Paper Report

DDPM Denoising Diffusion Probabilistic Models, NeurIPS'20

@ 2022/09 Chia-Jen, Yeh

Report Structure

Introduction

- The diffusion model is a novel model that has beaten GAN in image generation in 2021.
- This paper presents high quality image synthesis results using diffusion probabilistic models.
- The diffusion model is based on Variational Inference.
- We use DDPM as short name of this paper propose model.

What is diffusion model?

x_0

What is diffusion model?

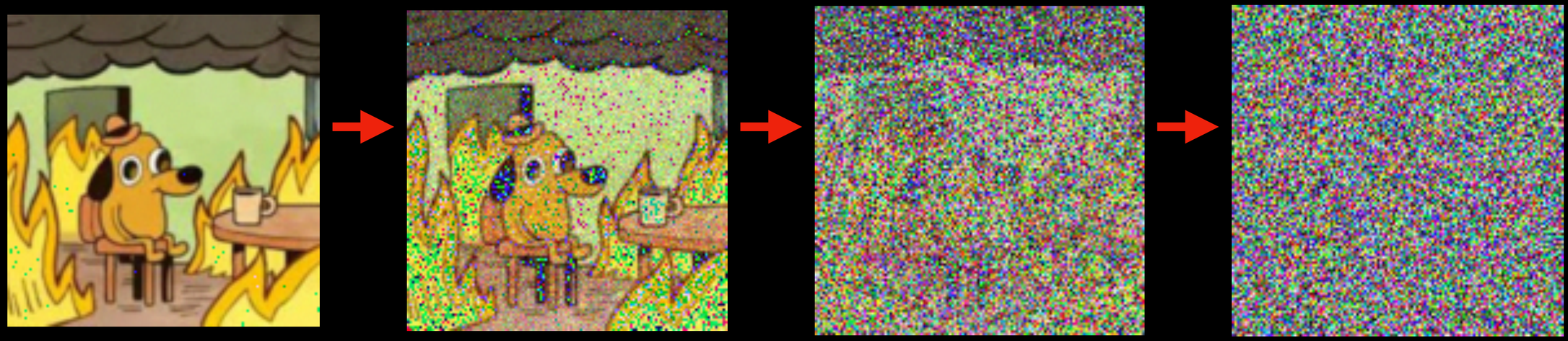
x_0

What is diffusion model?

x_0

What is diffusion model?

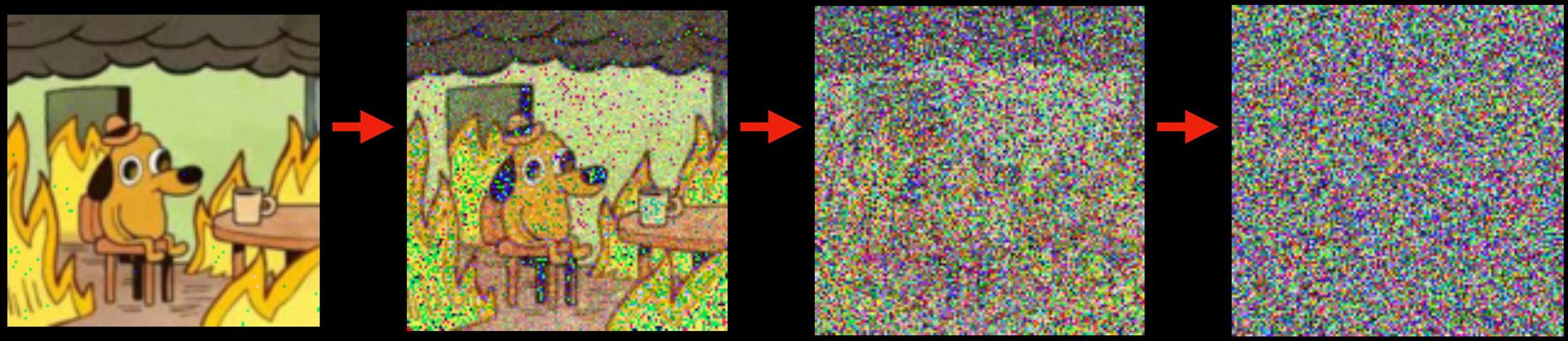
Gaussian Noise



x_0 x_T

What is diffusion model?

Gaussian Noise



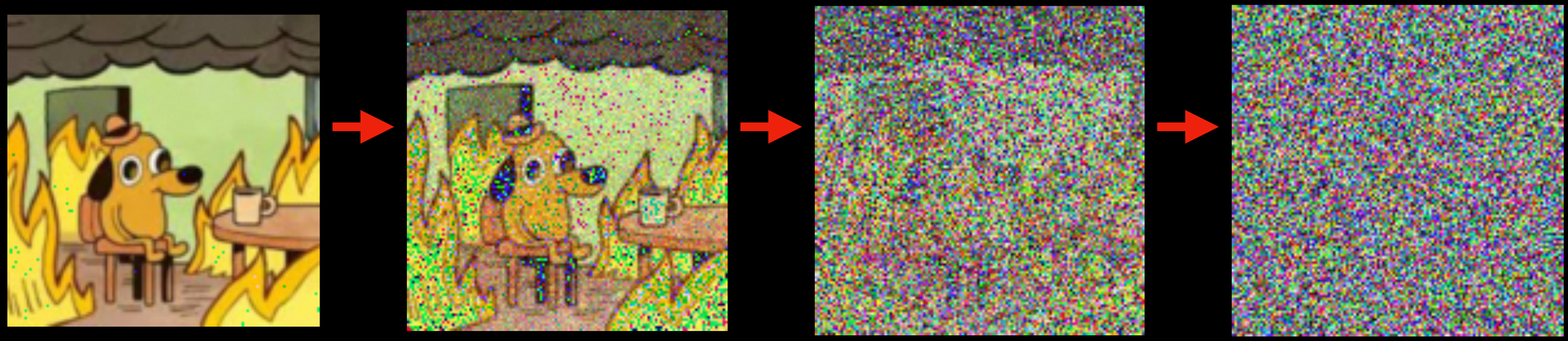
x_0

Markov chain

x_T

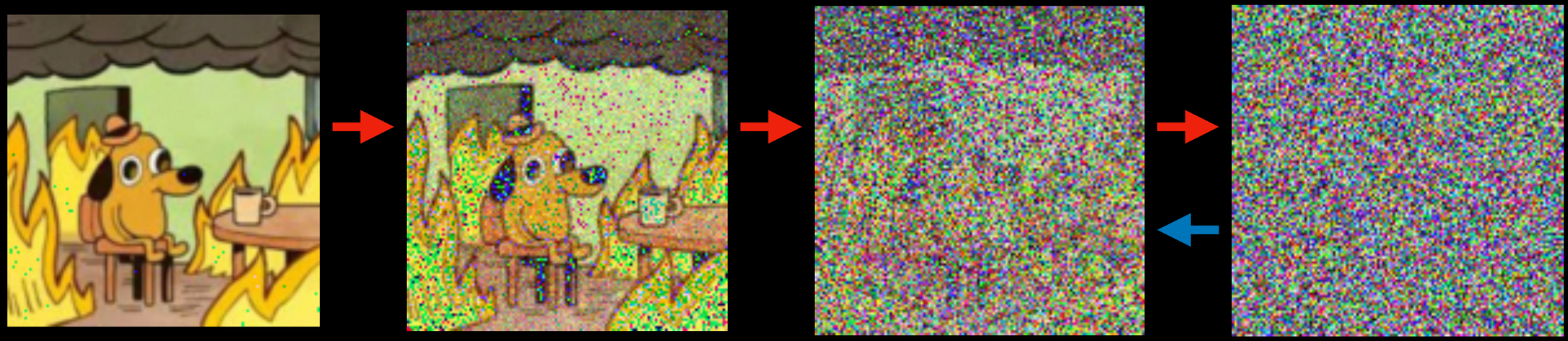
What is diffusion model?

Forward Process q



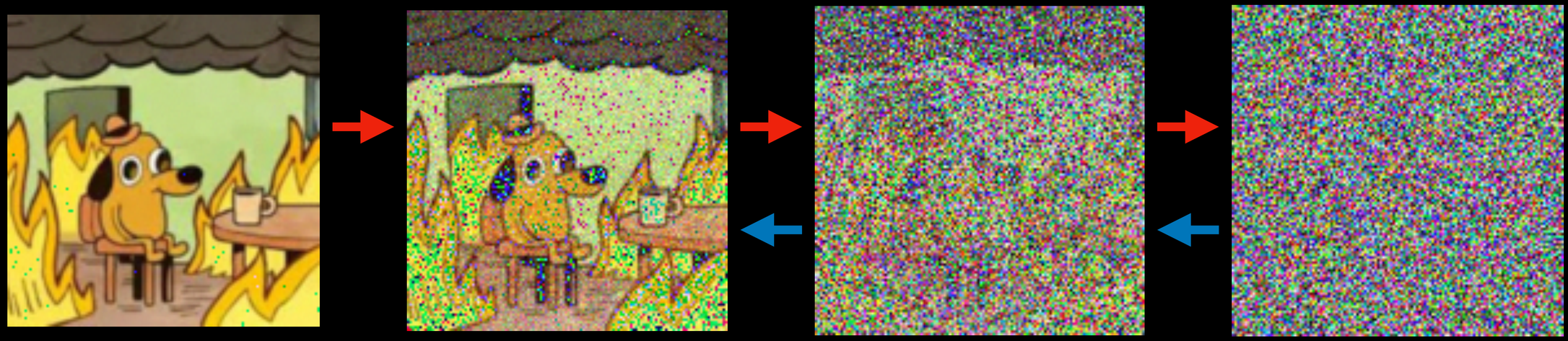
x_0 x_T

What is diffusion model?



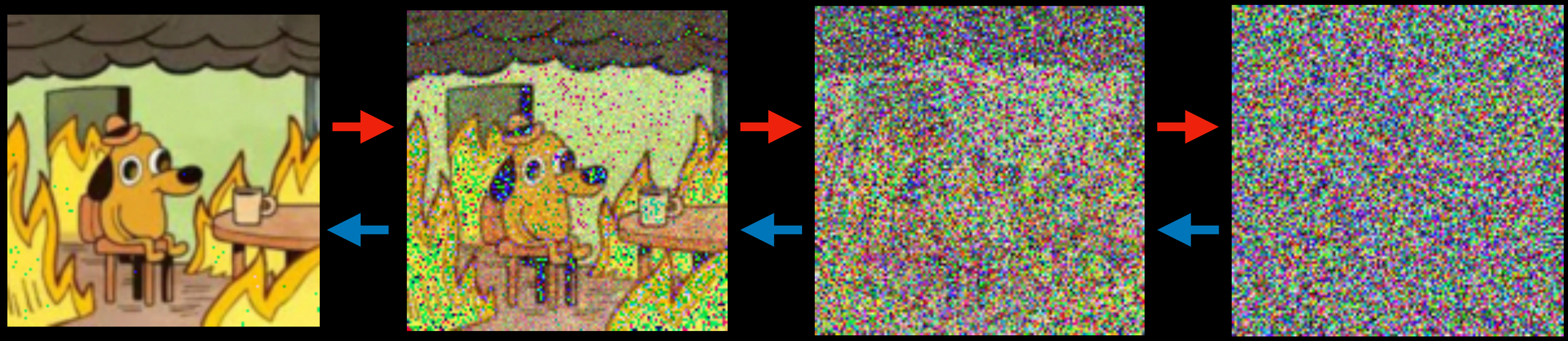
x_0 x_T

What is diffusion model?



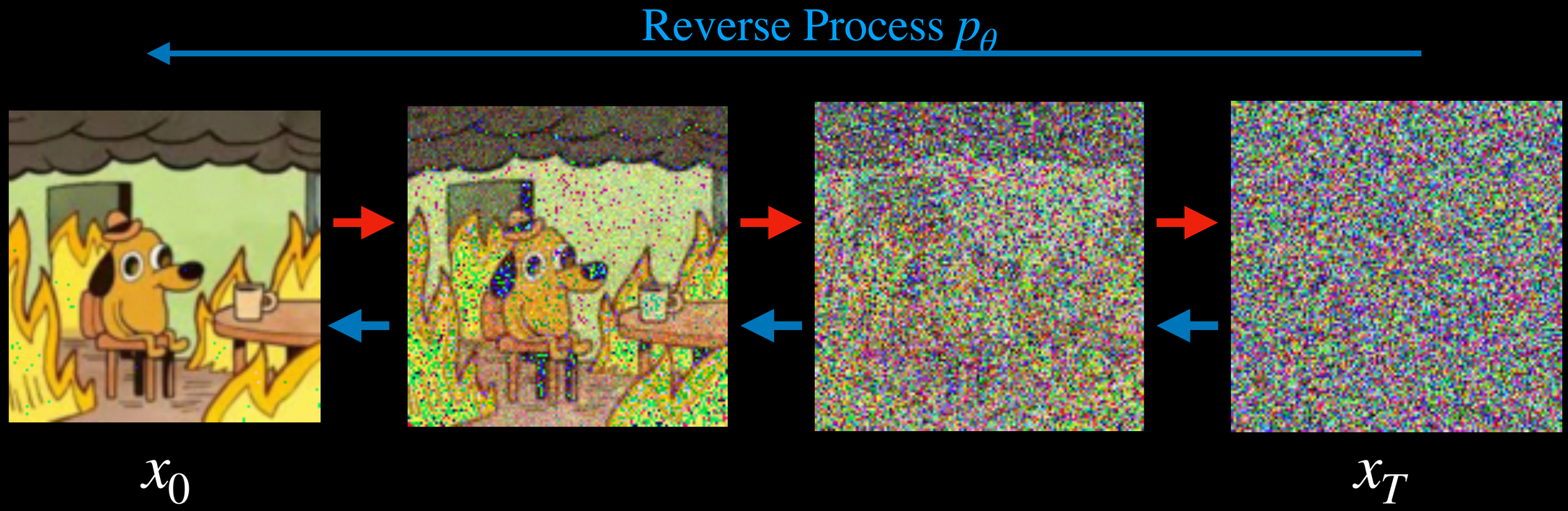
x_0 x_T

What is diffusion model?



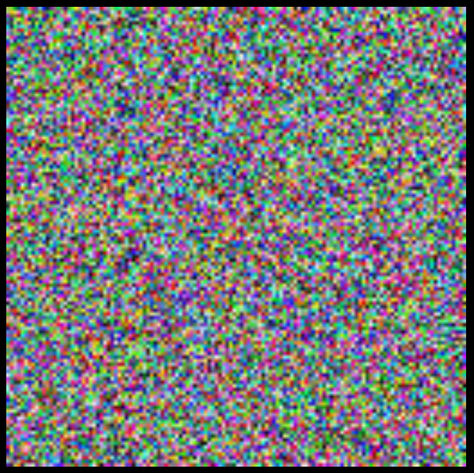
x_0 x_T

What is diffusion model?



