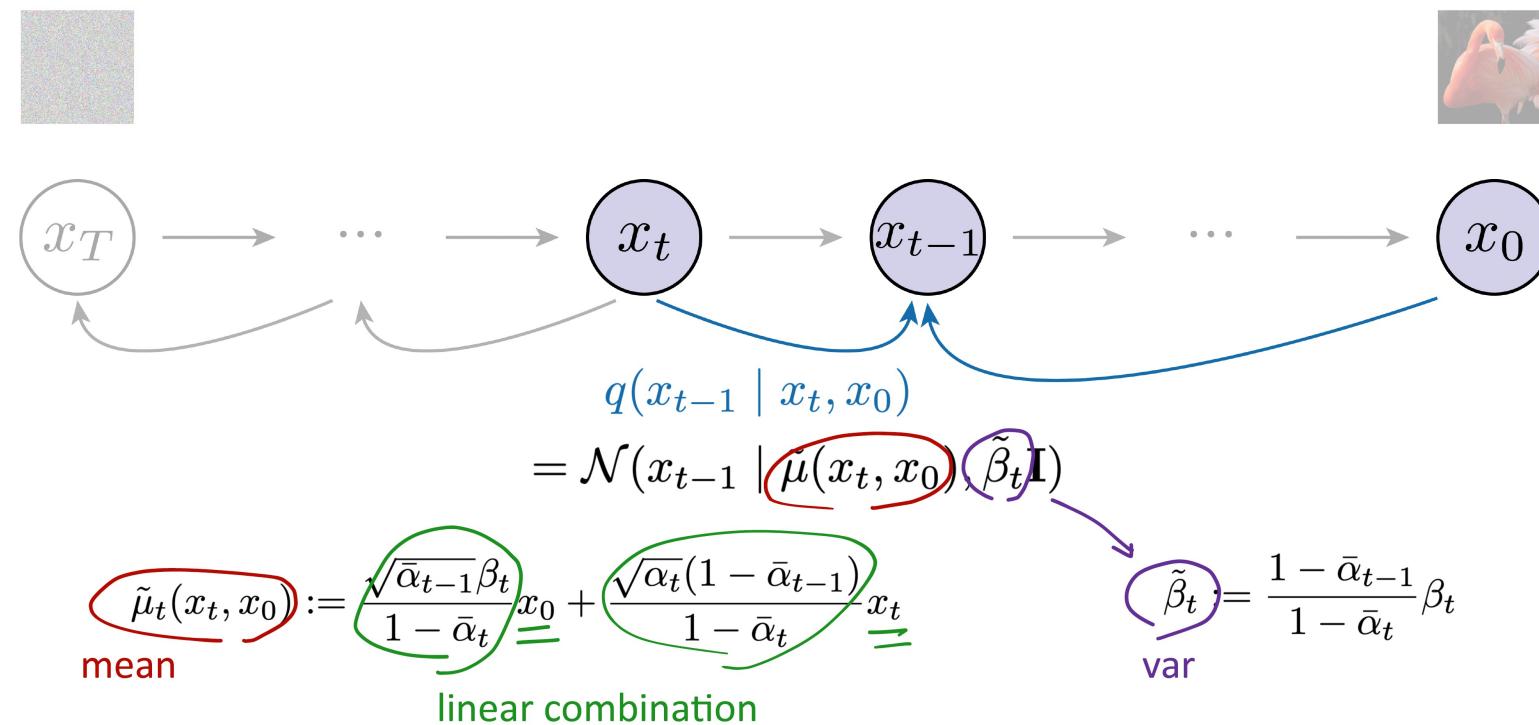
$$q(x_{t-1} | x_t, x_0) \propto \exp \left(-\frac{1}{2} \left[\frac{\|x_t - \sqrt{1 - \beta_t} \mathbf{x}_{t-1}\|^2}{\beta_t} + \frac{\|\mathbf{x}_{t-1} - \sqrt{\bar{\alpha}_{t-1}} x_0\|^2}{\bar{\beta}_{t-1}} \right] \right)$$



