



# 模式识别

# Pattern Recognition

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





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扩散模型简介

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前向和反向过程

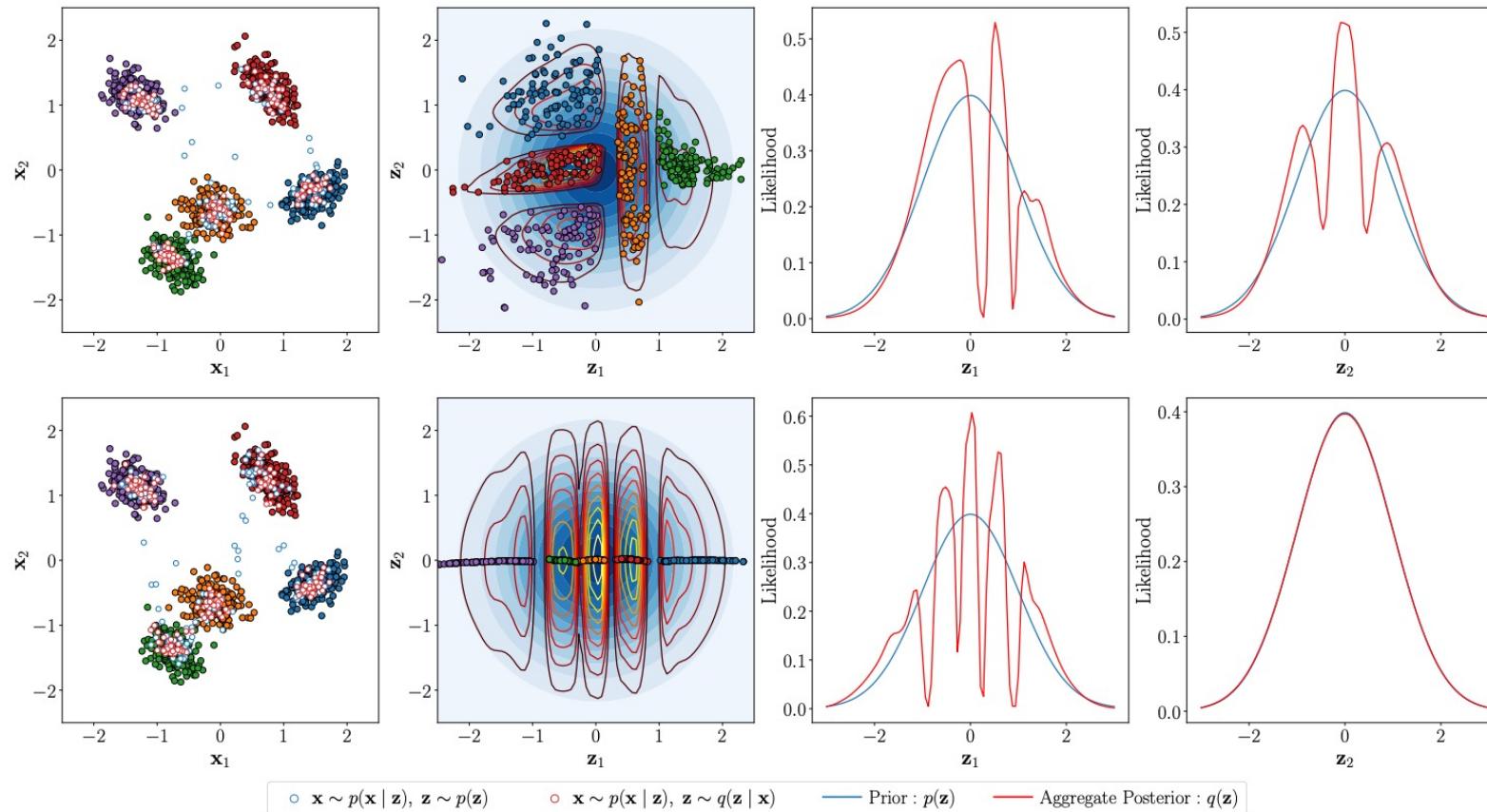
3

训练目标

4

多种参数化形式

- VAE的空洞问题：没采样到的样本很难生成

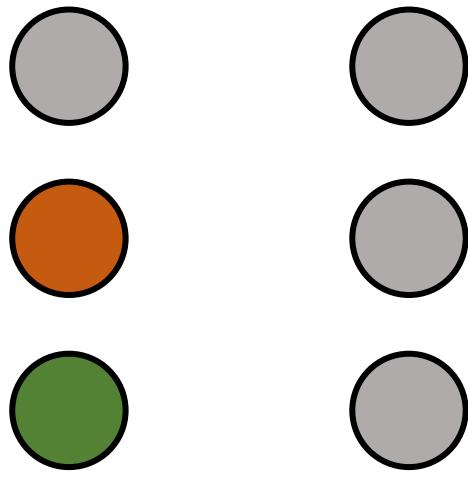


# 建模条件分布



VAE的空洞问题：

- 表征缺少相关性
- 难以建模没采样到的点



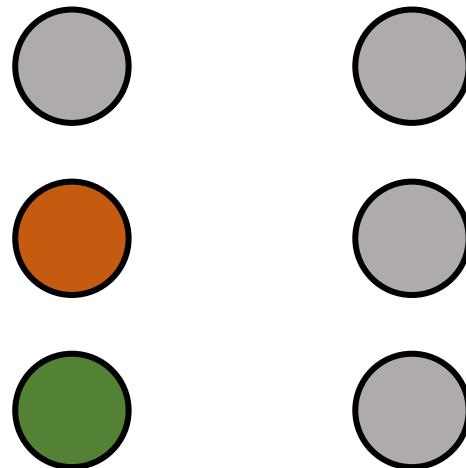
真实       采样



# 建模条件分布

VAE的空洞问题：

