

Diffusion Model Review

CAO Hanqun

Outlines

- Brief Introduction to diffusion model
- Viewing diffusion model through generative model development
- Diffusion model basic algorithm
- Enhancing Understanding from multi-view
- Algorithm improvement
- Applications
- Further Directions and Discussions

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Diffusion Model is Striking Right Now!

Stable
Diffusion



Midjourney



Explosive Growth of Diffusion Model

Denoising diffusion probabilistic models

[J Ho](#), [A Jain](#), [P Abbeel](#) - Advances in neural information ..., 2020 - proceedings.neurips.cc

... This paper presents progress in **diffusion probabilistic models** [53]. A **diffusion probabilistic model** (which we will call a “**diffusion model**” for brevity) is a parameterized Markov chain ...

☆ 保存 引用 被引用次数: 3640 相关文章 所有 6 个版本 导入BibTeX 》》

Score-based generative modeling through stochastic differential equations

[Y Song](#), [J Sohl-Dickstein](#), [DP Kingma](#), [A Kumar](#)... - arXiv preprint arXiv ..., 2020 - arxiv.org

... Figure 1: Solving a reversion-time **SDE** yields a **score**-based generative model. Transforming ... a continuous-time **SDE**. This **SDE** can be reversed if we know the **score** of the distribution at ...

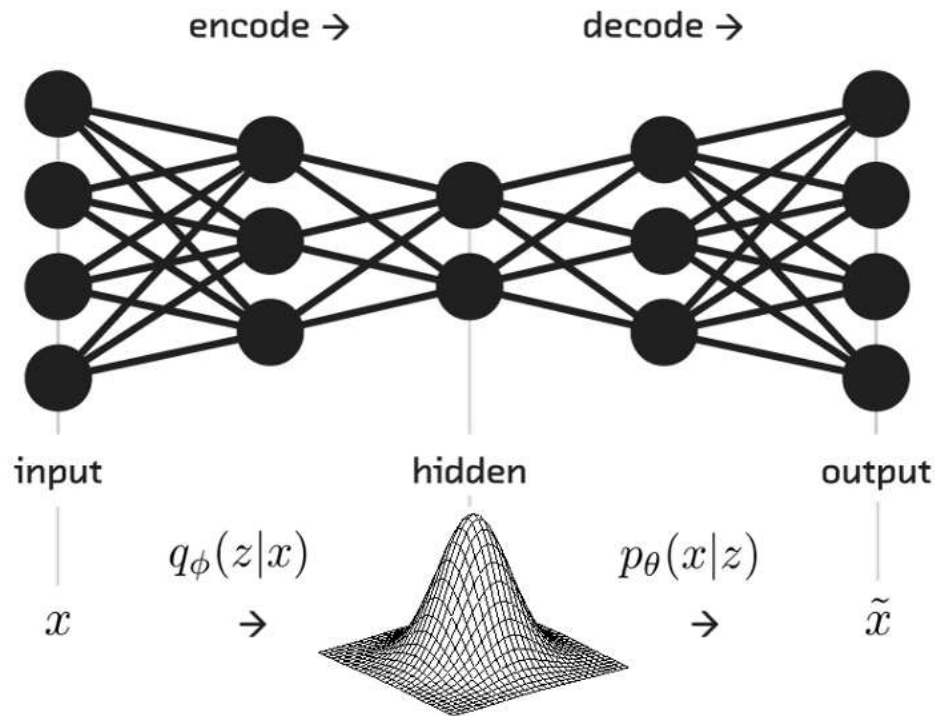
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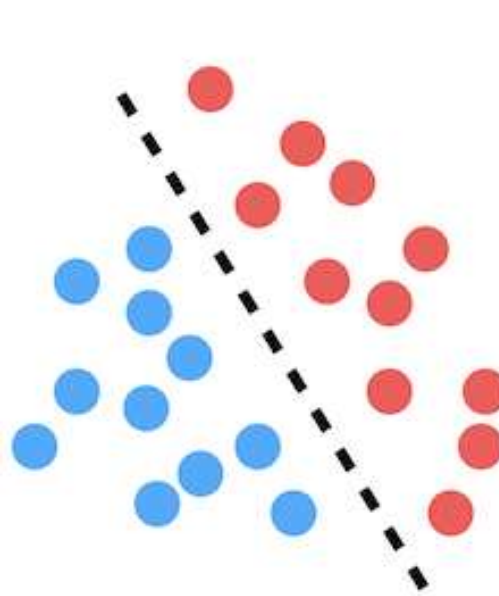
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From Generative Model to Diffusion Model

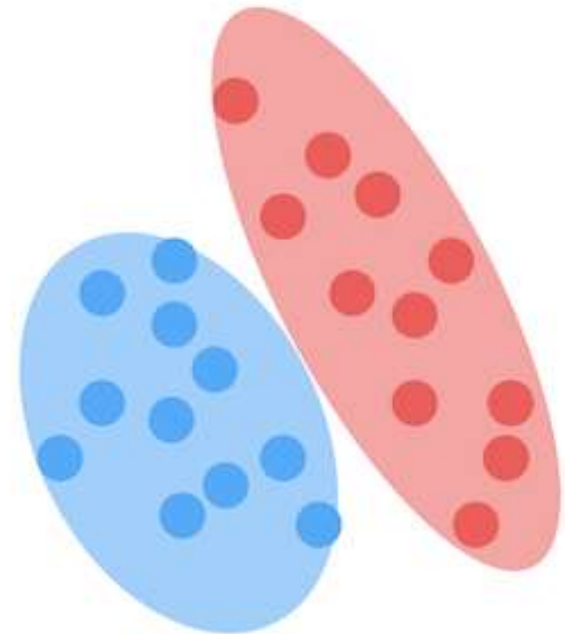
- Given data x , generating samples following distribution $p(x)$



Discriminative

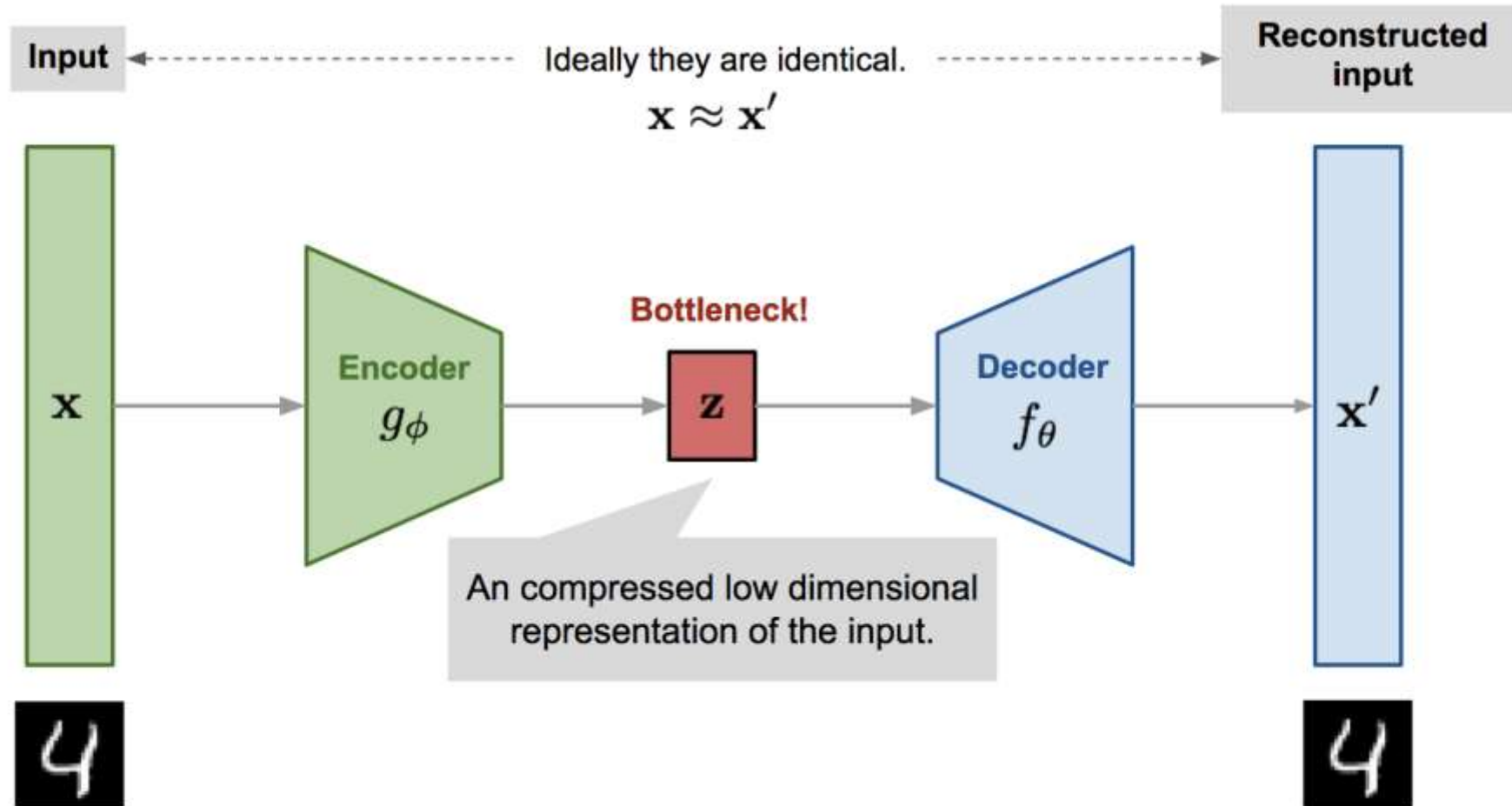


Generative



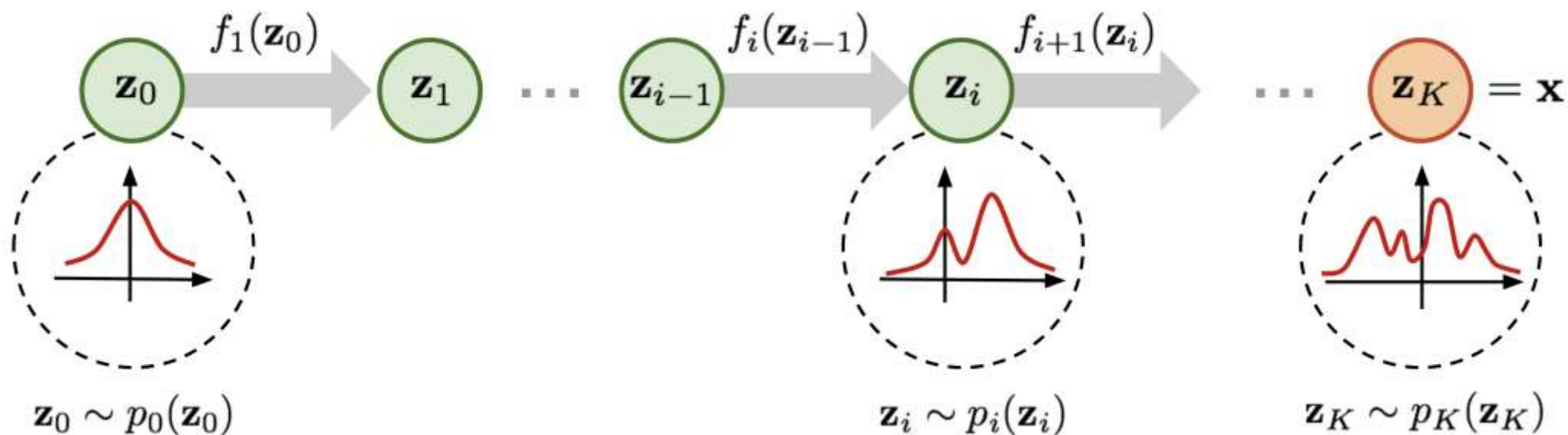
From VAE to NF, to Diffusion Model

How to accurately and efficiently express the distribution remains to be a challenge



VAE suffers from an information loss when conducting encoding

From VAE to NF, to Diffusion Model

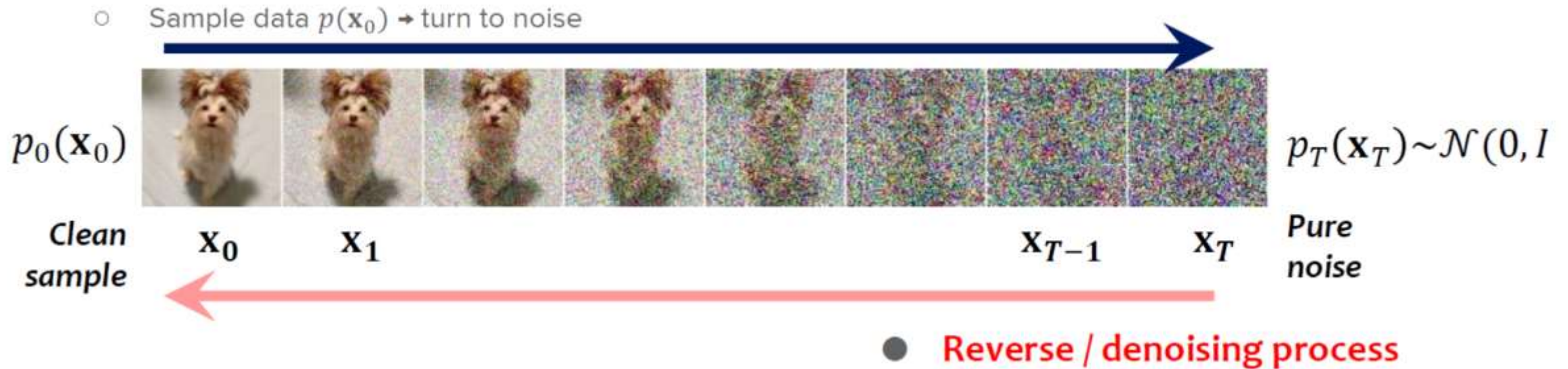


Normalizing Flow (NF) suffers from complicated modeling and training

From VAE to NF, to Diffusion Model

No information loss -> equal-dimension transformation

Efficient Modeling -> Markovian process

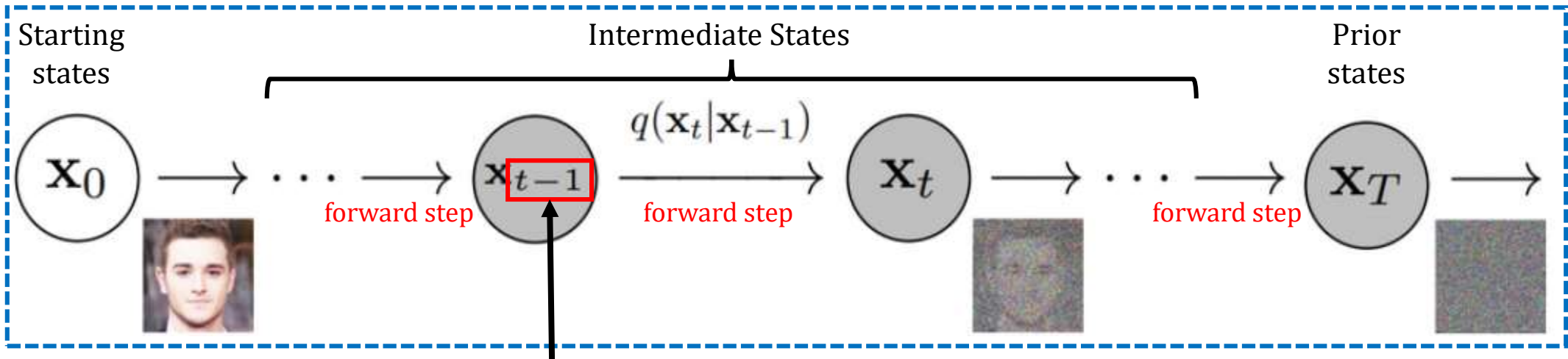


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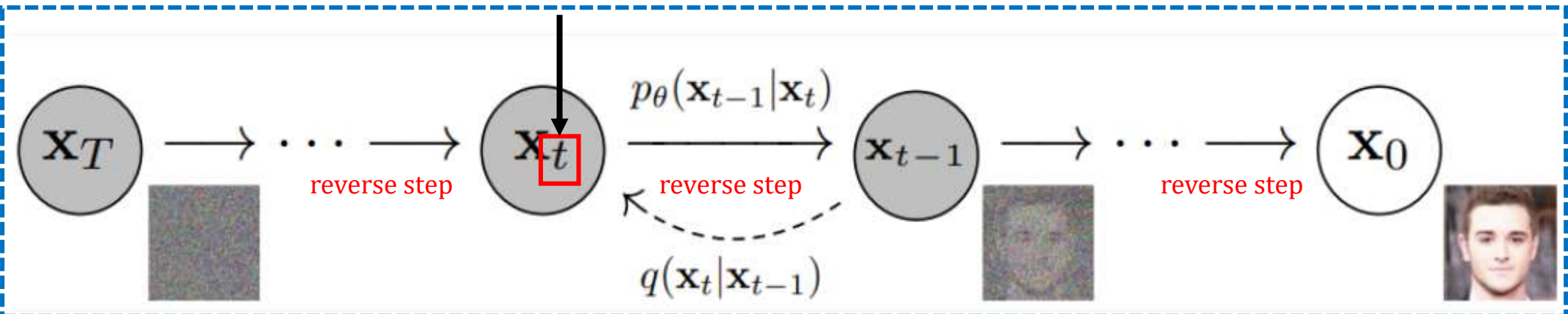
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Basic Definitions

Forward Process



Backward Process



Landmark Works: DDPM

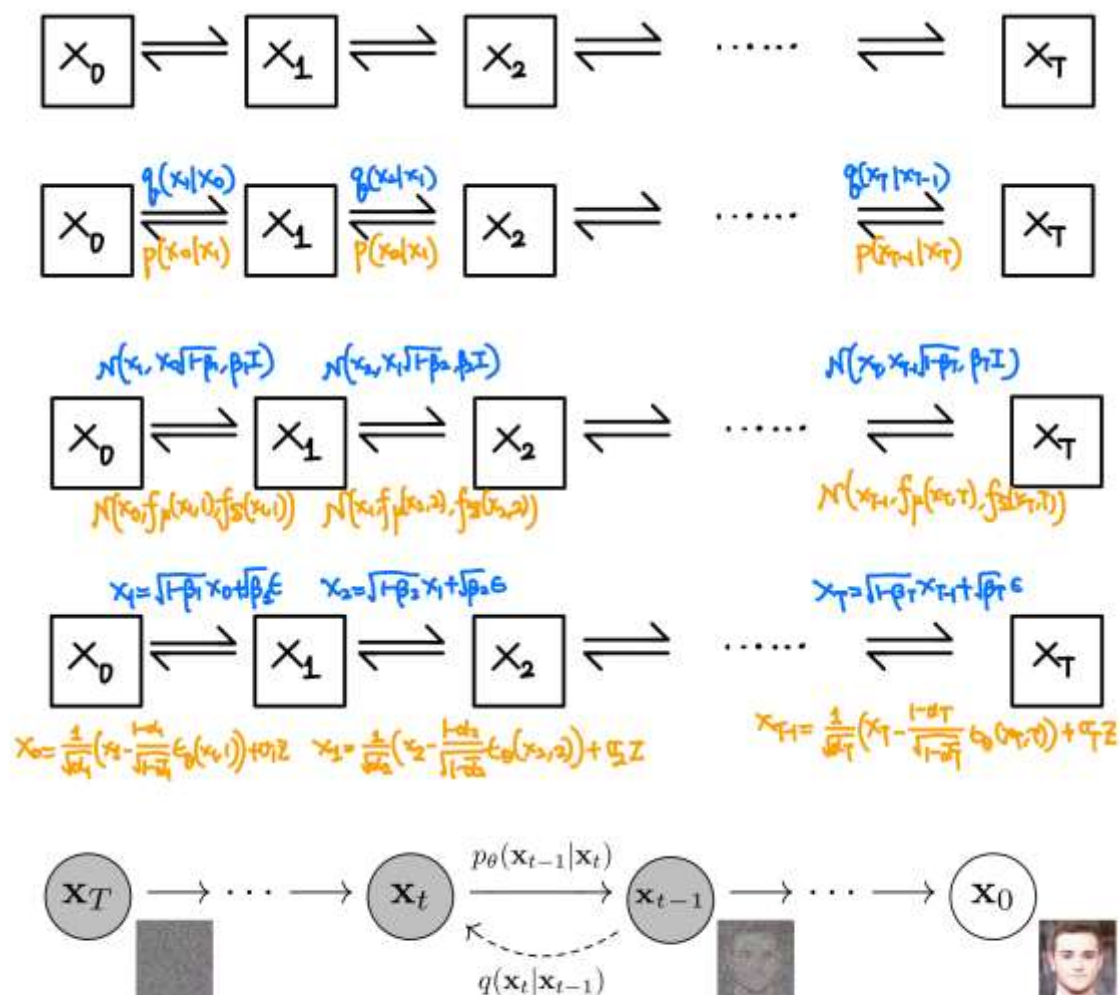


Figure 2: The directed graphical model considered in this work.

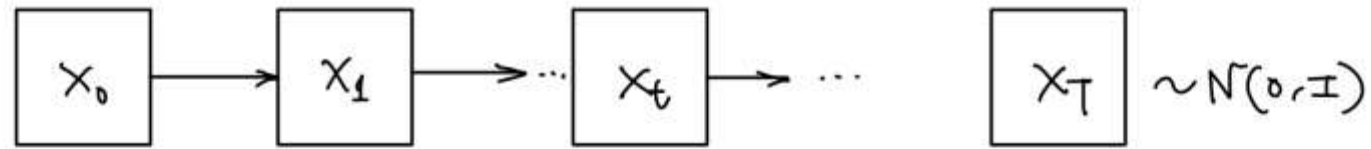
Algorithm 1 Training

- 1: **repeat**
- 2: $x_0 \sim q(x_0)$
- 3: $t \sim \text{Uniform}(\{1, \dots, T\})$
- 4: $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
- 5: Take gradient descent step on $\nabla_\theta \|\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t)\|^2$
- 6: **until** converged

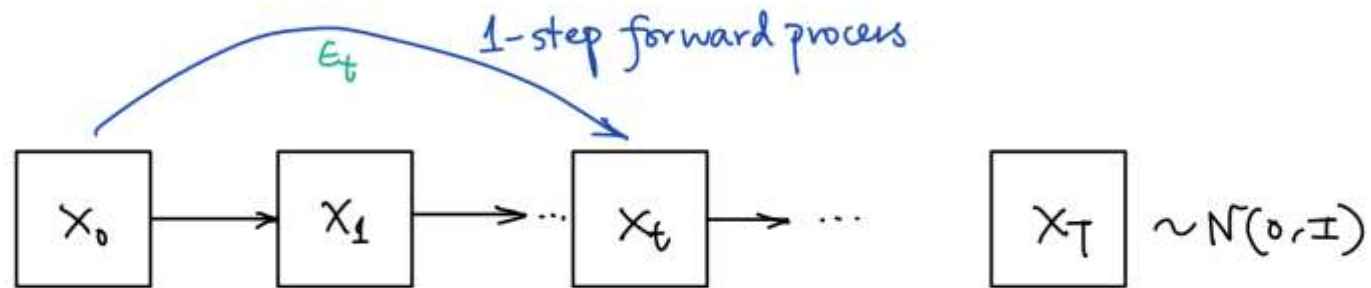
Algorithm 2 Sampling

- 1: $x_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
- 2: **for** $t = T, \dots, 1$ **do**
- 3: $z \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $z = \mathbf{0}$
- 4: $x_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(x_t - \frac{1-\alpha_t}{\sqrt{1-\alpha_t}} \epsilon_\theta(x_t, t) \right) + \sigma_t z$
- 5: **end for**
- 6: **return** x_0