反向过程



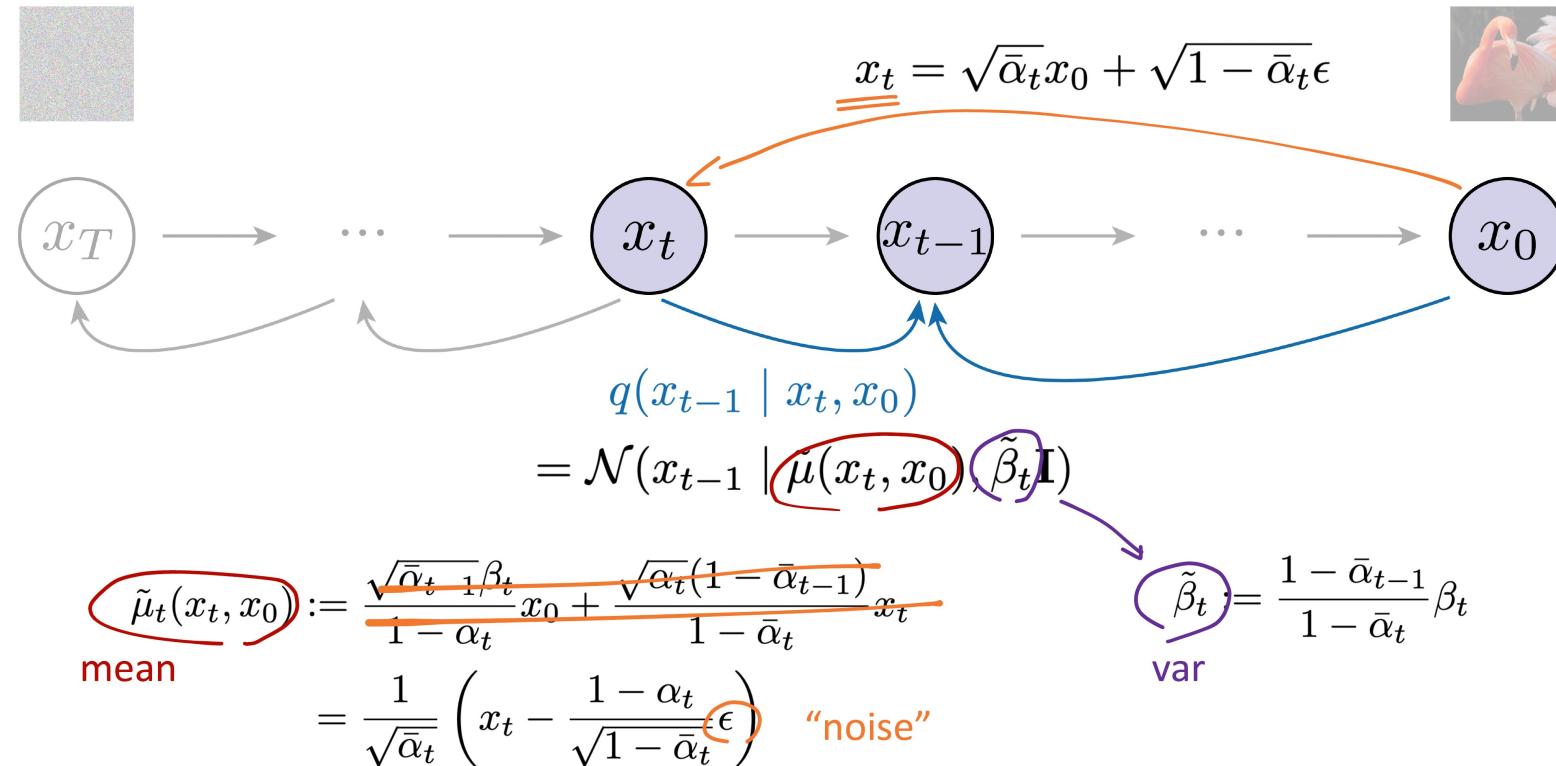
- 在 x_0 已知时，反向转移也是已知的高斯分布



反向过程



- 将 x_0 到 x_t 的过程整理成统一的噪声 ϵ

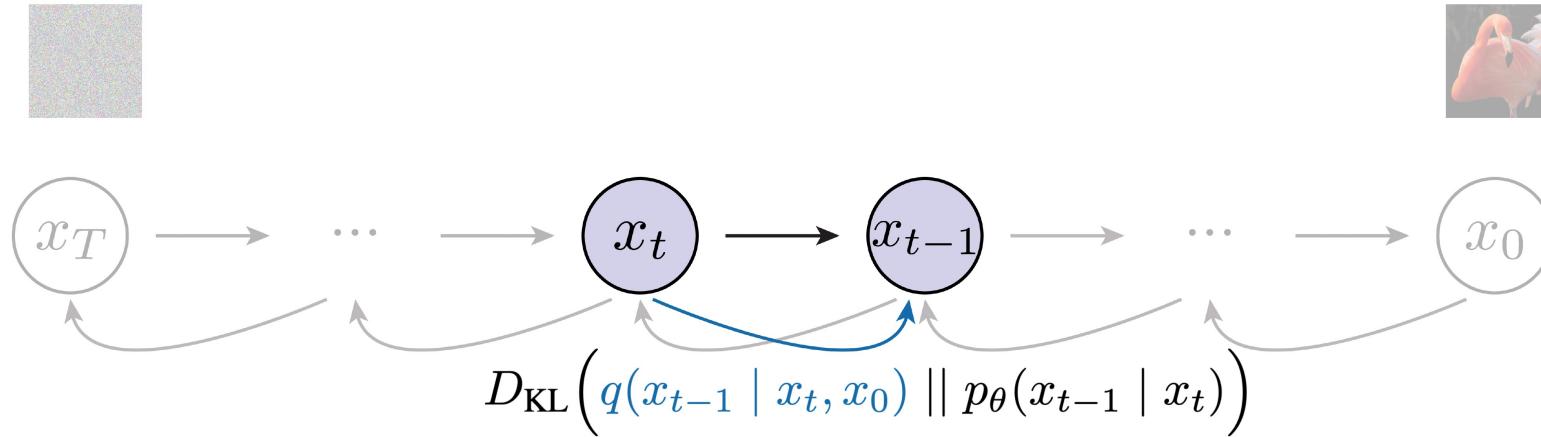


注意，这里的噪声是加在 x_0 上，用于得到 x_t 的

反向过程



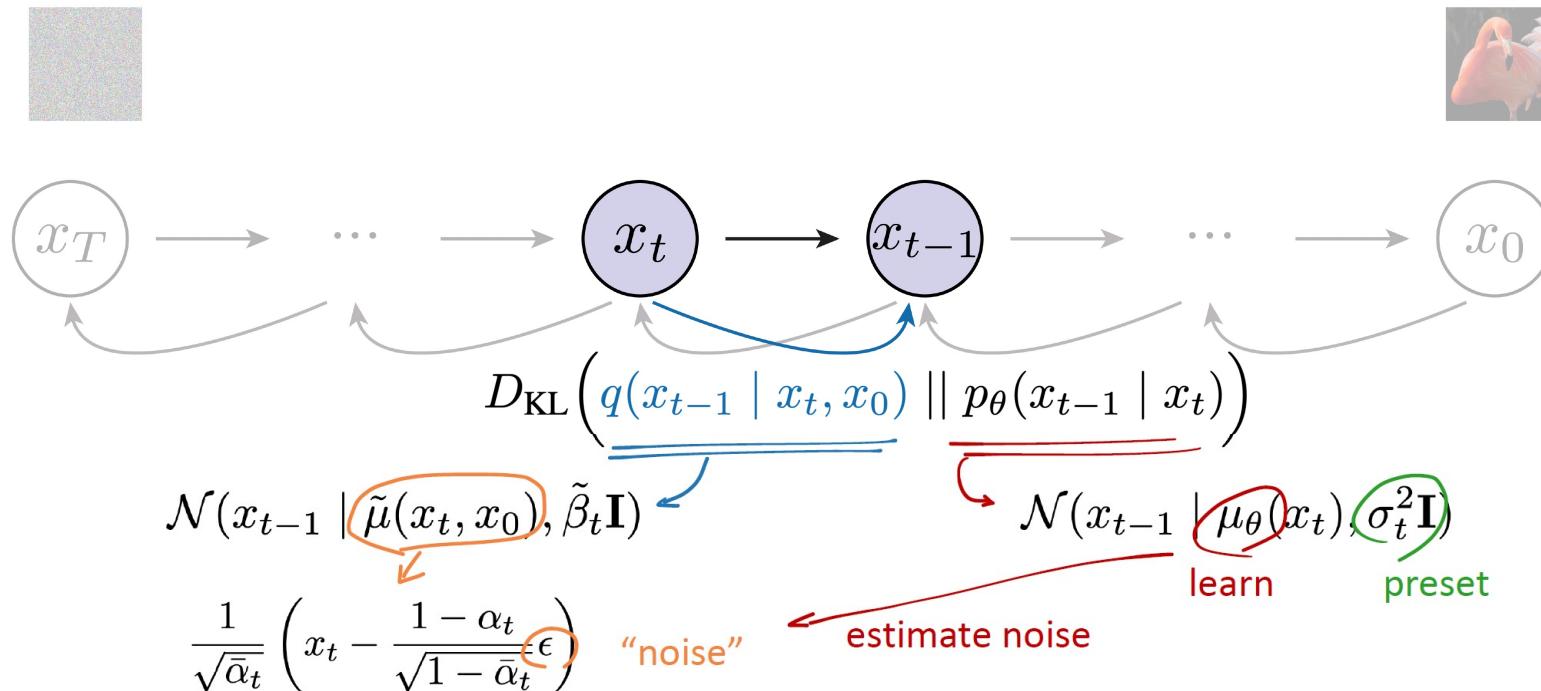
- 最小化KL散度



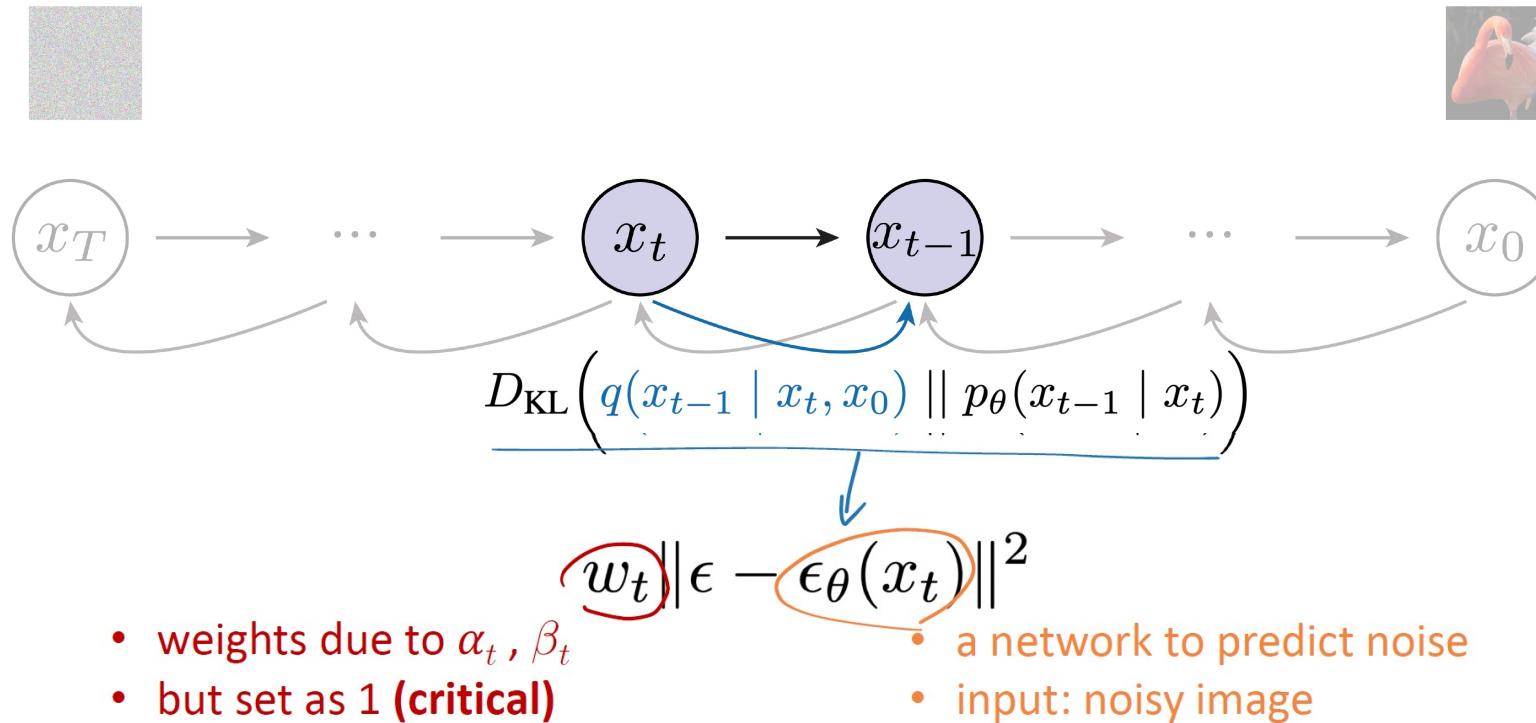
反向过程



- KL散度简化成噪声预测



- 噪声预测的L2损失



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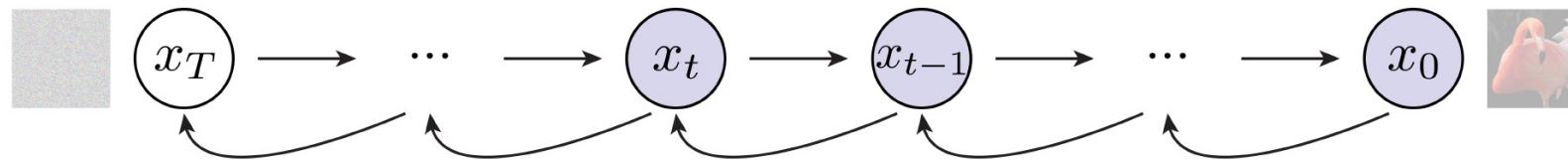
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多种参数化形式

- 所有时间步加和，通过引入近似后验分布来逼近真实后验
- 是一种ELBO衍生的损失



- variational lower bound
- like ELBO

$$\mathcal{L}_{\text{VLB}} := \mathcal{L}_T + \mathcal{L}_{T-1} + \dots + \mathcal{L}_0$$

$$\mathcal{L}_T := D_{\text{KL}}(q(x_T | x_0) || p_{\theta}(x_T))$$

只是为了完整，不需要训练

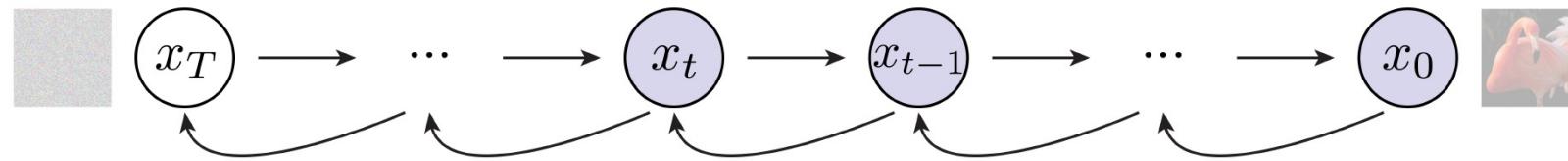