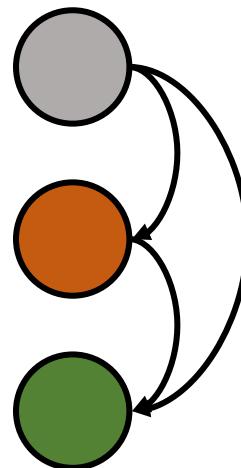
- 表征缺少相关性
- 难以建模没采样到的点



真实  采样

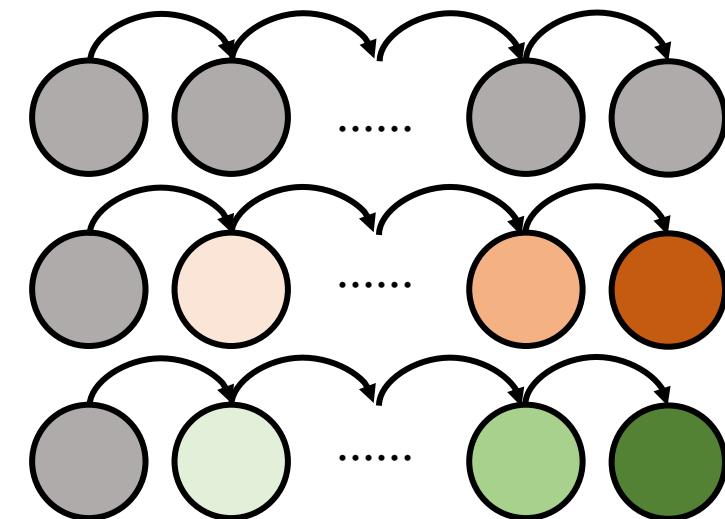
自回归模型：

- 基于时间建模
- 条件依赖，顺序建模

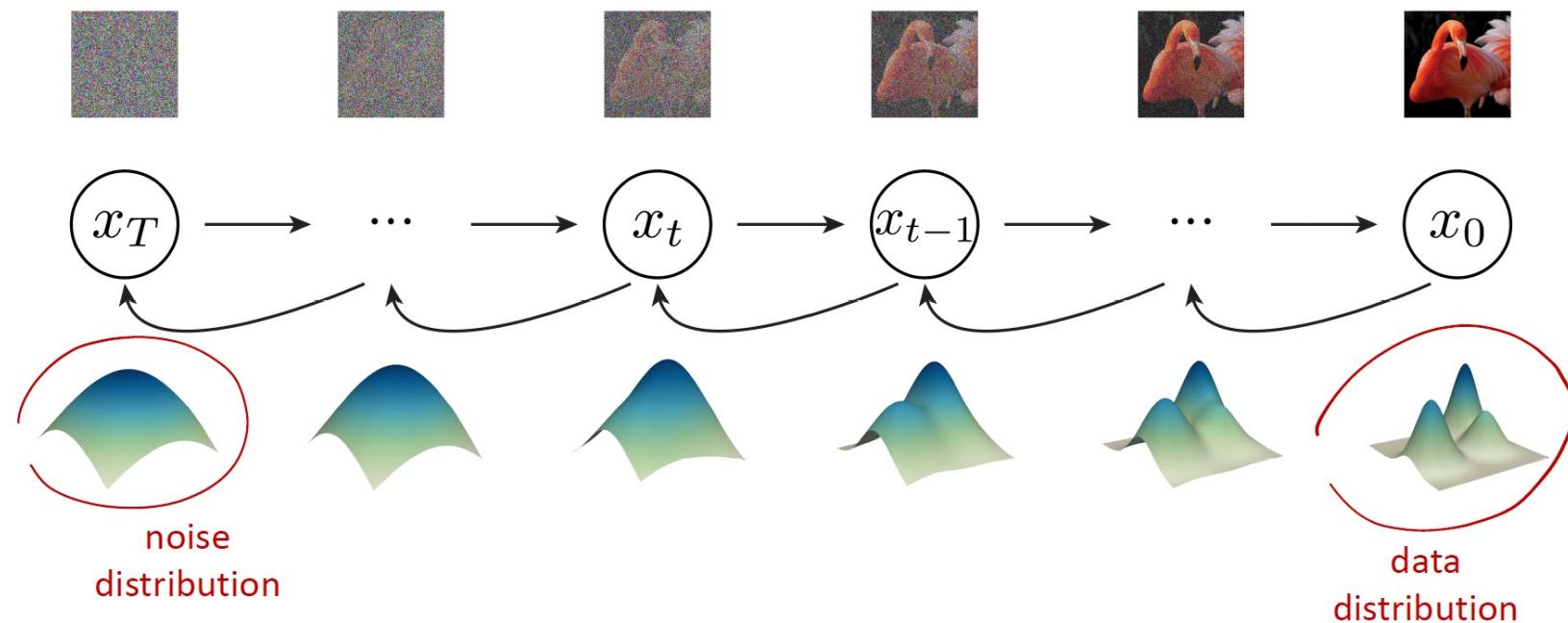


扩散模型：

- 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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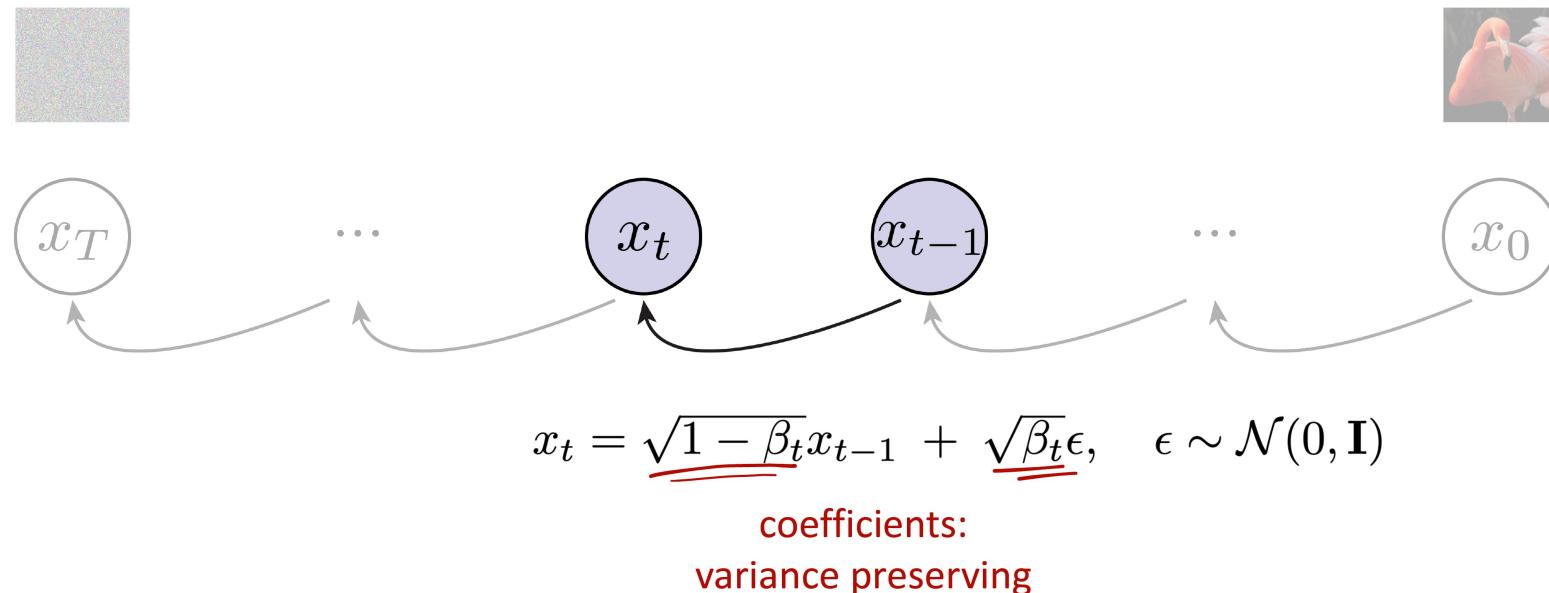
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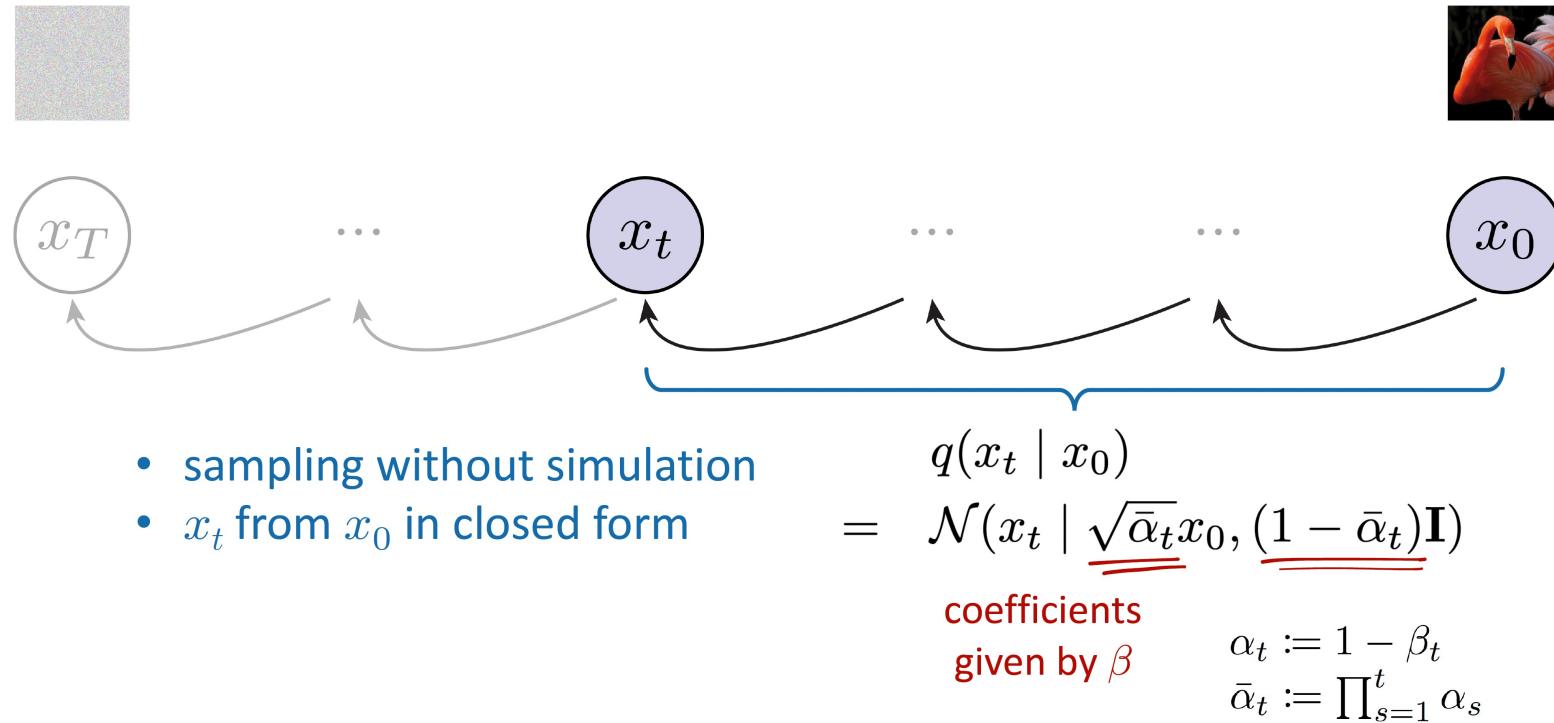
# 前向过程



- 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)