What is diffusion model?

Timestep 1~T



x_0 x_T

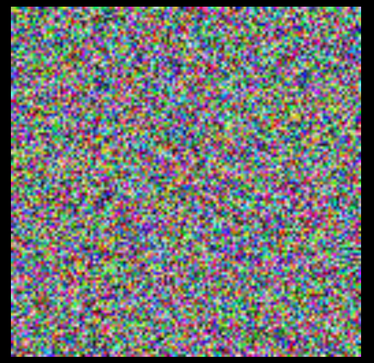
What is diffusion model?

Inference

Reverse Process

Sample Image

Diffusion Model



Initial Image

02
Model Structure

Define Question

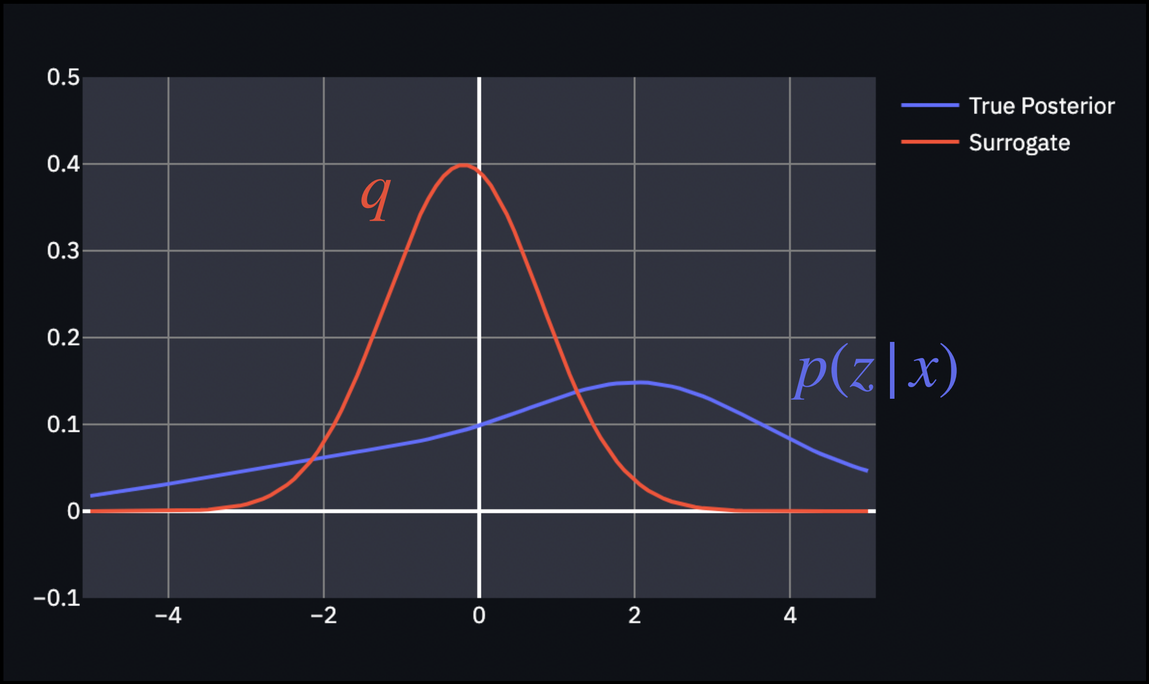
What is Variational Bayesian Inference?

What is Forward Process?

What is Reverse Process?

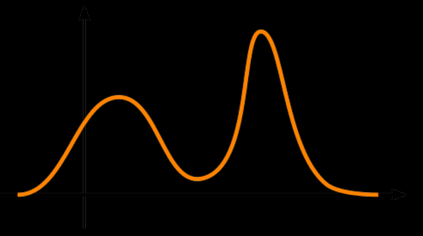
What is the Training Objective of the Diffusion Model?

What is Variational Bayesian Inference?

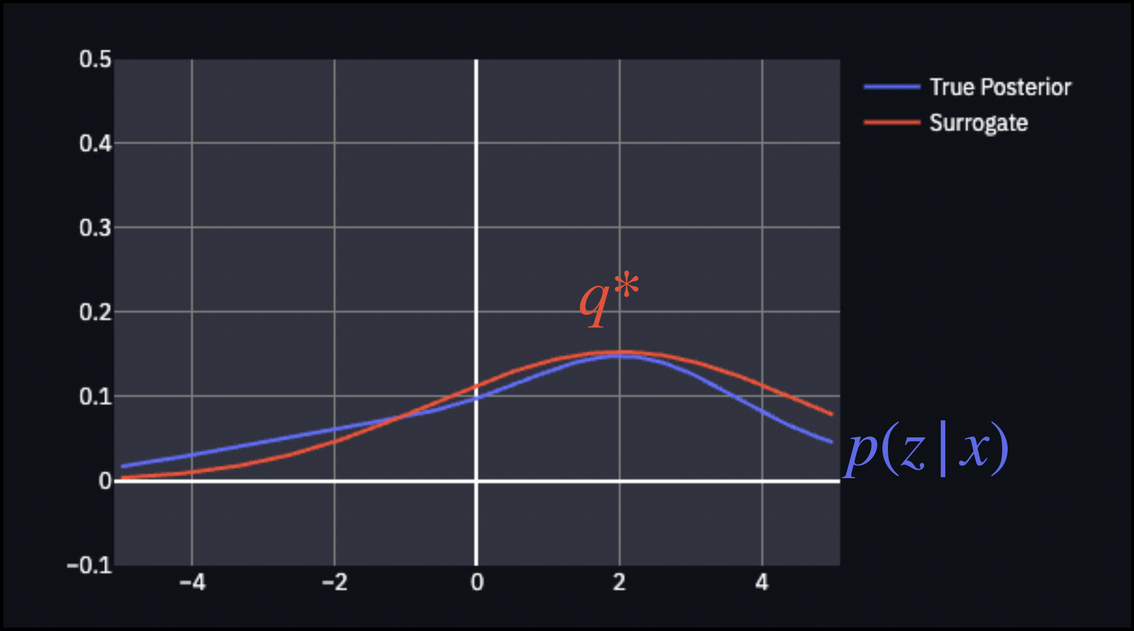


- Observed Variable x
- Latent Variable z
- Posterior Distribution $p(z \mid x)$

Posterior distribution $p(z \mid x)$ might be complex, so we use a Surrogate Normal Distribution q to fit $p(z \mid x)$



What is Variational Bayesian Inference?



- Observed Variable x
- Latent Variable z
- Posterior Distribution $p(z|x)$
- Surrogate Distribution q

We want q as similar to $p(z|x)$ as possible

$$q^* = \arg\min D_{KL}(q||p(z|x))$$

Variational Bayesian Inference in VAE

$$q(z\,|\,x) \quad \approx \quad p(z\,|\,x)$$

$$
\begin{aligned}
D_{\mathrm{KL}}(q_\phi(z|x)\|p_\theta(z|x)) &= \int q_\phi(z|x)\log\frac{q_\phi(z|x)}{p_\theta(z|x)}dz \\
&= \int q_\phi(z|x)\log\frac{q_\phi(z|x)p_\theta(x)}{p_\theta(z,x)}dz \\
&= \int q_\phi(z|x)\big(\log p_\theta(x)+\log\frac{q_\phi(z|x)}{p_\theta(z,x)}\big)dz \\
&= \log p_\theta(x)+\int q_\phi(z|x)\log\frac{q_\phi(z|x)}{p_\theta(z,x)}dz \\
&= \log p_\theta(x)+\int q_\phi(z|x)\log\frac{q_\phi(z|x)}{p_\theta(x|z)p_\theta(z)}dz \\
&= \log p_\theta(x)+\mathbb{E}_{z\sim q_\phi(z|x)}\Big[\log\frac{q_\phi(z|x)}{p_\theta(z)}-\log p_\theta(x|z)\Big] \\
&= \log p_\theta(x)+D_{\mathrm{KL}}(q_\phi(z|x)\|p_\theta(z))-\mathbb{E}_{z\sim q_\phi(z|x)}\log p_\theta(x|z)
\end{aligned}
$$

Variational Bayesian Inference in VAE

$$q(z\,|\,x) \quad \approx \quad p(z\,|\,x)$$

$$\boxed{D_{\mathrm{KL}}(q_\phi(z|x)\|p_\theta(z|x))} \geq 0$$

$$\begin{aligned}
&= \int q_\phi(z|x) \log \frac{q_\phi(z|x)}{p_\theta(z|x)} dz \\
&= \int q_\phi(z|x) \log \frac{q_\phi(z|x) p_\theta(x)}{p_\theta(z,x)} dz \\
&= \int q_\phi(z|x) \big(\log p_\theta(x) + \log \frac{q_\phi(z|x)}{p_\theta(z,x)} \big) dz \\
&= \log p_\theta(x) + \int q_\phi(z|x) \log \frac{q_\phi(z|x)}{p_\theta(z,x)} dz \\
&= \log p_\theta(x) + \int q_\phi(z|x) \log \frac{q_\phi(z|x)}{p_\theta(x|z) p_\theta(z)} dz \\
&= \log p_\theta(x) + \mathbb{E}_{z\sim q_\phi(z|x)} \Big[\log \frac{q_\phi(z|x)}{p_\theta(z)} - \log p_\theta(x|z) \Big] \\
&\boxed{= \log p_\theta(x) + D_{\mathrm{KL}}(q_\phi(z|x)\|p_\theta(z)) - \mathbb{E}_{z\sim q_\phi(z|x)} \log p_\theta(x|z)}
\end{aligned}$$

Variational Bayesian Inference in VAE

$$q(z\,|\,x) \quad \approx \quad p(z\,|\,x)$$

$$\rightarrow \quad \log p_\theta(x) + D_{\mathrm{KL}}(q_\phi(z|x)\|p_\theta(z)) - \mathbb{E}_{z\sim q_\phi(z|x)} \log p_\theta(x|z) \geq 0$$

$$\log p_\theta(x) \geq \mathbb{E}_{z\sim q_\phi(z|x)} \log p_\theta(x|z) - D_{\mathrm{KL}}(q_\phi(z|x)\|p_\theta(z))$$

Variational Bayesian Inference in VAE

$$q(z\,|\,x) \quad \approx \quad p(z\,|\,x)$$

$$\rightarrow \quad \log p_\theta(x) + D_{\mathrm{KL}}(q_\phi(z|x)\|p_\theta(z)) - \mathbb{E}_{z\sim q_\phi(z|x)} \log p_\theta(x|z) \geq 0$$

$$\boxed{\log p_\theta(x)} \geq \boxed{\mathbb{E}_{z\sim q_\phi(z|x)} \log p_\theta(x|z) - D_{\mathrm{KL}}(q_\phi(z|x)\|p_\theta(z))}$$

Log-likelihood

Evidence/Variational Lower Bound, ELBO

Variational Bayesian Inference in VAE

$$q(z|x) \approx p(z|x)$$

$$\log p_\theta(x) + D_{\mathrm{KL}}(q_\phi(z|x)\|p_\theta(z)) - \mathbb{E}_{z\sim q_\phi(z|x)} \log p_\theta(x|z) \geq 0$$

$$\log p_\theta(x) \geq \mathbb{E}_{z\sim q_\phi(z|x)} \log p_\theta(x|z) - D_{\mathrm{KL}}(q_\phi(z|x)\|p_\theta(z))$$

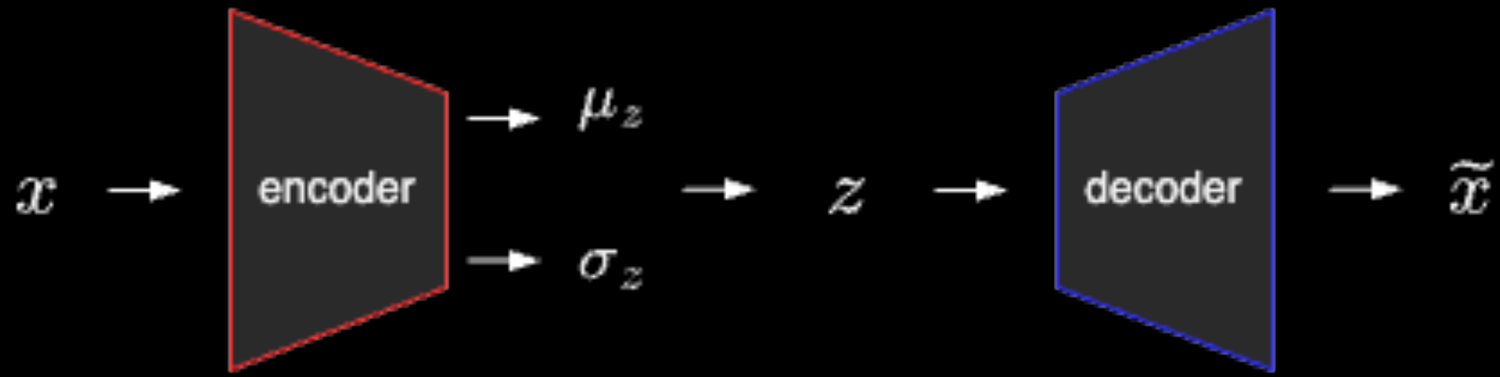
$$= \mathbb{E}_{q_\phi}\left[\log p_\theta(x|z) - D_{KL}\left(q_\phi(z|x) \,||\, p_\theta(z)\right)\right]$$

VAE's loss function

use Monte Carlo (sampling) method. In VAE, the sample num is 1.