$$\mathcal{L}_{t-1} := D_{\text{KL}}(q(x_{t-1} | x_t, x_0) || p_{\theta}(x_{t-1} | x_t))$$

学习如何一步步去噪（核心学习任务）

$$\mathcal{L}_0 := -\log p_{\theta}(x_0 | x_1)$$

最终的重构质量，被隐式忽略

- 可以直接简化成去噪任务



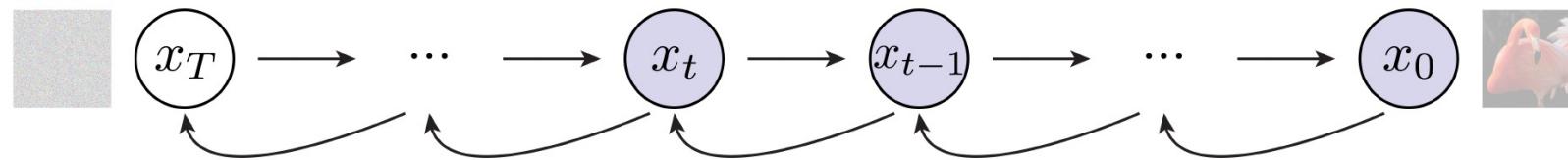
$$\mathcal{L} = \mathbb{E}_{x_0, t, \epsilon} \left[w_t \|\epsilon - \epsilon_\theta(x_t, t)\|^2 \right]$$

over p_{data}

over $[1, T]$

over $\mathcal{N}(0, \mathbf{I})$

- 理论上 $w_t = \frac{\beta_t^2}{2\sigma_t^2\alpha_t(1-\bar{\alpha}_t)}$ 在信噪比变化最快时间步权重高，高噪声水平权重小
- 理论最优 \neq 实践最佳**，实际上发现 $w_t = 1$ 表现更好



$$\mathcal{L} = \mathbb{E}_{x_0, t, \epsilon} [w_t \|\epsilon - \epsilon_\theta(x_t, t)\|^2]$$

set as 1 (critical)

Objective	IS	FID
L , learned diagonal Σ	—	—
L , fixed isotropic Σ	7.67 ± 0.13	$13.51 \leftarrow$
$\ \tilde{\epsilon} - \epsilon_\theta\ ^2$ (L_{simple})	9.46 ± 0.11	$3.17 \leftarrow$