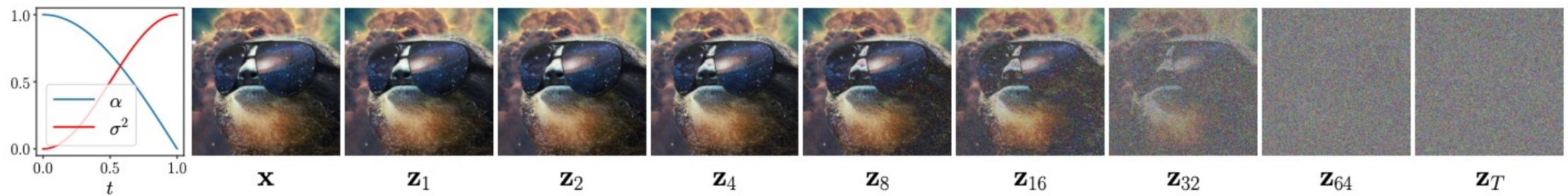
- 高斯分布再生性：多个独立高斯随机变量的和仍然是高斯分布
- 所以可以训练的时候随机取一步



# 前向过程



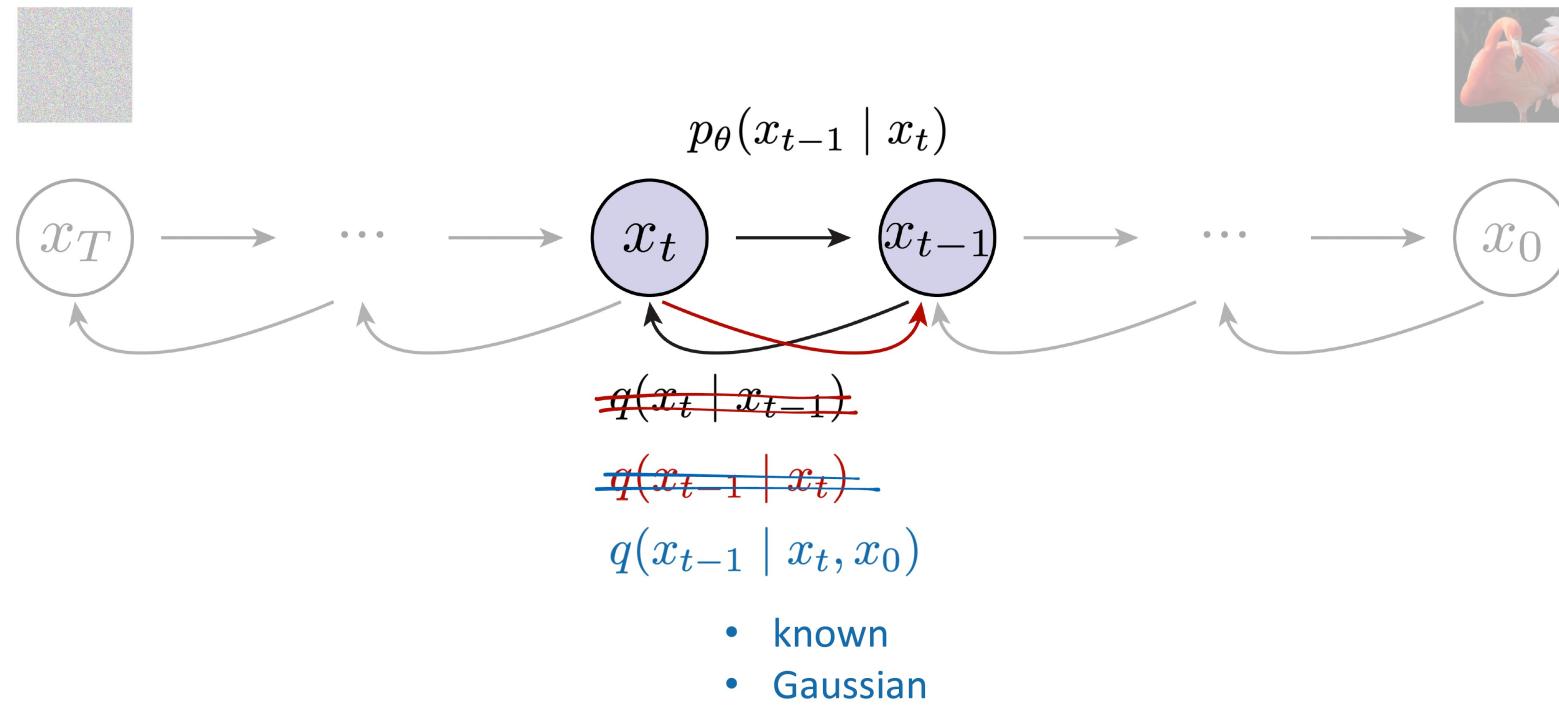
- 噪声在干净步骤均值最接近1，方差最小
- 噪声在噪声步骤均值最接近0，方差最大



# 反向过程



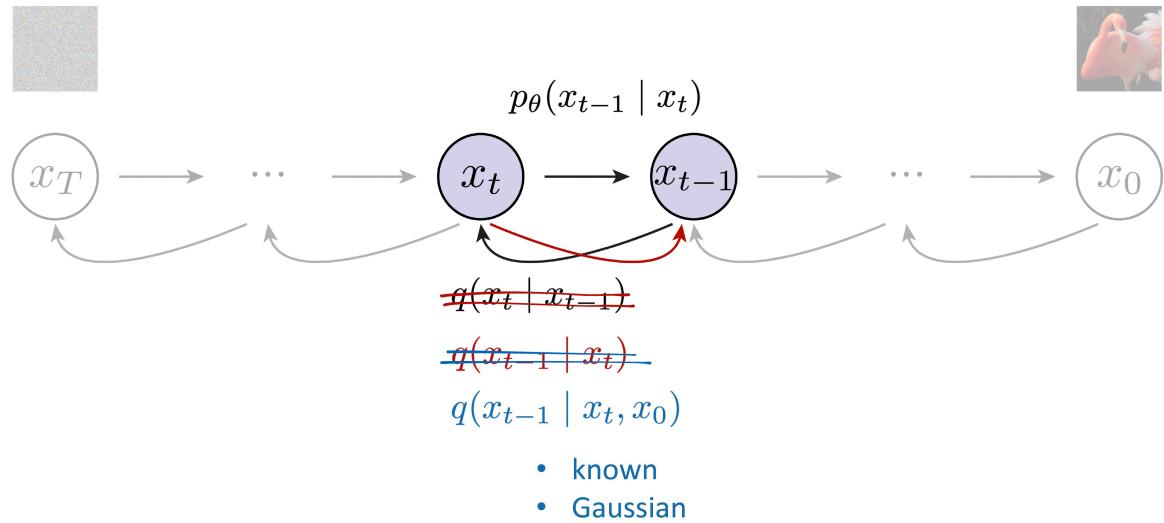
- 在同时观察到  $x_t$  和知道  $x_0$  的情况下，对  $x_{t-1}$  的估计



# 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  $\Rightarrow$

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

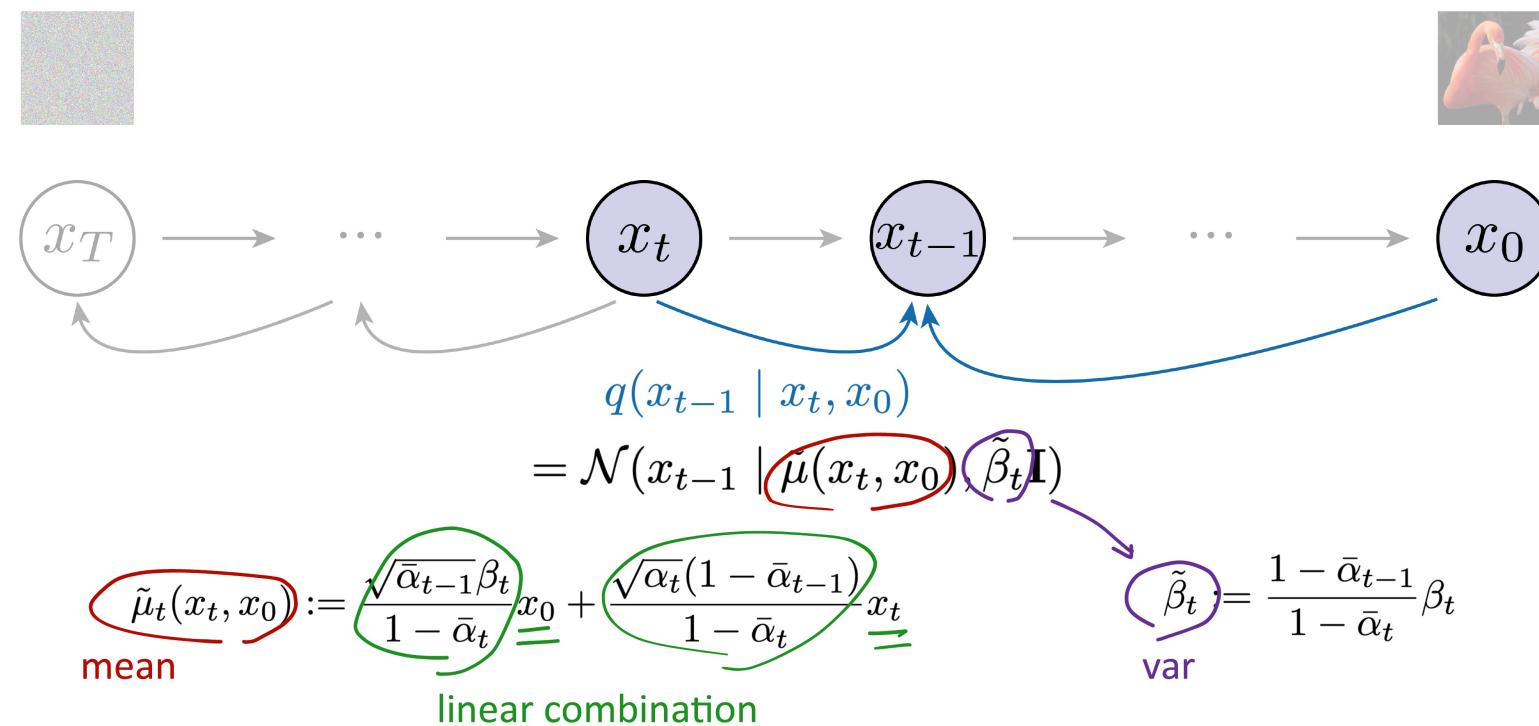
代入高斯分布，忽略与  $x_{t-1}$  无关常数  $\Rightarrow$