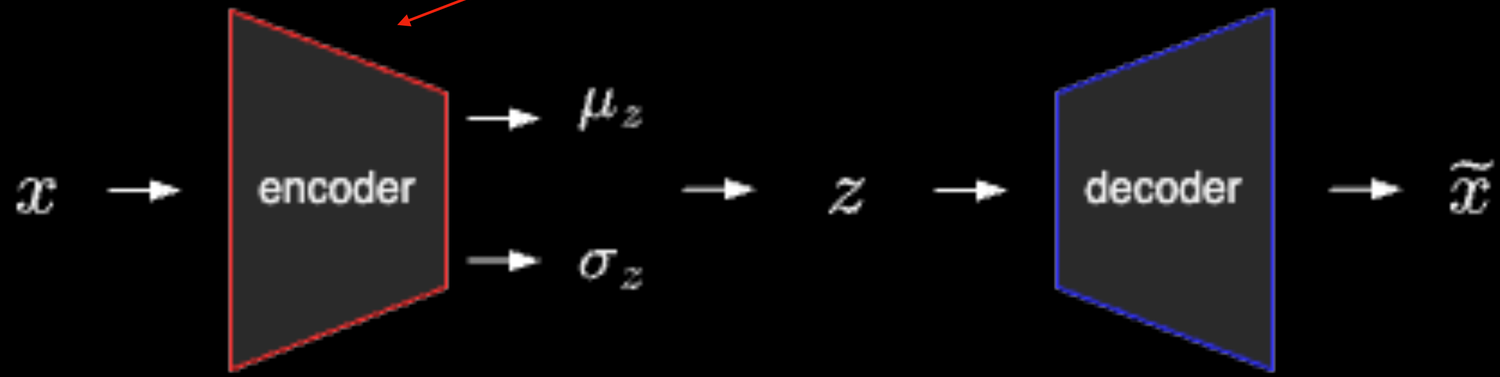
Variational Bayesian Inference in VAE

$$\mathbb{E}_{q_\phi}\Big[\log p_\theta(x\,|\,z) - D_{KL}\Big(q_\phi(z\,|\,x)\;||\;p_\theta(z)\Big)\Big]$$



Variational Bayesian Inference in VAE

$$\mathbb{E}_{q_\phi}\left[\log p_\theta(x\,|\,z) - D_{KL}\left(q_\phi(z\,|\,x)\,||\,p_\theta(z)\right)\right]$$



Variational Bayesian Inference in VAE

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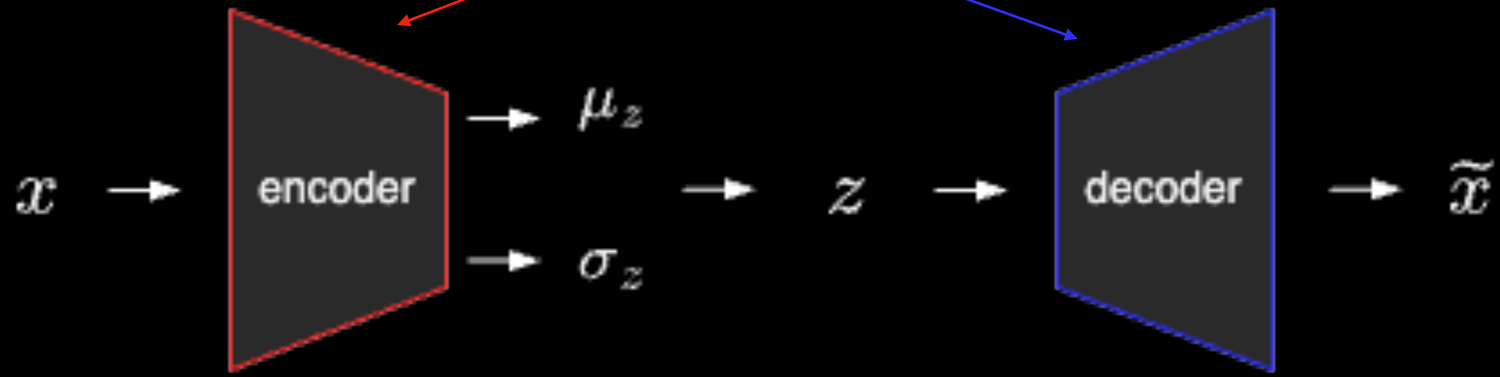
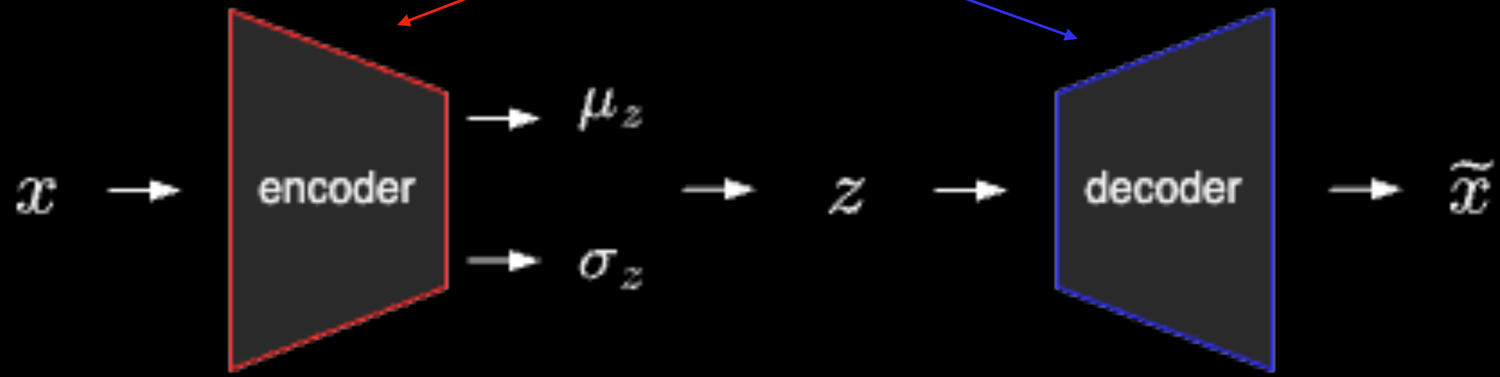


Variational Bayesian Inference in VAE

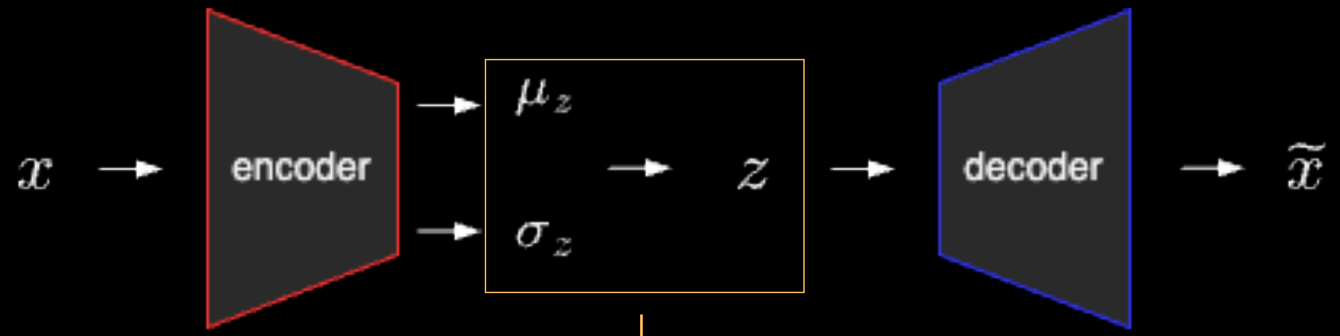
$$\mathbb{E}_{q_\phi}\left[\log p_\theta(x\,|\,z) - D_{KL}\left(q_\phi(z\,|\,x)\,||\,p_\theta(z)\right)\right]$$

$$\sim N(0,1)$$



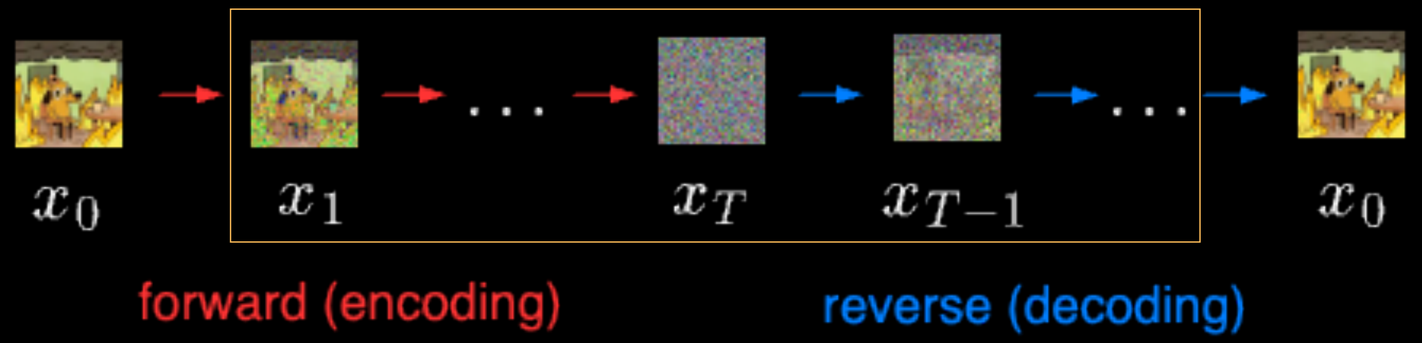
From VAE to Diffusion

VAE



DDPM

Replace latent variable z to $x_{1:T}$



From VAE to Diffusion

VAE

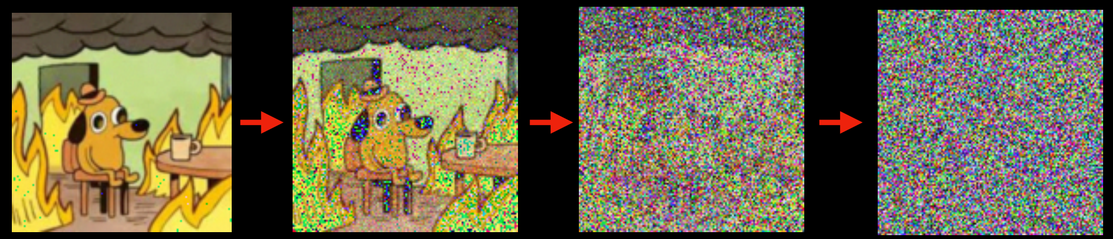
$$\mathbb{E}_{q_\phi}\left[\log p_\theta(x \mid z) - D_{KL}\left(q_\phi(z \mid x) \,||\, p_\theta(z)\right)\right]$$

Replace latent variable from z to $x_{1:T}$

DDPM

$$\mathbb{E}_{q}\left[\log p_\theta(x_0 \mid x_{1:T}) - D_{\mathsf{KL}}\left(q(x_{1:T} \mid x_0) \,||\, p_\theta(x_{1:T})\right)\right]$$

What is forward process?

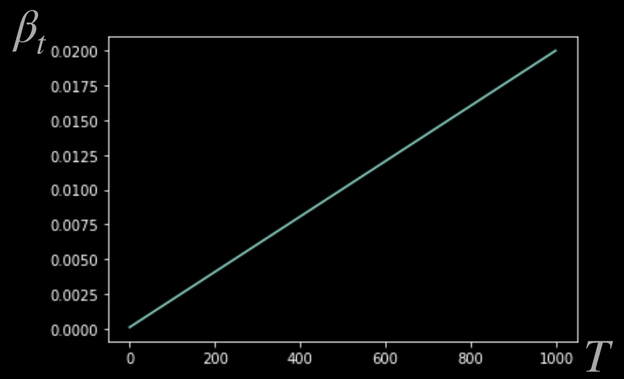


$$q(x_{1:T}|x_0) := \prod_{t=1}^{T} q(x_t|x_{t-1}),$$

$$q(x_t|x_{t-1}) := N(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t I)$$

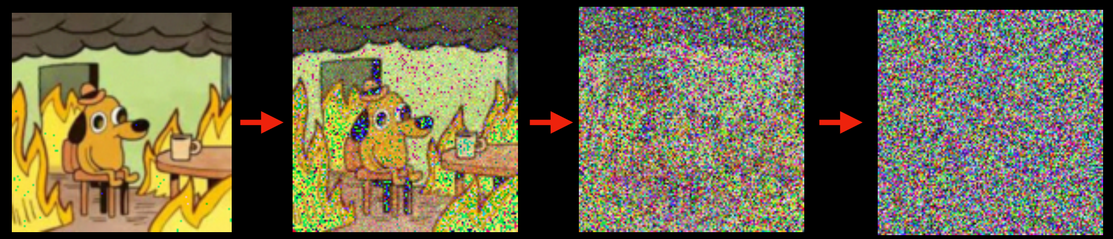
- Define a Markov chain of diffusion steps to slowly add random noise to the data according to a variance schedule $\beta_1, \ldots, \beta_T$

$$\beta_1 = 0.0001$$
$$\beta_T = 0.02$$



When T is bigger enough($T \to \infty$), the final x_T would become a random gaussian distribution

What is forward process?



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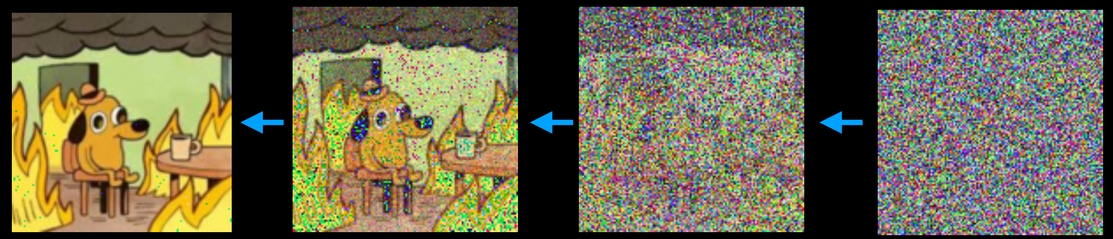
- Define a Markov chain of diffusion steps to slowly add random noise to the data according to a variance schedule $\beta_1, \ldots, \beta_T$
- The process is fixed throughout the process, has noting to do with model and training

VAE's ELBO	$\mathbb{E}_{q_\phi}\left[\log p_\theta(x|z) - D_{KL}\left(q_\phi(z|x) \,||\, p_\theta(z)\right)\right]$
Diffusion Model's ELBO	$\mathbb{E}_{q}\left[\log p_\theta(x_0|x_{1:T}) - D_{\mathrm{KL}}\left(q(x_{1:T}|x_0)||p_\theta(x_{1:T})\right)\right]$

What is reverse process?



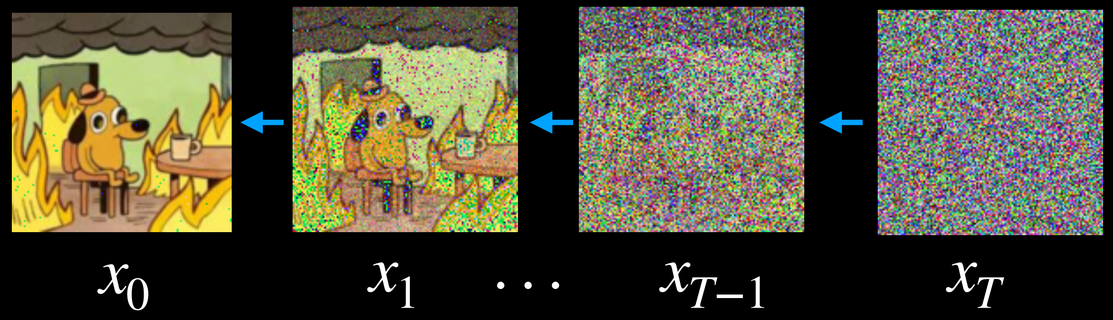
$$p_\theta(x_{0:T}) := p(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1} \mid x_t),$$

$$p_\theta(x_{t-1} \mid x_t) := N(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$$

- The reverse process is a model learn to reverse the diffusion process to construct desired data from the noise.
- Unlike VAE just use Linear Layer, DDPM use U-net as predict model

* U-Net is a convolutional neural network that was developed for biomedical image segmentation

What is reverse process?