[Ho et al. 2020]; see more in [Salimans & Ho, 2022]

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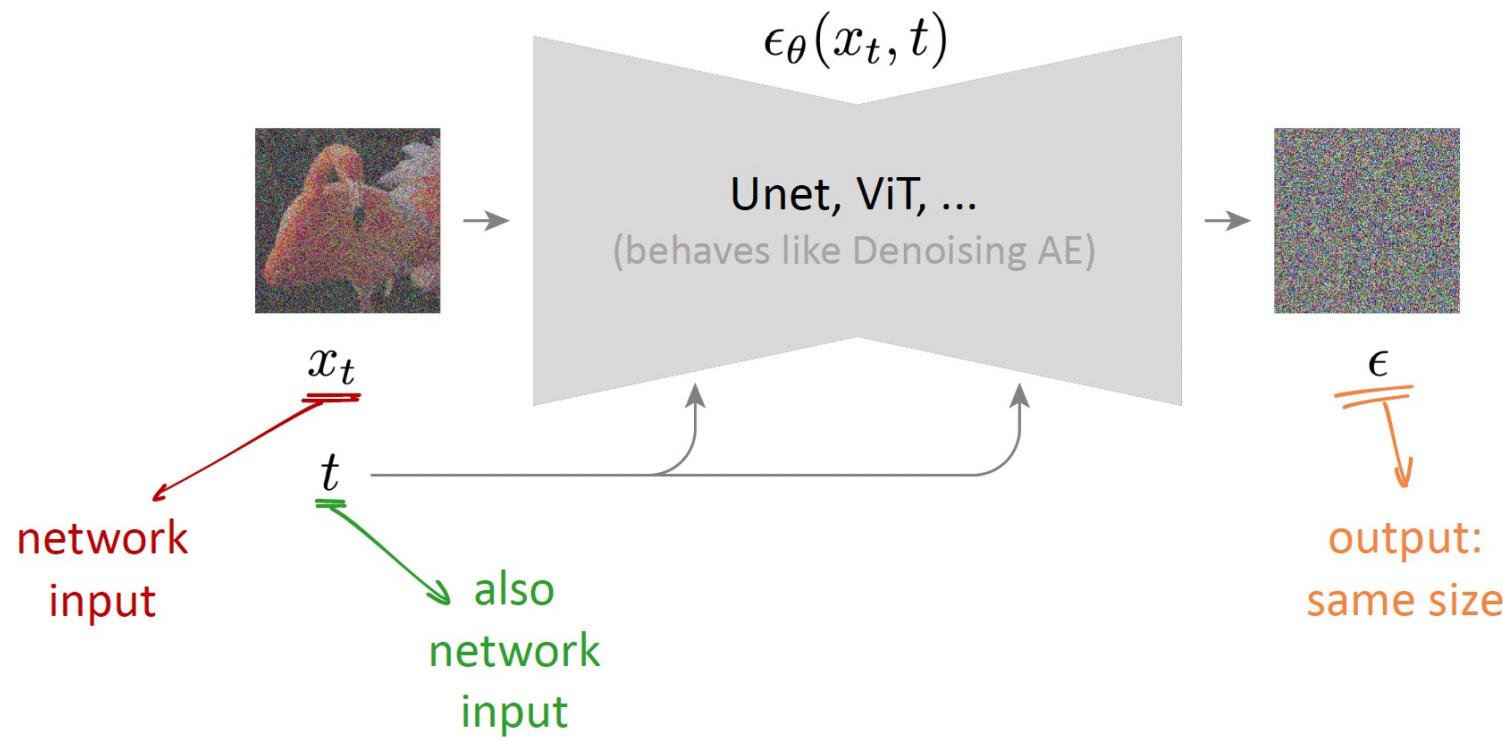
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多种参数化形式

噪声条件网络



- 利用同一个网络来预测所有时间步噪声 $p_\theta(x_{t-1}|x_t)$



- 基础扩散模型的训练和采样过程

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 $\nabla_{\theta} \|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\theta}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}) t\|^2$
- 6: **until** converged