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



# 反向过程

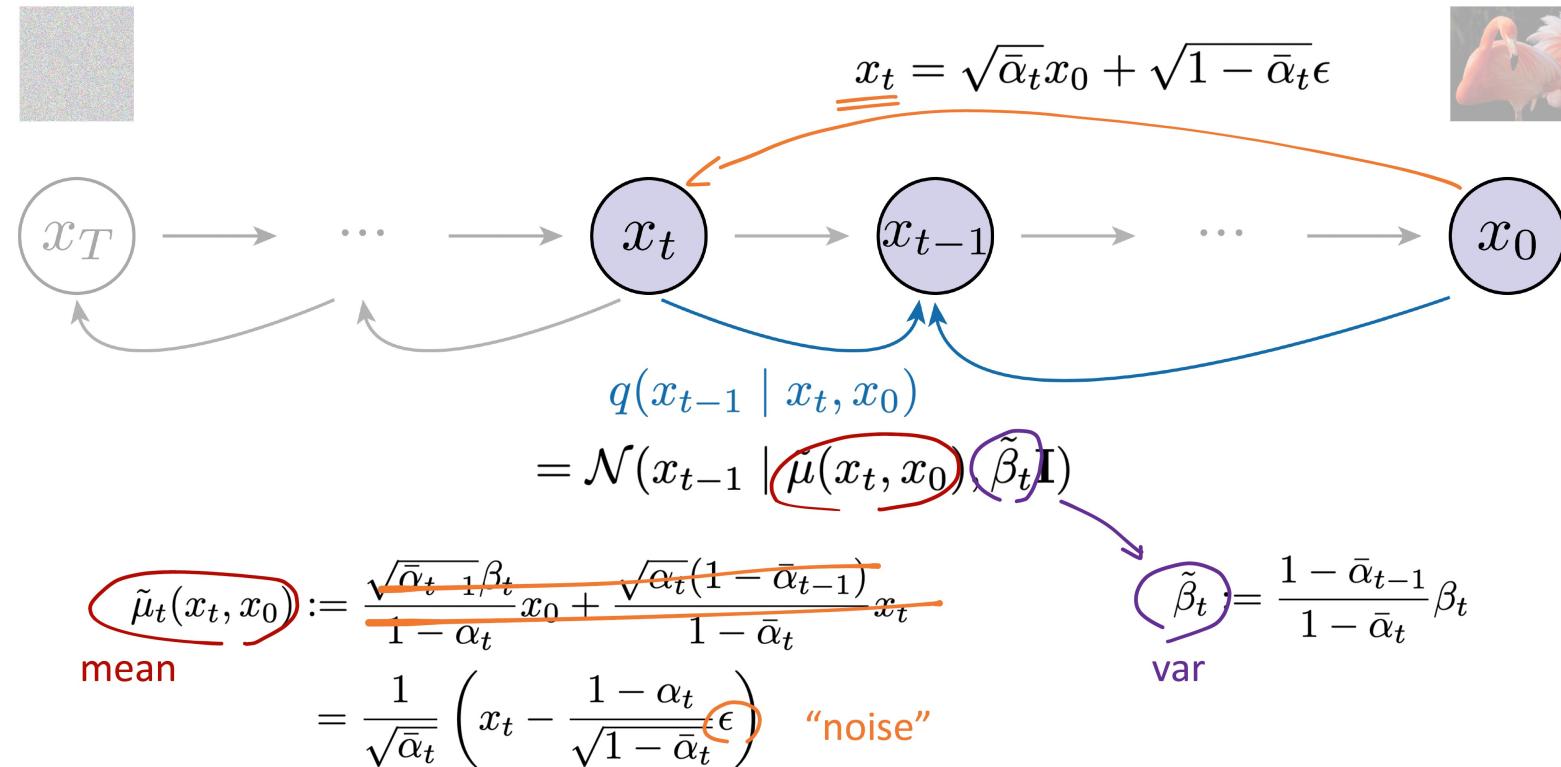
- 在  $x_0$  已知时，反向转移也是已知的高斯分布



# 反向过程



- 将  $x_0$  到  $x_t$  的过程整理成统一的噪声  $\epsilon$

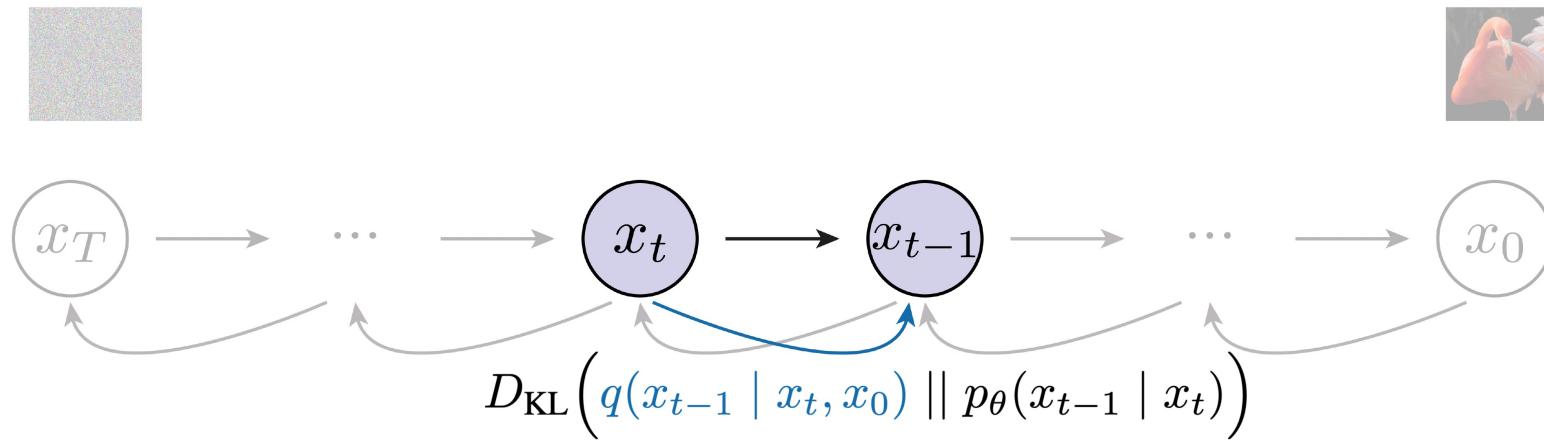


注意，这里的噪声是加在  $x_0$  上，用于得到  $x_t$  的



# 反向过程

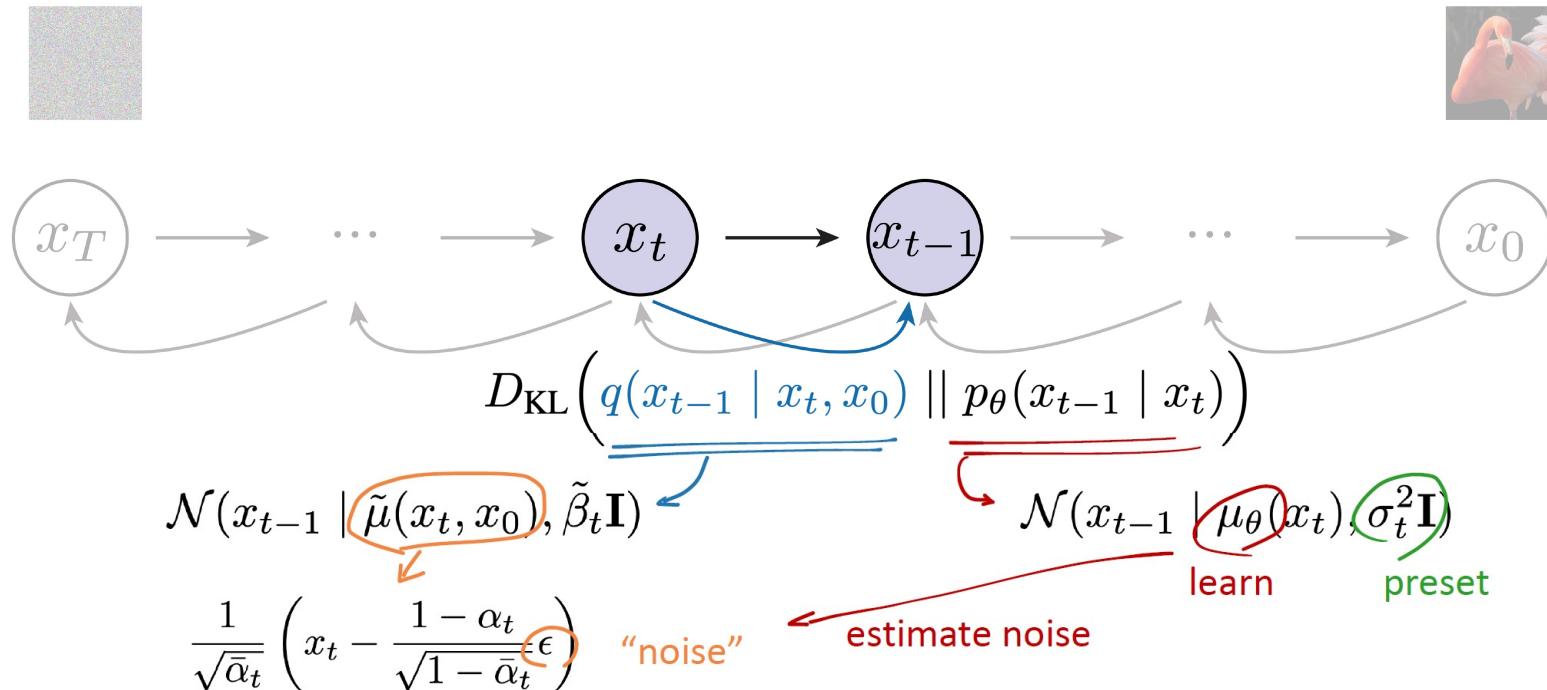
- 最小化KL散度



# 反向过程



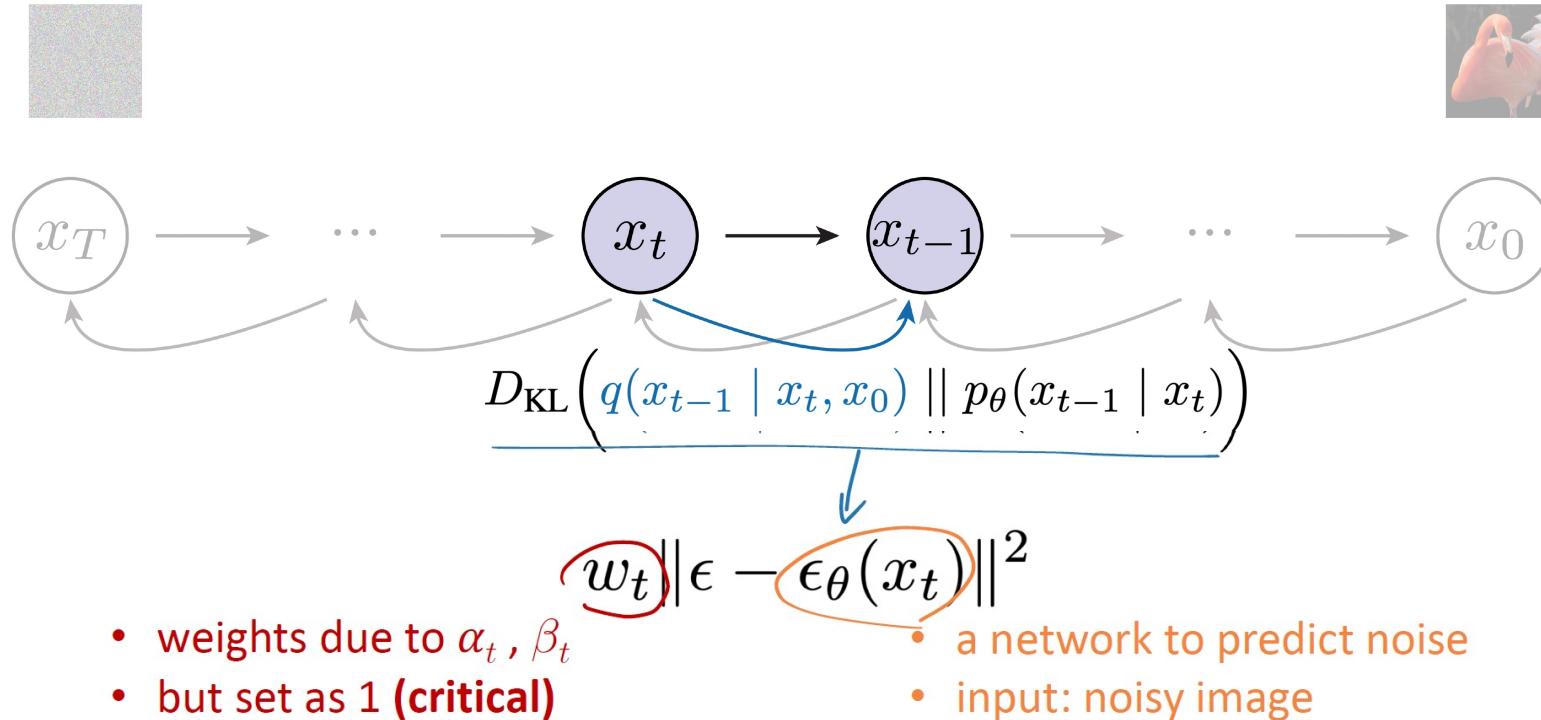