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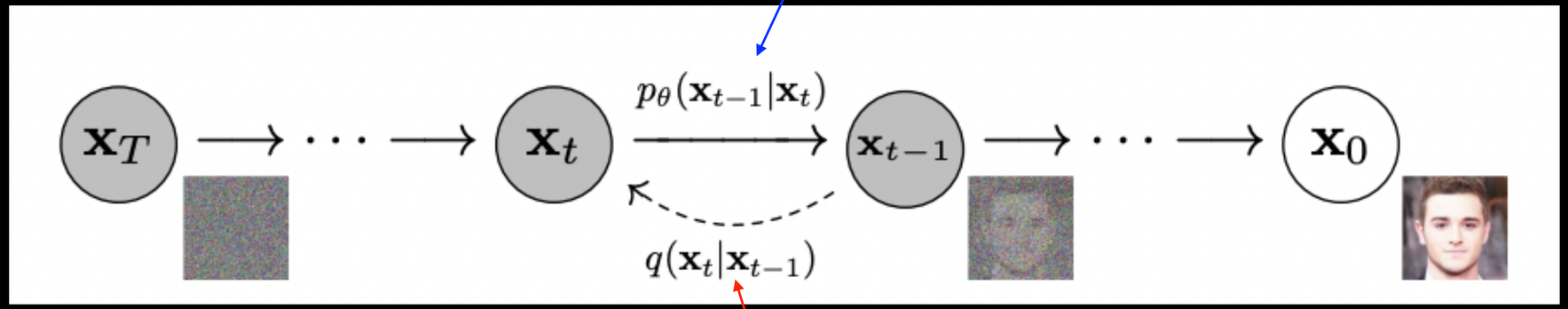
Can be fixed as forwarding's variance β_t, or been predicted by the model

- The reverse process is a model learn to reverse the diffusion process to construct desired data from the noise.
- Unlike VAE just use Linear Layer, DDPM use U-net as predict model

* U-Net is a convolutional neural network that was developed for biomedical image segmentation

The directed graphical model considered in this work.

$$p_\theta(x_{0:T}) := p(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1}\,|\,x_t), \quad p_\theta(x_{t-1}\,|\,x_t) := N(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$$



$$q(x_{1:T}\,|\,x_0) := \prod_{t=1}^{T} q(x_t\,|\,x_{t-1}), \quad q(x_t\,|\,x_{t-1}) := N(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t I)$$

What is the Training Objective of the Diffusion Model?

ELBO

$$\mathbb{E}_q\Big[\log p_\theta(x_0 \mid x_{1:T}) - D_{\mathrm{KL}}\Big(q(x_{1:T} \mid x_0) \,||\, p_\theta(x_{1:T})\Big)\Big]$$

↓

Predict μ_θ

Learned Σ_θ :

$$L_{t-1} = \mathbb{E}_q\Big[\frac{1}{2||\Sigma_\theta||_2^2}||\tilde{\mu}(x_t, x_0) - \mu_\theta(x_t, t)||^2\Big]$$

Fixed Σ as σ_t, $\sigma_t^2 = \beta_t$ or $\frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t$:

$$L_{t-1} = \mathbb{E}_q\Big[\frac{1}{2\sigma_t^2}||\tilde{\mu}(x_t, x_0) - \mu_\theta(x_t, t)||^2\Big]$$

↓

Predict ϵ_θ

Noise

$$\mathbb{E}_{x_0,\epsilon}\Big[\frac{\beta_t^2}{2\sigma_t^2\alpha_t(1-\bar{\alpha}_t)}||\epsilon - \epsilon_\theta(x_t, t)||^2\Big] \xrightarrow{\text{Simplify}} \mathbb{E}_{x_0,\epsilon,t}\Big[||\epsilon - \epsilon_\theta(x_t, t)||^2\Big]$$

(MSE of noise)

What is the Training Objective of the Diffusion Model?

ELBO

$$\mathbb{E}_q\Big[\log p_\theta(x_0 \mid x_{1:T}) - D_{\mathrm{KL}}\Big(q(x_{1:T} \mid x_0) \,||\, p_\theta(x_{1:T})\Big)\Big]$$

↓

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↓

Predict ϵ_θ

Noise

$$\mathbb{E}_{x_0,\epsilon}\Big[\frac{\beta_t^2}{2\sigma_t^2\alpha_t(1-\bar{\alpha}_t)}||\epsilon - \epsilon_\theta(x_t, t)||^2\Big] \xrightarrow{\text{Simplify}} \mathbb{E}_{x_0,\epsilon,t}\Big[||\epsilon - \epsilon_\theta(x_t, t)||^2\Big]$$

(MSE of noise)

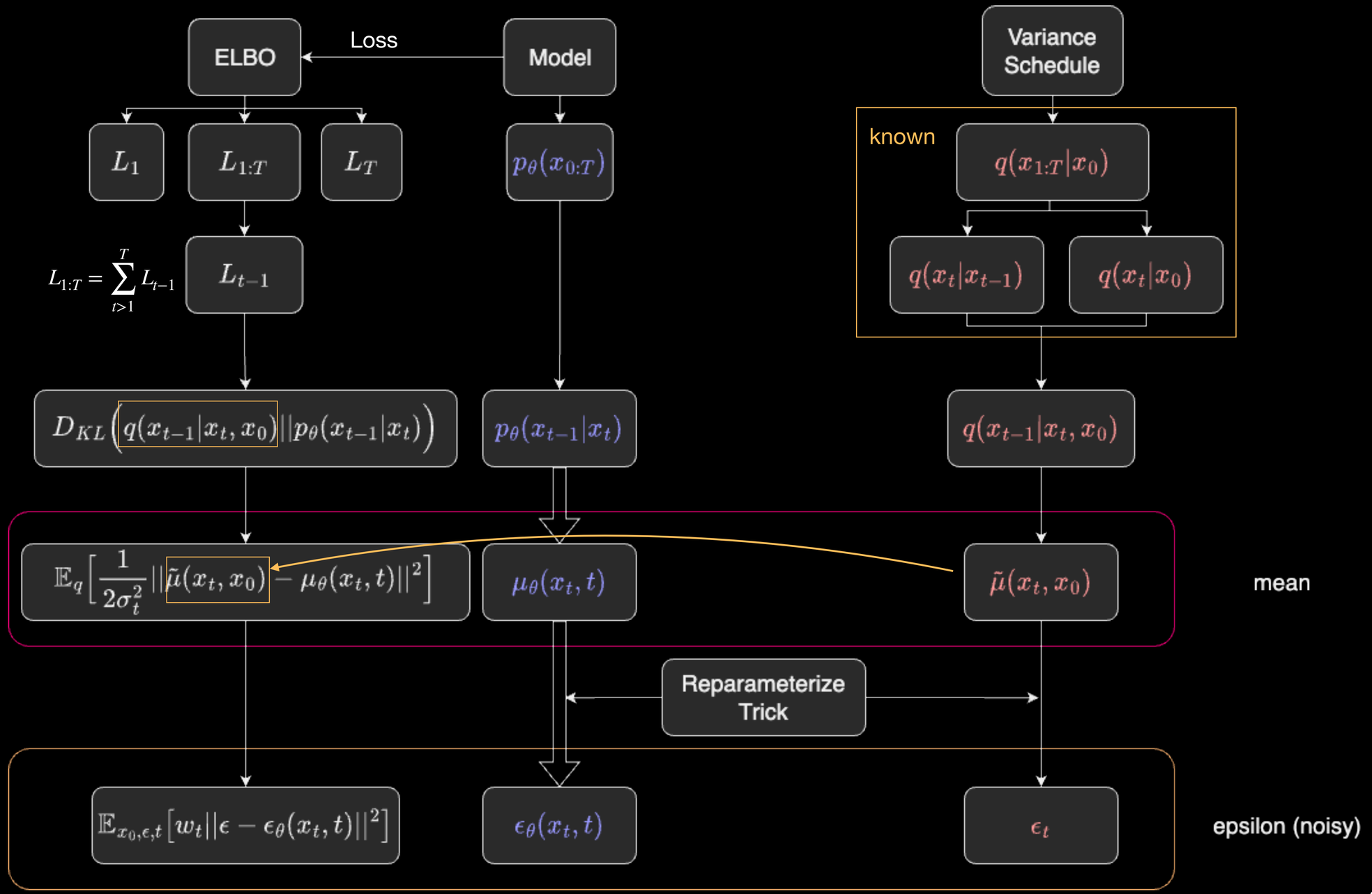
Derivation flow chart

1.Split ELBO loss to different time step, and Ignore L_0 and L_T, we can focus on the loss between each step.

2. Use Bayes' Rule and Probability Density Function to derivate $q(x_{t-1}|x_t)$ when conditioned on x_0.

3. We can represent the distribution in μ and σ format when compute the KLD between two normal distribution

4. Use Reparameterize Trick Convert $\tilde{\mu}_t$ to ϵ_t form



03
Experiments

Measure Method

Inception Score, IS

Frechet Inception Distance, FID

Both:

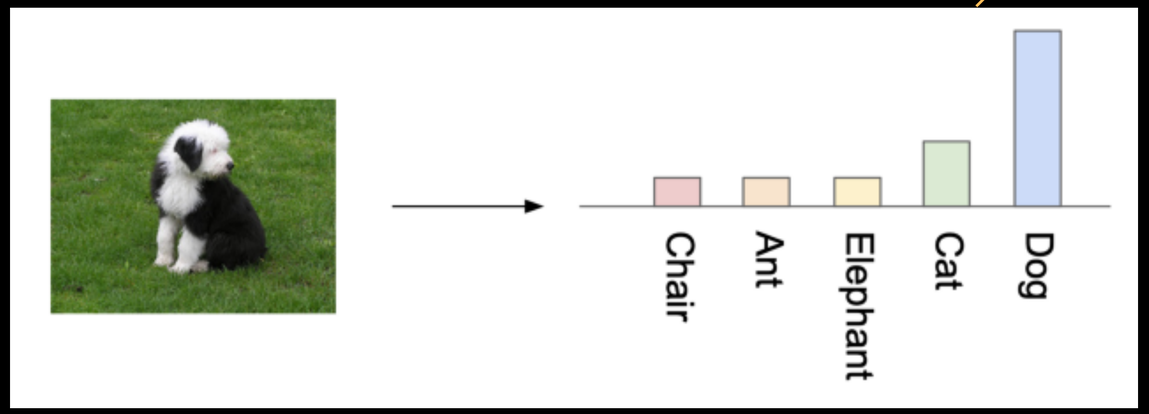
- Measure of how realistic a generated image is.
- Use Inception V3 (Google’s model trained on ImageNet Dataset)

Inception Score

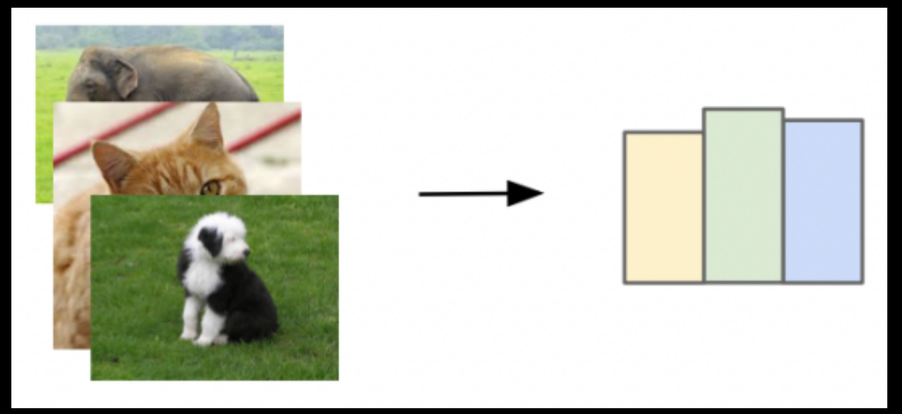
Inception v3 model p

Generated image x

$$\text{IS} = exp\Big(\mathbb{E}_{x \sim p_g} D_{KL}\big(p(y \mid x) \,||\, p(y)\big) \Big)$$



Distinct

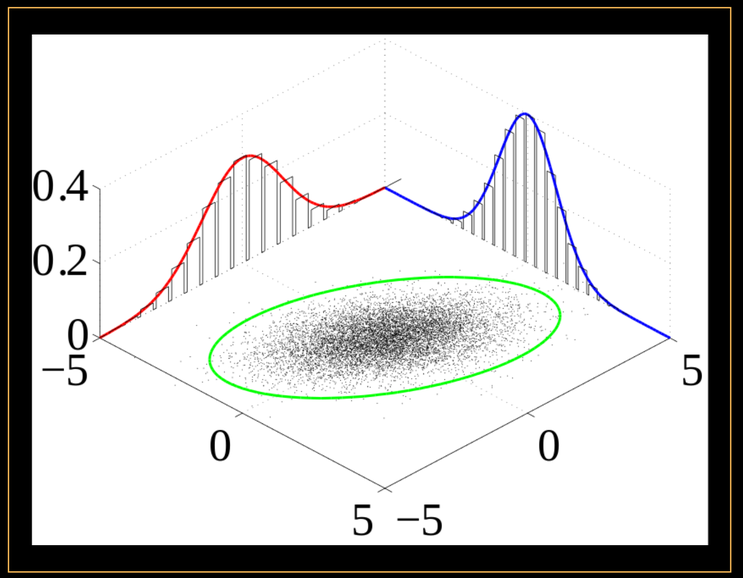


Diversity (look all input x)