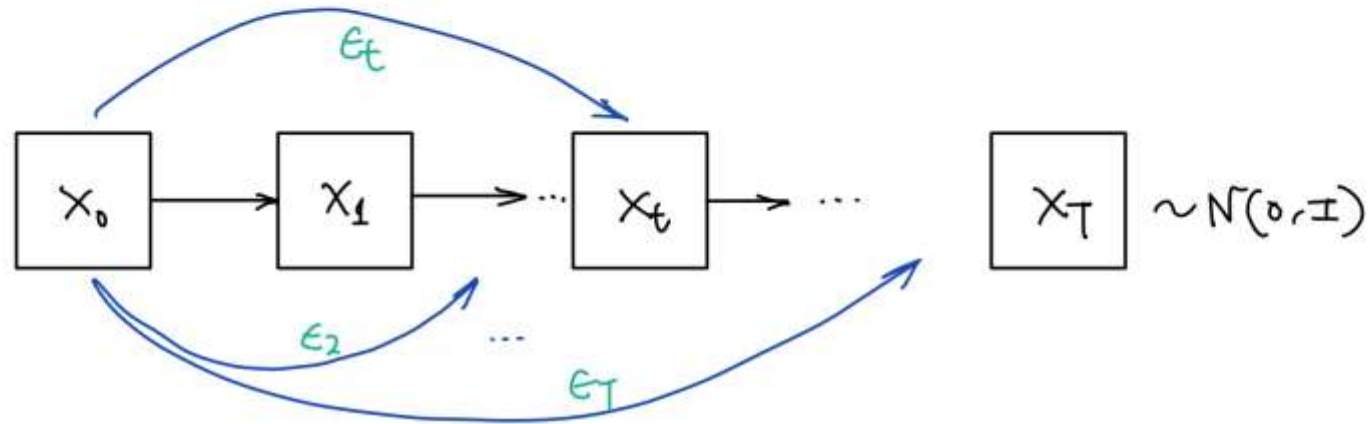
Landmark Works: DDPM



Initialization

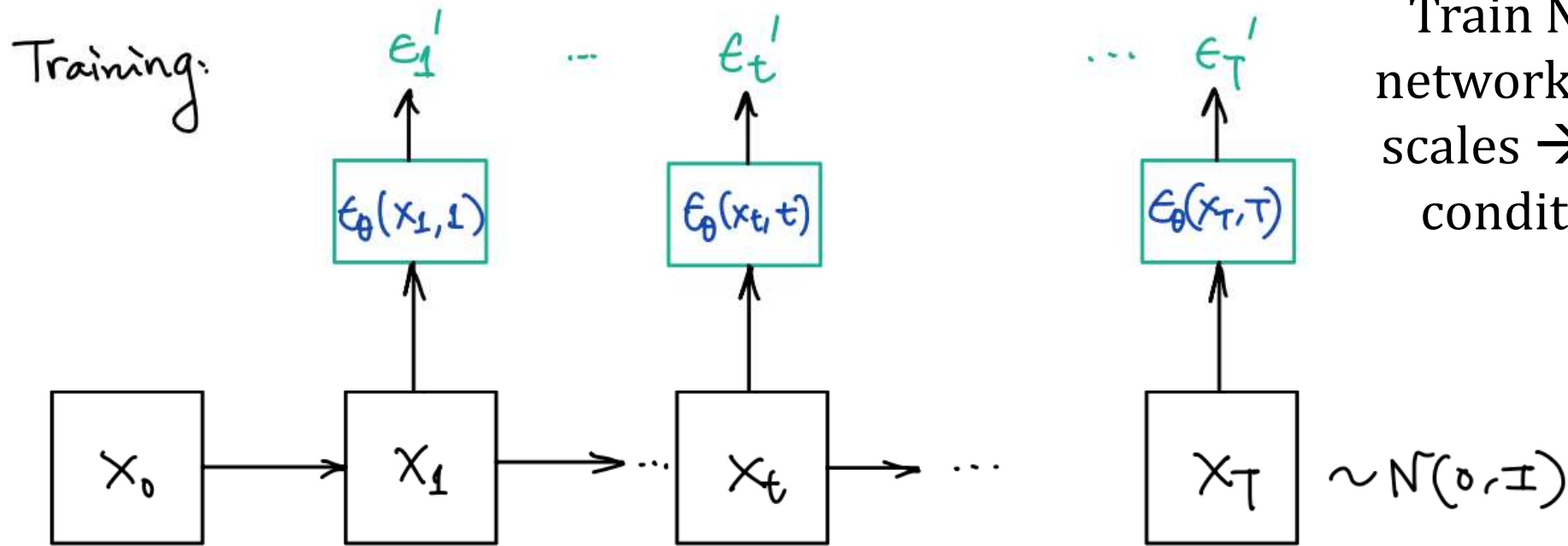


Forward step with
random noise



Forward steps with
diverse random noise

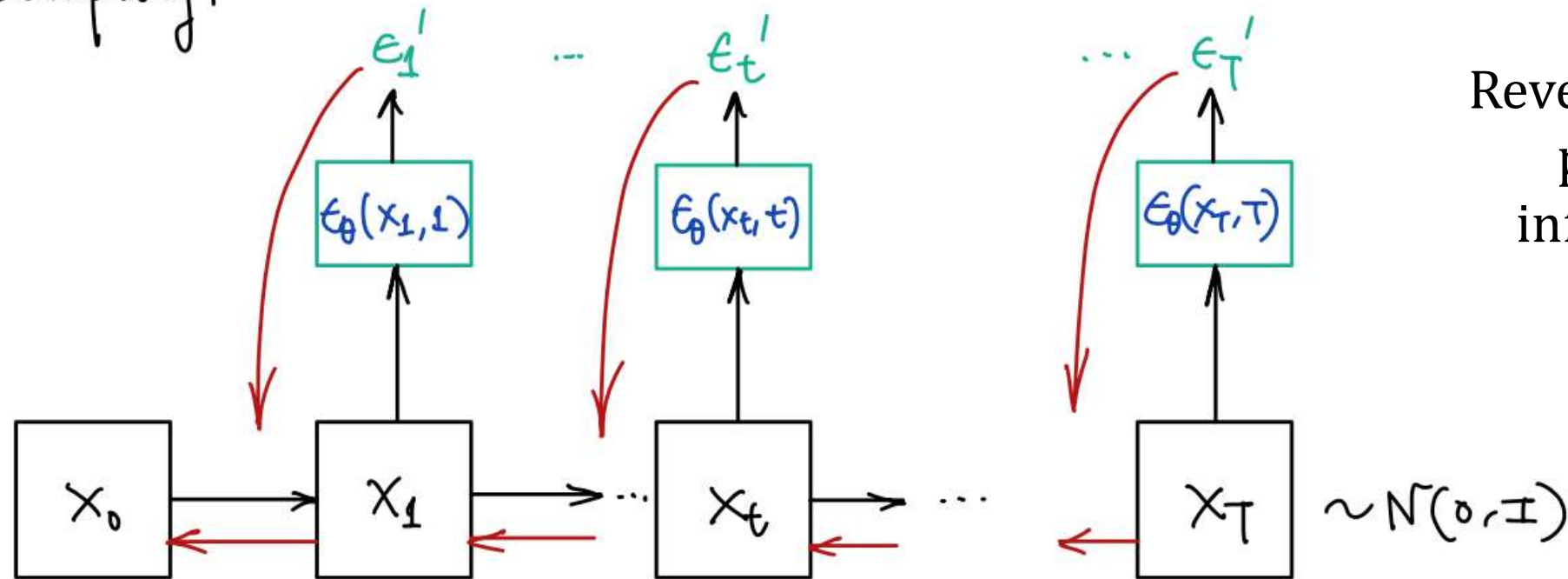
Landmark Works: DDPM



Train NOISE PREDICTION network to fit different noise scales \rightarrow time is treated as a condition to the network

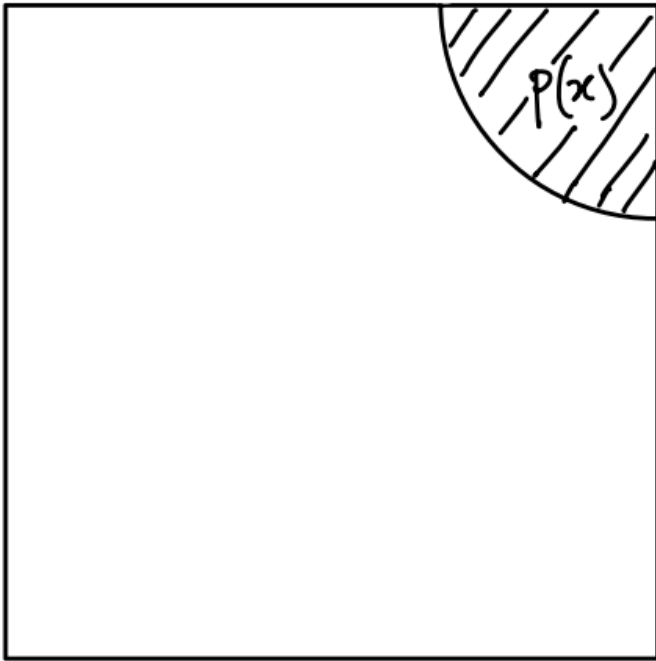
Landmark Works: DDPM

Sampling:

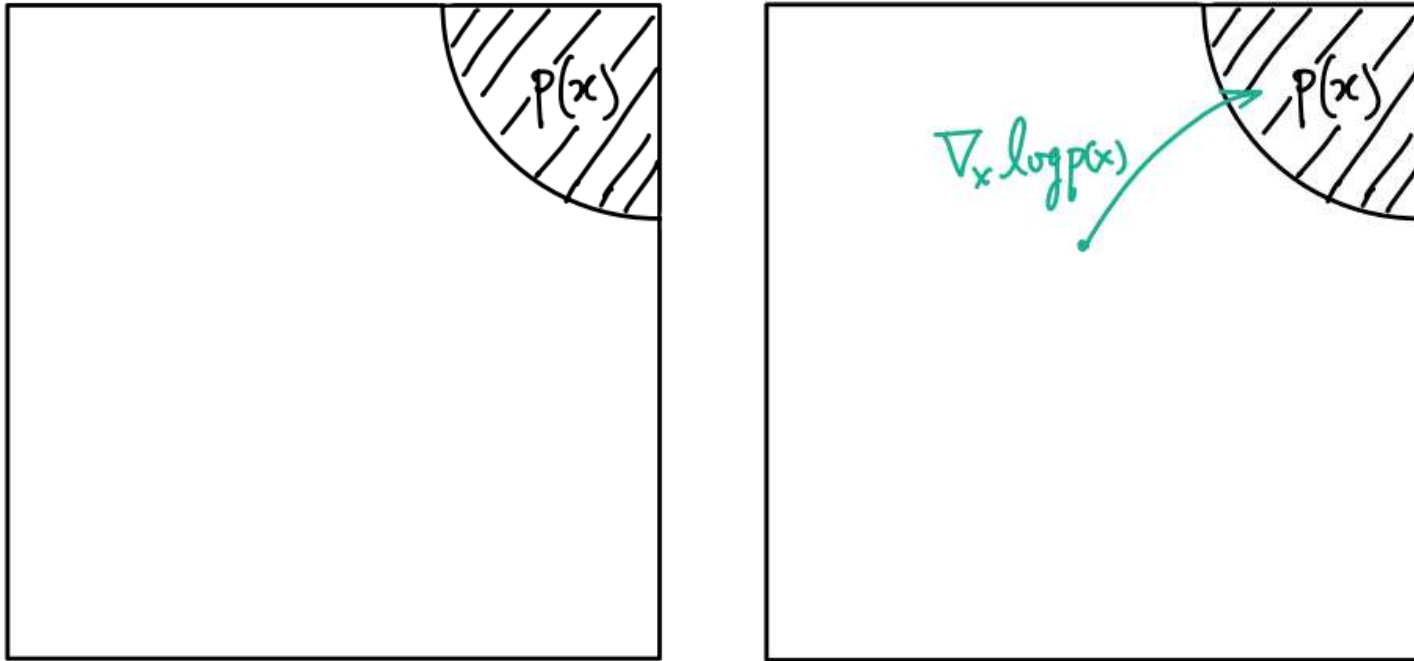


Reverse the forward
process with
inference noises

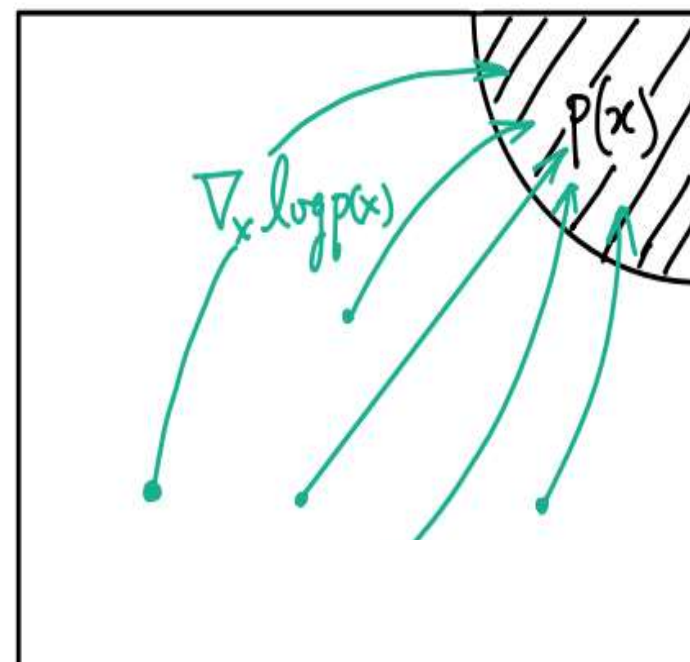
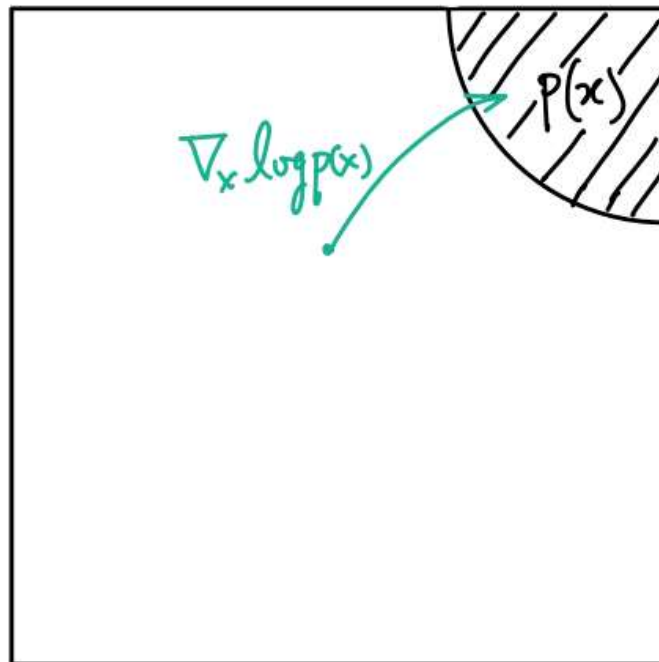
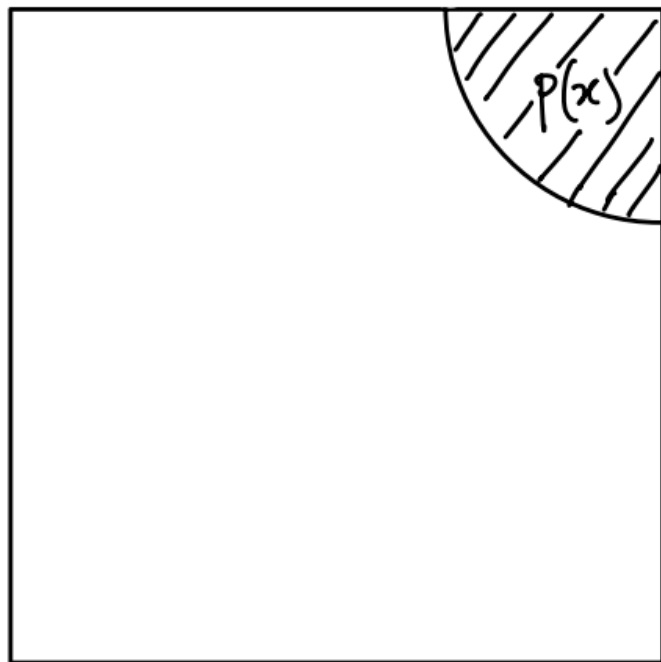
Landmark Works: Score Network



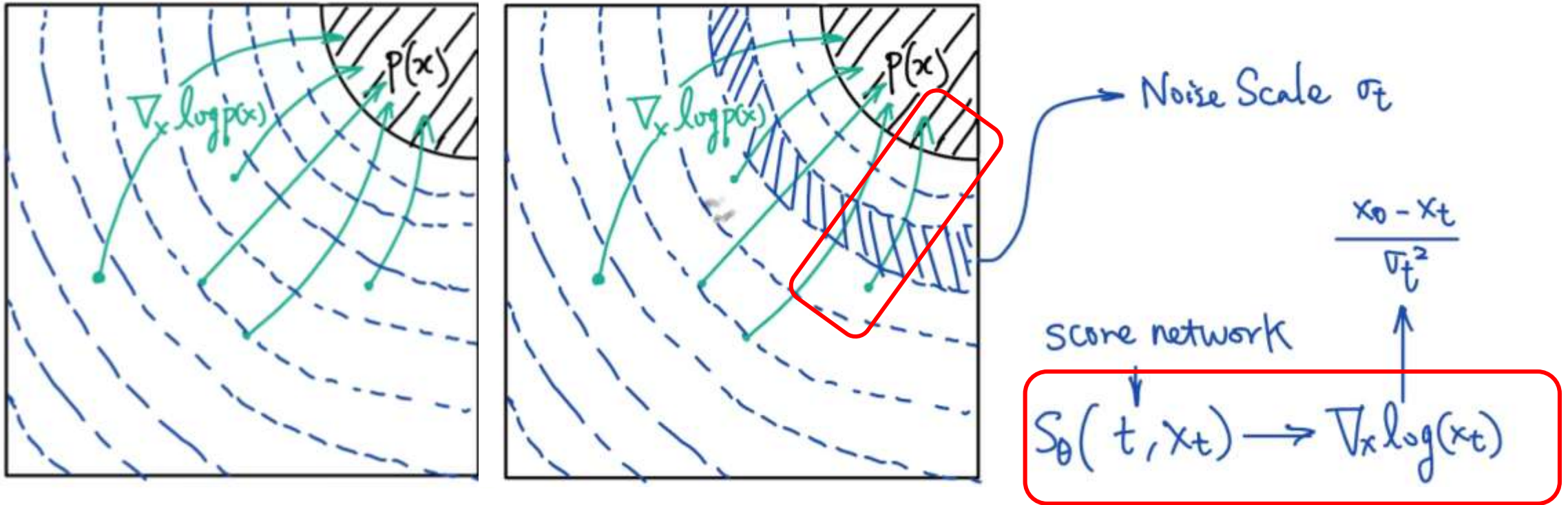
Landmark Works: Score Network



Landmark Works: Score Network



Landmark Works: Score Network



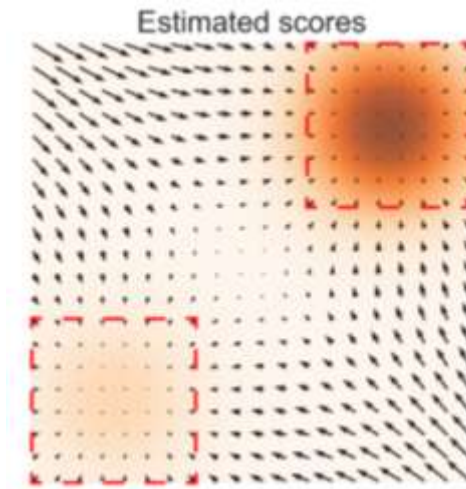
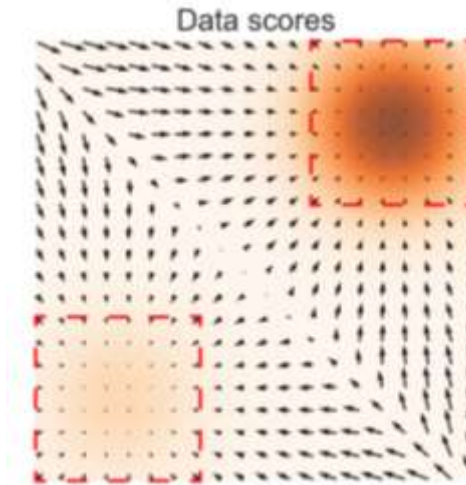
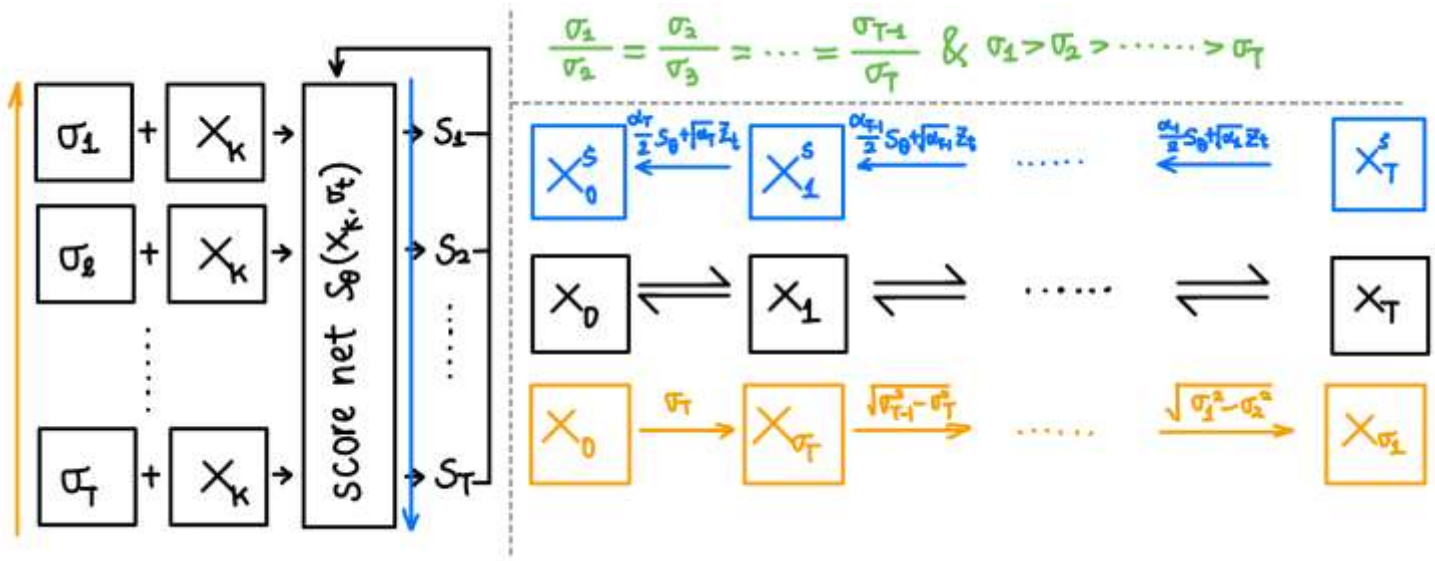
Landmark Works: Score Network

Obtaining distributions by estimating its gradients

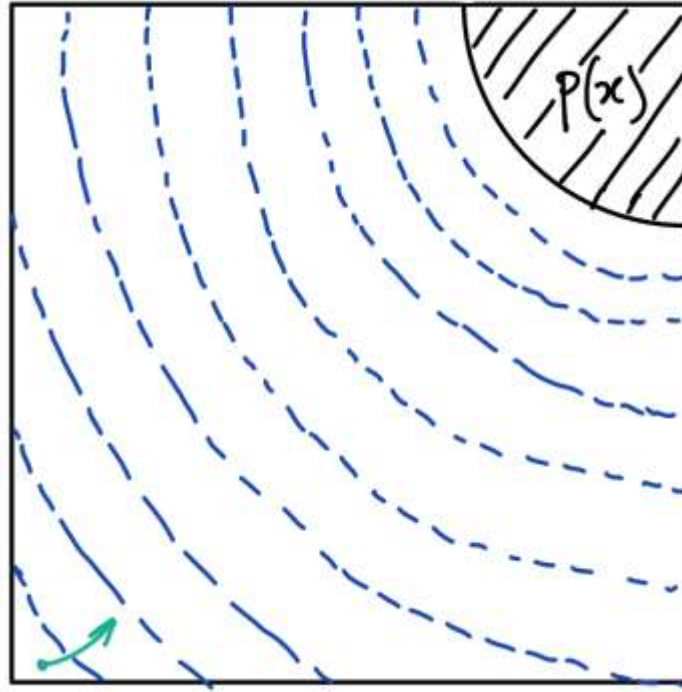
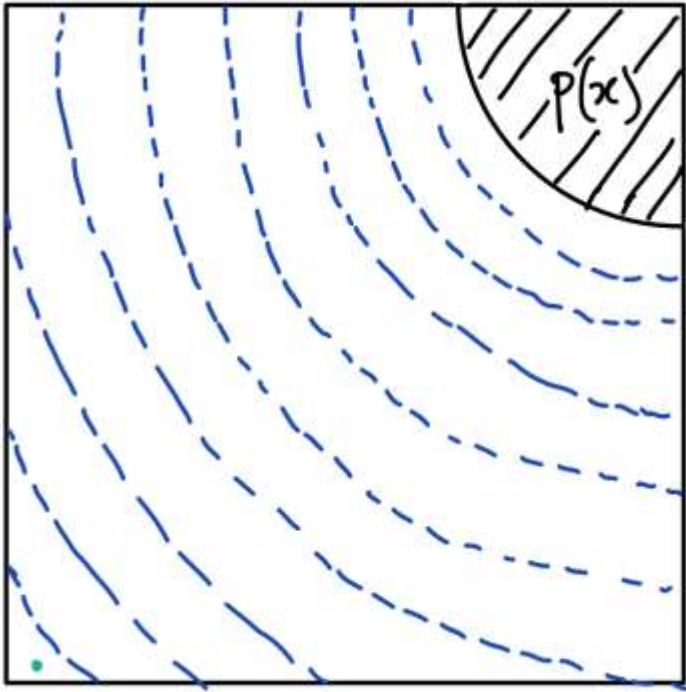
Score

$$s_{\theta}(\mathbf{x}) = \nabla_{\mathbf{x}} \log p_{\theta}(\mathbf{x}) = -\nabla_{\mathbf{x}} f_{\theta}(\mathbf{x}) - \underbrace{\nabla_{\mathbf{x}} \log Z_{\theta}}_{=0} = -\nabla_{\mathbf{x}} f_{\theta}(\mathbf{x}).$$