- KL散度简化成噪声预测



# 反向过程



- 噪声预测的L2损失



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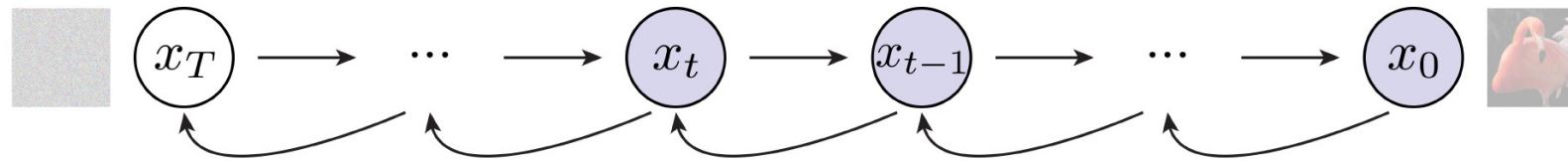
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训练目标

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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）

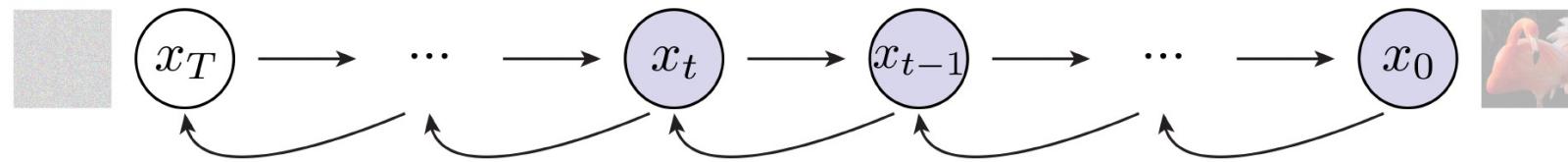
$$\mathcal{L}_0 := -\log p_\theta(x_0 | x_1)$$