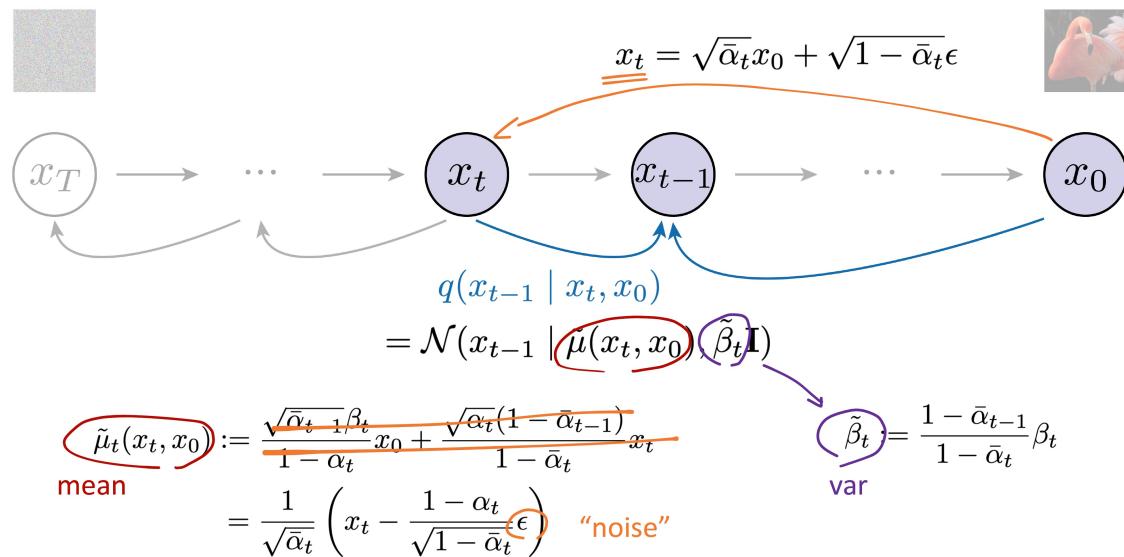
Algorithm 2 Sampling

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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:    $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left( \mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \epsilon_{\theta}(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$ 
5: end for
6: return  $\mathbf{x}_0$ 

```

estimated μ



扩散模型的设计空间



- 扩散模型的成功很大程度归功于大规模的工程实践与集体技术攻坚

Table 1: Specific design choices employed by different model families. N is the number of ODE solver iterations that we wish to execute during sampling. The corresponding sequence of time steps is $\{t_0, t_1, \dots, t_N\}$, where $t_N = 0$. If the model was originally trained for specific choices of N and $\{t_i\}$, the originals are denoted by M and $\{u_j\}$, respectively. The denoiser is defined as $D_\theta(\mathbf{x}; \sigma) = c_{\text{skip}}(\sigma)\mathbf{x} + c_{\text{out}}(\sigma)F_\theta(c_{\text{in}}(\sigma)\mathbf{x}; c_{\text{noise}}(\sigma))$; F_θ represents the raw neural network layers.

	VP [49]	VE [49]	iDDPM [37] + DDIM [47]	Ours (“EDM”)
Sampling (Section 3)				
ODE solver	Euler	Euler	Euler	2 nd order Heun
Time steps	$t_{i < N} = 1 + \frac{i}{N-1}(\epsilon_s - 1)$	$\sigma_{\max}^2 (\sigma_{\min}^2 / \sigma_{\max}^2)^{\frac{i}{N-1}}$	$u_{\lfloor j_0 + \frac{M-1-j_0}{N-1}i + \frac{1}{2} \rfloor}$, where $u_M = 0$ $u_{j-1} = \sqrt{\frac{u_j^2 + 1}{\max(\bar{\alpha}_{j-1}/\bar{\alpha}_j, C_1)} - 1}$	$(\sigma_{\max}^{\frac{1}{\rho}} + \frac{i}{N-1}(\sigma_{\min}^{\frac{1}{\rho}} - \sigma_{\max}^{\frac{1}{\rho}}))^{\rho}$
Schedule	$\sigma(t) = \sqrt{e^{\frac{1}{2}\beta_d t^2 + \beta_{\min} t} - 1}$	\sqrt{t}	t	t
Scaling	$s(t) = 1 / \sqrt{e^{\frac{1}{2}\beta_d t^2 + \beta_{\min} t}}$	1	1	1
Network and preconditioning (Section 5)				
Architecture of F_θ	DDPM++	NCSN++	DDPM	(any)
Skip scaling $c_{\text{skip}}(\sigma)$	1	1	1	$\sigma_{\text{data}}^2 / (\sigma^2 + \sigma_{\text{data}}^2)$
Output scaling $c_{\text{out}}(\sigma)$	$-\sigma$	σ	$-\sigma$	$\sigma \cdot \sigma_{\text{data}} / \sqrt{\sigma_{\text{data}}^2 + \sigma^2}$
Input scaling $c_{\text{in}}(\sigma)$	$1 / \sqrt{\sigma^2 + 1}$	1	$1 / \sqrt{\sigma^2 + 1}$	$1 / \sqrt{\sigma^2 + \sigma_{\text{data}}^2}$