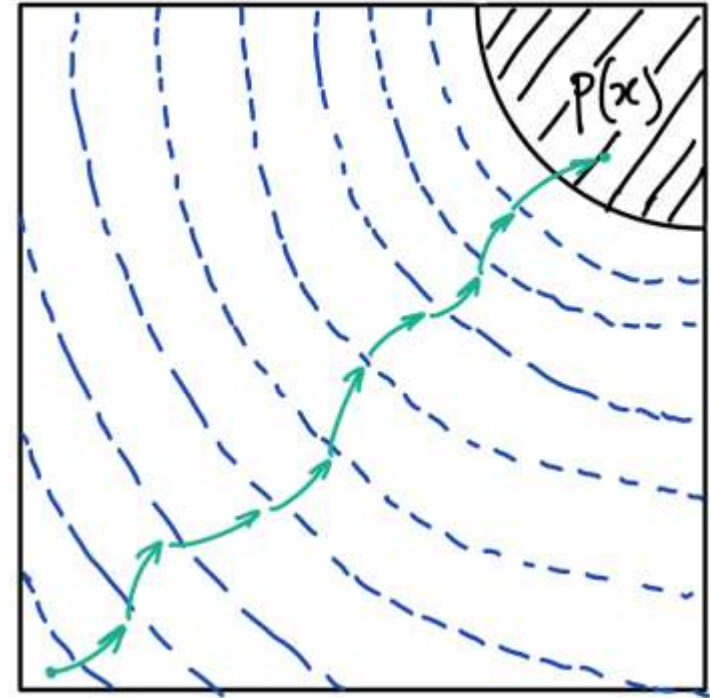
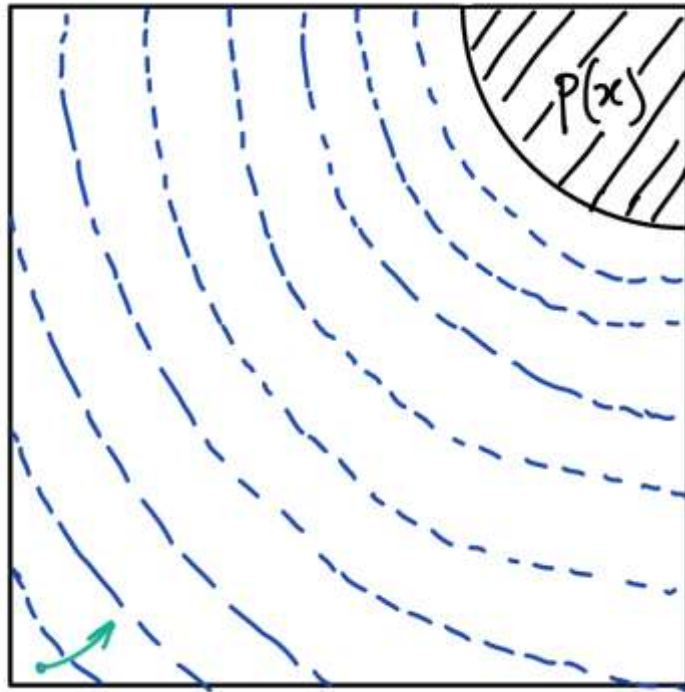
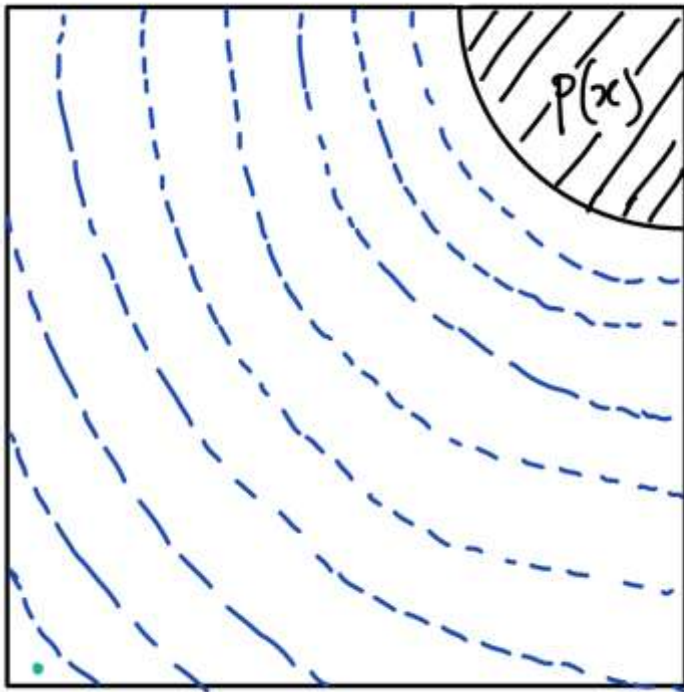
$$\mathbf{x}_{i+1} \leftarrow \mathbf{x}_i + \epsilon \nabla_{\mathbf{x}} \log p(\mathbf{x}) + \sqrt{2\epsilon} \mathbf{z}_i, \quad i = 0, 1, \dots, K,$$



Landmark Works: Score Network

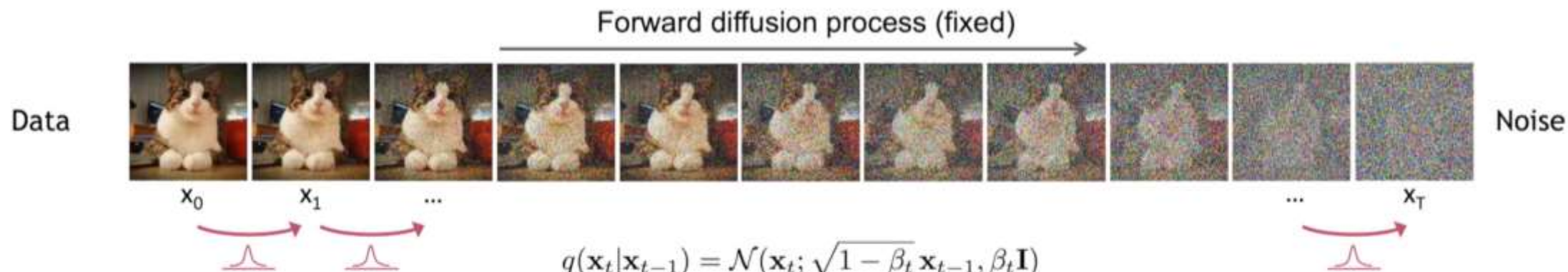


Landmark Works: Score Network



Landmark Works: From discrete to Continuous

Consider the limit of many small steps:



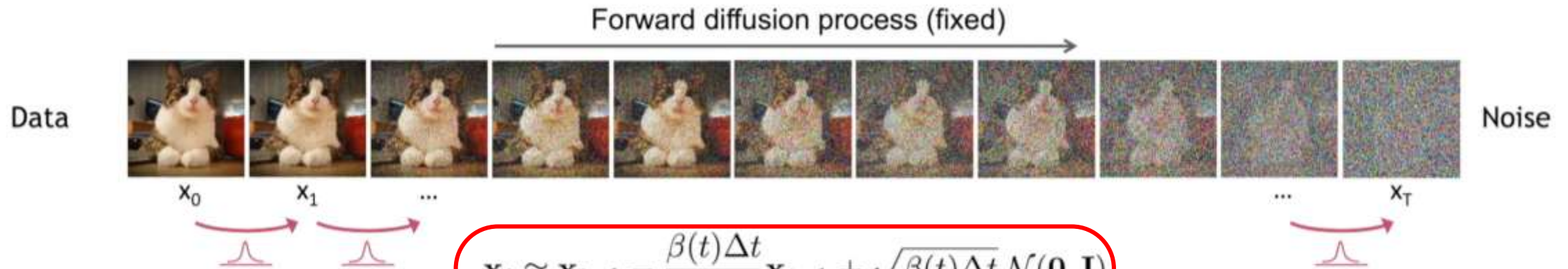
$$\begin{aligned} \mathbf{x}_t &= \sqrt{1 - \beta_t} \mathbf{x}_{t-1} + \sqrt{\beta_t} \mathcal{N}(\mathbf{0}, \mathbf{I}) \\ &= \sqrt{1 - \beta(t)\Delta t} \mathbf{x}_{t-1} + \sqrt{\beta(t)\Delta t} \mathcal{N}(\mathbf{0}, \mathbf{I}) \end{aligned} \quad (\beta_t := \beta(t)\Delta t)$$



$$\approx \mathbf{x}_{t-1} - \frac{\beta(t)\Delta t}{2} \mathbf{x}_{t-1} + \sqrt{\beta(t)\Delta t} \mathcal{N}(\mathbf{0}, \mathbf{I}) \quad \text{(Taylor expansion)}$$

Landmark Works: ScoreSDE

Consider the limit of many small steps:



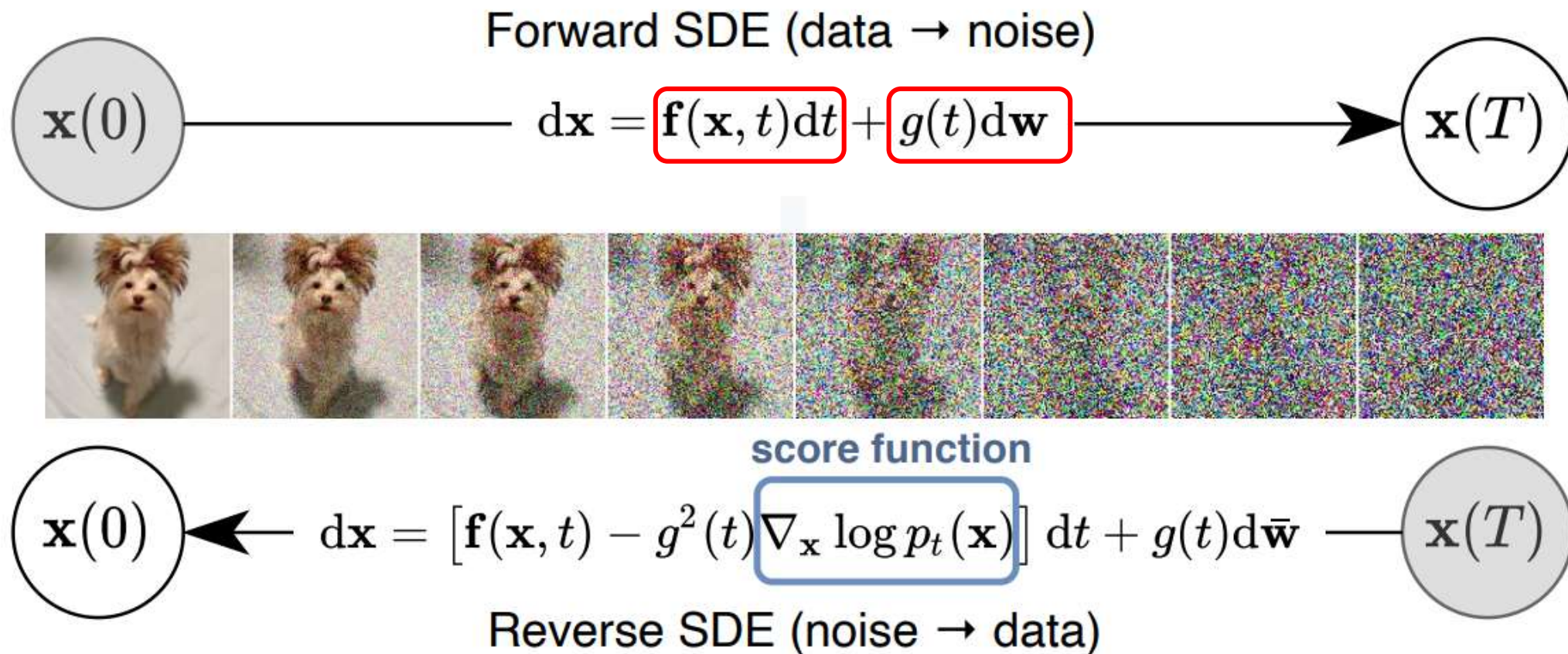
$$\mathbf{x}_t \approx \mathbf{x}_{t-1} - \frac{\beta(t)\Delta t}{2}\mathbf{x}_{t-1} + \sqrt{\beta(t)\Delta t}\mathcal{N}(\mathbf{0}, \mathbf{I})$$



$$d\mathbf{x}_t = -\frac{1}{2}\beta(t)\mathbf{x}_t dt + \sqrt{\beta(t)} d\omega_t$$

Stochastic Differential Equation (SDE)
describing the diffusion in infinitesimal limit

Landmark Works: ScoreSDE



Landmark Works: Differential Equation Views

$$p_{0t}(\mathbf{x}(t) \mid \mathbf{x}(0)) = \begin{cases} \mathcal{N}(\mathbf{x}(t); \mathbf{x}(0), [\sigma^2(t) - \sigma^2(0)]\mathbf{I}), & \text{(VE SDE)} \\ \mathcal{N}(\mathbf{x}(t); \mathbf{x}(0)e^{-\frac{1}{2}\int_0^t \beta(s)ds}, \mathbf{I} - \mathbf{I}e^{-\int_0^t \beta(s)ds}) & \text{(VP SDE)} \\ \mathcal{N}(\mathbf{x}(t); \mathbf{x}(0)e^{-\frac{1}{2}\int_0^t \beta(s)ds}, [1 - e^{-\int_0^t \beta(s)ds}]^2\mathbf{I}) & \text{(sub-VP SDE)} \end{cases}$$

Algorithm 2 PC sampling (VE SDE)

```

1:  $\mathbf{x}_N \sim \mathcal{N}(\mathbf{0}, \sigma_{\max}^2 \mathbf{I})$ 
2: for  $i = N - 1$  to  $0$  do
3:    $\mathbf{x}'_i \leftarrow \mathbf{x}_{i+1} + (\sigma_{i+1}^2 - \sigma_i^2)\mathbf{s}_{\theta*}(\mathbf{x}_{i+1}, \sigma_{i+1})$ 
4:    $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
5:    $\mathbf{x}_i \leftarrow \mathbf{x}'_i + \sqrt{\sigma_{i+1}^2 - \sigma_i^2}\mathbf{z}$ 
6:   for  $j = 1$  to  $M$  do
7:      $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
8:      $\mathbf{x}_i \leftarrow \mathbf{x}_i + \epsilon_i \mathbf{s}_{\theta*}(\mathbf{x}_i, \sigma_i) + \sqrt{2\epsilon_i}\mathbf{z}$ 
9: return  $\mathbf{x}_0$ 

```

Algorithm 3 PC sampling (VP SDE)

```

1:  $\mathbf{x}_N \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
2: for  $i = N - 1$  to  $0$  do
3:    $\mathbf{x}'_i \leftarrow (2 - \sqrt{1 - \beta_{i+1}})\mathbf{x}_{i+1} + \beta_{i+1}\mathbf{s}_{\theta*}(\mathbf{x}_{i+1}, i + 1)$ 
4:    $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
5:    $\mathbf{x}_i \leftarrow \mathbf{x}'_i + \sqrt{\beta_{i+1}}\mathbf{z}$  Predictor
6:   for  $j = 1$  to  $M$  do Corrector
7:      $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
8:      $\mathbf{x}_i \leftarrow \mathbf{x}_i + \epsilon_i \mathbf{s}_{\theta*}(\mathbf{x}_i, i) + \sqrt{2\epsilon_i}\mathbf{z}$ 
9: return  $\mathbf{x}_0$ 

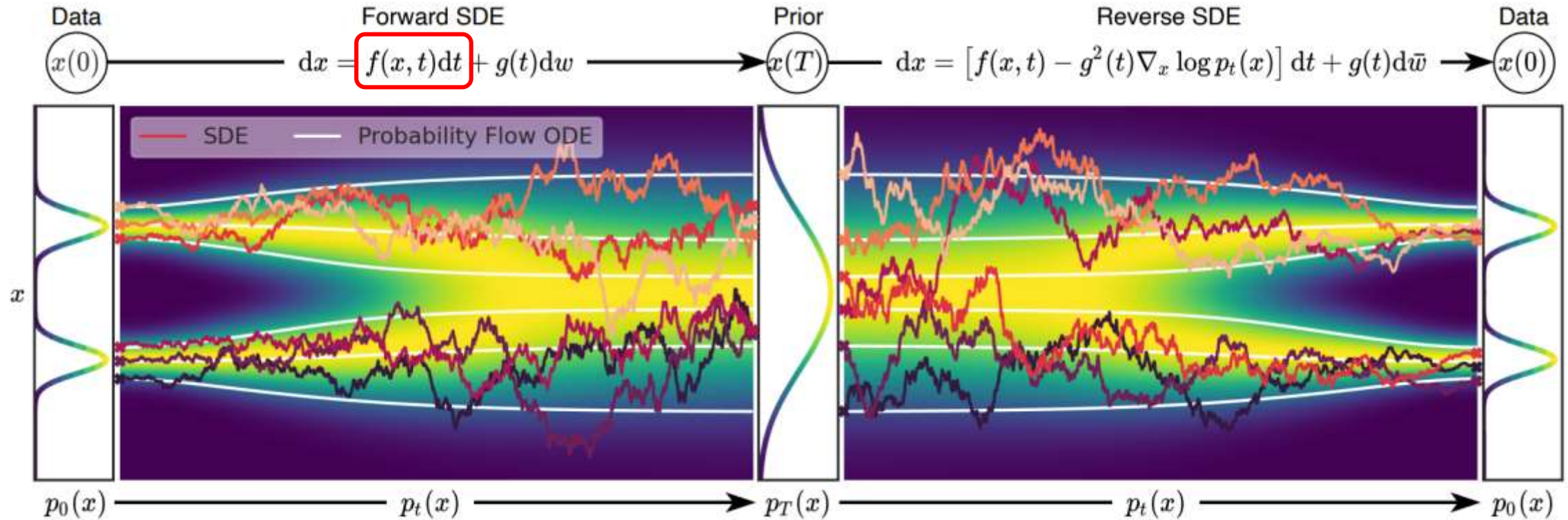
```

-- Sampling along the reverse trajectory is actually finding the numerical solution of differential equations.

Outlines

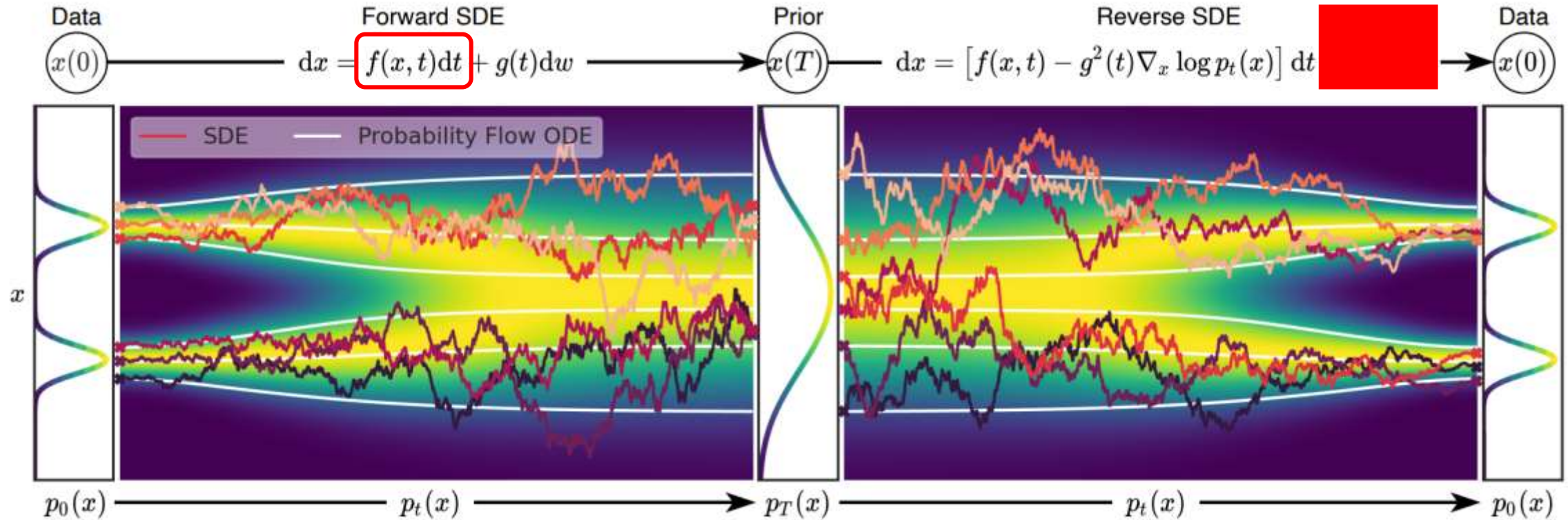
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Stochastic or Deterministic?



- SDE: Higher Performance
- ODE: Higher Speed

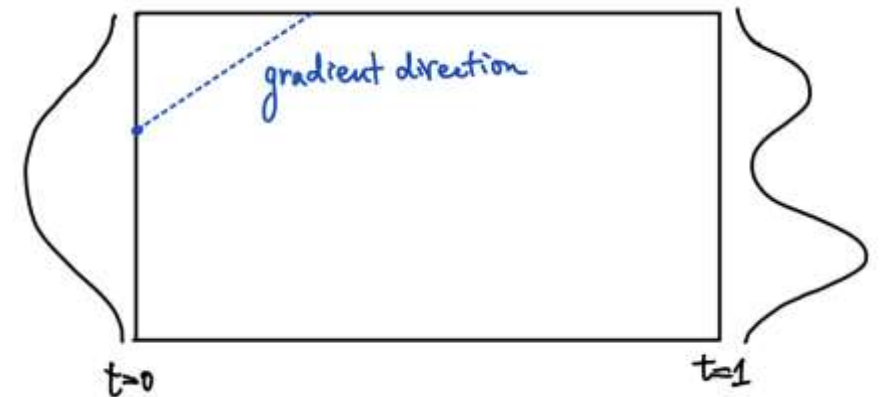
Stochastic or Deterministic?



- SDE: Higher Performance
- ODE: Higher Speed

Stochastic or Deterministic?

- Deterministic sampling is not equivalent to no diversity
 - > there are infinite random points which can be sampled from prior distributions
- Why ODEs are faster?
 - > no randomness leads to larger steps
 - > but the error would accumulate
- Regarding SDE
 - > small steps leads to more steps
 - > random noise for each steps brings less error



Label Conditional Diffusion

Algorithm 1 Classifier guided diffusion sampling, given a diffusion model $(\mu_\theta(x_t), \Sigma_\theta(x_t))$, classifier $p_\phi(y|x_t)$, and gradient scale s .

Input: class label y , gradient scale s

$x_T \leftarrow$ sample from $\mathcal{N}(0, \mathbf{I})$

for all t from T to 1 **do**

$\mu, \Sigma \leftarrow \mu_\theta(x_t), \Sigma_\theta(x_t)$

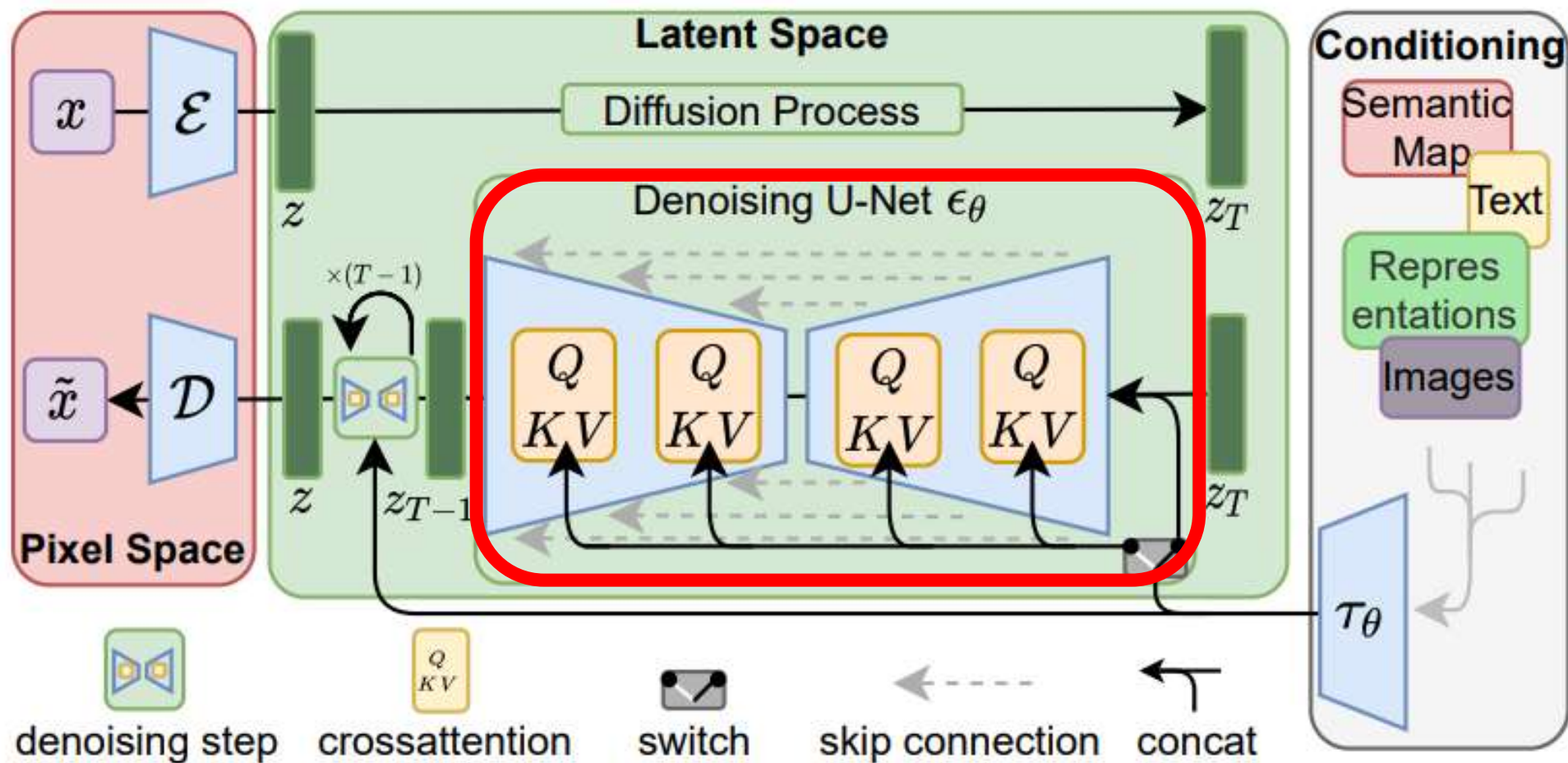
$x_{t-1} \leftarrow$ sample from $\mathcal{N}(\mu + s\Sigma \nabla_{x_t} \log p_\phi(y|x_t), \Sigma)$

end for

return x_0

$$\begin{aligned} p(x_t | x_{t+1}, y) &= \frac{p(x_t | x_{t+1})p(y | x_t, x_{t+1})}{p(y | x_{t+1})} \\ &= \frac{p(x_t | x_{t+1})p(y | x_t)}{p(y | x_{t+1})}, \end{aligned}$$