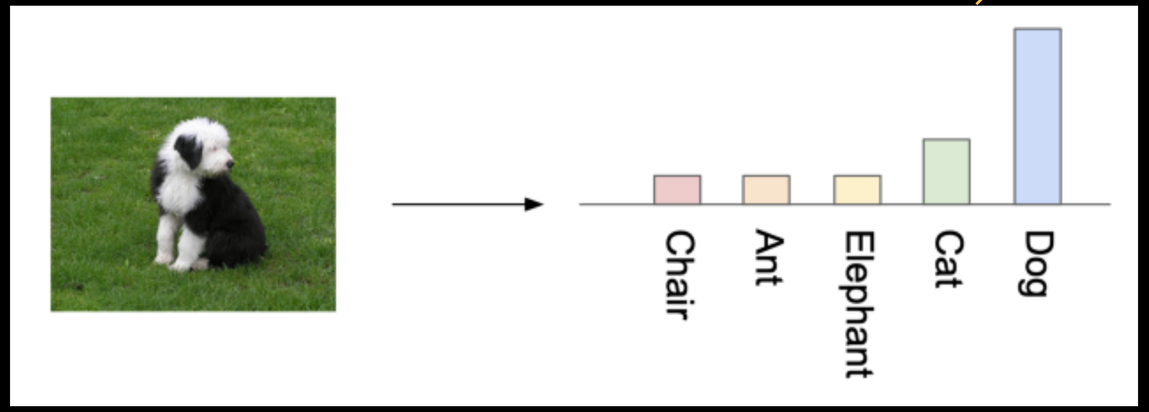
The bigger the better

Inception Score

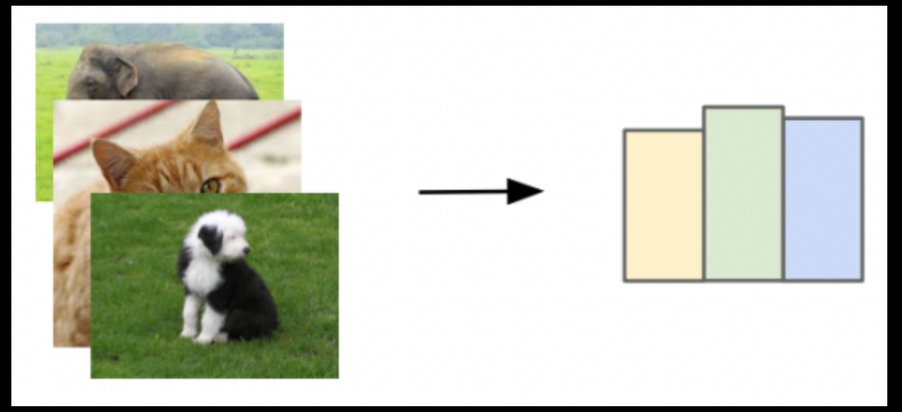
$$\text{IS} = exp\Big(\mathbb{E}_{x\sim p_g} D_{KL}\big(p(y\,|\,x)\,||\,p(y)\big)\Big)$$



Marginal distribution when seen all x



Distinct



Diversity (look all input x)

The bigger the better

Frechet Inception Distance

$$\text{FID} = ||\mu_x - \mu_Y||^2 - Tr\left(\Sigma_X + \Sigma_Y - 2\Sigma_X\Sigma_Y\right)$$

Real Images Embeddings X

Fake Images Embeddings Y

(Assumed X, Y to be two multivariate normal distributions)

Trace of the matrix Tr

The smaller the better

Ablation study

Objective	IS	FID
$\tilde{\mu}$ prediction (baseline)		
L, learned diagonal Σ	7.28 ± 0.10	23.69
L, fixed isotropic Σ	8.06 ± 0.09	13.22
$\|\|\tilde{\mu} - \tilde{\mu}_\theta\|\|^2$	–	–
ϵ prediction (ours)		
L, learned diagonal Σ	–	–
L, fixed isotropic Σ	7.67 ± 0.13	13.51
$\|\|\tilde{\epsilon} - \epsilon_\theta\|\|^2$ (L_{simple})	$\mathbf{9.46 \pm 0.11}$	**3.17**

Blank entries were unstable to train and generated poor samples

- $\tilde{\mu}$ only works well on the true ELBO
- ϵ prediction approximately as well as prediction $\tilde{\mu}$ when Σ is fixed
- ϵ prediction without w_t get the best results

What is the Training Objective of the Diffusion Model?

ELBO

$$\mathbb{E}_q\Big[\log p_\theta(x_0 \mid x_{1:T}) - D_{\mathrm{KL}}\Big(q(x_{1:T} \mid x_0) \,||\, p_\theta(x_{1:T})\Big)\Big]$$

Predict μ_θ

Learned Σ_θ :

$$L_{t-1} = \mathbb{E}_q\Big[\frac{1}{2\sigma_t^2}||\tilde{\mu}(x_t, x_0) - \mu_\theta(x_t, t)||^2\Big]$$

Fixed Σ as σ_t, $\sigma_t^2 = \beta_t$ or $\frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t$:

$$L_{t-1} = \mathbb{E}_q\Big[\frac{1}{2\sigma_t^2}||\tilde{\mu}(x_t, x_0) - \mu_\theta(x_t, t)||^2\Big]$$

Predict ϵ_θ

$$\mathbb{E}_{x_0,\epsilon}\Big[\frac{\beta_t^2}{2\sigma_t^2\alpha_t(1-\bar{\alpha}_t)}||\epsilon - \epsilon_\theta(x_t, t)||^2\Big] \xrightarrow{\text{Simplify}} \mathbb{E}_{x_0,\epsilon,t}\Big[||\epsilon - \epsilon_\theta(x_t, t)||^2\Big]$$

(MSE of noise)

Ablation study

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ϵ prediction (ours)		
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- ϵ prediction without w_t get the best results

Compare with SOTAs

Table 1: CIFAR10 results. NLL measured in bits/dim.

Model	IS	FID	NLL Test (Train)
Conditional			
EBM [11]	8.30	37.9	
JEM [17]	8.76	38.4	
BigGAN [3]	9.22	14.73	
StyleGAN2 + ADA (v1) [29]	**10.06**	**2.67**	
Unconditional			
Diffusion (original) [53]			≤ 5.40
Gated PixelCNN [59]	4.60	65.93	3.03 (2.90)
Sparse Transformer [7]			**2.80**
PixelIQN [43]	5.29	49.46	
EBM [11]	6.78	38.2	
NCSNv2 [56]		31.75	
NCSN [55]	8.87 ± 0.12	25.32	
SNGAN [39]	8.22 ± 0.05	21.7	
SNGAN-DDLS [4]	9.09 ± 0.10	15.42	
StyleGAN2 + ADA (v1) [29]	**9.74** $\pm$ 0.05	3.26	
Ours (L, fixed isotropic $\mathbf{\Sigma}$)	7.67 ± 0.13	13.51	≤ 3.70 (3.69)
Ours (L_{simple})	9.46 ± 0.11	**3.17**	≤ 3.75 (3.72)

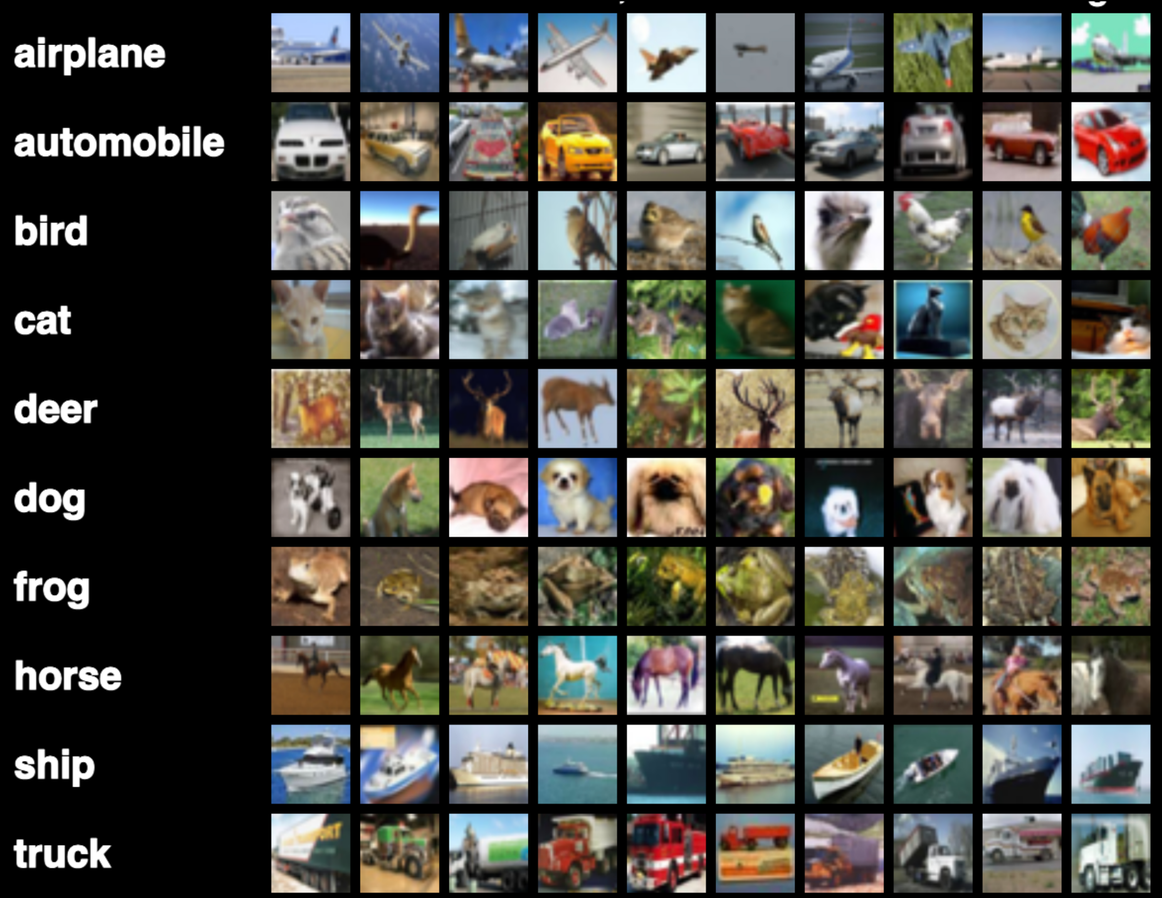
Conditional image synthesis

create an image according to some multi-modal guidance in the forms of textual descriptions, reference images, etc.

- L_{simple} only worse than the model proposed from Training generative adversarial networks with limited data, NeurIPS'20

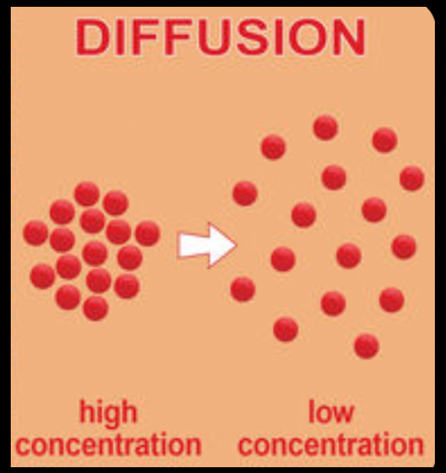
CIFAR-10 Datasets

CIFAR-10 dataset consists of 60000 32x32 colour images in 10 classes



Questions

- Q1. Why called diffusion?



Diffusion is a direct result of the second law of entropy.
The molecules spread out in all directions, lowering the molecules' concentrations in the original space.

The system state changed from Low entropy to High entropy.

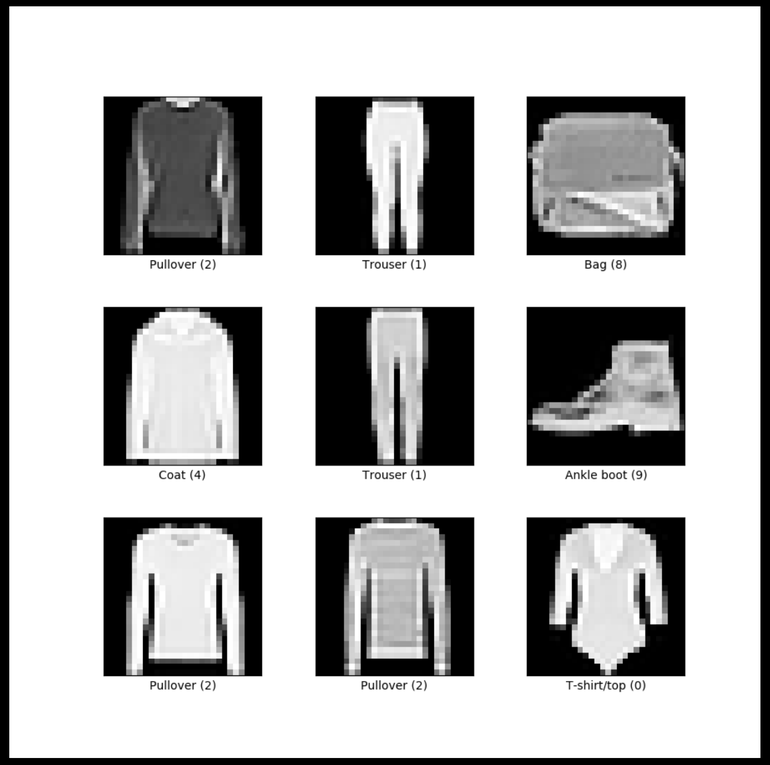
- Q2. What's the difference between DDPM and Diffusion Model 2015?

  1. Use the ϵ as the training objective to explicit connection between diffusion models and denoting score matching.
  2. The model structure used in the reverse process is different:
  DDPM use U-Net and Diffusion Model 2015 use the other CNN model propose in "Volumetric Semantic Segmentation Using Pyramid Context Features, IEEE'13 "

SWOT

Strengths	Weaknesses
• Variational inference can have better performance in the case of fewer data and the case of data generation. • The idea that use Markov chain as latent variable can achieve High performance on image synthesis.	• Sample Speed is low. • Hard to use in Discrete Data.
Opportunities	**Threats**
• Any situation that can combined with Variational Inference. • The idea of diffusion process may be used for recommender system	• How to apply the diffusion model to discrete tradings data is a complex problem.

My Experiments

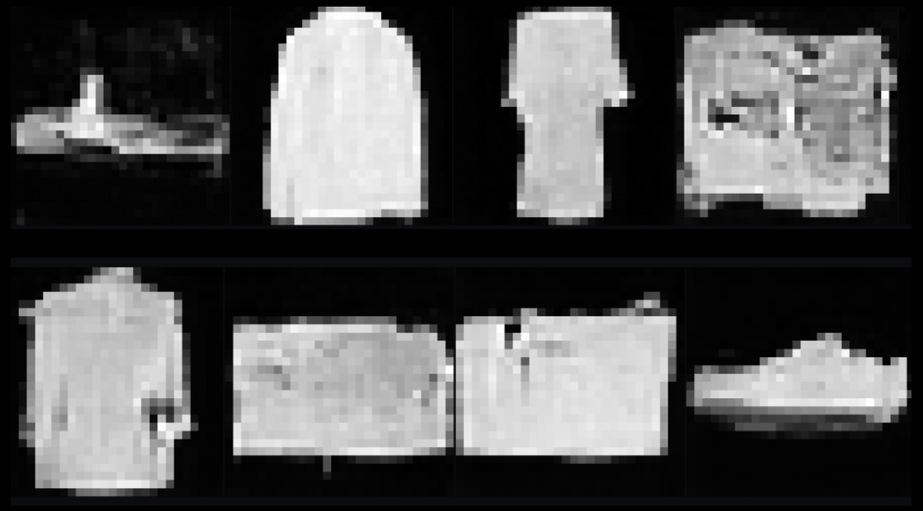


Fashion_mnist Dataset

Each example is a 28x28 grayscale image, associated with a label from 10 classes.