最终的重构质量，被隐式忽略

# 训练目标



- 可以直接简化成去噪任务



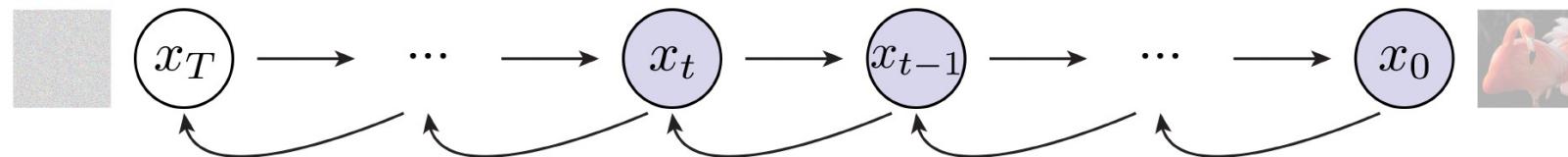
$$\mathcal{L} = \mathbb{E}_{x_0, t, \epsilon} \left[ w_t \|\epsilon - \epsilon_\theta(x_t, t)\|^2 \right]$$

over  $p_{data}$       over  $[1, T]$       over  $\mathcal{N}(0, \mathbf{I})$



# 训练目标

- 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 $\Sigma$	-	-
$L$ , fixed isotropic $\Sigma$	$7.67 \pm 0.13$	$13.51 \leftarrow$
$\ \tilde{\epsilon} - \epsilon_\theta\ ^2$ ( $L_{\text{simple}}$ )	$9.46 \pm 0.11$	$3.17 \leftarrow$

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



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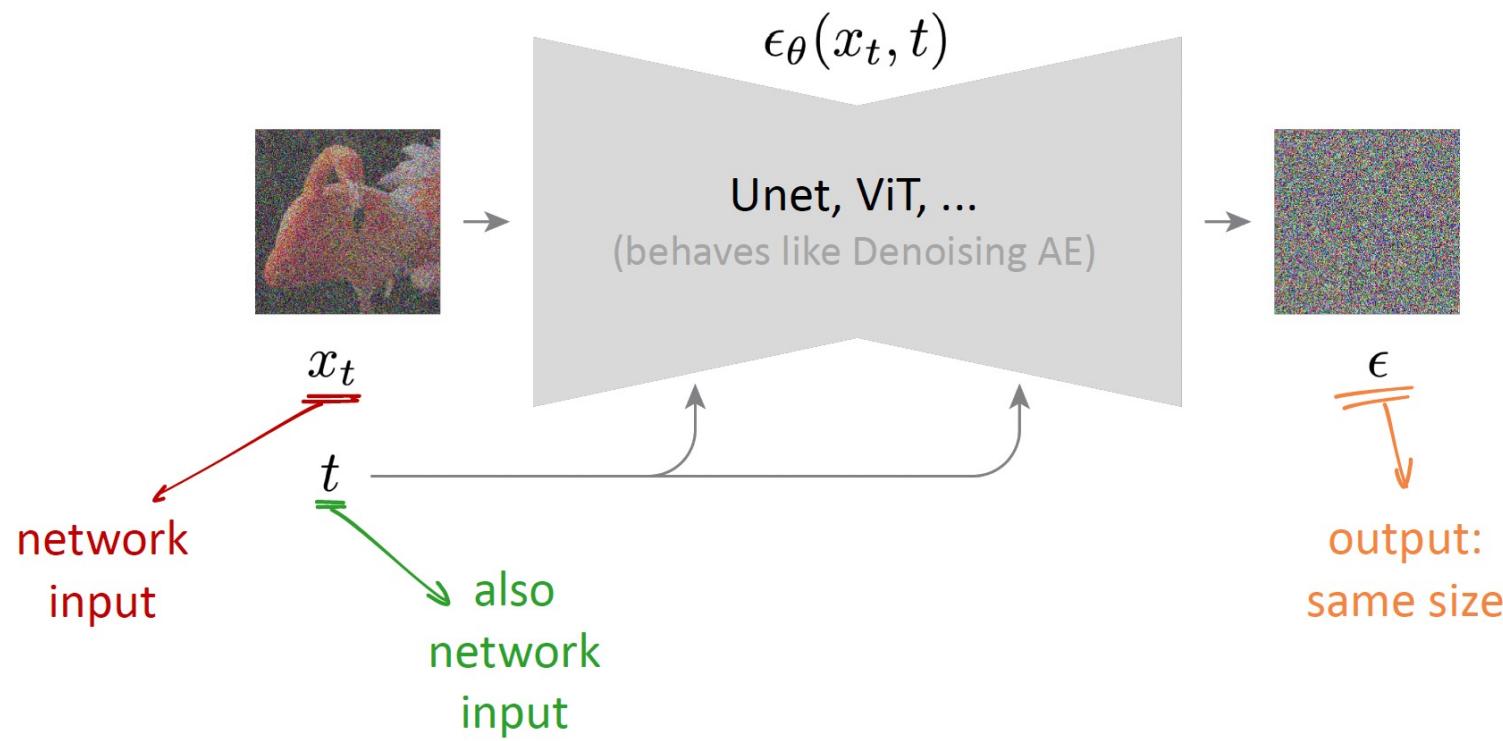
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多种参数化形式

# 噪声条件网络



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



# 噪声条件网络



- 基础扩散模型的训练和采样过程

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**Algorithm 1** Training

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```

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  $x_t$   


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

6: until converged

```

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**Algorithm 2** Sampling

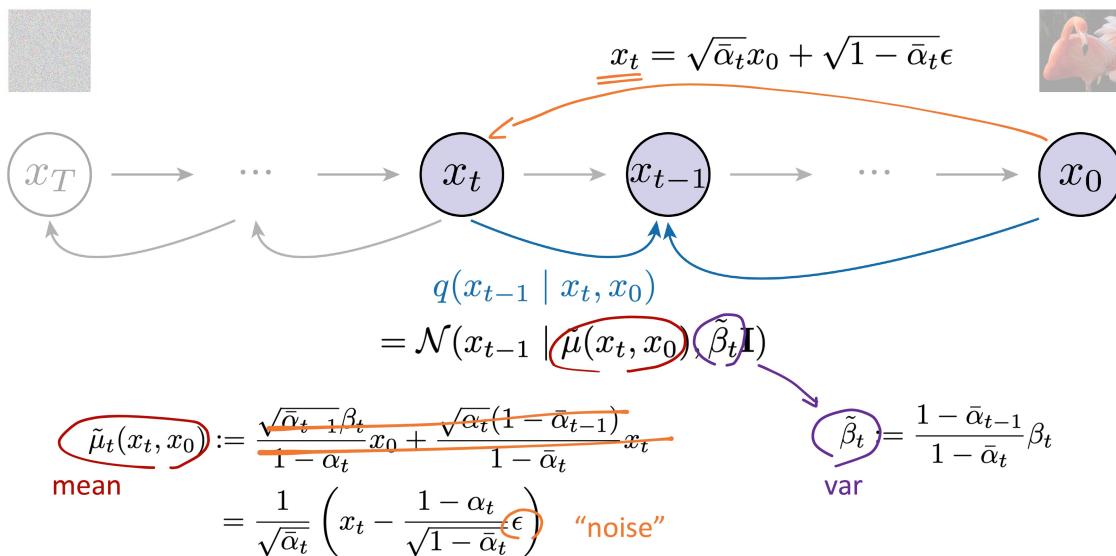
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```

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

```

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estimated  $\mu$   
 sampling from  
 estimated distribution



# 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  $D_\theta(\mathbf{x}; \sigma) = c_{\text{skip}}(\sigma)\mathbf{x} + c_{\text{out}}(\sigma)F_\theta(c_{\text{in}}(\sigma)\mathbf{x}; c_{\text{noise}}(\sigma))$ ;  $F_\theta$  represents the raw neural network layers.

	VP [49]	VE [49]	iDDPM [37] + DDIM [47]	Ours (“EDM”)
<b>Sampling (Section 3)</b>				
ODE solver	Euler	Euler	Euler	2 <sup>nd</sup> order Heun
Time steps	$t_{i < N} = 1 + \frac{i}{N-1}(\epsilon_s - 1)$	$\sigma_{\max}^2 (\sigma_{\min}^2 / \sigma_{\max}^2)^{\frac{i}{N-1}}$	$u_{\lfloor j_0 + \frac{M-1-j_0}{N-1} i + \frac{1}{2} \rfloor}, \text{ where } u_M = 0$ $u_{j-1} = \sqrt{\frac{u_j^2 + 1}{\max(\bar{\alpha}_{j-1}/\bar{\alpha}_j, C_1)} - 1}$	$(\sigma_{\max}^{\frac{1}{\rho}} + \frac{i}{N-1}(\sigma_{\min}^{\frac{1}{\rho}} - \sigma_{\max}^{\frac{1}{\rho}}))^{\rho}$
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
<b>Network and preconditioning (Section 5)</b>				
Architecture of $F_\theta$	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 $c_{\text{out}}(\sigma)$	$-\sigma$	$\sigma$	$-\sigma$	$\sigma \cdot \sigma_{\text{data}} / \sqrt{\sigma_{\text{data}}^2 + \sigma^2}$
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 $	$\frac{1}{4} \ln(\sigma)$
<b>Training (Section 5)</b>				
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: *)	$(\sigma^2 + \sigma_{\text{data}}^2) / (\sigma \cdot \sigma_{\text{data}})^2$
<b>Parameters</b>				
	$\beta_d = 19.9, \beta_{\min} = 0.1$	$\sigma_{\min} = 0.02$	$\bar{\alpha}_j = \sin^2(\frac{\pi}{2} \frac{j}{M(C_2+1)})$	$\sigma_{\min} = 0.002, \sigma_{\max} = 80$
	$\epsilon_s = 10^{-3}, \epsilon_t = 10^{-5}$	$\sigma_{\max} = 100$	$C_1 = 0.001, C_2 = 0.008$	$\sigma_{\text{data}} = 0.5, \rho = 7$
	$M = 1000$		$M = 1000, j_0 = 8^\dagger$	$P_{\text{mean}} = -1.2, P_{\text{std}} = 1.2$