Data Conditional Diffusion



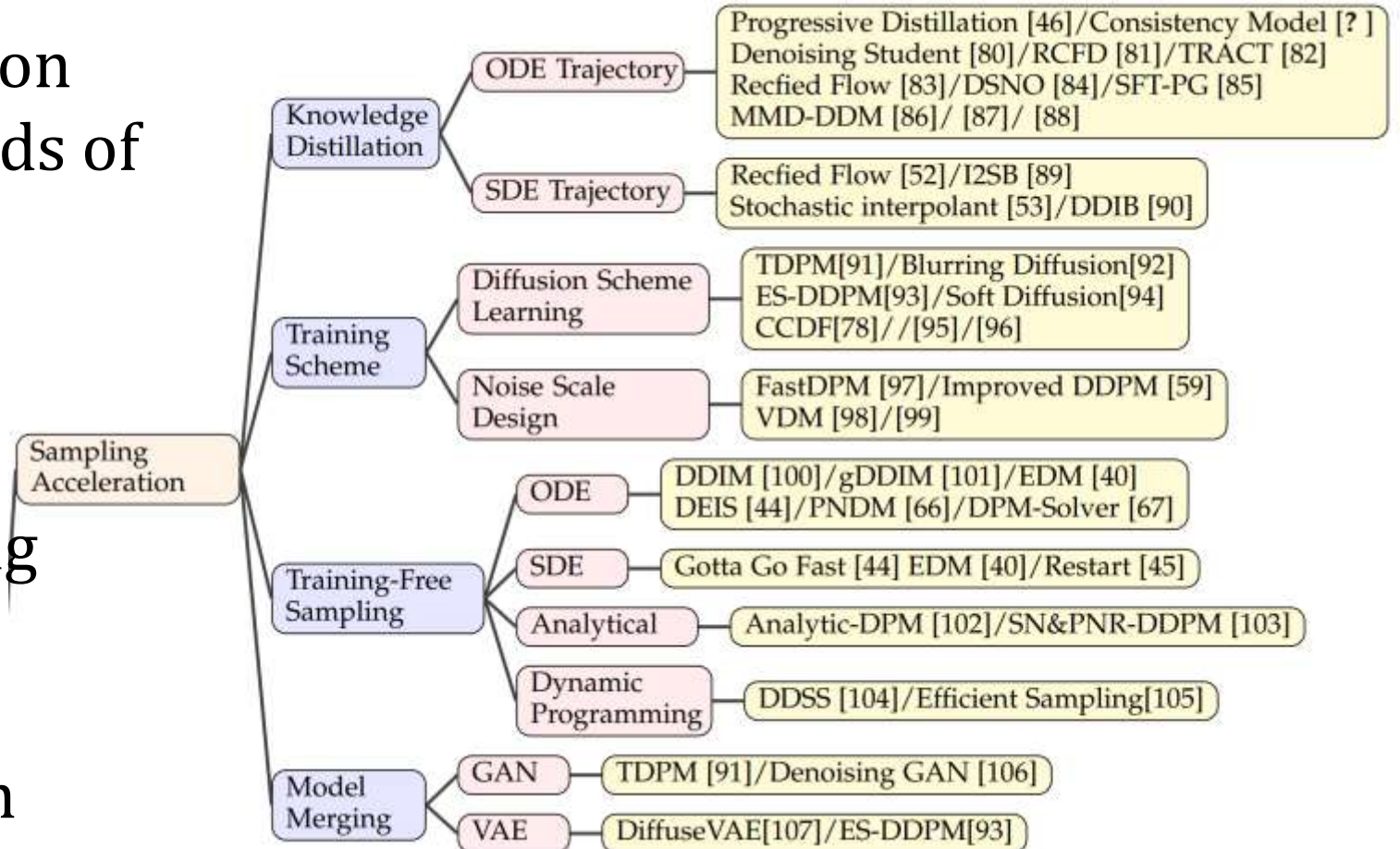
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Diffusion Needs Improvements

- Gaussian-based diffusion sampler takes thousands of steps to sample.

1. Training Scheme
2. Training-Free Sampling
3. Model Merging
4. Knowledge Distillation

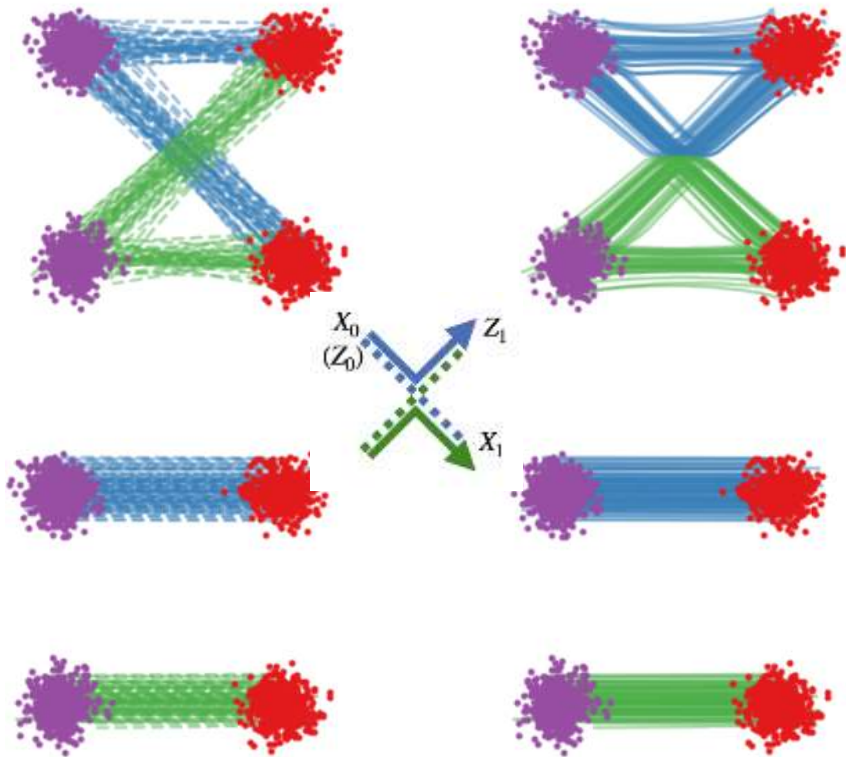


Diffusion Needs Improvements

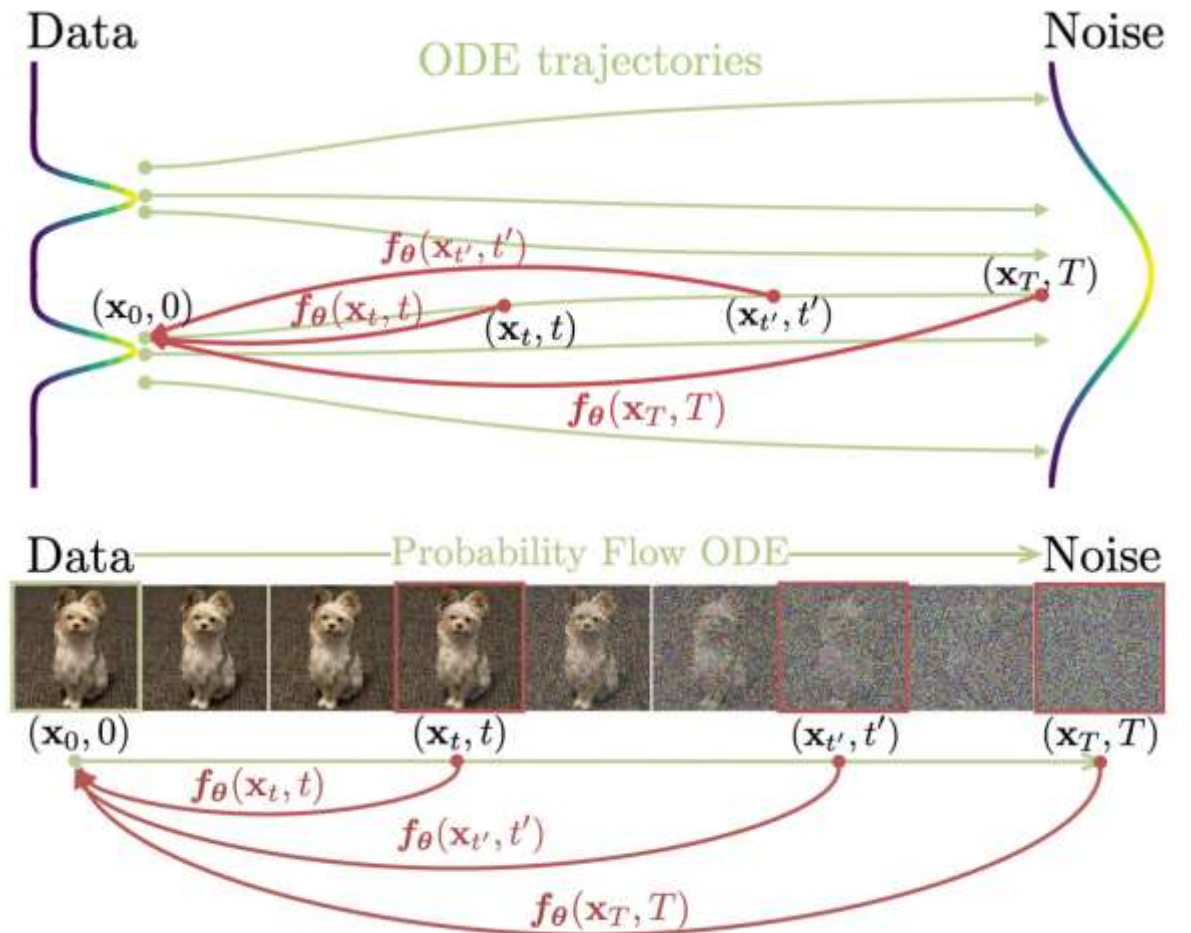
- | | |
|--------------------------------|---------------------------|
| 1. Slow sampling | ➤ Sampling Acceleration |
| 2. High-Dimensional Space | ➤ New Forward Process |
| 3. Conditional sampling | ➤ Likelihood Optimization |
| 4. Wide range data application | ➤ Bridging Diffusion |

Training-Free Sampling: Distillation

Path-based distillation



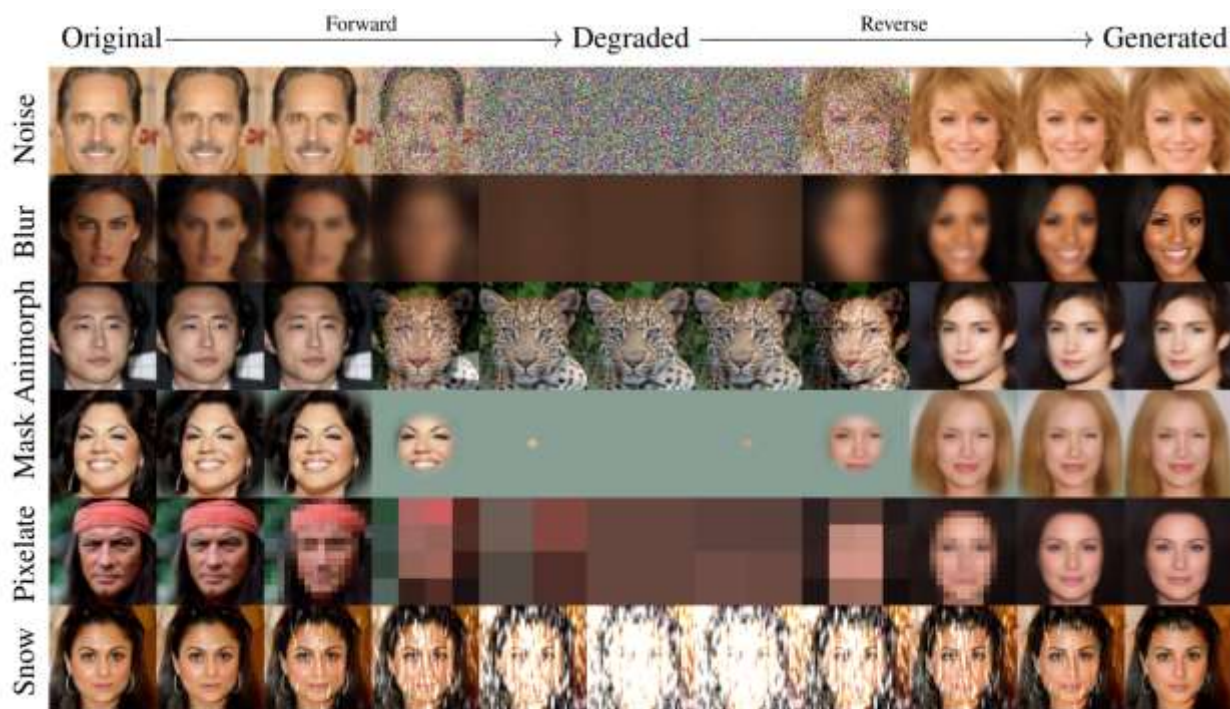
Objective-based distillation



Training Scheme: Diffusion Scheme Learning

Incomplete forward and sampling process \rightarrow Non-Gaussian noise but a starting distribution from other distribution

Forward Path

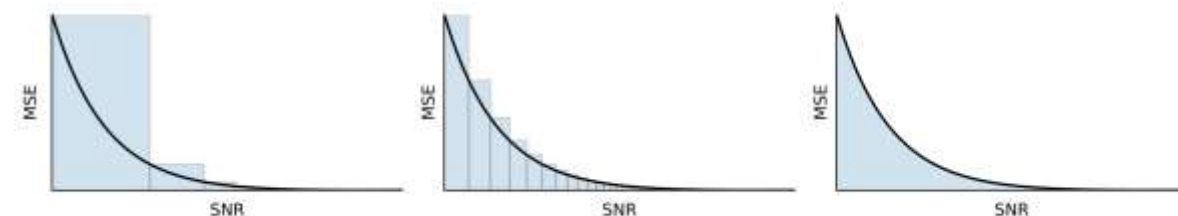


Efficient Noise

$$\text{SNR}(t) := \alpha_t^2 / \beta_t^2 = \exp(\gamma_\eta(t)), \quad \sigma_t^2 = \text{sigmoid}(\gamma_\eta(t)) \quad (16)$$

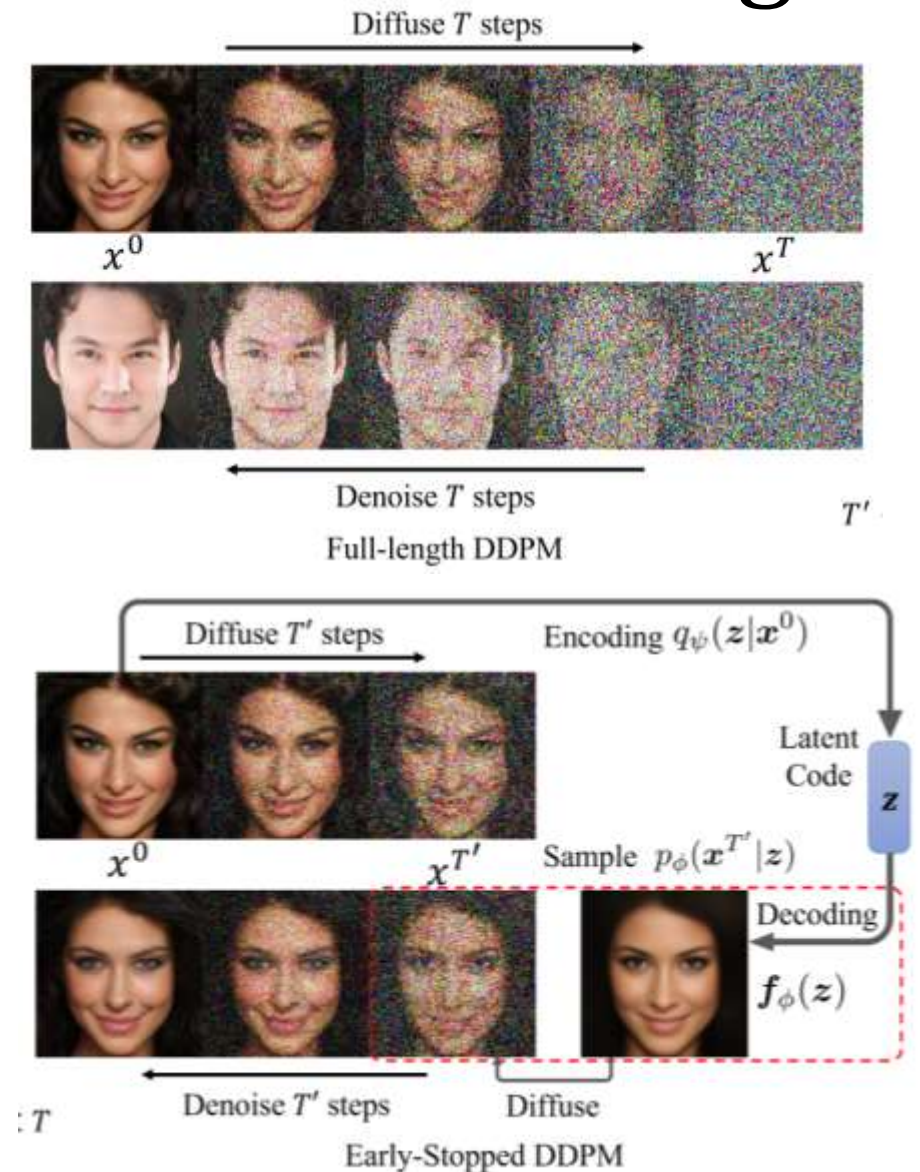
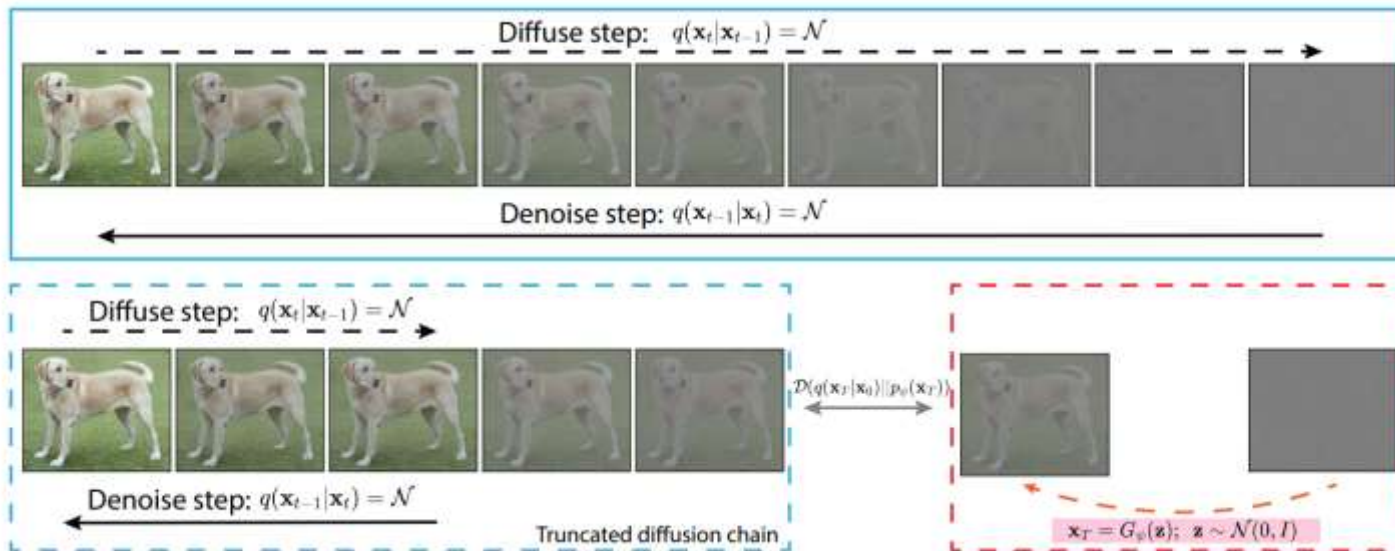
$$\mathcal{L}_T(\mathbf{x}) = \frac{T}{2} \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} [(\text{SNR}(s) - \text{SNR}(t)) \|\mathbf{x} - \hat{\mathbf{x}}_\theta(\mathbf{z}_t; t)\|_2^2]$$

$$\mathcal{L}_\infty(\mathbf{x}) = \frac{1}{2} \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \int_{\text{SNR}_{\min}}^{\text{SNR}_{\max}} \|\mathbf{x} - \tilde{\mathbf{x}}_\theta(\mathbf{z}_v, v)\|_2^2 dv \quad (17)$$



Training Scheme: Diffusion Scheme Learning

Incomplete forward and sampling process \rightarrow From intermediate states generated by other fast generative models (such as GAN and VAE)



Training Scheme: Noise Scale Design

- FastDPM: link noise with time t with bijective map

$$\mathcal{R}(t) = (\Delta\beta)^{\frac{t}{2}} \Gamma(\hat{\beta} + 1)^{\frac{1}{2}} \Gamma(\hat{\beta} - t + 1)^{-\frac{1}{2}}.$$

- VDM: link noise with time t with bijective map

$$\sigma_t^2 = \text{sigmoid}(\gamma_\eta(t)) \quad \alpha_t^2 = \text{sigmoid}(-\gamma_\eta(t))$$

guide the training with SNR: $\text{SNR}(t) = \exp(-\gamma_\eta(t))$

$$\mathcal{L}_T(\mathbf{x}) = \frac{T}{\gamma} \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I}), i \sim U\{1, T\}} [(\text{SNR}(s) - \text{SNR}(t)) \|\mathbf{x} - \hat{\mathbf{x}}_\theta(\mathbf{z}_t; t)\|_2^2],$$

$$\mathcal{L}_\infty(\mathbf{x}) = \frac{1}{2} \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \int_{\text{SNR}_{\min}}^{\text{SNR}_{\max}} \|\mathbf{x} - \tilde{\mathbf{x}}_\theta(\mathbf{z}_v, v)\|_2^2 dv,$$

- Improved DDPM: learn noise scale by new loss function

$$L_{\text{hybrid}} = L_{\text{simple}} + \lambda L_{\text{vlb}}$$

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

Training-Free Sampling: DE In General

- Differential equation based samplers are actually numerical solvers for differential equations. Network's output is actually the step gradient for each steps
- The number of sampling steps depends on the errors during sampling
 - > Euler Method: $y_{n+1} = y_n + hf(t_n + y_n)$
 - > h : step size
 - > $f(t_n + y_n)$: estimated gradient
- Advanced sampler means advanced numerical solvers
 - > higher-order solvers: more accurate gradient -> larger step -> faster sampling
 - > multi-step solvers: multi-step results -> accurate predictions -> faster sampling

Training-Free Sampling: Other Techniques

Analytic Solvers

- Analytical DPM: Start from vlb optimization to explore analytical solutions
- Extended Analytical DPM: Suppose that reverse mean is independent of reverse noise, finding optimal mean and noise

Theorem 1. (Score representation of the optimal solution to Eq. (4), proof in Appendix A.2)

The optimal solution $\mu_n^*(\mathbf{x}_n)$ and σ_n^{*2} to Eq. (4) are

$$\mu_n^*(\mathbf{x}_n) = \tilde{\mu}_n \left(\mathbf{x}_n, \frac{1}{\sqrt{\alpha_n}} (\mathbf{x}_n + \bar{\beta}_n \nabla_{\mathbf{x}_n} \log q_n(\mathbf{x}_n)) \right),$$
$$\sigma_n^{*2} = \lambda_n^2 + \left(\sqrt{\frac{\bar{\beta}_n}{\alpha_n}} - \sqrt{\bar{\beta}_{n-1} - \lambda_n^2} \right)^2 \left(1 - \bar{\beta}_n \mathbb{E}_{q_n(\mathbf{x}_n)} \frac{\|\nabla_{\mathbf{x}_n} \log q_n(\mathbf{x}_n)\|^2}{d} \right),$$