(Pullover, Trouser, Bag, Coat…)

Train & Sample



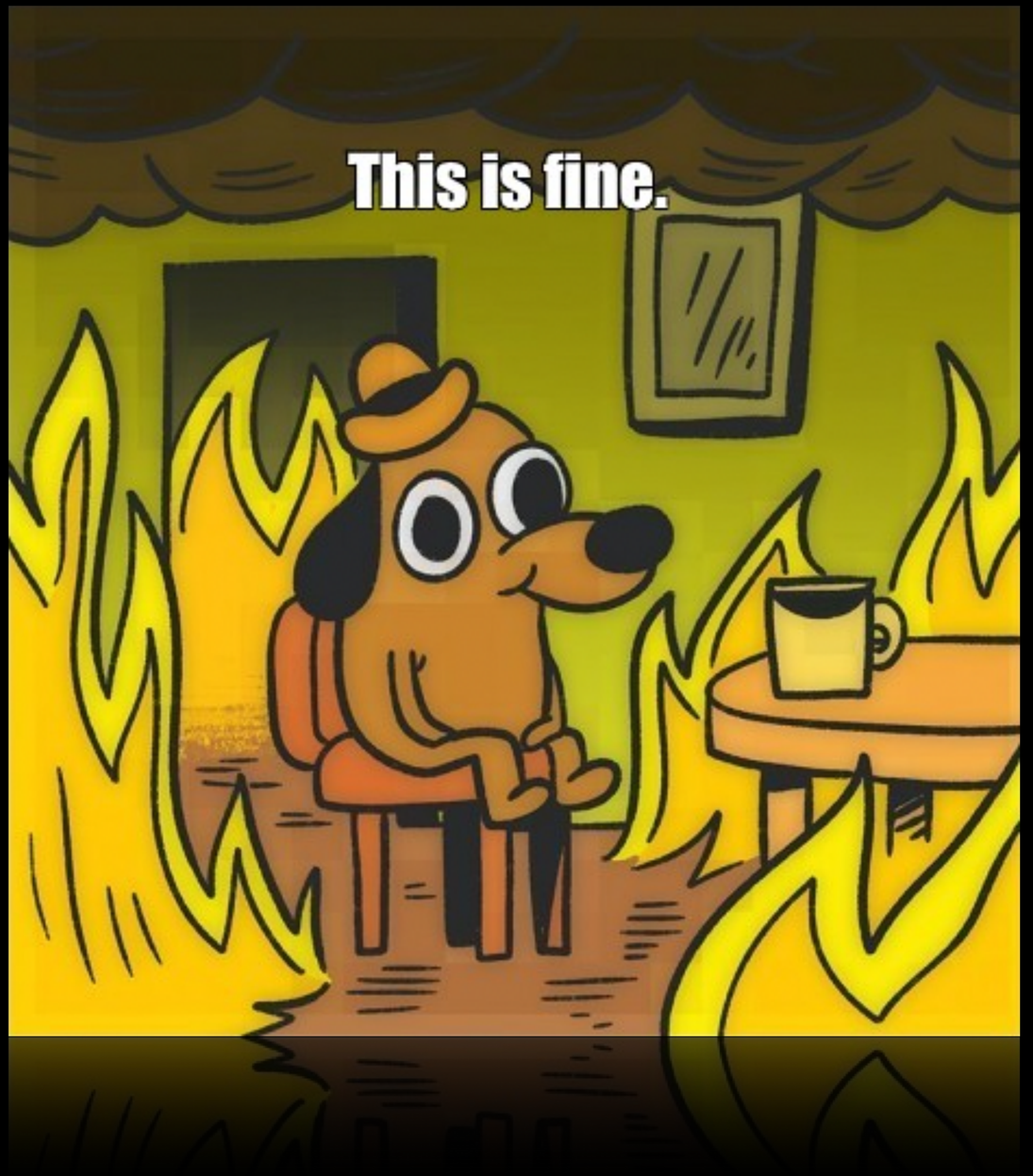
GeForce RTX 2070
Linear Variance schedule
epochs = 10
timesteps = 1000
training took 8m 28.2s
sampling 8 images took 10.2s
Memory usage 2749MiB

References

- Deep Unsupervised Learning using Nonequilibrium Thermodynamics, ICML'15
  https://arxiv.org/pdf/1503.03585.pdf
- Denoising Diffusion Probabilistic Models, NIPS'20
  https://arxiv.org/pdf/2006.11239.pdf
- Volumetric Semantic Segmentation using Pyramid Context Features, IEEE’13
  https://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=6751540
- From Autoencoder to Beta-VAE
  https://lilianweng.github.io/posts/2018-08-12-vae/
- What are Diffusion Models?
  https://lilianweng.github.io/posts/2021-07-11-diffusion-models/
- Hung-yiLee VAE Tutorial
  https://www.youtube.com/watch?v=8zomhgKrsmQ&ab_channel=Hung-yiLee

404

Appendix



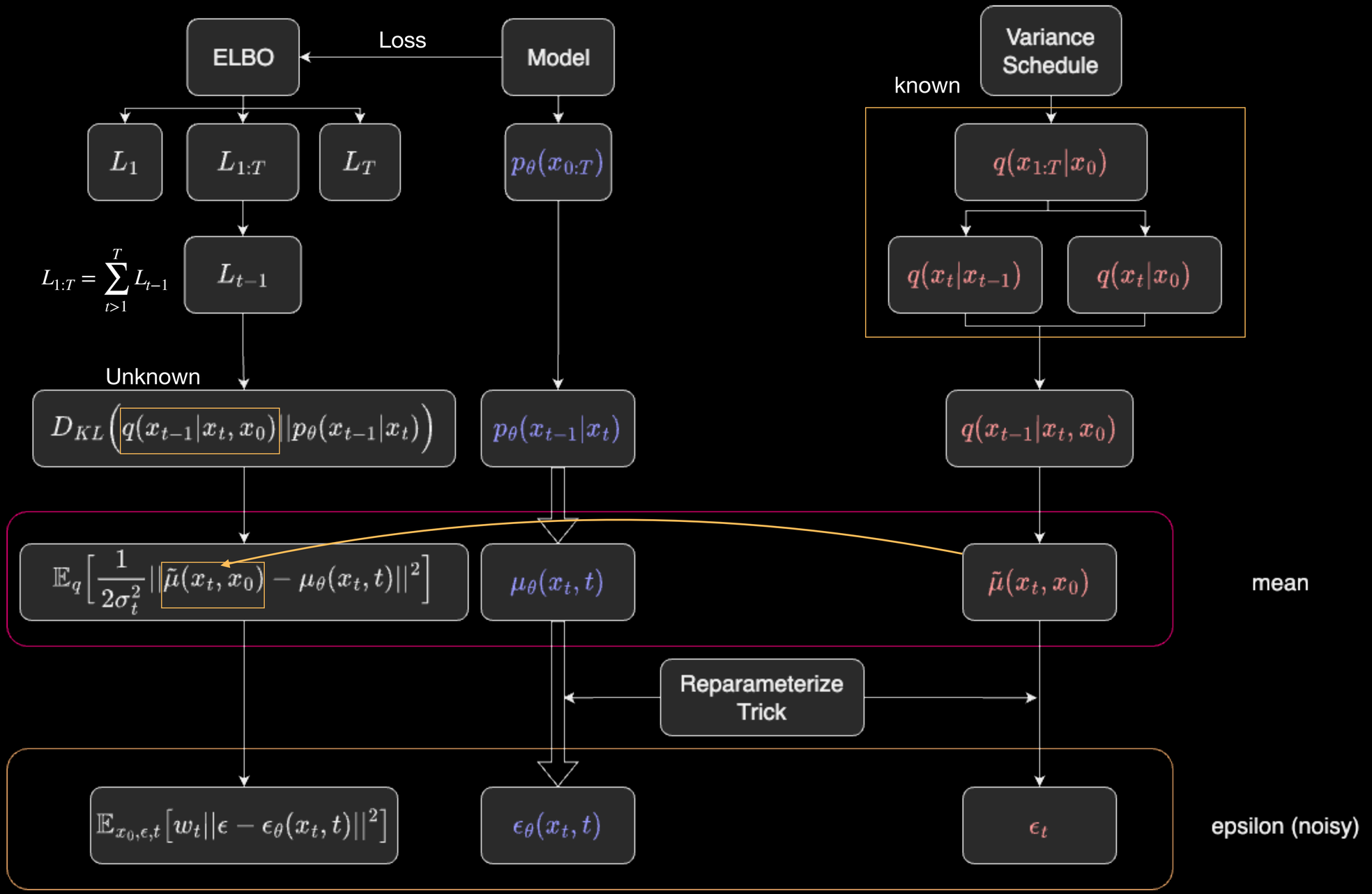
Derivation
flow chart

1.Split ELBO loss to different time step, and Ignore L_0 and L_T, we can focus on the loss between each step.

2. Use Bayes' Rule and Probability Density Function to derivate $q(x_{t-1}|x_t)$ when conditioned on x_0.

3. We can represent the distribution in μ and σ format when compute the KLD between two normal distribution

4. Use Reparameterize Trick Convert $\tilde{\mu}_t$ to ϵ_t form



Step1. Split ELBO loss to different time step: $L = L_T + L_{1:T} + L_0$

From $x_{1:T}$ to the form of conditional probability

Reverse Process

$$p_\theta(x_{0:T}) := p(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1} \mid x_t),$$

$$p_\theta(x_{t-1} \mid x_t) := N(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$$

$$\mathbb{E}_q \Big[\log p_\theta(x_0|x_{1:T}) - D_{\mathrm{KL}} \Big(q(x_{1:T}|x_0) || p_\theta(x_{1:T}) \Big) \Big]$$

$$= \mathbb{E}_q \Big[\log p_\theta(x_0|x_{1:T}) - \log \frac{q(x_{1:T}|x_0)}{p_\theta(x_{1:T})} \Big]$$

$$= \mathbb{E}_q \Big[\log p_\theta(x_0|x_{1:T}) + \log \frac{p_\theta(x_{1:T})}{q(x_{1:T}|x_0)} \Big]$$

$$= \mathbb{E}_q \Big[\log \frac{p_\theta(x_{0:T})}{q(x_{1:T}|x_0)} \Big]$$

$$= \mathbb{E}_q \Big[\log \frac{p_\theta(x_T) p_\theta(x_0|x_1) \dots p_\theta(x_{T-1}|x_T)}{q(x_1|x_0) q(x_2|x_1) \dots q(x_T|x_{T-1})} \Big]$$

$$= \mathbb{E}_q \Big[\log p_\theta(x_T) + \sum_{t \geq 1} \log \frac{p_\theta(x_{t-1}|x_t)}{q(x_t|x_{t-1})} \Big]$$

Step1. Split ELBO loss to different time step: $L = L_T + L_{1:T} + L_0$

According to the Paper, split L into different parts: $L_T, L_{1:T}, L_0$

$$
\begin{aligned}
L &= -\mathbb{E}_q\Big[\log p(x_T) + \sum_{t\geq 1}\log\frac{p_\theta(x_{t-1}|x_t)}{q(x_t|x_{t-1})}\Big] \\
&= -\mathbb{E}_q\Big[\log p(x_T) + \sum_{t>1}\log\frac{p_\theta(x_{t-1}|x_t)}{q(x_t|x_{t-1})} + \log\frac{p_\theta(x_0|x_1)}{q(x_1|x_0)}\Big] \\
&= -\mathbb{E}_q\Big[\log p(x_T) + \sum_{t>1}\log\frac{p_\theta(x_{t-1}|x_t)}{q(x_{t-1}|x_t)}\cdot\frac{q(x_{t-1}|x_0)}{q(x_t|x_0)} + \log\frac{p_\theta(x_0|x_1)}{q(x_1|x_0)}\Big] \\
&= -\mathbb{E}_q\Big[\log p(x_T) + \sum_{t>1}\log\frac{p_\theta(x_{t-1}|x_t)}{q(x_{t-1}|x_t)} + \log\frac{q(x_1|x_0)}{q(x_2|x_0)}\cdot\frac{q(x_2|x_0)}{q(x_3|x0)}\cdot\ldots\cdot\frac{q(x_{T-1}|x_0)}{q(x_T|x_0)} + \log\frac{p_\theta(x_0|x_1)}{q(x_1|x_0)}\Big] \\
&= -\mathbb{E}_q\Big[\log p(x_T) + \sum_{t>1}\log\frac{p_\theta(x_{t-1}|x_t)}{q(x_{t-1}|x_t)} + \log\frac{q(x_1|x_0)}{q(x_T|x_0)} + \log\frac{p_\theta(x_0|x_1)}{q(x_1|x_0)}\Big] \\
&= -\mathbb{E}_q\Big[\log\frac{p(x_T)}{q(x_T|x_0)} + \sum_{t>1}\log\frac{p_\theta(x_{t-1}|x_t)}{q(x_{t-1}|x_t)} + \log p_\theta(x_0|x_1)\Big] \\
&= \mathbb{E}_q\Big[D_{\mathrm{KL}}(q(x_T|x_0)||p(x_T)) + \sum_{t>1}D_{\mathrm{KL}}(q(x_{t-1}|x_t,x_0)||p_\theta(x_{t-1}|x_t)) - \log p_\theta(x_0|x_1)\Big] \\
&= L_T + L_{1:T} + L_0
\end{aligned}
$$

Step1. Split ELBO loss to different time step: $L = L_T + L_{1:T} + L_0$

Ignore L_T and L_0

$$= \mathbb{E}_q \Big[D_{\mathrm{KL}}(q(x_T|x_0)||p(x_T)) + \sum_{t>1} D_{\mathrm{KL}}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t)) - \log p_\theta(x_0|x_1) \Big]$$