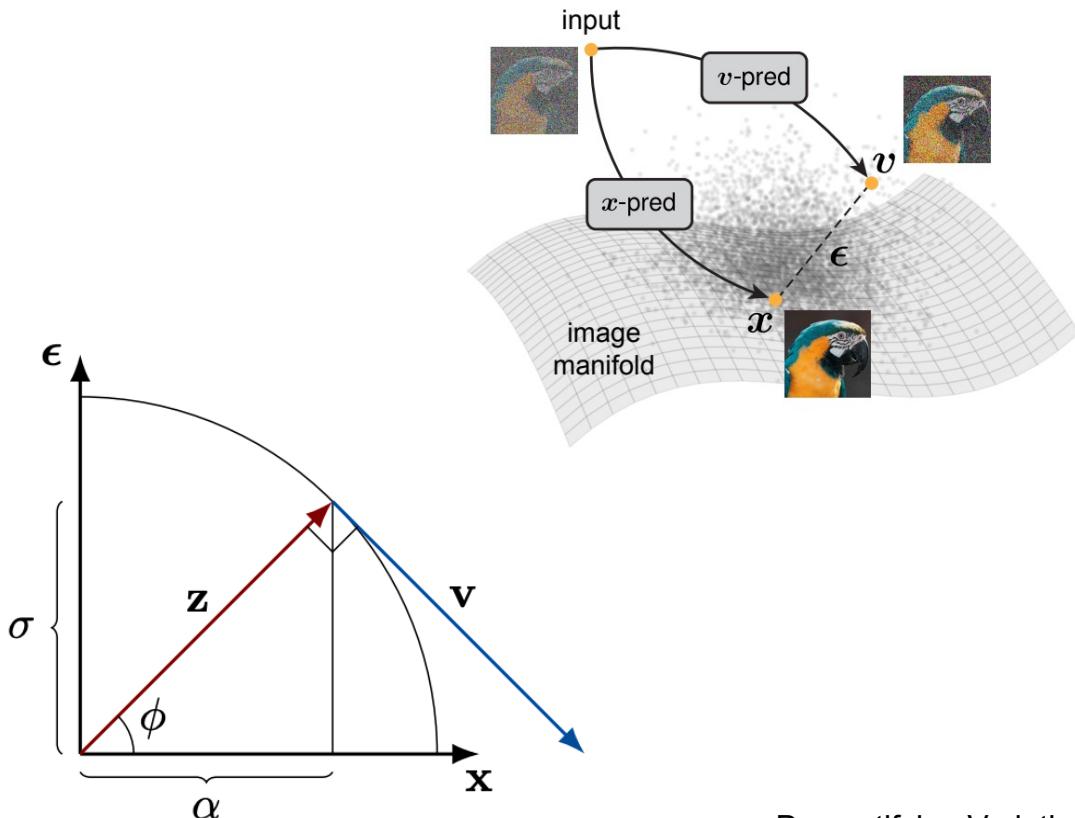
\* iDDPM also employs a second loss term  $L_{\text{vib}}$

† 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



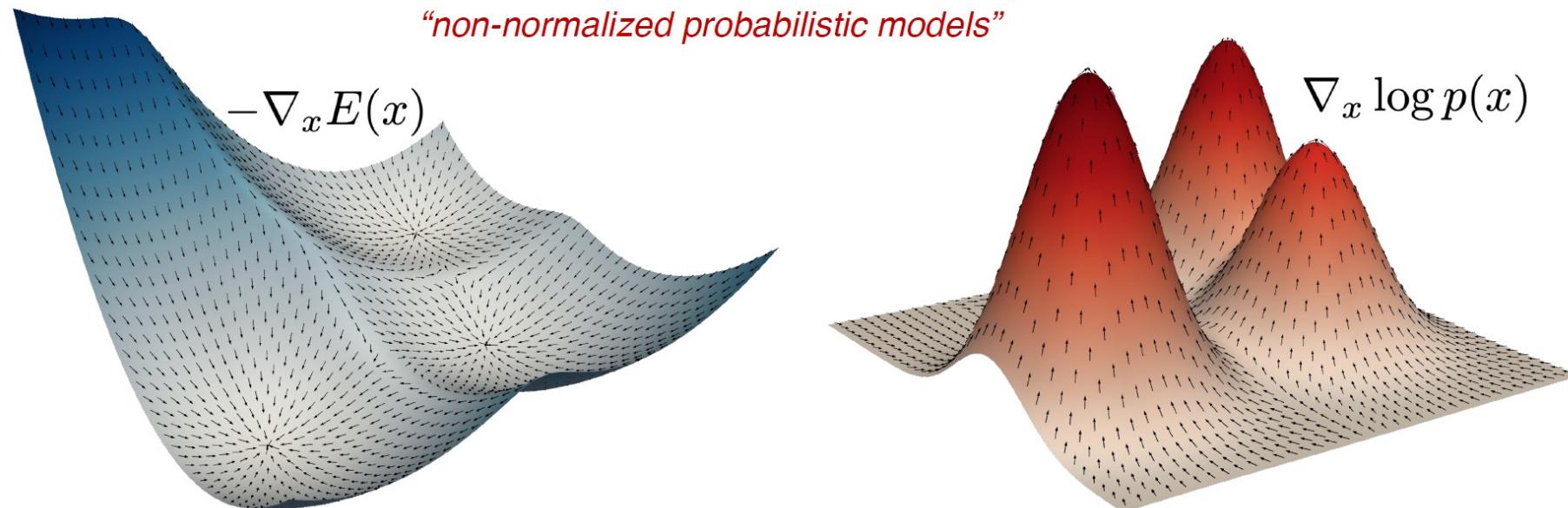
Model	Posterior Mean $\mu_{\theta}(\mathbf{z}_t; s, t)$
Image Denoising $\hat{\mathbf{x}}_{\theta}(\mathbf{z}_t; t)$	$\frac{\alpha_{t s}\sigma_s^2}{\sigma_t^2}\mathbf{z}_t + \frac{\alpha_s\sigma_{t s}^2}{\sigma_t^2}\hat{\mathbf{x}}_{\theta}(\mathbf{z}_t; t)$ ] 预测原图
Noise Prediction $\hat{\boldsymbol{\epsilon}}_{\theta}(\mathbf{z}_t;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