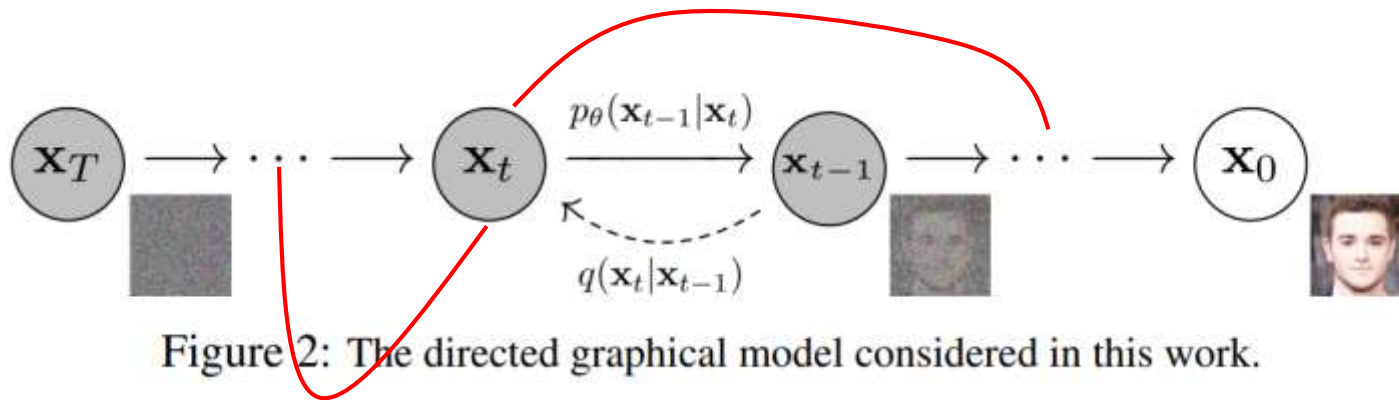
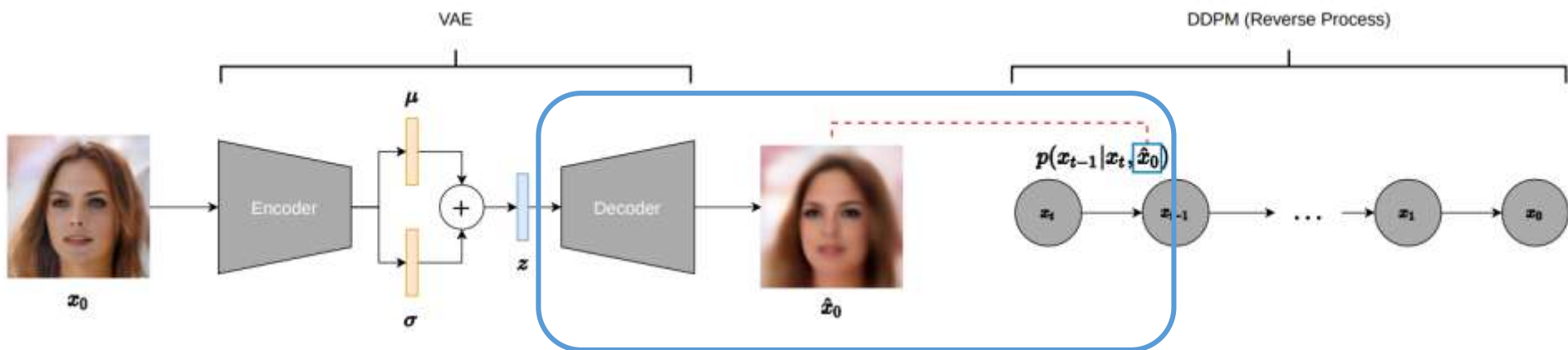
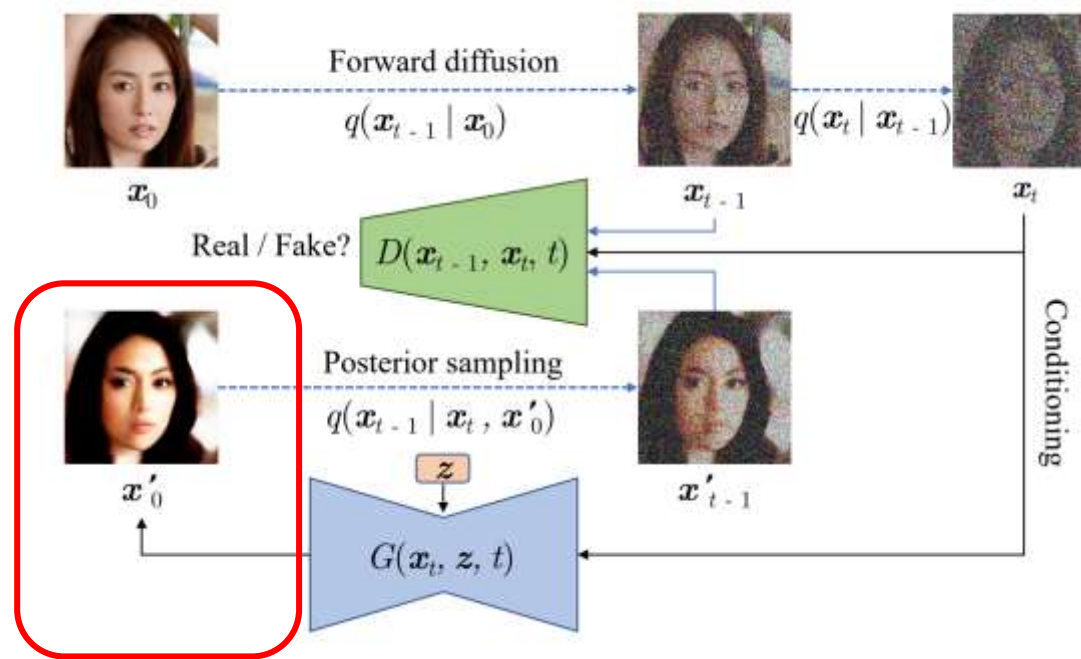
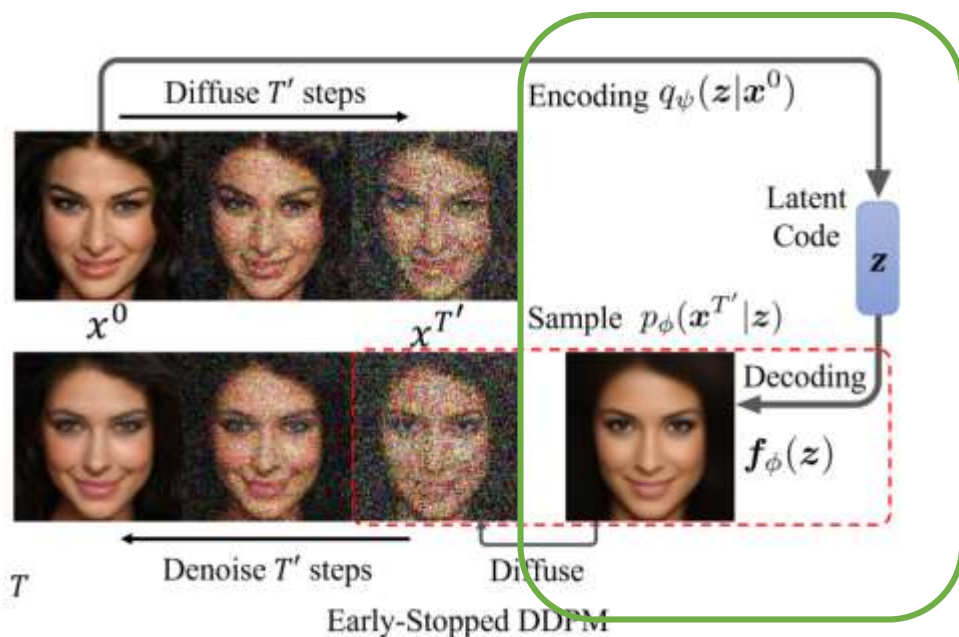


Figure 2: The directed graphical model considered in this work.

Dynamic Programming

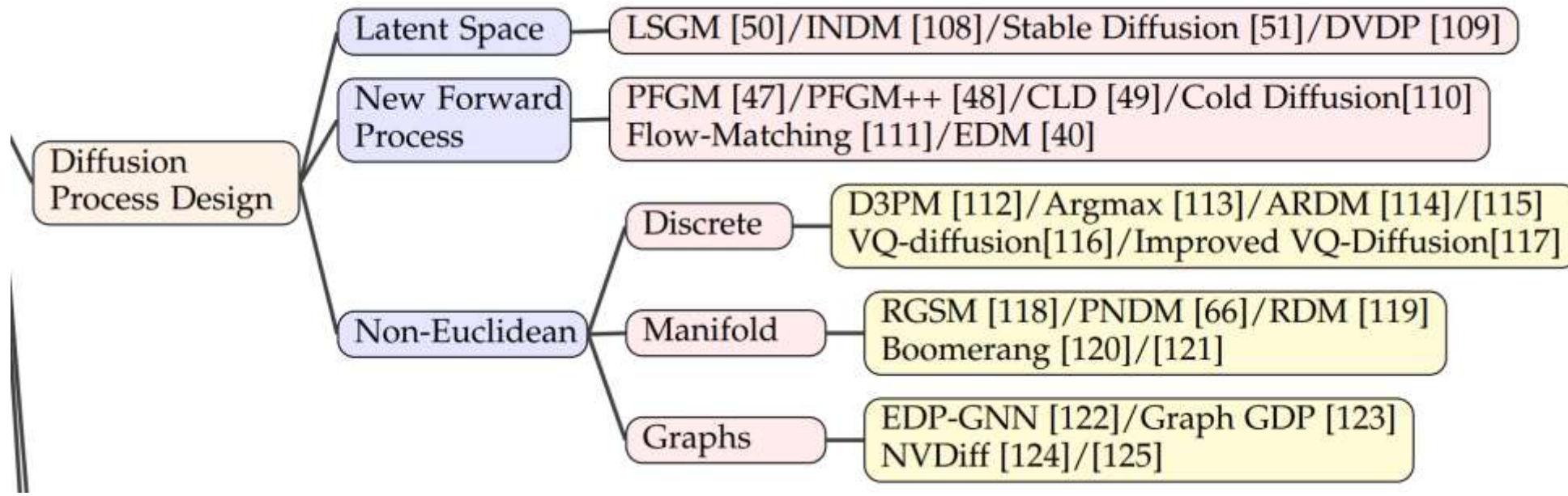
- Construct a refinement path composed of K sampling steps according to the log-likelihood losses.

Model Merging: Acceleration

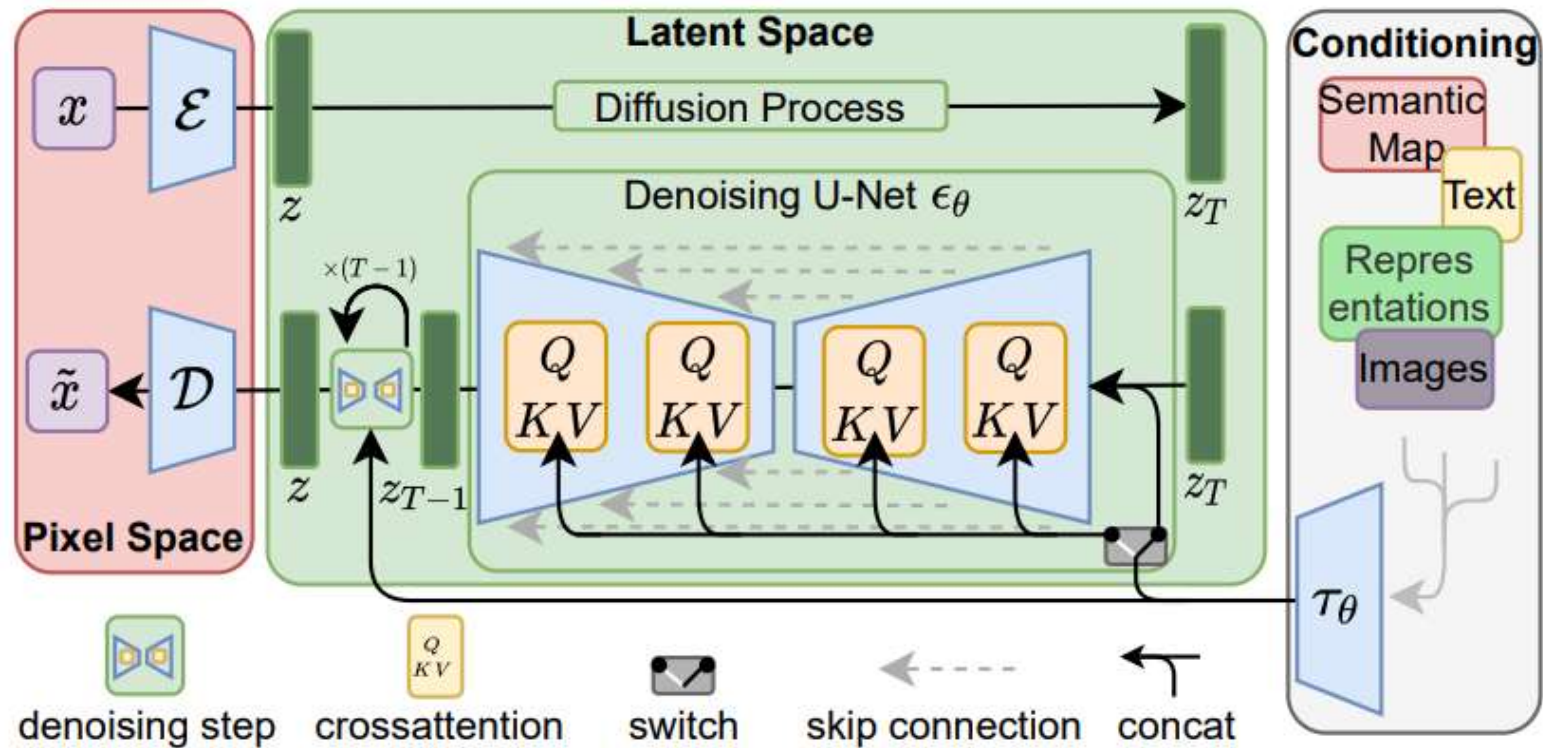


Diffusion Needs Improvements

Designing advanced process for wider application, including:
diverse data types, cross-modality generation, cross distribution



Diffusion Process Design: Latent Space

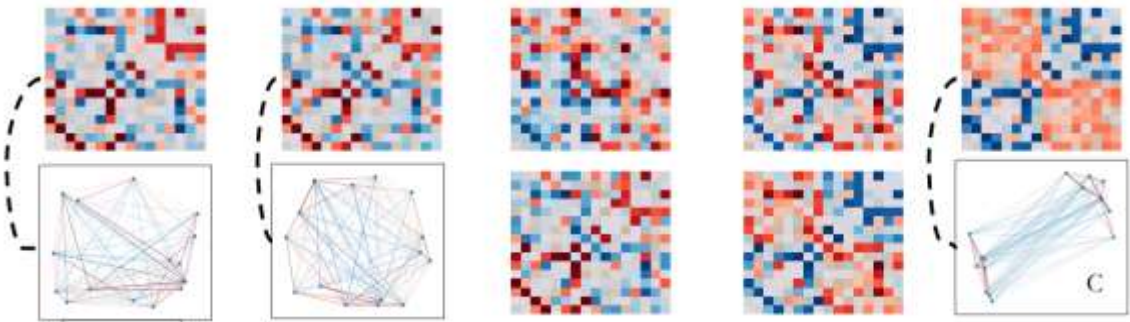


Latent Diffusion: Conducting diffusion process on latent space

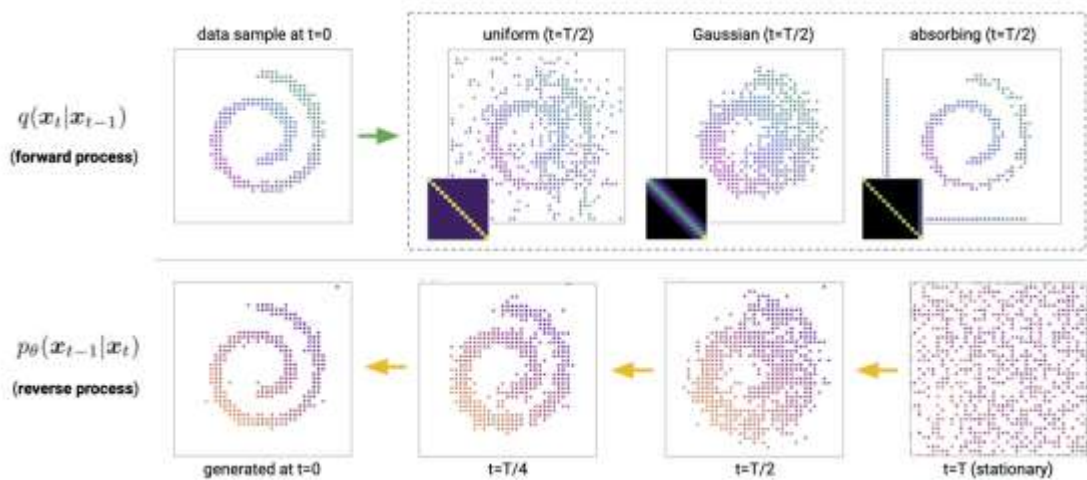
- Faster convergence
- Multi-condition guidance
- Prior knowledge from Encoders & Decoders

Diffusion Process Design: Wider Range

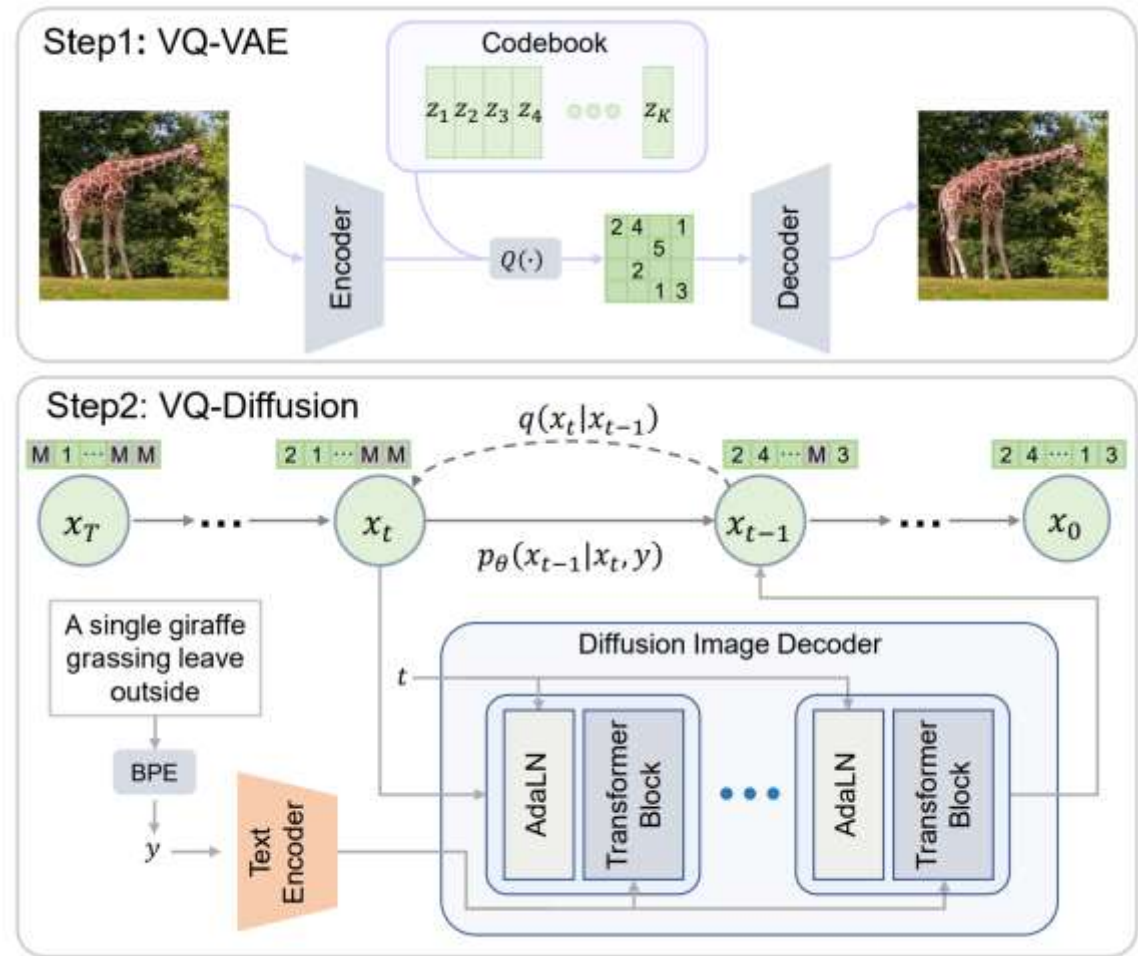
Graph



Categorical data

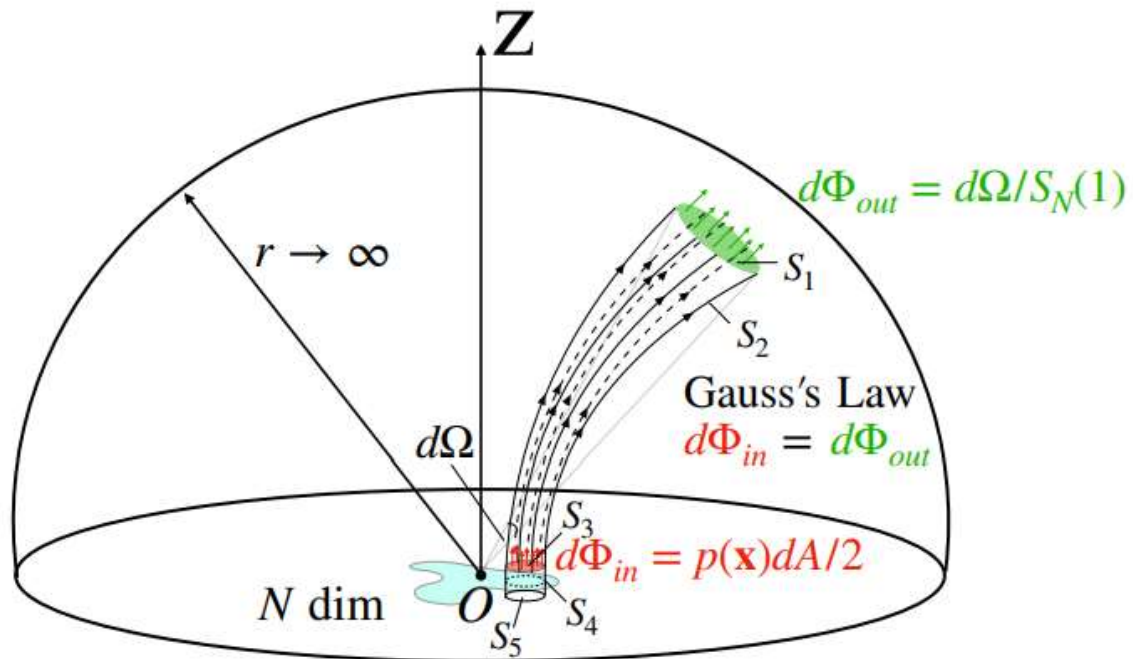


Vector-Quantized: Cross modality

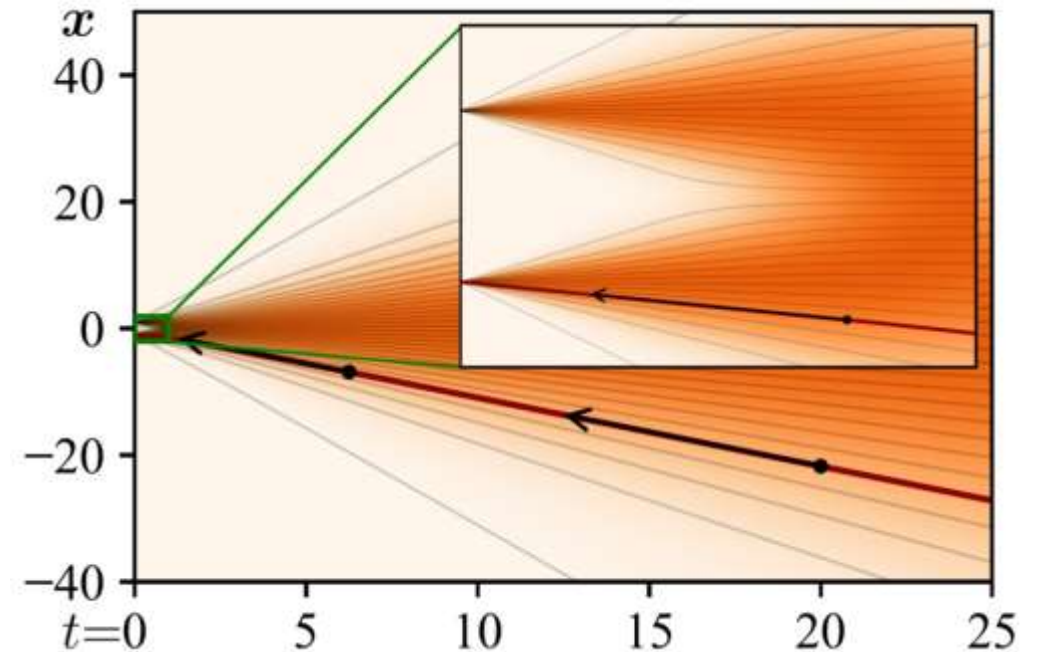


Diffusion Process Design: Advanced Forward

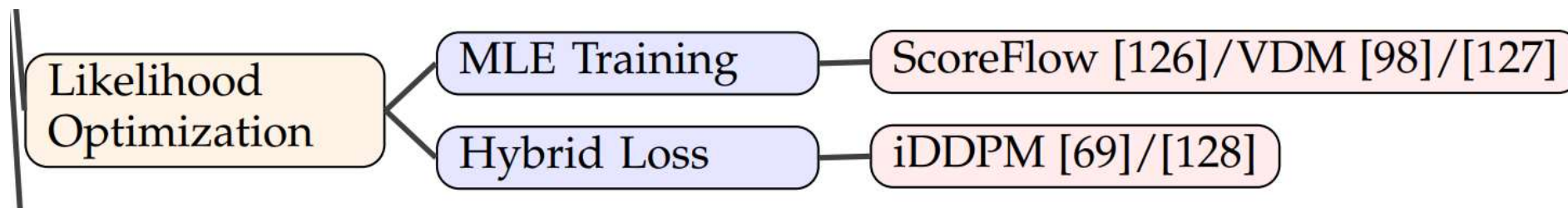
Physics-inspired forward process



Self-designed sampling space



Diffusion Needs Improvements



Enhance the continuous diffusion training from the perspective of

- Directly optimizing the likelihood instead of
- Minimizing the lower bound of log-likelihood

Likelihood Optimization: Advanced ELBO

Theorem 3. Let $p_{0t}(\mathbf{x}' | \mathbf{x})$ denote the transition distribution from $p_0(\mathbf{x})$ to $p_t(\mathbf{x})$ for the SDE in Eq. (1). With the same notations and conditions in Theorem 1, we have

$$-\log p_{\theta}^{\text{SDE}}(\mathbf{x}) \leq \mathcal{L}_{\theta}^{\text{SM}}(\mathbf{x}) = \mathcal{L}_{\theta}^{\text{DSM}}(\mathbf{x}), \quad (11)$$

Score Connection:

Represent ELBO based on score-matching loss

where $\mathcal{L}_{\theta}^{\text{SM}}(\mathbf{x})$ is defined as

$$-\mathbb{E}_{p_{0T}(\mathbf{x}'|\mathbf{x})}[\log \pi(\mathbf{x}')] + \frac{1}{2} \int_0^T \mathbb{E}_{p_{0t}(\mathbf{x}'|\mathbf{x})} \left[2g(t)^2 \nabla_{\mathbf{x}'} \cdot \mathbf{s}_{\theta}(\mathbf{x}', t) + g(t)^2 \|\mathbf{s}_{\theta}(\mathbf{x}', t)\|_2^2 - 2\nabla_{\mathbf{x}'} \cdot \mathbf{f}(\mathbf{x}', t) \right] dt,$$

and $\mathcal{L}_{\theta}^{\text{DSM}}(\mathbf{x})$ is given by

$$\begin{aligned} & -\mathbb{E}_{p_{0T}(\mathbf{x}'|\mathbf{x})}[\log \pi(\mathbf{x}')] + \frac{1}{2} \int_0^T \mathbb{E}_{p_{0t}(\mathbf{x}'|\mathbf{x})} \left[g(t)^2 \|\mathbf{s}_{\theta}(\mathbf{x}', t) - \nabla_{\mathbf{x}'} \log p_{0t}(\mathbf{x}' | \mathbf{x})\|_2^2 \right] dt \\ & - \frac{1}{2} \int_0^T \mathbb{E}_{p_{0t}(\mathbf{x}'|\mathbf{x})} \left[g(t)^2 \|\nabla_{\mathbf{x}'} \log p_{0t}(\mathbf{x}' | \mathbf{x})\|_2^2 + 2\nabla_{\mathbf{x}'} \cdot \mathbf{f}(\mathbf{x}', t) \right] dt. \end{aligned}$$

$$L_{\text{hybrid}} = L_{\text{simple}} + \lambda L_{\text{vlb}}$$

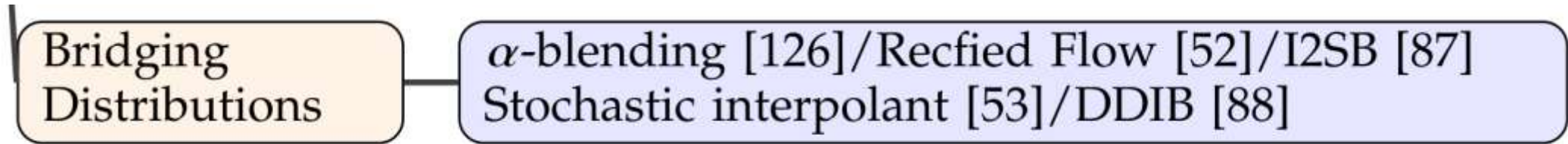
$$\mathcal{L}_T(\mathbf{x}) = \frac{T}{2} \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I}), i \sim U\{1, T\}} \left[(\text{SNR}(s) - \text{SNR}(t)) \|\mathbf{x} - \hat{\mathbf{x}}_{\theta}(\mathbf{z}_t; t)\|_2^2 \right],$$

$$\mathcal{L}_{\infty}(\mathbf{x}) = \frac{1}{2} \mathbb{E}_{\epsilon \sim \mathcal{N}(0, \mathbf{I})} \int_{\text{SNR}_{\min}}^{\text{SNR}_{\max}} \|\mathbf{x} - \tilde{\mathbf{x}}_{\theta}(\mathbf{z}_v, v)\|_2^2 dv,$$

Re-Design:

Design vlb loss from a different perspective to obtain better convergence

Diffusion Needs Improvements



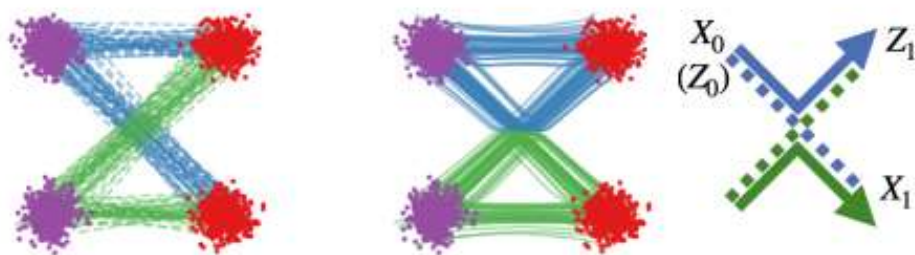
From one-direction translation to bi-directional translation:

- Image-to-image translation
- Cell distribution transportation

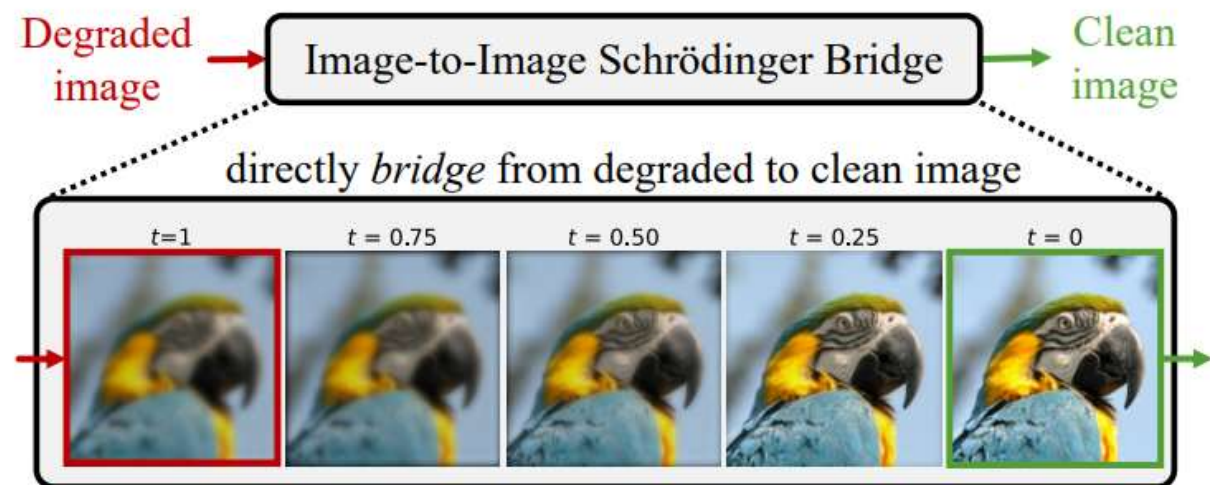
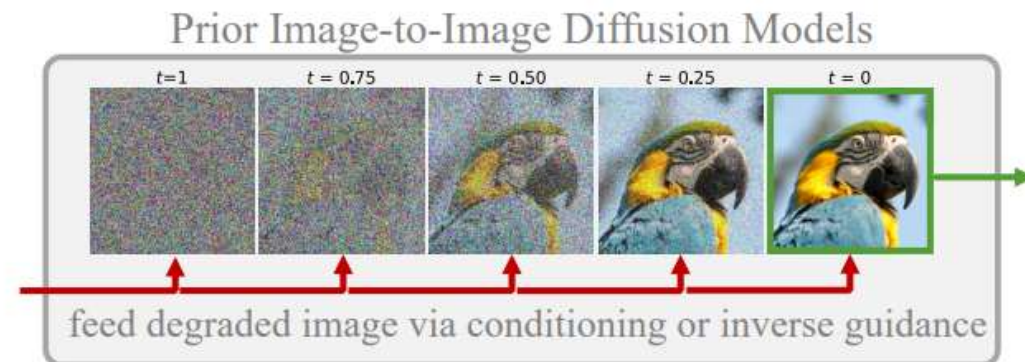
Bridging Distributions: Multi-directional

Connecting two distributions:

- Design transportation maps based on score-matching objective
- Apply Schrodinger bridge for the connection



Optimal Transport

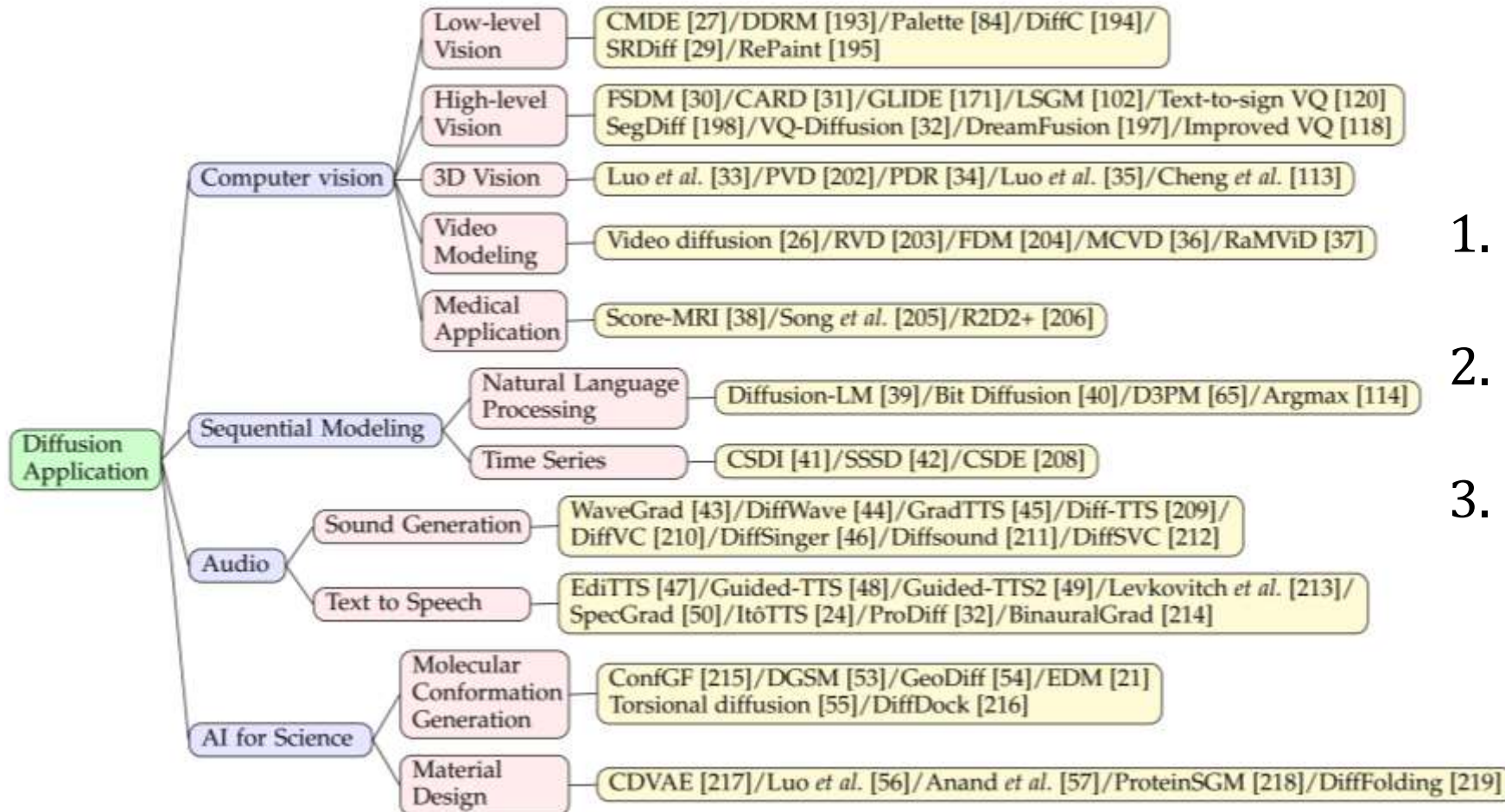


Schrodinger Bridge

Outlines

- Brief Introduction to diffusion model
- Viewing diffusion model through generative model development
- Diffusion model basic algorithms
- Enhancing Understanding from multi-view
- Algorithm improvement
- **Applications**
- Further Directions and Discussions

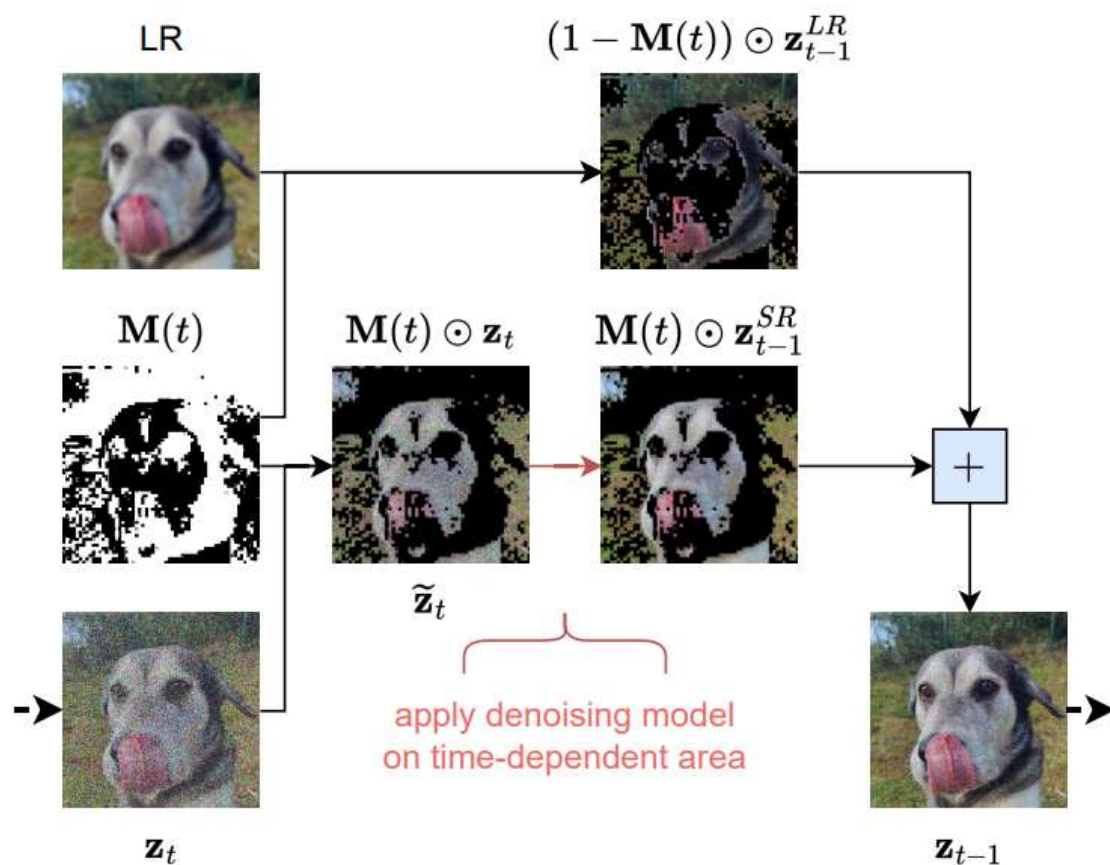
Diffusion Applications



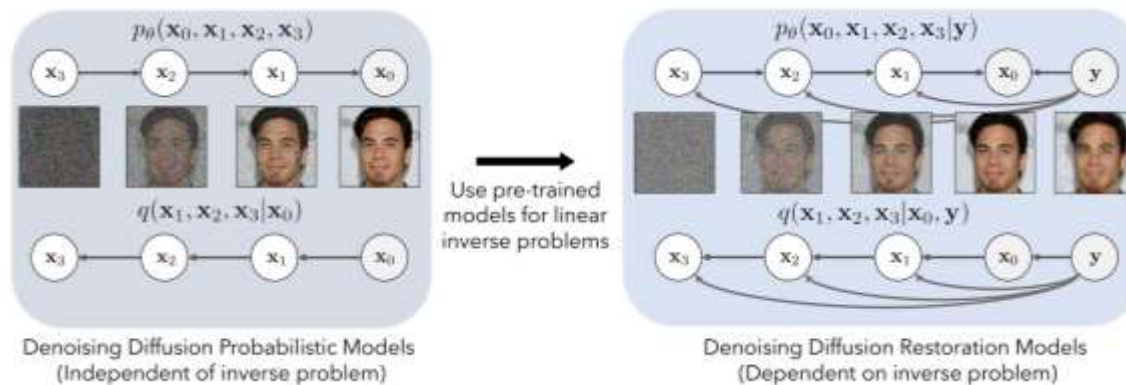
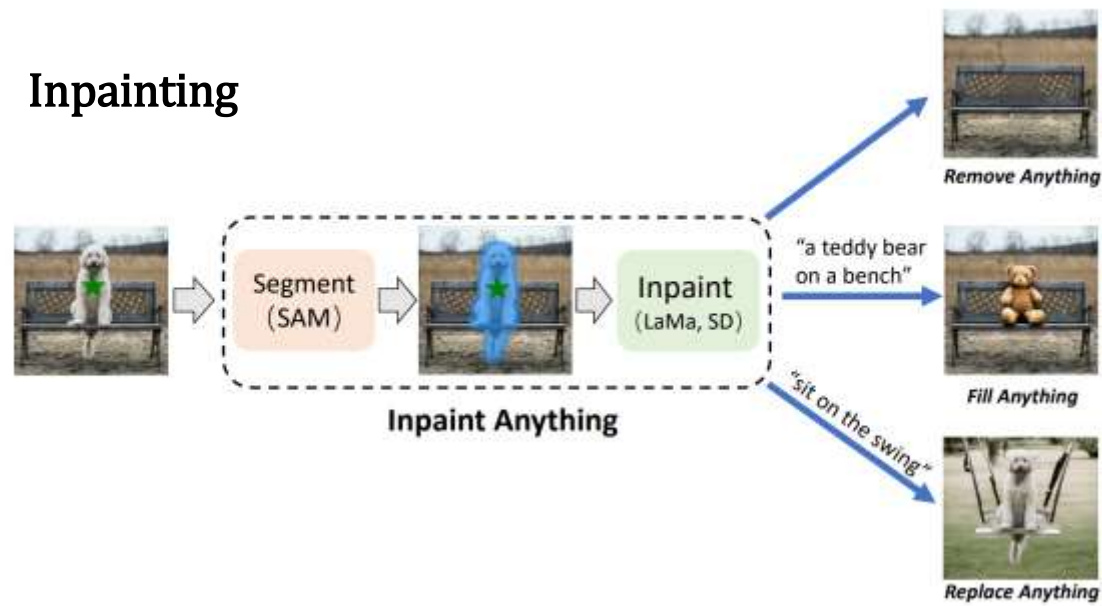
1. Mechanisms behind the better performance
2. Key-point technique in the implementation
3. Current challenges and future directions

Low-Level Vision

Super-Resolution



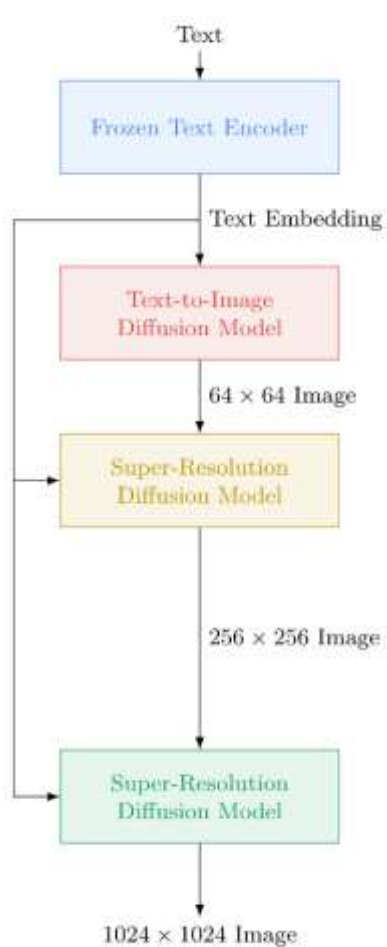
Inpainting



Restoration

High-Level Vision

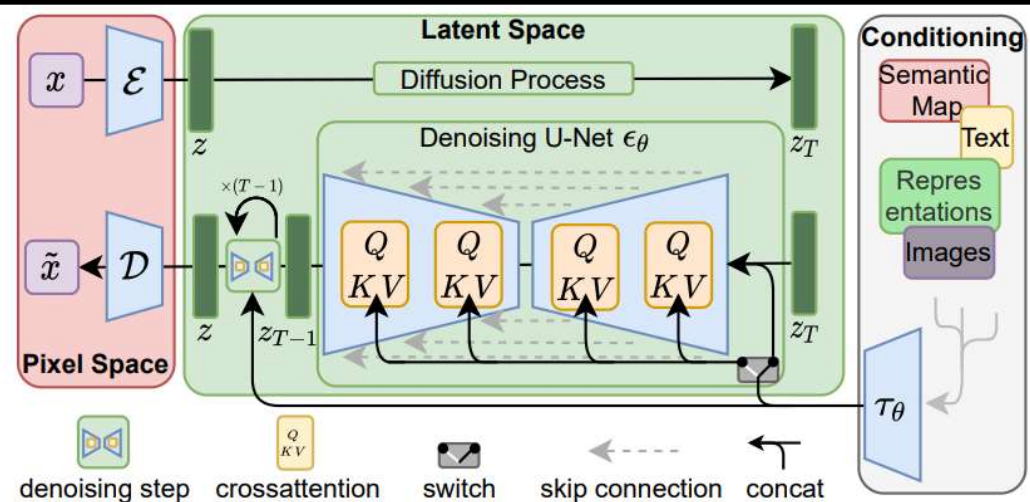
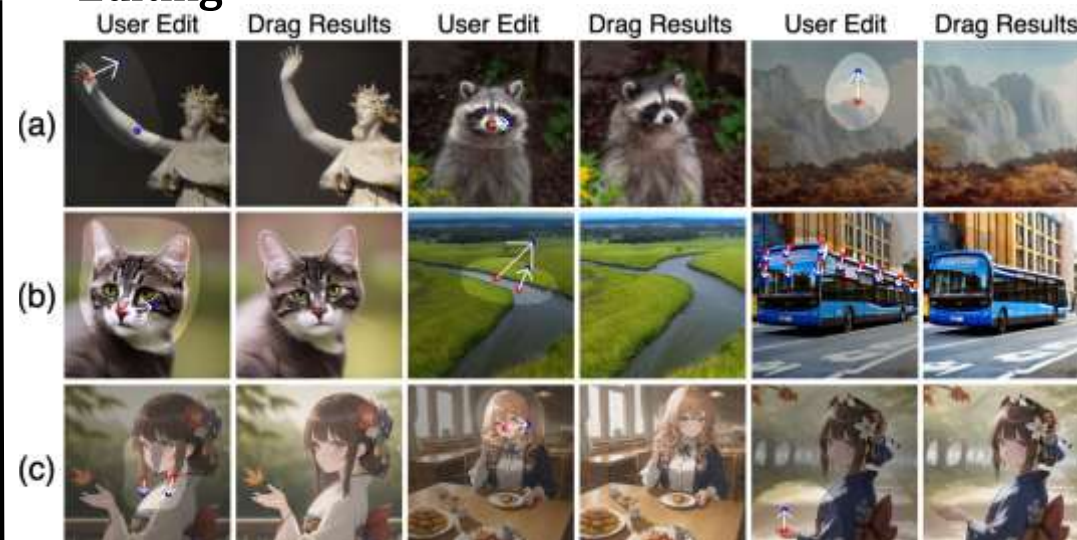
Generation



"A Golden Retriever dog wearing a blue checkered beret and red dotted turtleneck."

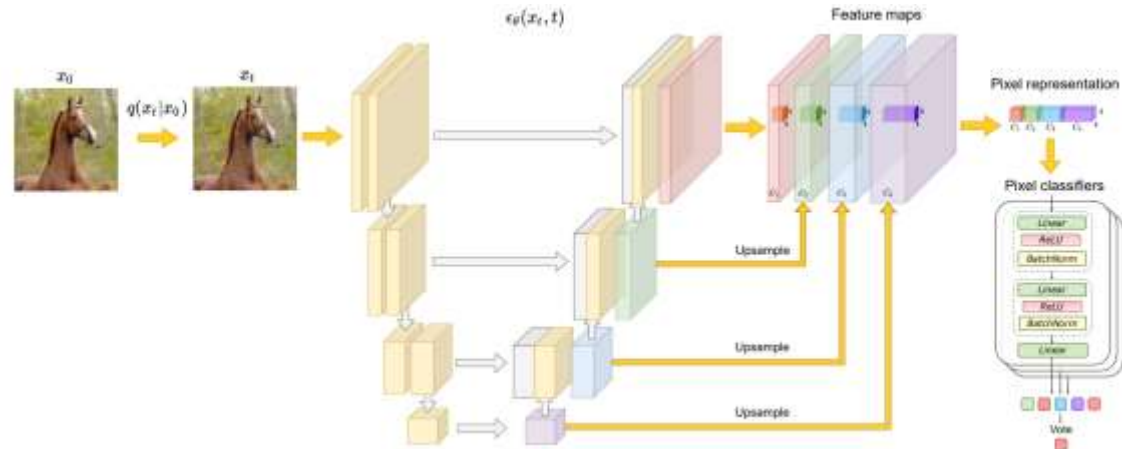


Editing

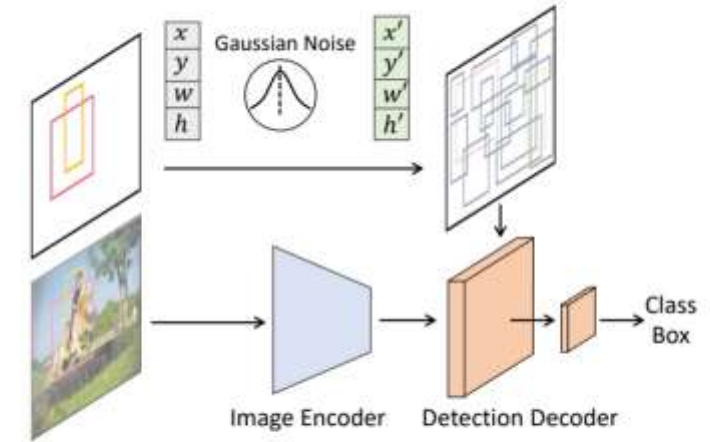


High-Level Vision

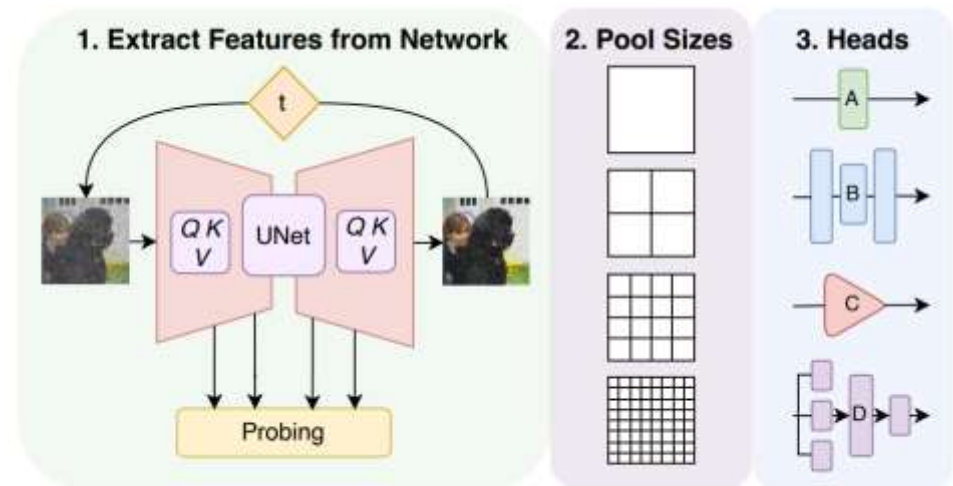
Segmentation



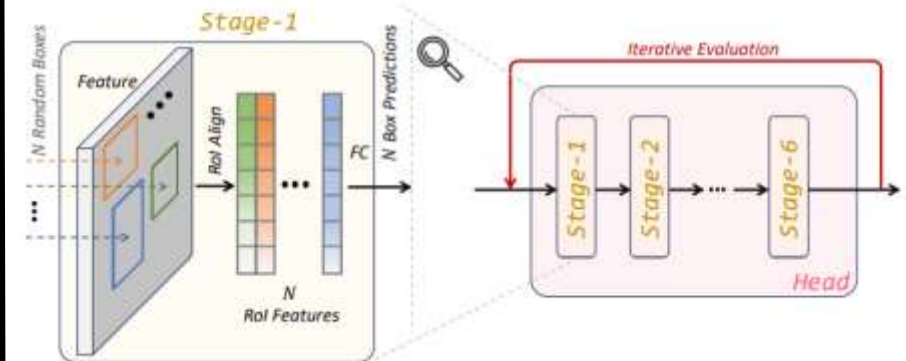
Detection



(a) Overall pipeline.