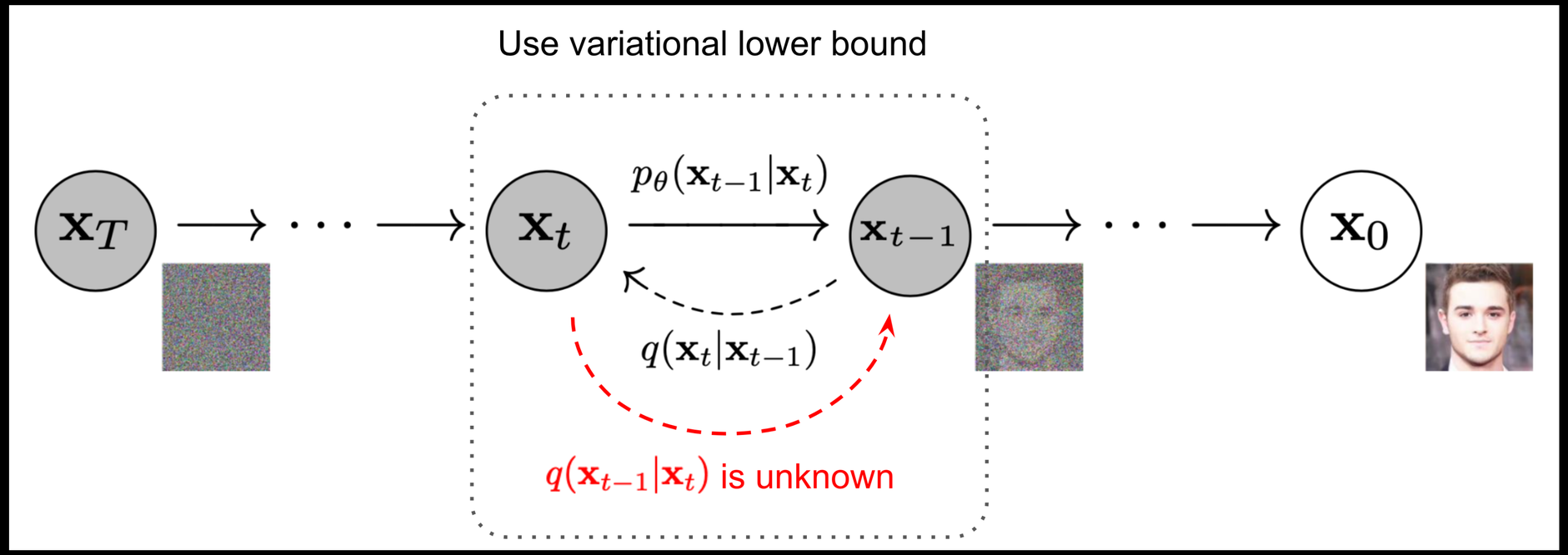
$$= \cancel{L_T} + L_{1:T} + \cancel{L_0}$$

$q(x_T|x_0)$ & $p(x_T)$ is fixed, and no parameters θ need to be trained, so L_T is a const and can be ignore.

$$L_{t-1} = D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t))$$

Step1. Split ELBO loss to different time step: $L = L_T + L_{1:T} + L_0$

To compute the L_{t-1}, we have to know $q(x_{t-1} \mid x_t)$ first

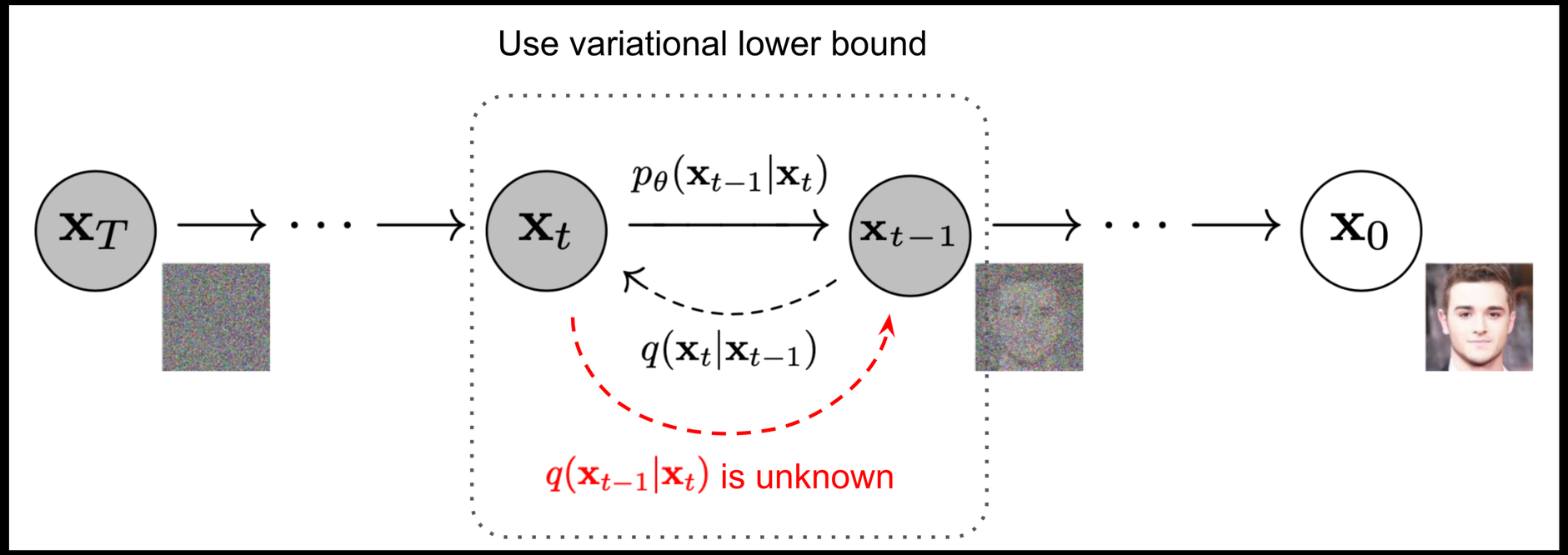


$$L_{t-1} = D_{KL}(q(x_{t-1} \mid x_t) \,||\, p_\theta(x_{t-1} \mid x_t))$$

unknown

Step1. Split ELBO loss to different time step: $L = L_T + L_{1:T} + L_0$

In forward process, we know that $q(x_{t-1} \mid x_t)$ can be tractable when conditioned on x_0



$$L_{t-1} = D_{KL}(q(x_{t-1} \mid x_t, x_0) \,||\, p_\theta(x_{t-1} \mid x_t))$$

tractable when conditioned on x_0

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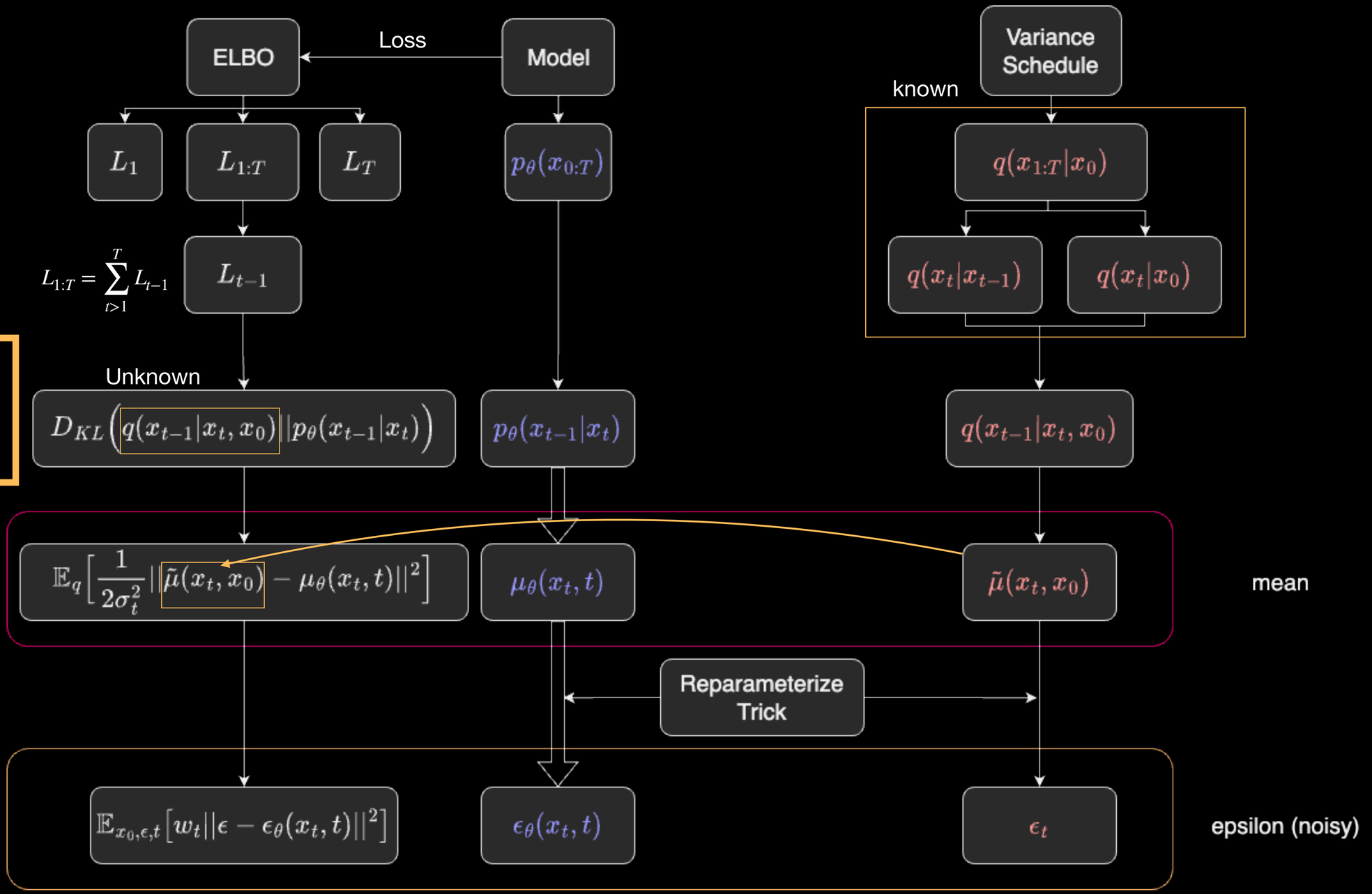


Step2. Use Bayes' Rule and Probability density function to derivate $q(x_{t-1} \mid x_t)$ when conditioned on x_0

Assume

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

Known

$$q(x_t|x_{t-1}) := N(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t I)$$

$$\alpha_t := 1 - \beta_t, \quad \bar{\alpha}_t = \prod_{s=1} \alpha_s$$

$$q(x_t|x_0) = N(x_t; \sqrt{\bar{\alpha}_t}x_0, (1-\bar{\alpha}_t)I)$$

PDF: $\frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^2}$

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

$$\propto \exp\Big(-\frac{1}{2}\big(\frac{(x_t - \sqrt{\alpha_t}x_{t-1})^2}{\beta_t} + \frac{(x_{t-1} - \sqrt{\bar{\alpha}_{t-1}}x_0)^2}{1-\bar{\alpha}_{t-1}} - \frac{(x_t - \sqrt{\bar{\alpha}_t}x_0)^2}{1-\bar{\alpha}_t}\big)\Big)$$

$$= \exp\Big(-\frac{1}{2}\big(\frac{\mathbf{x}_t^2 - 2\sqrt{\alpha_t}\mathbf{x}_t\mathbf{x}_{t-1} + \alpha_t\mathbf{x}_{t-1}^2}{\beta_t} + \frac{\mathbf{x}_{t-1}^2 - 2\sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0\mathbf{x}_{t-1} + \bar{\alpha}_{t-1}\mathbf{x}_0^2}{1-\bar{\alpha}_{t-1}} - \frac{(\mathbf{x}_t - \sqrt{\bar{\alpha}_t}\mathbf{x}_0)^2}{1-\bar{\alpha}_t}\big)\Big)$$

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

Step2. Use Bayes' Rule and Probability density function to derivate $q(x_{t-1} \mid x_t)$ when conditioned on x_0

Assume

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

Known

$$q(x_t|x_{t-1}) := N(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t I)$$

$$\alpha_t := 1 - \beta_t, \quad \bar{\alpha}_t = \prod_{s=1} \alpha_s$$

$$q(x_t|x_0) = N(x_t; \sqrt{\bar{\alpha}_t}x_0, (1-\bar{\alpha}_t)I)$$

PDF: $\frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^2}$

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

$$\propto \exp\Big(-\frac{1}{2}\big(\frac{(x_t - \sqrt{\alpha_t}x_{t-1})^2}{\beta_t} + \frac{(x_{t-1} - \sqrt{\bar{\alpha}_{t-1}}x_0)^2}{1-\bar{\alpha}_{t-1}} - \frac{(x_t - \sqrt{\bar{\alpha}_t}x_0)^2}{1-\bar{\alpha}_t}\big)\Big)$$

$$= \exp\Big(-\frac{1}{2}\big(\frac{\mathbf{x}_t^2 - 2\sqrt{\alpha_t}\mathbf{x}_t\mathbf{x}_{t-1} + \alpha_t\mathbf{x}_{t-1}^2}{\beta_t} + \frac{\mathbf{x}_{t-1}^2 - 2\sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0\mathbf{x}_{t-1} + \bar{\alpha}_{t-1}\mathbf{x}_0^2}{1-\bar{\alpha}_{t-1}} - \frac{(\mathbf{x}_t - \sqrt{\bar{\alpha}_t}\mathbf{x}_0)^2}{1-\bar{\alpha}_t}\big)\Big)$$

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

Left term of PDF

$$\frac{1}{\sigma_{q(x_t|x_{t-1},x_0)}\sqrt{2\pi}} \frac{1}{\sigma_{q(x_{t-1}|x_0)}\sqrt{2\pi}} \frac{1}{\sigma_{q(x_t|x_0)}\sqrt{2\pi}}$$

$$= \frac{1}{\beta_t\sqrt{2\pi}} \frac{1}{(1-\bar{\alpha}_{t-1})\sqrt{2\pi}} \frac{1}{(1-\bar{\alpha}_t)\sqrt{2\pi}}$$

Step2. Use Bayes' Rule and Probability density function to derivate $q(x_{t-1} \mid x_t)$ when conditioned on x_0

Assume

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

Known

PDF $\frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^2}$

$$\exp\Big(-\frac{1}{2}\big(\big(\frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}}\big)\mathbf{x}_{t-1}^2 - \big(\frac{2\sqrt{\alpha_t}}{\beta_t}\mathbf{x}_t + \frac{2\sqrt{\bar{\alpha}_{t-1}}}{1-\bar{\alpha}_{t-1}}\mathbf{x}_0\big)\mathbf{x}_{t-1} + C(\mathbf{x}_t, \mathbf{x}_0)\big)\Big)$$

$$\tilde{\beta}_t = 1/\big(\frac{\alpha_t}{\beta_t} + \frac{1}{1-\bar{\alpha}_{t-1}}\big) = 1/\big(\frac{\alpha_t - \bar{\alpha}_t + \beta_t}{\beta_t(1-\bar{\alpha}_{t-1})}\big) = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t} \cdot \beta_t$$