Noise cond. $c_{\text{noise}}(\sigma)$	$(M-1) \sigma^{-1}(\sigma)$	$\ln(\frac{1}{2}\sigma)$	$M-1 - \arg \min_j u_j - \sigma $	$\frac{1}{4} \ln(\sigma)$
Training (Section 5)				
Noise distribution	$\sigma^{-1}(\sigma) \sim \mathcal{U}(\epsilon_t, 1)$	$\ln(\sigma) \sim \mathcal{U}(\ln(\sigma_{\min}), \ln(\sigma_{\max}))$	$\sigma = u_j, \quad j \sim \mathcal{U}\{0, M-1\}$	$\ln(\sigma) \sim \mathcal{N}(P_{\text{mean}}, P_{\text{std}}^2)$
Loss weighting $\lambda(\sigma)$	$1/\sigma^2$	$1/\sigma^2$	$1/\sigma^2$ (note: *)	$(\sigma^2 + \sigma_{\text{data}}^2) / (\sigma \cdot \sigma_{\text{data}})^2$
Parameters				
	$\beta_d = 19.9, \beta_{\min} = 0.1$	$\sigma_{\min} = 0.02$	$\bar{\alpha}_j = \sin^2(\frac{\pi}{2} \frac{j}{M(C_2+1)})$	$\sigma_{\min} = 0.002, \sigma_{\max} = 80$
	$\epsilon_s = 10^{-3}, \epsilon_t = 10^{-5}$	$\sigma_{\max} = 100$	$C_1 = 0.001, C_2 = 0.008$	$\sigma_{\text{data}} = 0.5, \rho = 7$
	$M = 1000$		$M = 1000, j_0 = 8^\dagger$	$P_{\text{mean}} = -1.2, P_{\text{std}} = 1.2$

* iDDPM also employs a second loss term L_{vlb}

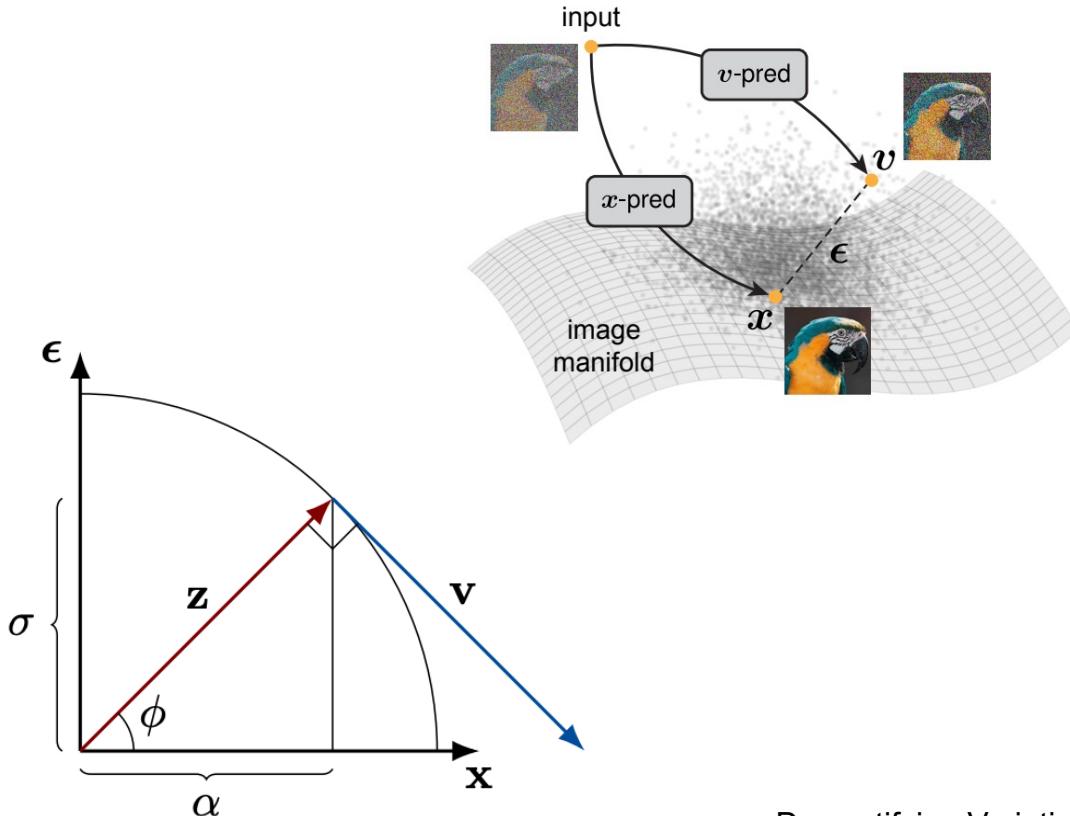
† In our tests, $j_0 = 8$ yielded better FID than $j_0 = 0$ used by iDDPM



多种参数化方法



- 不一定预测噪声，可以不同成分建模
- 去噪过程略有不同



Demystifying Variational Diffusion Models

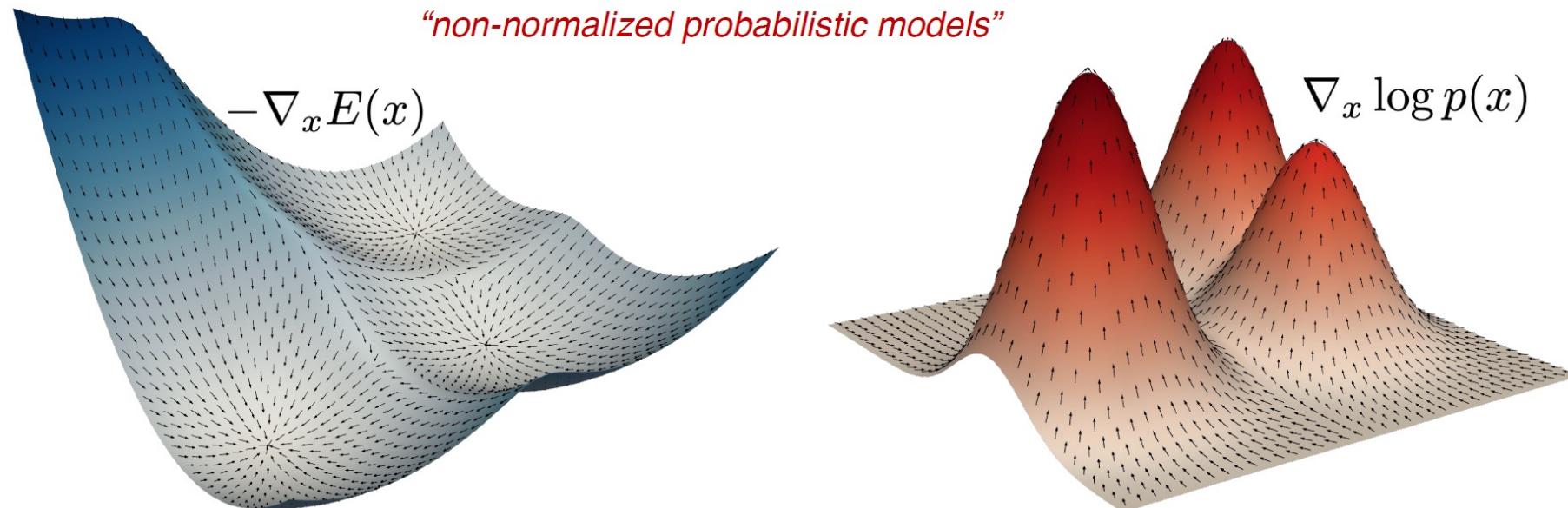
Model	Posterior Mean $\mu_{\theta}(\mathbf{z}_t; s, t)$
Image Denoising $\hat{\mathbf{x}}_{\theta}(\mathbf{z}_t; t)$	$\frac{\alpha_{t s}\sigma_s^2}{\sigma_t^2}\mathbf{z}_t + \frac{\alpha_s\sigma_{t s}^2}{\sigma_t^2}\hat{\mathbf{x}}_{\theta}(\mathbf{z}_t; t)$] 预测原图
Noise Prediction $\hat{\epsilon}_{\theta}(\mathbf{z}_t; t)$	$\frac{1}{\alpha_{t s}}\mathbf{z}_t - \frac{\sigma_{t s}^2}{\alpha_{t s}\sigma_t}\hat{\epsilon}_{\theta}(\mathbf{z}_t; t)$] 预测噪声
Score-based $\mathbf{s}_{\theta}(\mathbf{z}_t; t)$	$\frac{1}{\alpha_{t s}}\mathbf{z}_t + \frac{\sigma_{t s}^2}{\alpha_{t s}}\mathbf{s}_{\theta}(\mathbf{z}_t; t)$
Energy-based $E_{\theta}(\mathbf{z}_t; t)$	$\frac{1}{\alpha_{t s}}\mathbf{z}_t - \frac{\sigma_{t s}^2}{\alpha_{t s}}\nabla_{\mathbf{z}_t}E_{\theta}(\mathbf{z}_t; t)$