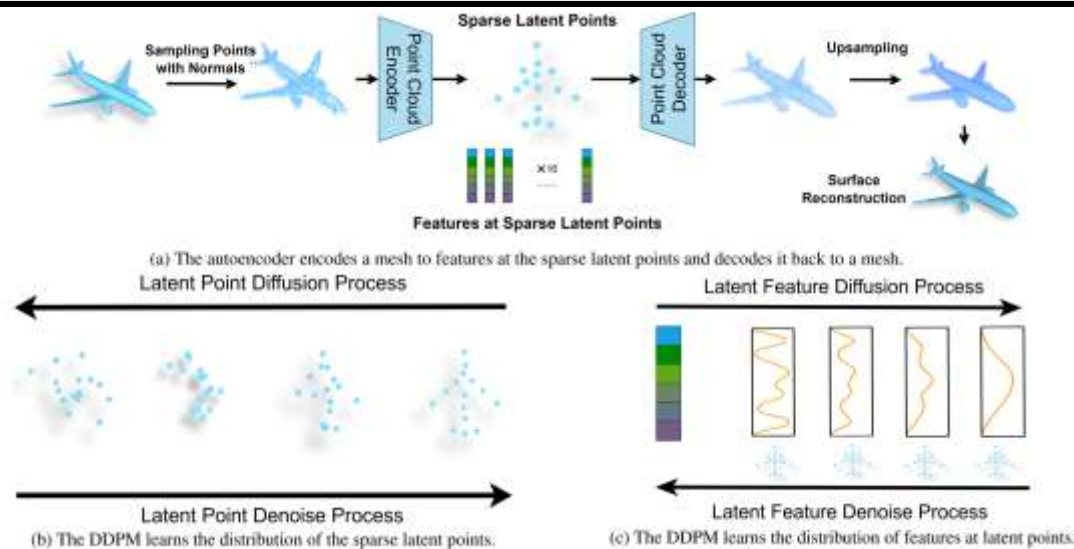
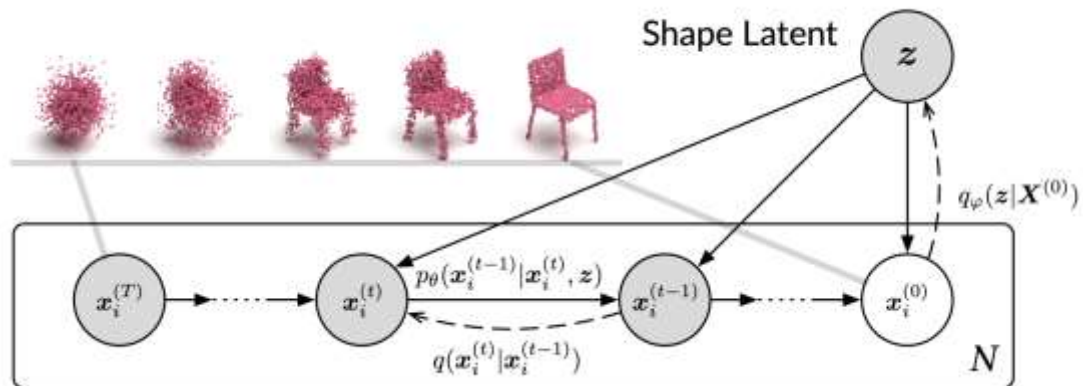
Classification



(b) Details of the detection decoder/head.

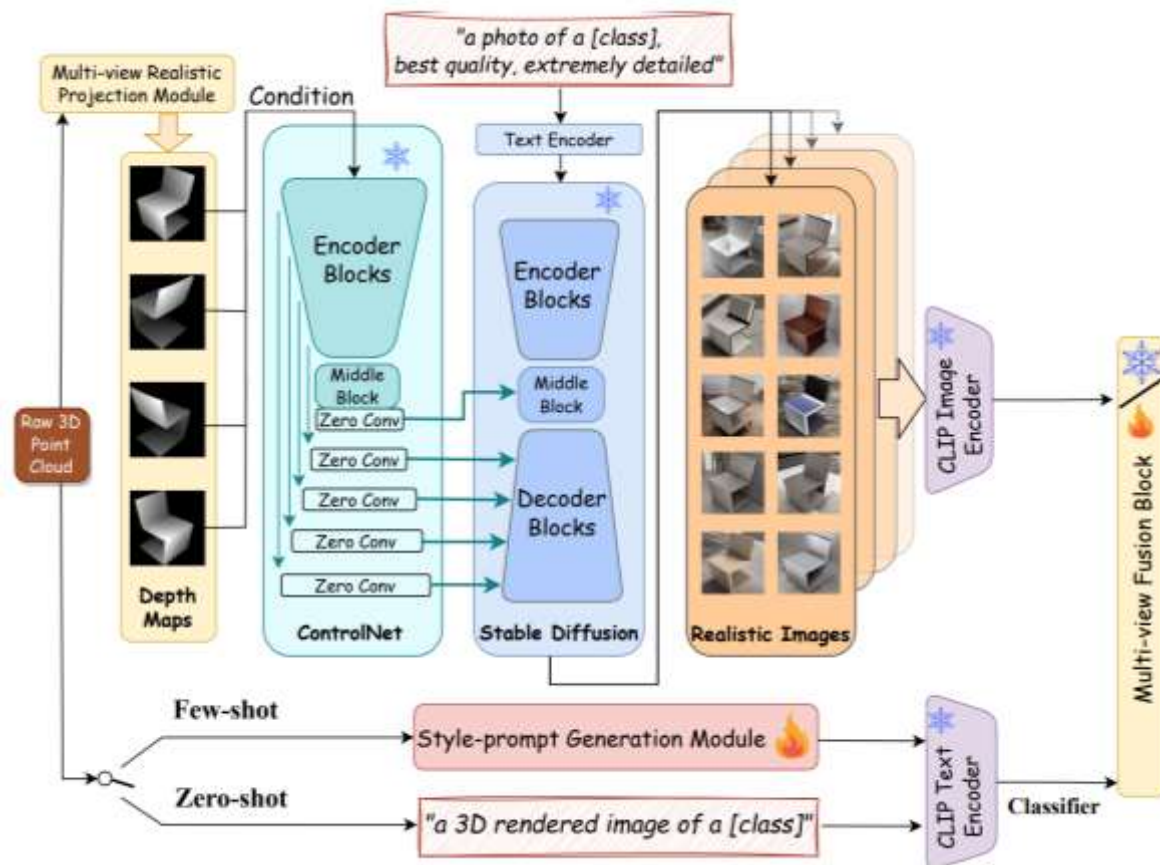
3D Vision

Unconditional Generation

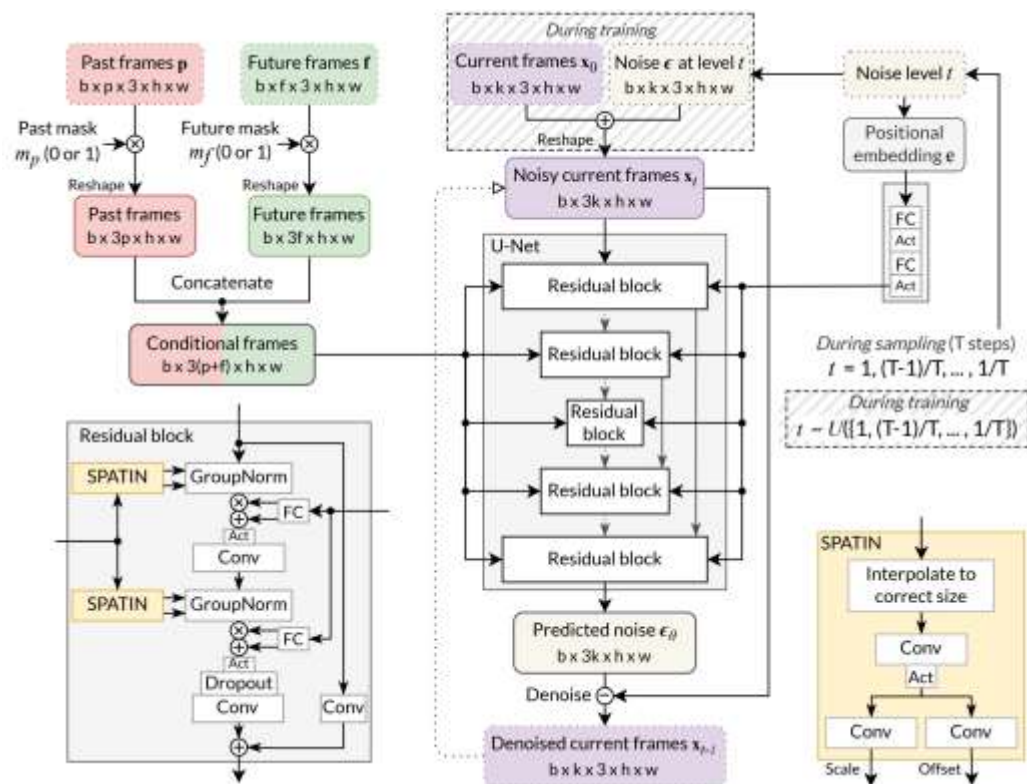


Completion

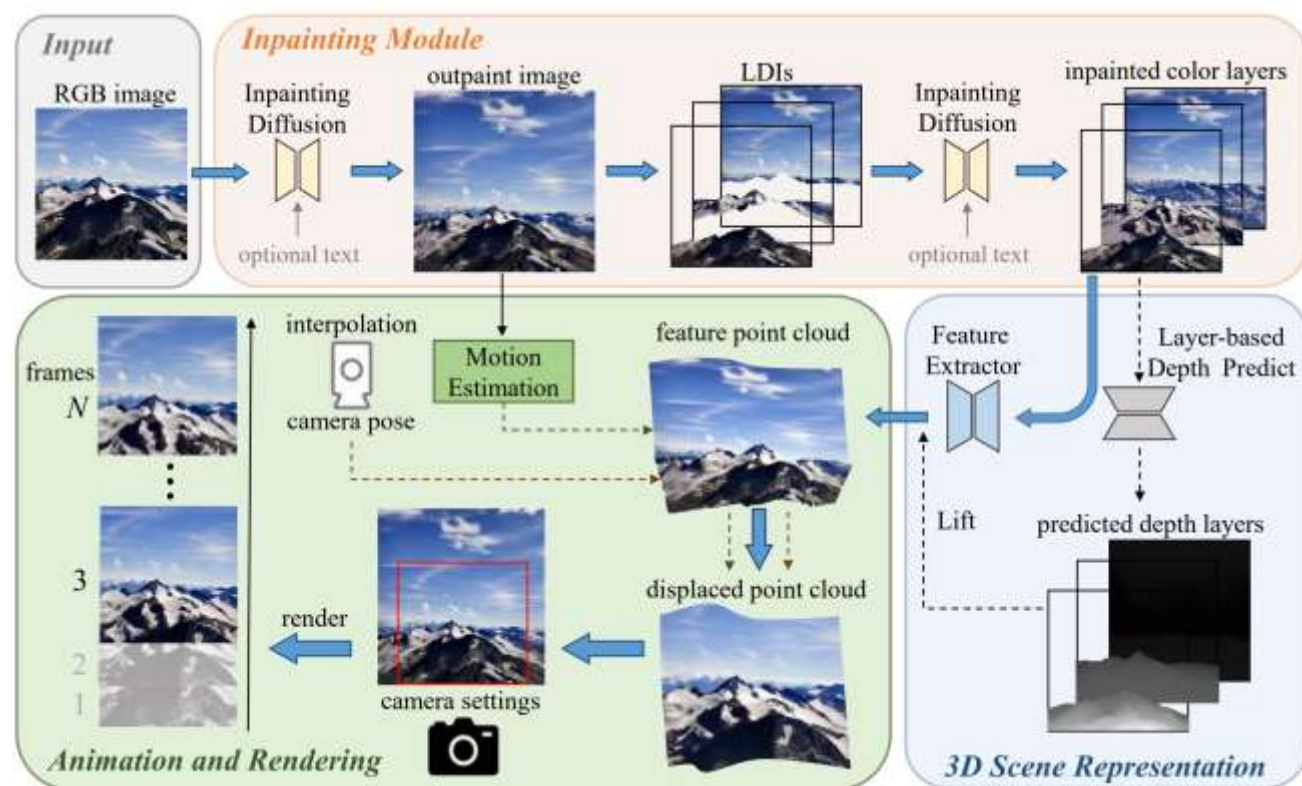
Multi-Conditional Generation



Video Modeling

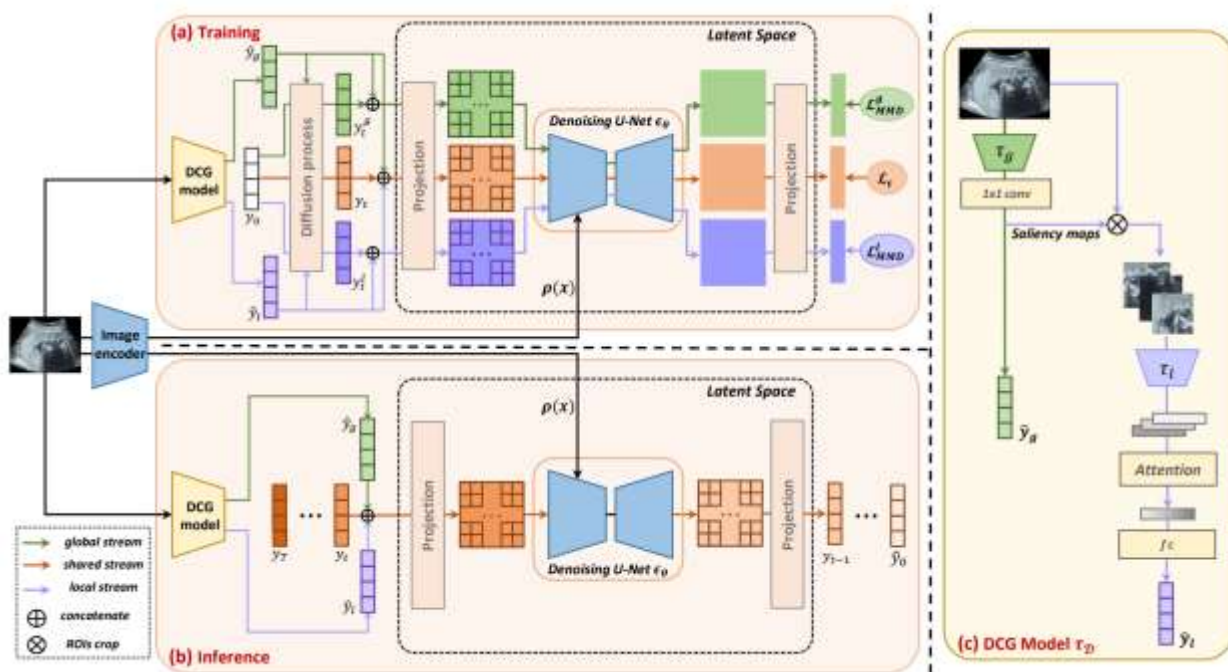


Generation



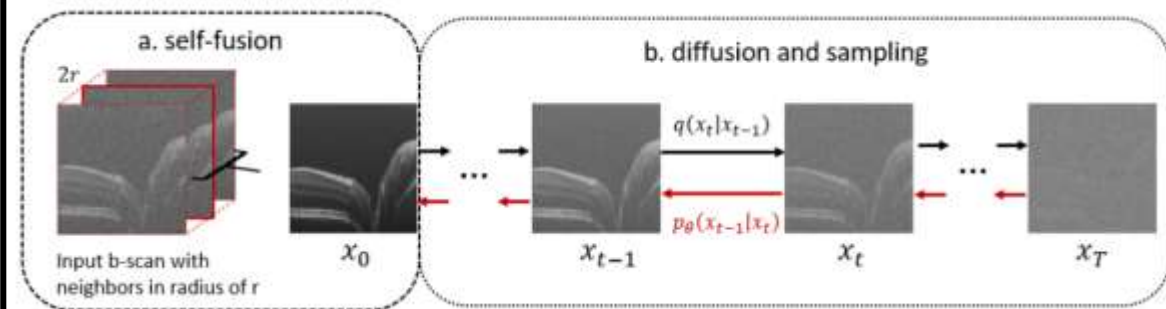
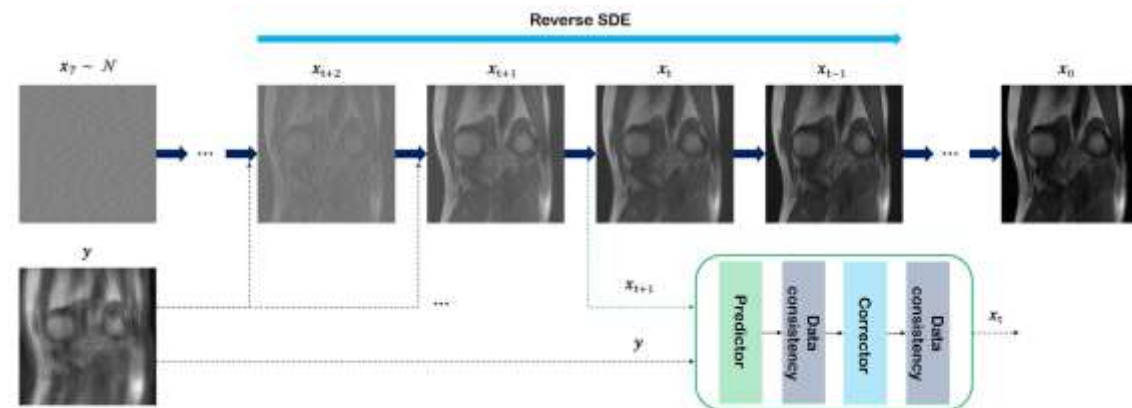
Editing

Medical Image Processing: Single Distribution



Classification

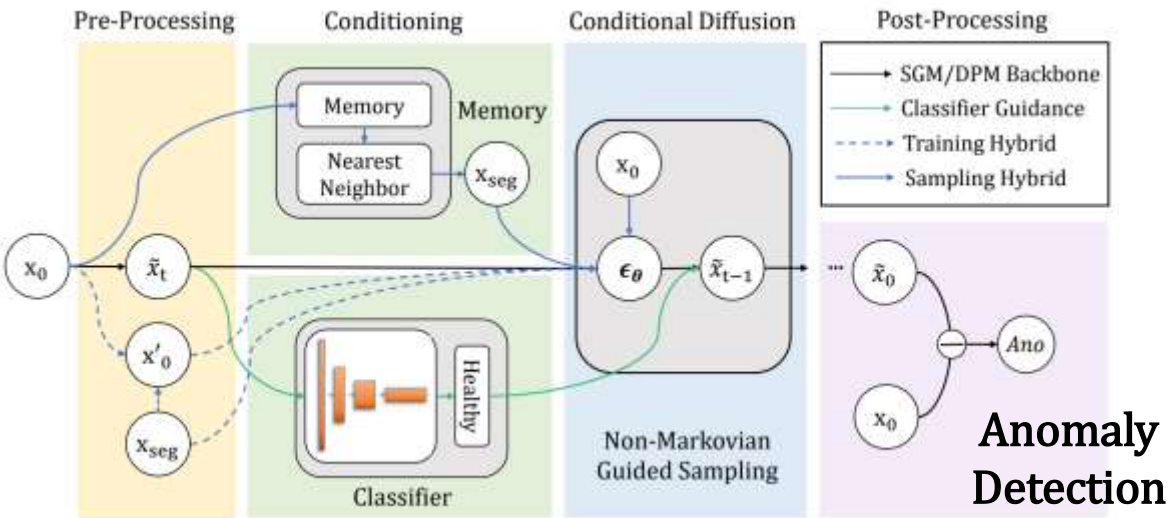
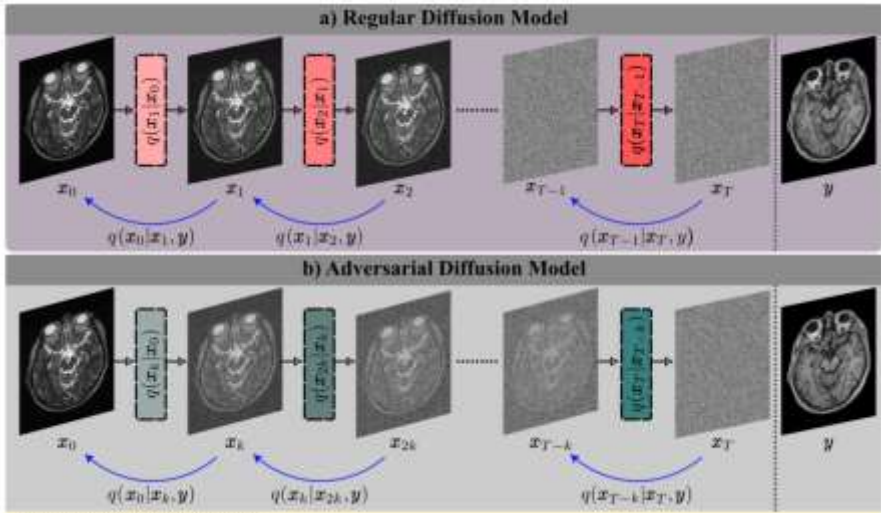
Reconstruction



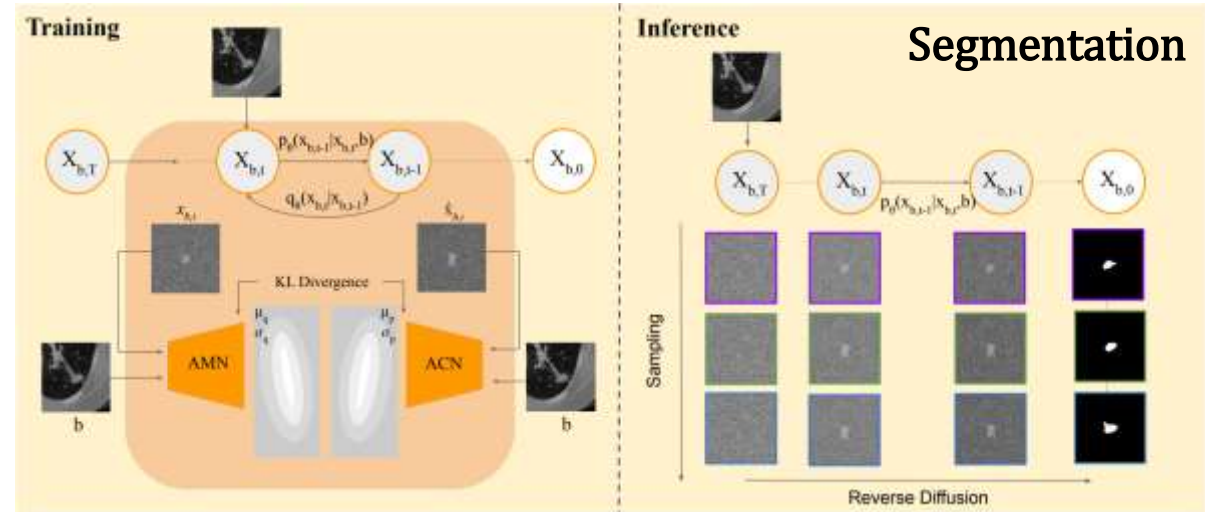
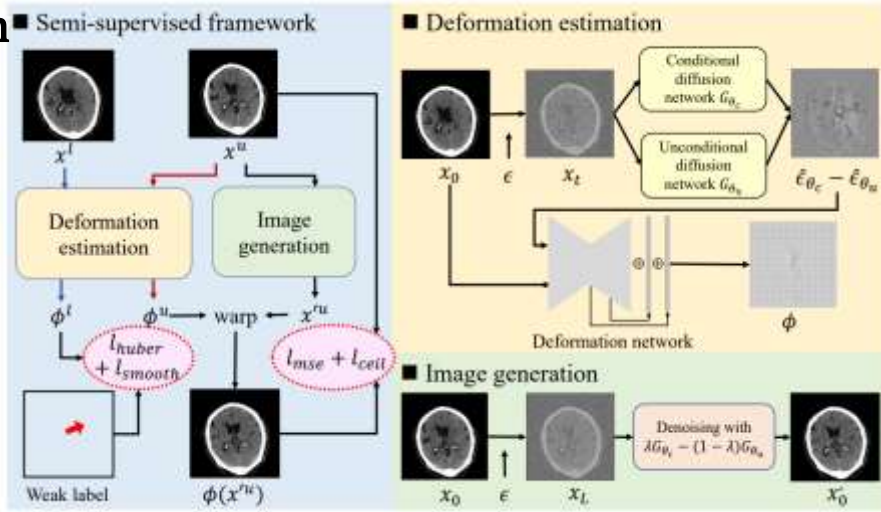
Denoising