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

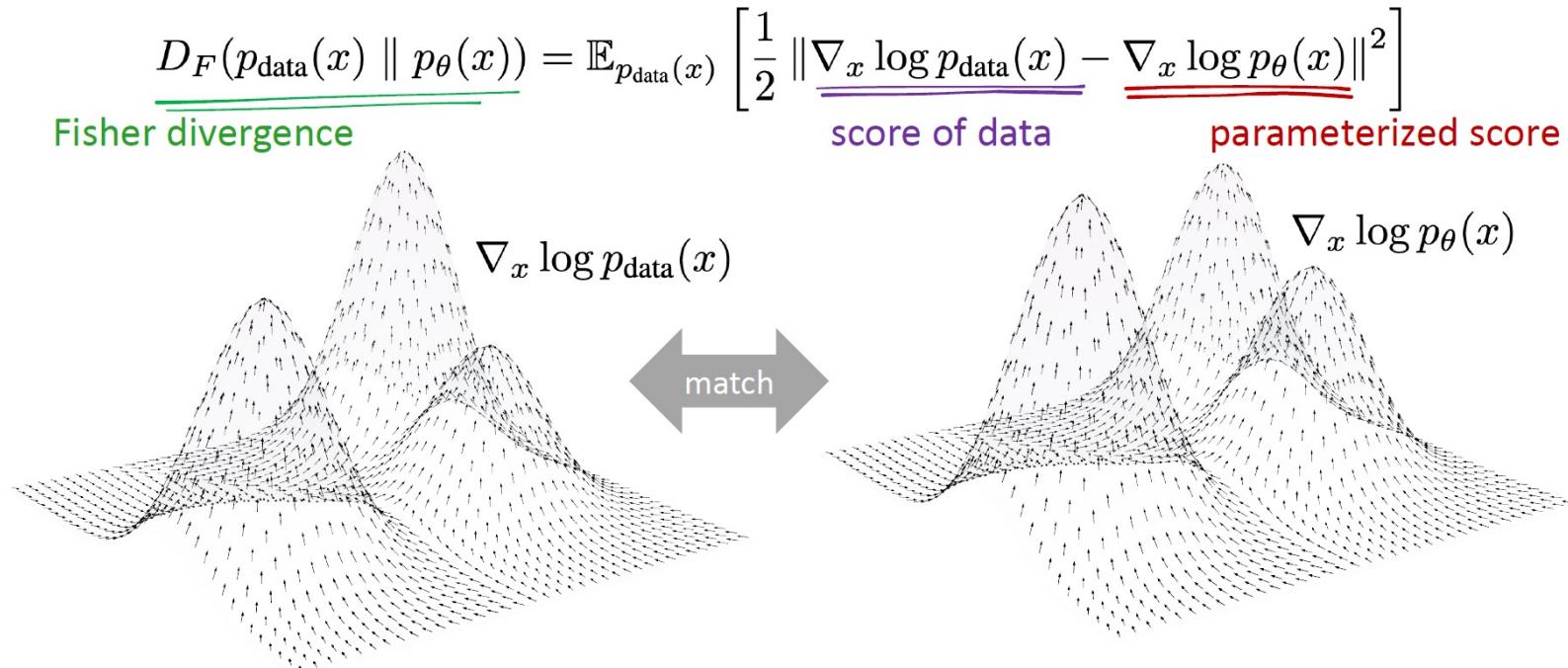
- 得分函数：概率的对数梯度
- 得分指向能量下降最快的方向

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

*“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

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

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

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

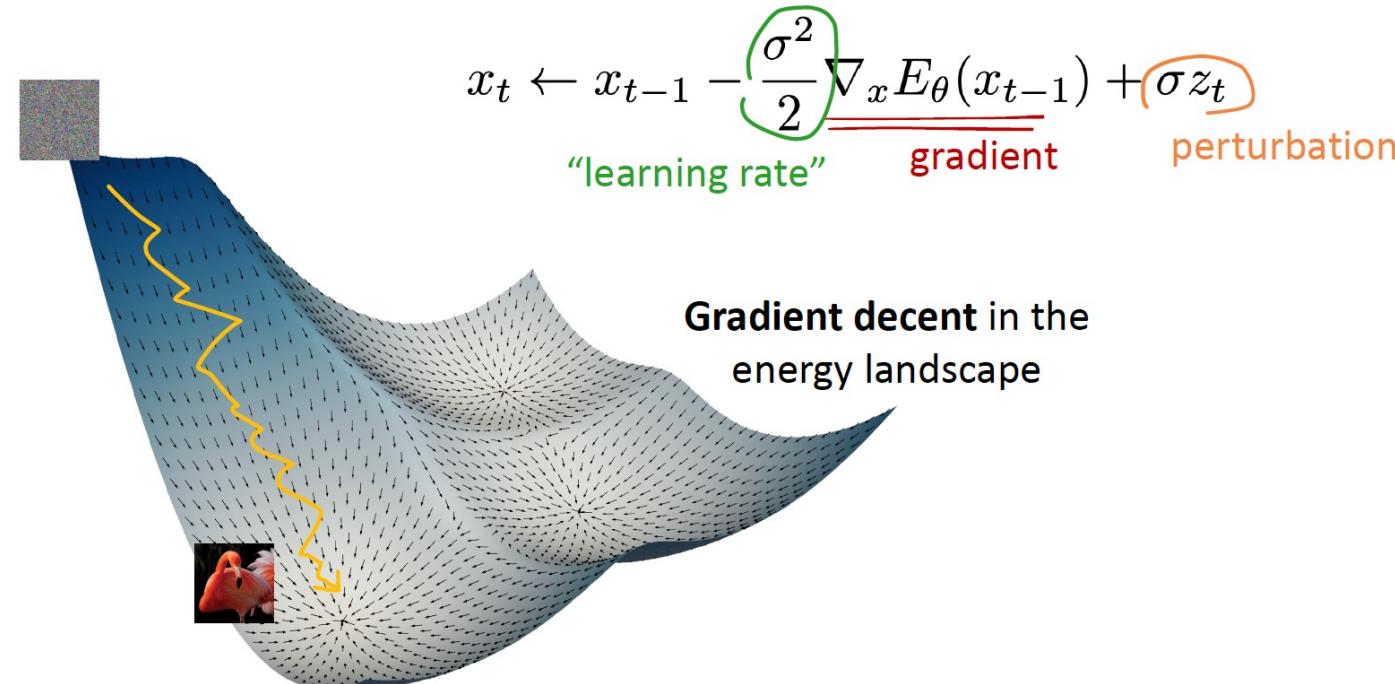
Gaussian noise:  

$$= \frac{1}{\sigma^2} (x - \tilde{x})$$

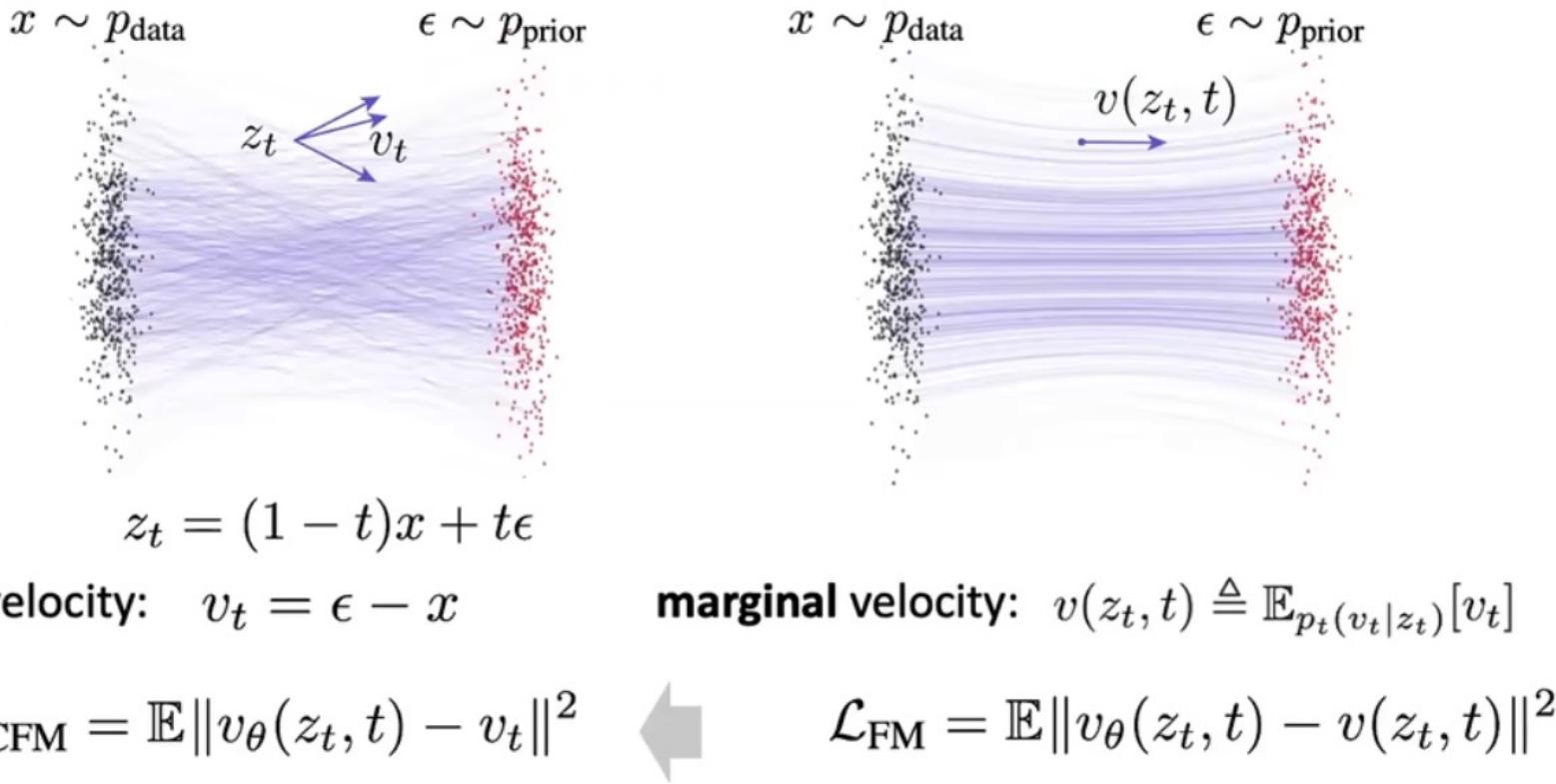
a network to predict  
 (negative) noise  
 $-\epsilon$



- 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	$\sigma_t^2 / \alpha_t^2$	$\sigma_t^2$
$\ \epsilon - \hat{\epsilon}_{\theta}(\mathbf{z}_t; t)\ _2^2$	$\alpha_t^2 / \sigma_t^2$	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