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

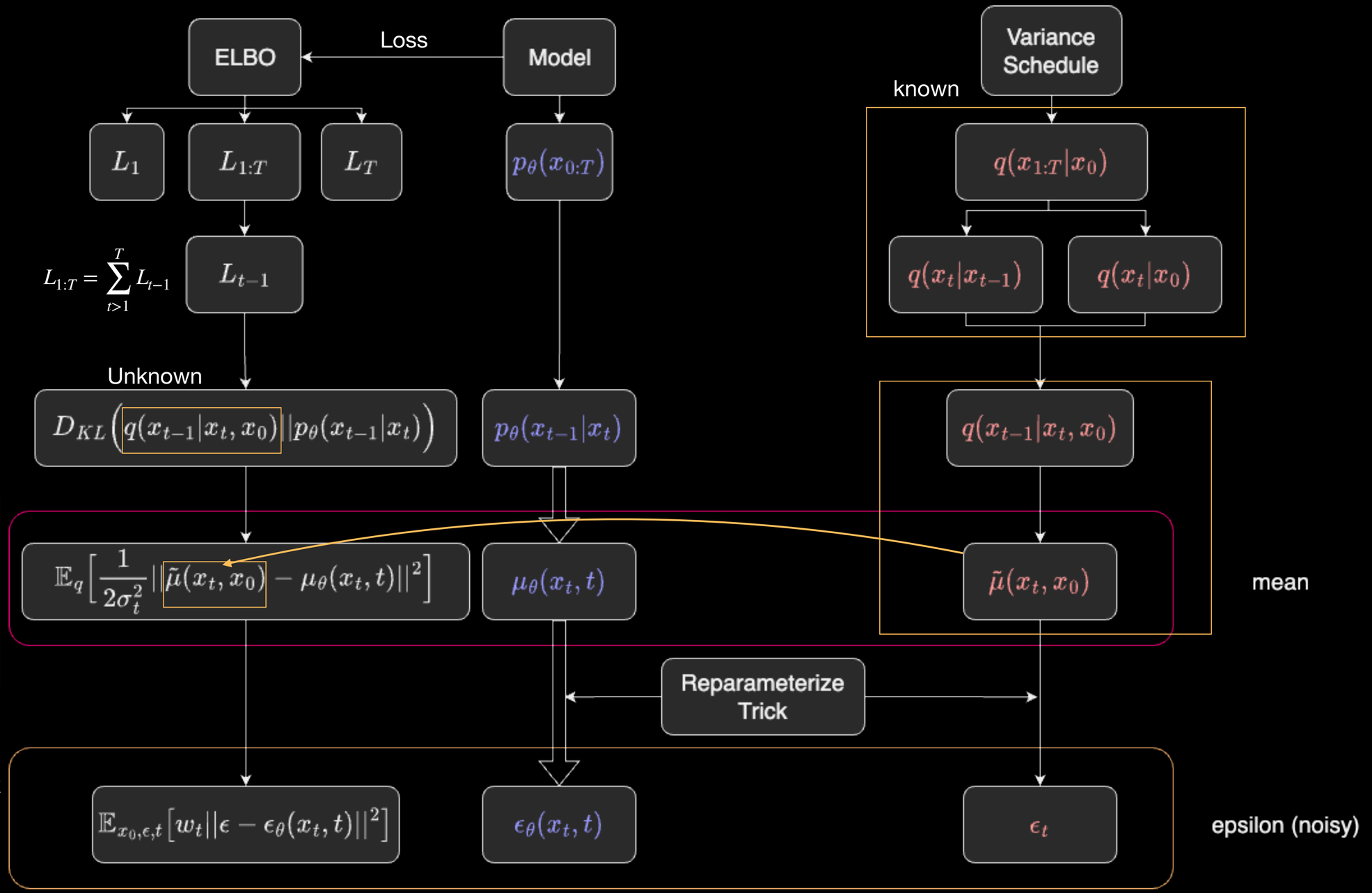
Derivation
flow chart

1.Split ELBO loss to different time step, and Ignore L_0 and L_T, we can focus on the loss between each step.

2. Use Bayes' Rule and Probability Density Function to derivate $q(x_{t-1}|x_t)$ when conditioned on x_0.

3. We can represent the distribution in μ and σ format when compute the KLD between two normal distribution

4. Use Reparameterize Trick Convert $\tilde{\mu}_t$ to ϵ_t form



Step3. KLD between two normal distribution

Use formula of KLD between two normal distribution to derivate KLD into μ form

Formula of KLD between to Normal Distribution

$$\log\frac{\sigma_2}{\sigma_1}+\frac{\sigma_1^2+(\mu_1-\mu_2)^2}{2\sigma_2^2}-\frac{1}{2}$$

when $\sigma_1=\sigma_2$

$$\log\frac{\sigma_1}{\sigma_1}+\frac{\sigma_1^2+(\mu_1-\mu_2)^2}{2\sigma_1^2}-\frac{1}{2}=\boxed{\frac{1}{2\sigma_1^2}(\mu_1-\mu_2)^2}$$

$$L_{t-1}=D_{KL}(q(x_{t-1}\,|\,x_t,x_0)\,||\,p_\theta(x_{t-1}\,|\,x_t))$$

$$=\mathbb{E}_q\left[\frac{1}{2\sigma_t^2}\,||\,\tilde{\mu}(x_t,x_0)-\mu_\theta(x_t,t)\,||^2\right]$$

Fixed Σ as σ_t, $\sigma_t^2=\beta_t$ or $\frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t$:

Derivation
flow chart

1.Split ELBO loss to different time step, and Ignore L_0 and L_T, we can focus on the loss between each step.

2. Use Bayes' Rule and Probability Density Function to derivate $q(x_{t-1}|x_t)$ when conditioned on x_0.

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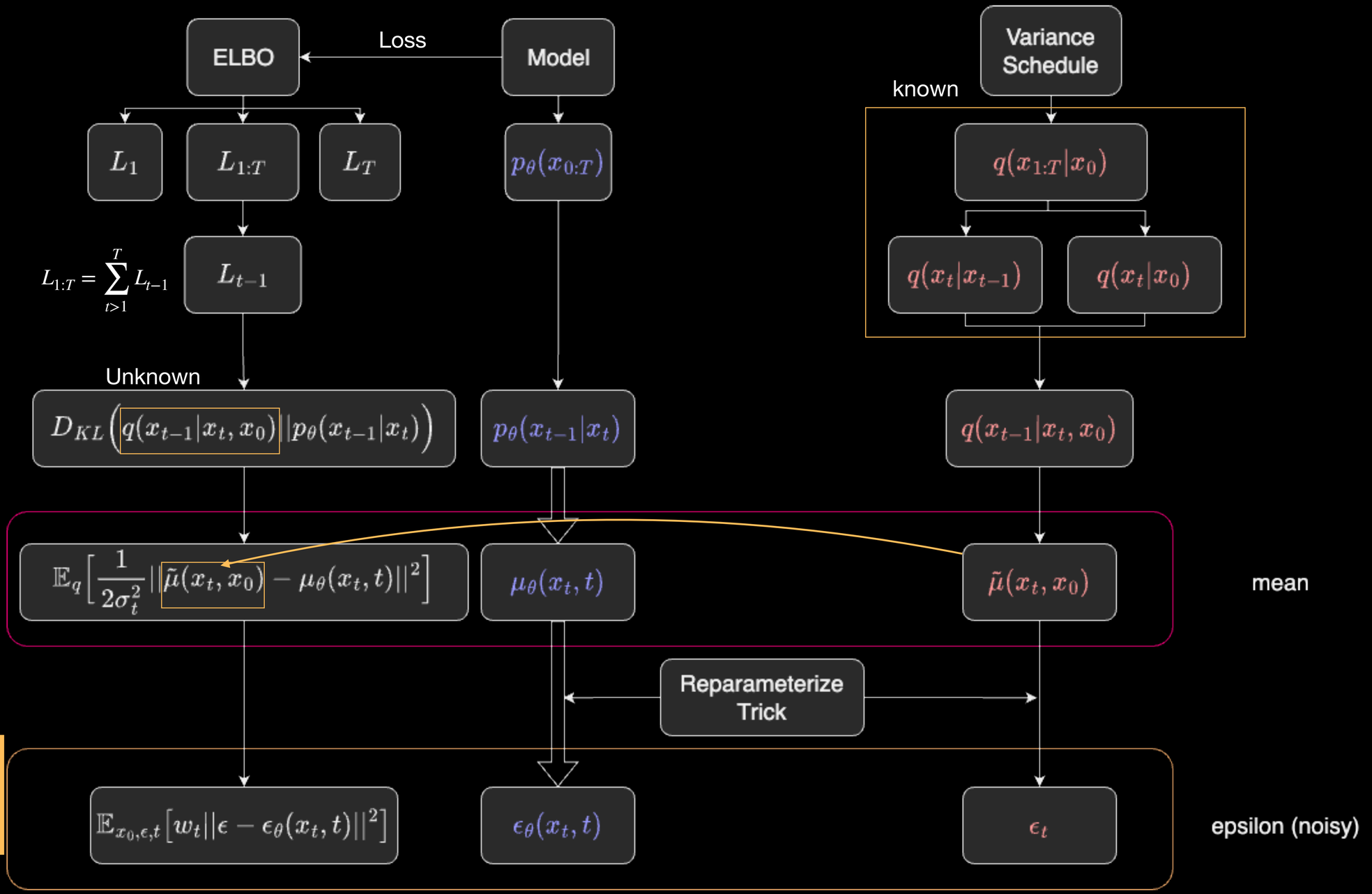

Use Reparameterize Trick Convert $\tilde{\mu}_t$ to ϵ_t form

Reparameterize Trick

$$z \sim q_\phi(z|x) = N(z; \mu, \sigma^2 I)$$
$$z = \mu + \sigma \odot \epsilon$$
$$\epsilon \sim N(0, I)$$

Forward process's property

$$q(x_{1:T}|x_0) := \prod_{t=1}^{T} q(x_t|x_{t-1}),$$
$$q(x_t|x_{t-1}) := N(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t I)$$

Use this trick,
we can simply use ϵ to represent μ and ϵ

$$\begin{aligned}
x_t &= \sqrt{1-\beta_t}x_{t-1} + \sqrt{\beta_t}\epsilon_{t-1} \\
&= \sqrt{\alpha_t}x_{t-1} + \sqrt{1-\alpha_t}\epsilon_{t-1} \\
&= \sqrt{\alpha_t\alpha_{t-1}}x_{t-2} + \sqrt{1-\alpha_t\alpha_{t-1}}\bar{\epsilon}_{t-2} \\
&= \dots \\
&= \sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon \\
x_0 &= \frac{1}{\sqrt{\bar{\alpha}_t}}(x_t - \sqrt{1-\bar{\alpha}_t}\epsilon)
\end{aligned}$$

Use Reparameterize Trick Convert $\tilde{\mu}_t(x_t, x_0)$ to ϵ_t form

Now we have:

$$x_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}(x_t - \sqrt{1-\bar{\alpha}_t}\epsilon)$$

Put x_0 into $\tilde{\mu}_t(x_t, x_0)$ to represent $\tilde{\mu}_t(x_t, x_0)$ in ϵ from

$$\begin{aligned}
\tilde{\mu}_t(x_t, x_0) &= \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}x_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}x_0 \\
&= \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{x}_t + \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\frac{1}{\sqrt{\bar{\alpha}_t}}(\mathbf{x}_t - \sqrt{1-\bar{\alpha}_t}\epsilon_t) \\
&= \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon\right)
\end{aligned}$$

Use Reparameterize Trick Convert $\tilde{\mu}_t(x_t, x_0)$ to ϵ_t form

$$\tilde{\boldsymbol{\mu}}_t(x_t, x_0) = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_t\right)$$

Then set our training objective from $\mu_\theta(x_t, x_0)$ to $\epsilon_\theta(x_t, t)$

$$\mu_\theta(x_t, t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(x_t, t)\right)$$

Use Reparameterize Trick Convert $\tilde{\mu}_t(x_t, x_0)$ to ϵ_t form

Rewrite L_{t-1} with ϵ

$$
\begin{aligned}
L_{t-1} &= \mathbb{E}_q\left[\frac{1}{2\sigma_t^2}||\tilde{\mu}(x_t, x_0) - \mu_\theta(x_t, t)||^2\right] \\
&= \mathbb{E}_{\mathbf{x}_0,\epsilon}\left[\frac{1}{2\sigma_t^2}\|\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}\right) - \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right)\|^2\right] \\
&= \mathbb{E}_{\mathbf{x}_0,\epsilon}\left[\frac{(1-\alpha_t)^2}{2\sigma_t^2\alpha_t(1-\bar{\alpha}_t)}\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\|^2\right] \\
&= \mathbb{E}_{\mathbf{x}_0,\epsilon}\left[\frac{(1-\alpha_t)^2}{2\sigma_t^2}\alpha_t(1-\bar{\alpha}_t)\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t)\|^2\right]
\end{aligned}
$$

Simplified step-specific weighting from ELBO

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

- DDPM find that a simpler version of the variational bound that discards the term weights that appear in the original bound led to better sample quality.

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

#

Use Reparameterize Trick Convert $\tilde{\mu}_t(x_t, x_0)$ to ϵ_t form

Rewrite L_{t-1} with ϵ

$$
\begin{aligned}
L_{t-1} &= \mathbb{E}_q\left[\frac{1}{2\sigma_t^2}||\tilde{\mu}(x_t, x_0) - \mu_\theta(x_t, t)||^2\right] \\
&= \mathbb{E}_{\mathbf{x}_0,\epsilon}\left[\frac{1}{2\sigma_t^2}\left\|\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon\right) - \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(\mathbf{x}_t, t)\right)\right\|^2\right] \\
&= \mathbb{E}_{\mathbf{x}_0,\epsilon}\left[\frac{(1-\alpha_t)^2}{2\sigma_t^2\alpha_t(1-\bar{\alpha}_t)}\|\epsilon - \epsilon_\theta(\mathbf{x}_t, t)\|^2\right] \\
&= \mathbb{E}_{\mathbf{x}_0,\epsilon}\left[\frac{(1-\alpha_t)^2}{2\sigma_t^2}\alpha_t(1-\bar{\alpha}_t)\|\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t)\|^2\right]
\end{aligned}
$$

Simplified step-specific weighting from ELBO

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

Objective	IS	FID
L, fixed isotropic $\mathbf{\Sigma}$	7.67 ± 0.13	13.51
$\|\tilde{\epsilon} - \epsilon_\theta\|^2$ (L_{simple})	$\mathbf{9.46 \pm 0.11}$	**3.17**

- DDPM find that a simpler version of the variational bound that discards the term weights that appear in the original bound led to better sample quality.

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

#