Medical Image Processing: I2I Translation

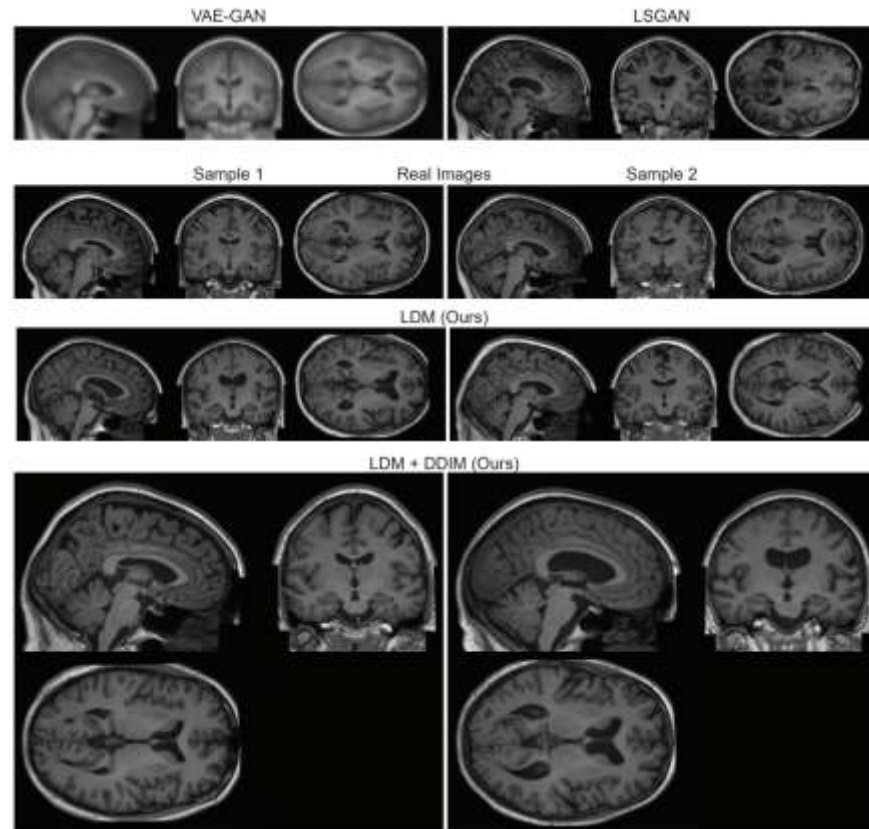
Data
Conversion



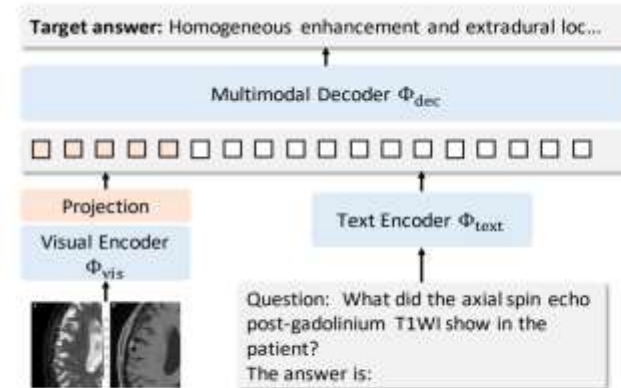
Deformation



Medical Image Processing: Applications

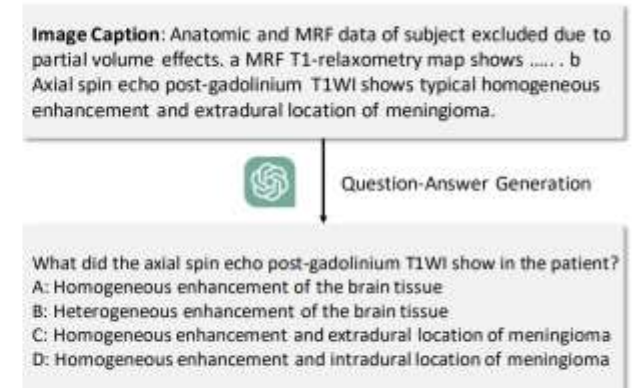


Synthesis

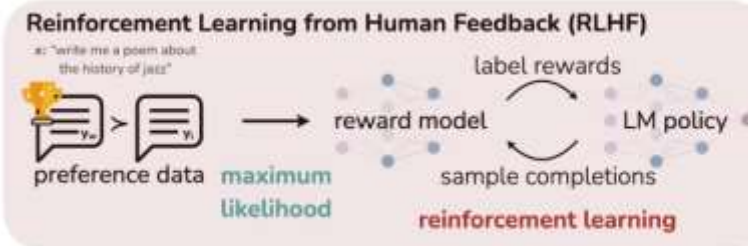


(a) Overall architecture of MedVInT

Multi-Modal System



(b) Pipeline for PMC-VQA generation



Medical GPT

Sequence Modeling: NLP

Discrete Modeling

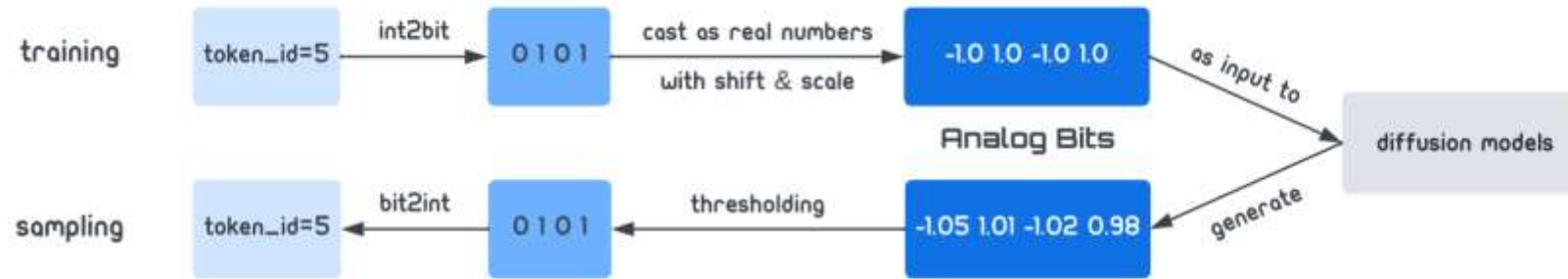
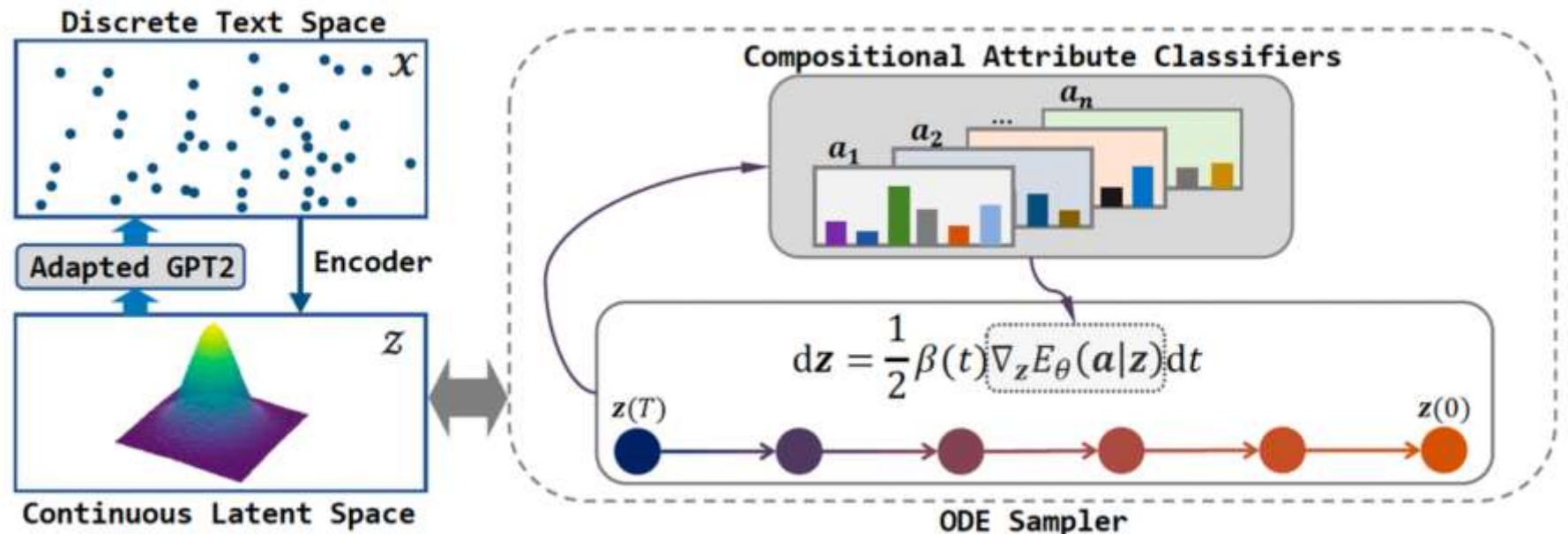


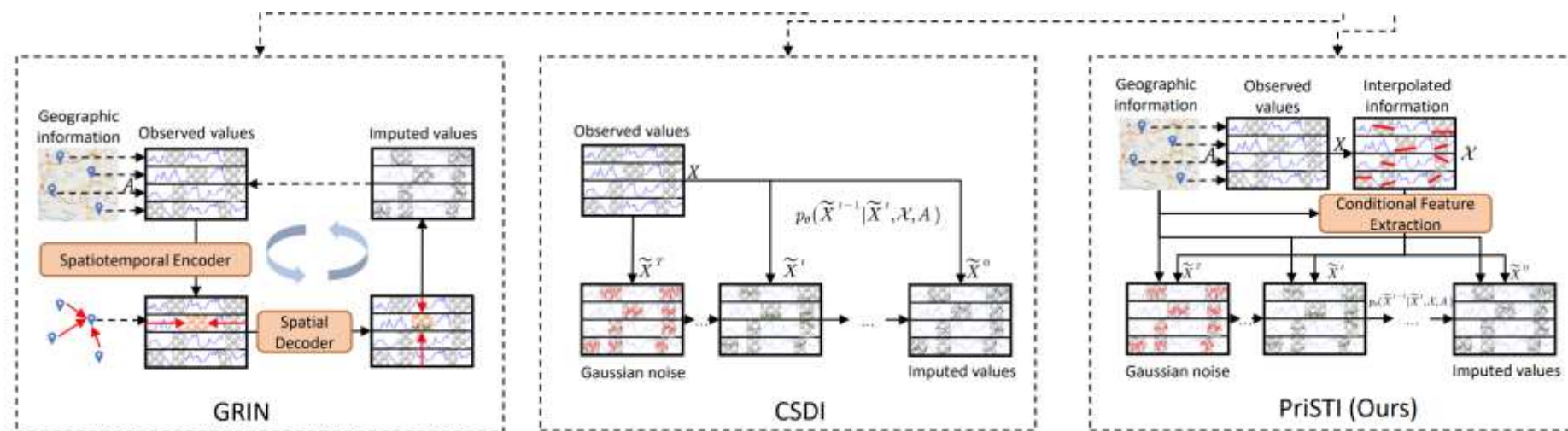
Figure 1: Bit Diffusion: modeling discrete data using continuous diffusion models with analog bits.

Latent Space Generation

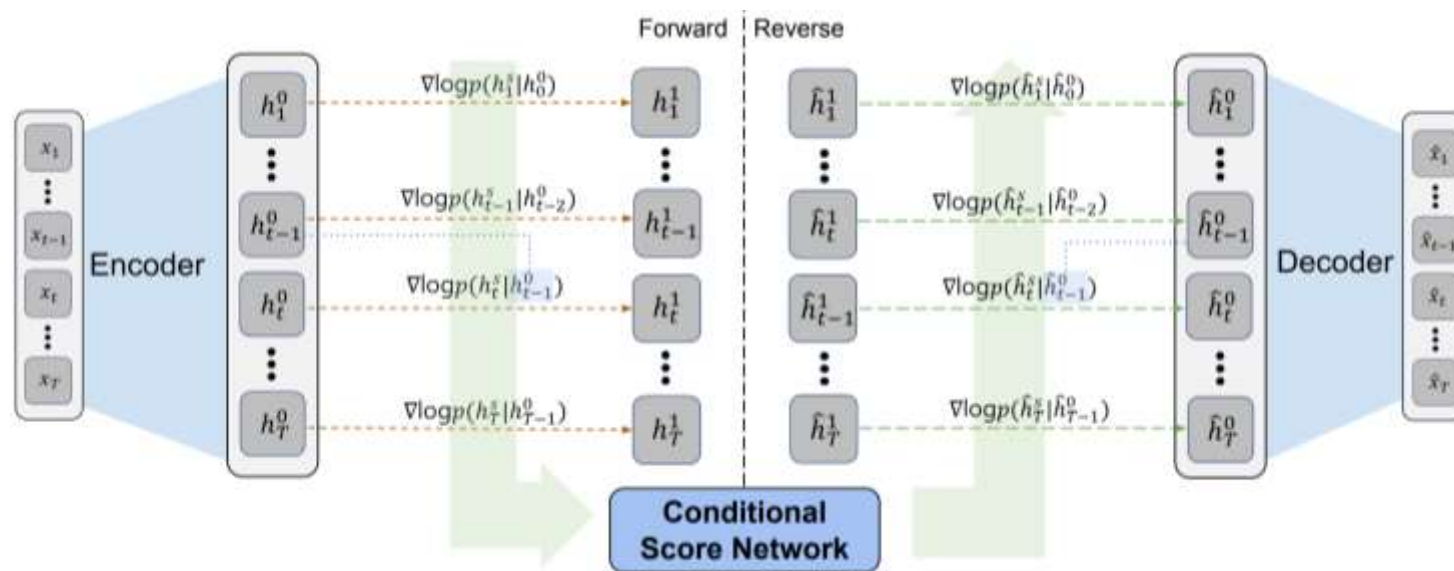


Sequence Modeling: Time Series

Imputation

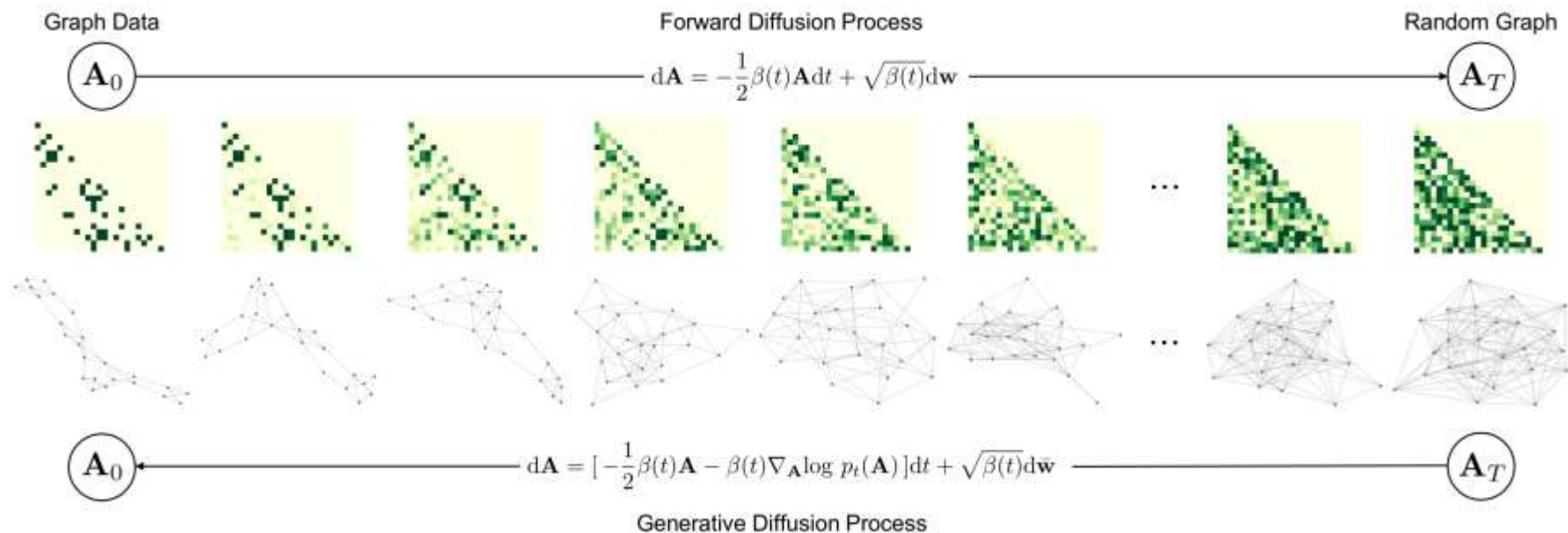
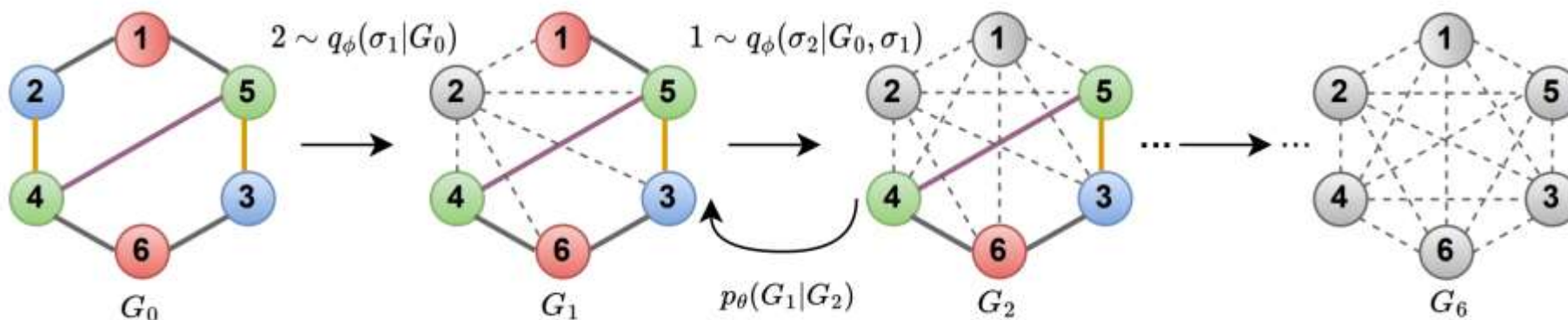


Generation



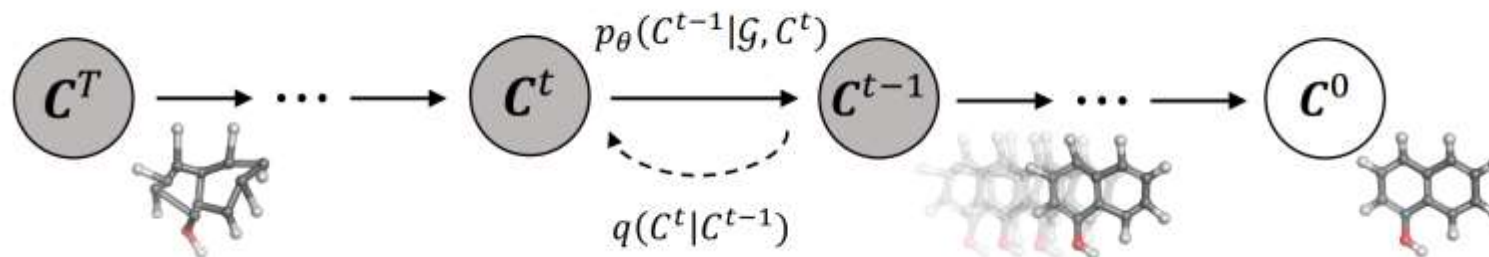
Graph Modeling: Graph

----- Masked edge ○ Masked node

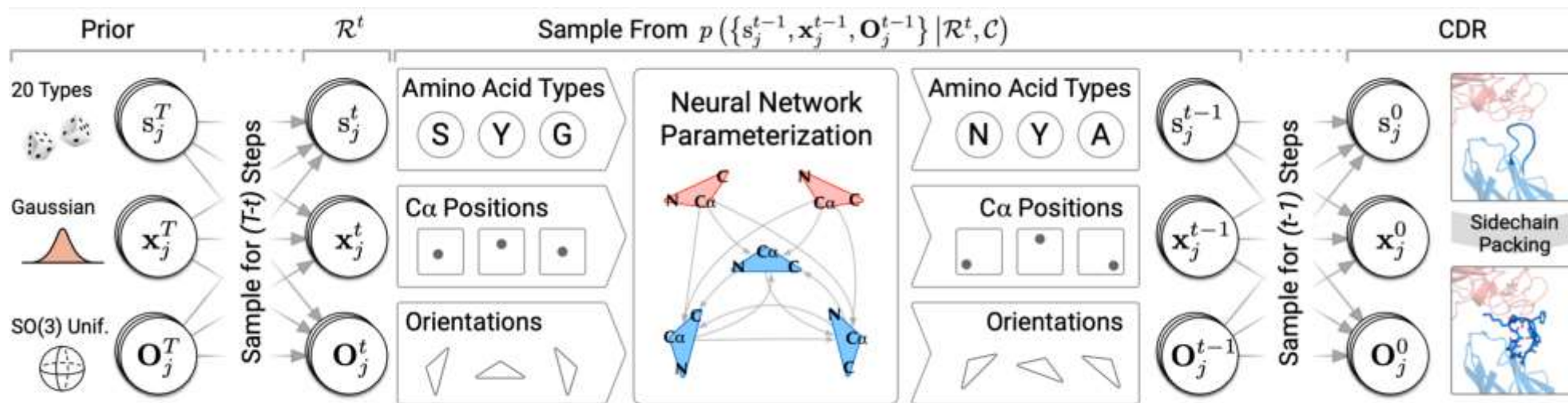


Graph Modeling: Molecular Generation

Monomer
Design



Complexes
Design



Outlines

- Brief Introduction to diffusion model
- Viewing diffusion model through generative model development
- Diffusion model basic algorithms
- Enhancing Understanding from multi-view
- Algorithm improvement
- Applications
- Further Directions and Discussions

How to equip diffusion Model?

Choose your framework

→ ODE: fast, deterministic & controllable generation

→ SDE: slow, high-fidelity and diverse sampling, unconditional generation

Data format & Model Architecture

→ Image / Discrete: UNet

→ Sequential data: Transformer, LSTM, RNN

→ Graph data: Invariant / Equivariant GNNs

How to equip diffusion Model?

Data Amount

→ Not enough: Latent diffusion, Data Augmentation, other types of generative model

Sampling Techniques

→ Unconditional: depend on the training loss (fast solver or traditional)

→ Conditional: classifier-based, pixel-level, latent space

Other Techniques

→ Domain distribution shift, early stop, distillation

Further Directions (Oct 2022):

- Attention on diffusion model class:
 - Prior distribution, transition kernel, sampling algorithm, and diffusion schemes
- Training objective & evaluation metric:
 - Evaluation mismatch, Improved objective for MLE
- Application and inductive bias:
 - Inductive bias, more practice

Further Directions (Oct 2023):

- Generation Quality & Speed:
 - Advanced distillation on ODE & SDE solvers
- Combined with Large Pre-trained Models:
 - Act as a re-generator for more diverse samples
- Cross-Modality Generation:
 - Aligning latent features from multiple modalities

Further Directions (Oct 2023):

- AIGC Era:
 - Generating highly reliable data for training enhancement
 - Generating Out-Of-Distribution samples for exploration and attack-defense
- Combined with other fields of ML:
 - Semi-supervised learning: generated data w./w.o labels ,
 - Reinforcement learning: reinforcement-guided sampling
 - Domain Transfer: cross-domain generation

Useful Resources

- Paper source:

<https://github.com/diff-usion/Awesome-Diffusion-Models>

- Codebases on huggingface:

<https://huggingface.co/docs/diffusers/index>

- Chinese version of detailed introduction:

<https://spaces.ac.cn/author/1/5/>

- Great Labs:

<https://scholar.google.com/citations?user=axsP38wAAAAJ&hl=zh-CN>

<https://scholar.google.com/citations?user=Ao4gtsYAAAAJ&hl=en>

https://scholar.google.co.uk/citations?user=o_J2CroAAAAJ&hl=en

Finally: Thanks for listening

Paper: <https://arxiv.org/abs/2209.02646>

GitHub: <https://github.com/chq1155/A-Survey-on-Generative-Diffusion-Model>

Be a contributor, Involve in diffusion research,
conduct diffusion applications!



Thanks for listening
and discussion!