Velocity Prediction $\hat{\mathbf{v}}_{\theta}(\mathbf{z}_t; t)$	$\frac{1 - \sigma_{t s}^2}{\alpha_{t s}}\mathbf{z}_t - \frac{\sigma_{t s}^2\alpha_s}{\sigma_t}\hat{\mathbf{v}}_{\theta}(\mathbf{z}_t; t)$] 预测速度
Flow-based $\hat{\mathbf{u}}_{\theta}(\mathbf{z}_t; t)$	$\frac{\sigma_t - \sigma_{t s}^2}{\alpha_{t s}\sigma_t}\mathbf{z}_t - \frac{\sigma_{t s}^2\alpha_s}{\sigma_t}\hat{\mathbf{u}}_{\theta}(\mathbf{z}_t; t)$

注意，这里的定义与之前稍有不同 $q(z_t|x) = \mathcal{N}(z_t|\alpha_t x, \sigma_t^2 \mathbf{I})$

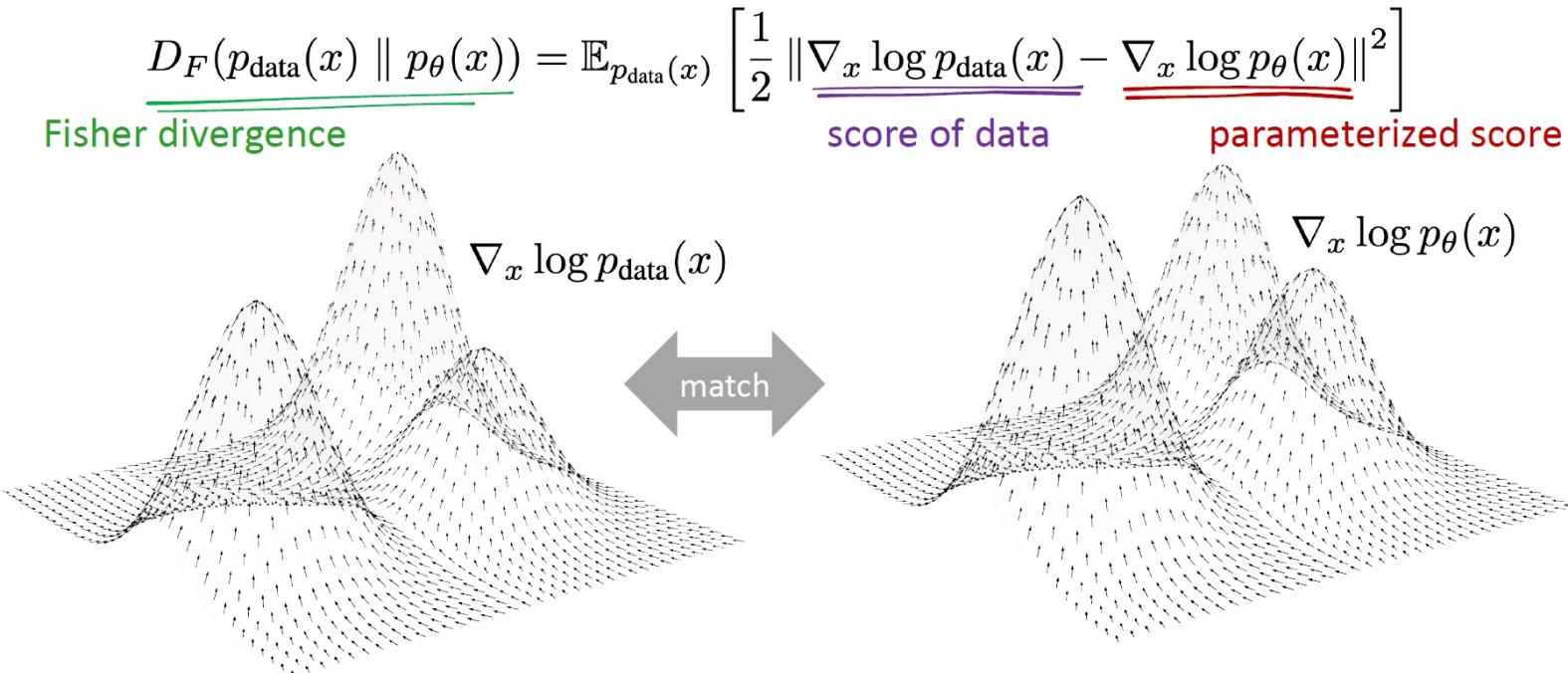
- 得分函数：概率的对数梯度
- 得分指向能量下降最快的方向

$$\nabla_x \log p(x) = -\nabla_x E(x)$$

“non-normalized probabilistic models”



- 建模真实分布难，直接对得分函数进行建模



- 若数据是加噪的形式

$$\underline{D_F(q(\tilde{x}) \parallel p_\theta(\tilde{x}))} = \mathbb{E}_{\underline{q(x, \tilde{x})}} \left[\frac{1}{2} \left\| \underline{\nabla_{\tilde{x}} \log q(\tilde{x} \mid x)} - \underline{\nabla_{\tilde{x}} \log p_\theta(\tilde{x})} \right\|^2 \right] + \text{constant}$$

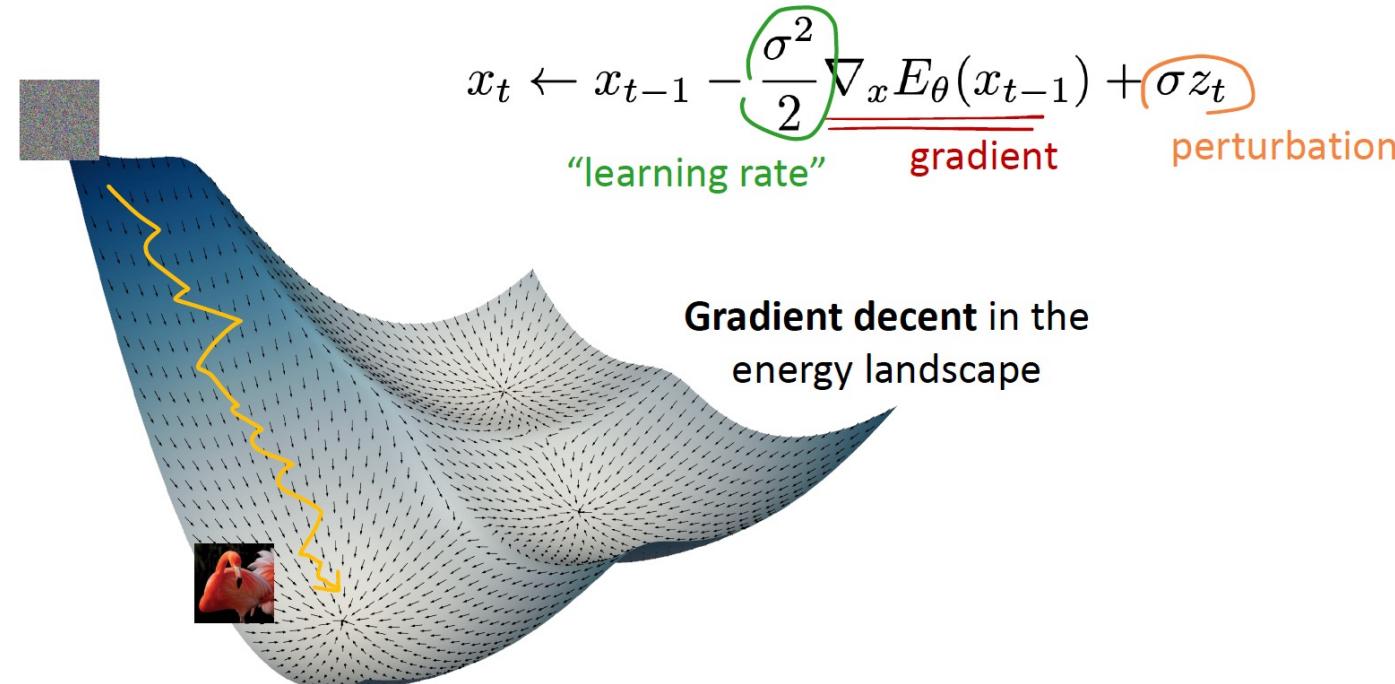
Fisher divergence joint distribution score of conditional parameterized score
 of noised data distribution

- 如果是高斯噪声，其等价于预测噪声

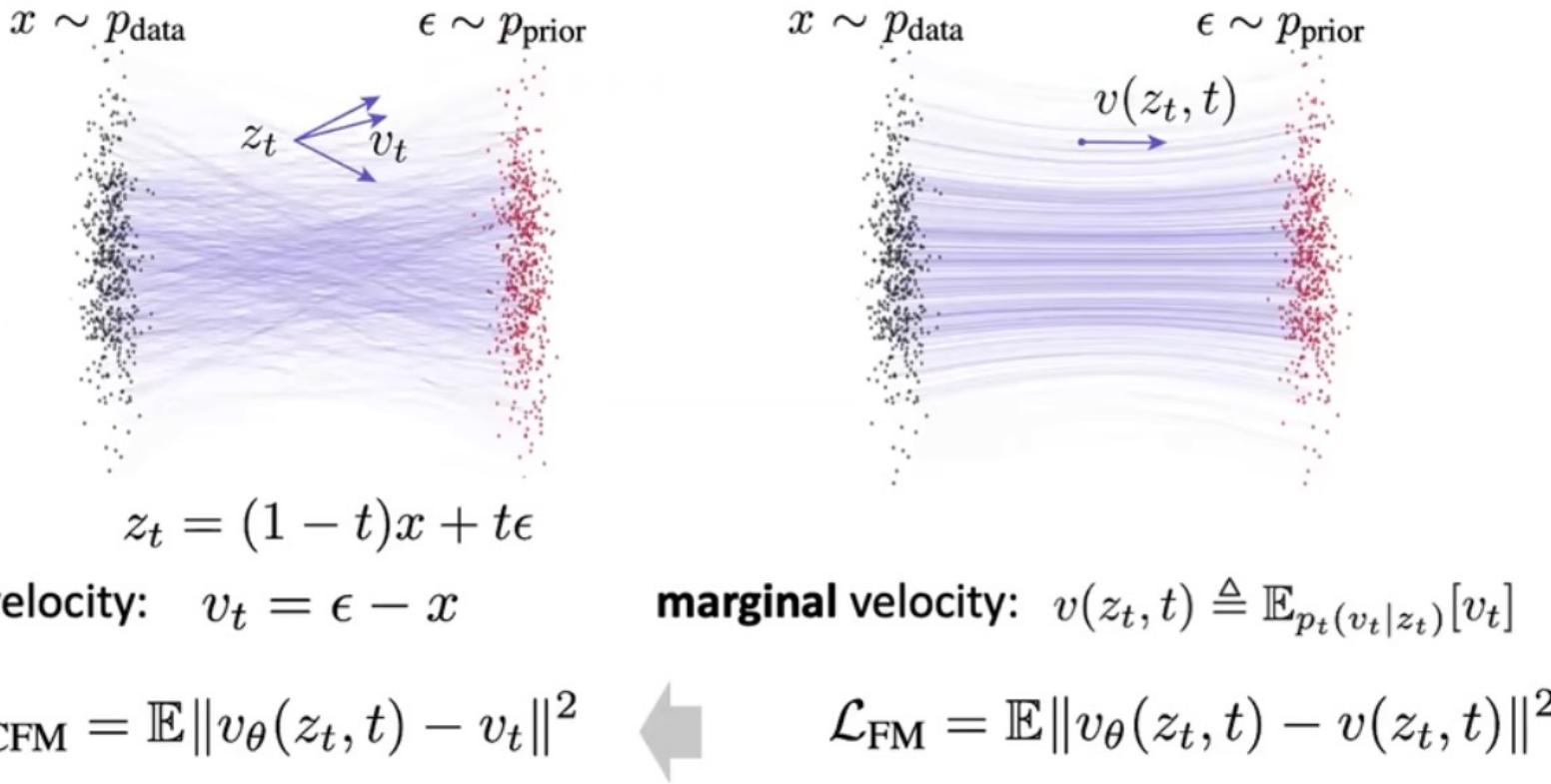
$$D_F(q(\tilde{x}) \parallel p_\theta(\tilde{x})) = \mathbb{E}_{q(x, \tilde{x})} \left[\frac{1}{2} \left\| \underline{\nabla_{\tilde{x}} \log q(\tilde{x} \mid x)} - \underline{\nabla_{\tilde{x}} \log p_\theta(\tilde{x})} \right\|^2 \right] + \text{constant}$$

Gaussian noise:
$$= \frac{1}{\sigma^2} (x - \tilde{x})$$
 a network to predict (negative) noise
 \downarrow
 \downarrow
 $-\epsilon$

- 学习到得分函数之后，可以对样本进行迭代采样
- 提供理论解释：预测噪声 \Rightarrow 学习得分函数 \Rightarrow 近似真实数据分布的对数梯度
- 基于得分函数的朗之万动力学：采样时能量最小



- 直接学习两个分布之间插值的速度场
- 学习到的是最近路径，并且采样更快



多种参数化方法



- 不同参数化方法，是可以相互转换的

Model	Equivalent Reparameterization				
	$\hat{\mathbf{x}}_{\theta}(\mathbf{z}_t; t)$	$\hat{\epsilon}_{\theta}(\mathbf{z}_t; t)$	$\mathbf{s}_{\theta}(\mathbf{z}_t; t)$	$\hat{\mathbf{v}}_{\theta}(\mathbf{z}_t; t)$	$\hat{\mathbf{u}}_{\theta}(\mathbf{z}_t; t)$
Image Denoising $\hat{\mathbf{x}}_{\theta}(\mathbf{z}_t; t)$	-	$\frac{\mathbf{z}_t - \sigma_t \hat{\epsilon}_{\theta}}{\alpha_t}$	$\frac{\mathbf{z}_t + \sigma_t^2 \mathbf{s}_{\theta}}{\alpha_t}$	$\alpha_t \mathbf{z}_t - \sigma_t \hat{\mathbf{v}}_{\theta}$	$\mathbf{z}_t - \sigma_t \hat{\mathbf{u}}_{\theta}$
Noise Prediction $\hat{\epsilon}_{\theta}(\mathbf{z}_t; t)$	$\frac{\mathbf{z}_t - \alpha_t \hat{\mathbf{x}}_{\theta}}{\sigma_t}$	-	$-\sigma_t \mathbf{s}_{\theta}$	$\sigma_t \mathbf{z}_t + \alpha_t \hat{\mathbf{v}}_{\theta}$	$\alpha_t \hat{\mathbf{u}}_{\theta} + \mathbf{z}_t$
Score-based $\mathbf{s}_{\theta}(\mathbf{z}_t; t)$	$\frac{\alpha_t \hat{\mathbf{x}}_{\theta} - \mathbf{z}_t}{\sigma_t^2}$	$\frac{-\hat{\epsilon}_{\theta}}{\sigma_t}$	-	$\frac{-\sigma_t \mathbf{z}_t + \alpha_t \hat{\mathbf{v}}_{\theta}}{\sigma_t}$	$\frac{-\alpha_t \hat{\mathbf{u}}_{\theta} + \mathbf{z}_t}{\sigma_t}$
Velocity Prediction $\hat{\mathbf{v}}_{\theta}(\mathbf{z}_t; t)$	$\frac{\alpha_t \mathbf{z}_t - \hat{\mathbf{x}}_{\theta}}{\sigma_t}$	$\frac{\hat{\epsilon}_{\theta} - \sigma_t \mathbf{z}_t}{\alpha_t}$	$\frac{-\sigma_t (\mathbf{z}_t + \mathbf{s}_{\theta})}{\alpha_t}$	-	$\hat{\mathbf{u}}_{\theta} - \mathbf{z}_t$
Flow-Based $\hat{\mathbf{u}}_{\theta}(\mathbf{z}_t; t)$	$\frac{\mathbf{z}_t - \hat{\mathbf{x}}_{\theta}}{\sigma_t}$	$\frac{\hat{\epsilon}_{\theta} (\alpha_t - \sigma_t) - \mathbf{z}_t}{\alpha_t}$	$\frac{\sigma_t \mathbf{s}_{\theta} (\sigma_t - \alpha_t) - \mathbf{z}_t}{\alpha_t}$	$\mathbf{z}_t + \hat{\mathbf{v}}_{\theta}$	-



多种参数化方法



- 不同损失参数化之间本质是样本加权方式不同

Loss	Image Denoising	Noise Prediction	Velocity Prediction
$\ \mathbf{x} - \hat{\mathbf{x}}_{\theta}(\mathbf{z}_t; t)\ _2^2$	$\ \mathbf{x} - \hat{\mathbf{x}}_{\theta}(\mathbf{z}_t; t)\ _2^2$	$\ \epsilon - \hat{\epsilon}_{\theta}(\mathbf{z}_t; t)\ _2^2$	$\ \mathbf{v} - \hat{\mathbf{v}}_{\theta}(\mathbf{z}_t; t)\ _2^2$
$\ \mathbf{x} - \hat{\mathbf{x}}_{\theta}(\mathbf{z}_t; t)\ _2^2$	1	σ_t^2 / α_t^2	σ_t^2
$\ \epsilon - \hat{\epsilon}_{\theta}(\mathbf{z}_t; t)\ _2^2$	α_t^2 / σ_t^2	1	$1 / \alpha_t^2$
$\ \mathbf{v} - \hat{\mathbf{v}}_{\theta}(\mathbf{z}_t; t)\ _2^2$	$\sigma_t^2 \left(\frac{\alpha_t^2}{\sigma_t^2} + 1 \right)^2$	$\alpha_t^2 \left(\frac{\sigma_t^2}{\alpha_t^2} + 1 \right)^2$	1



- 可解释性表征：让表征更加有意义
- 可解释性过程：确定性前向过程建模的因果表征，e.g. 概率流



- 扩散模型自回归模型殊途同归，最终都为了在 latent space 中创造出符合真实数据分布的、内部高度相关的、有意义的结构
- 相比自回归模型，扩散模型灵活性高，易于通过引导控制
- 扩散模型的前向和反向过程为对称的加噪和去噪
- 扩散模型的训练目标也是一种ELBO的变体
- 受益于高斯再生性，不同的扩散模型参数化是可以进行转换的