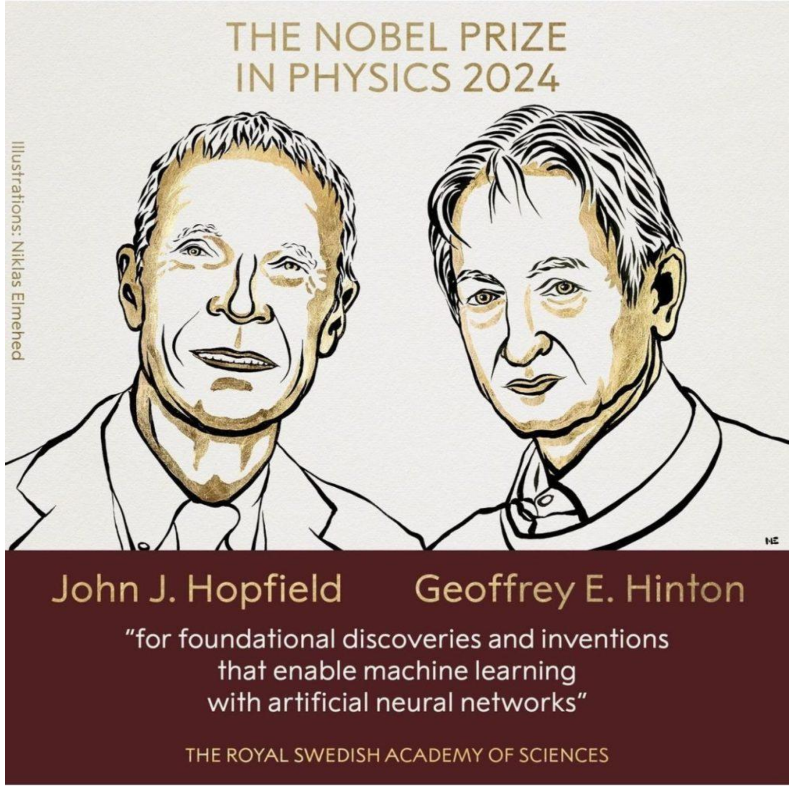
Probabilistic Foundation and Opportunities of Diffusion Models

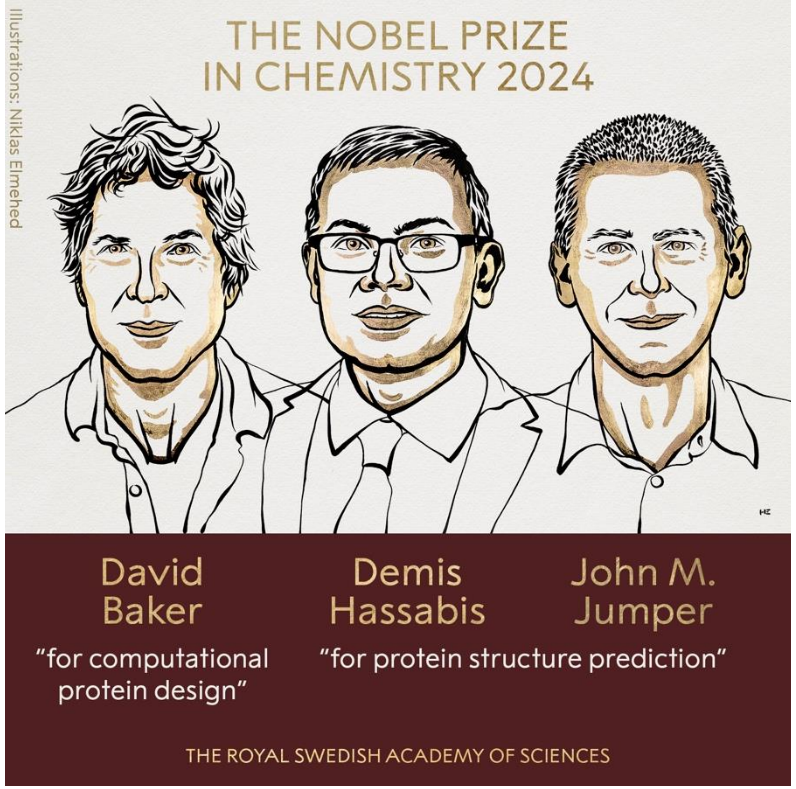
Mengdi Wang & Minshuo Chen

PRINCETON UNIVERSITY

Northwestern University

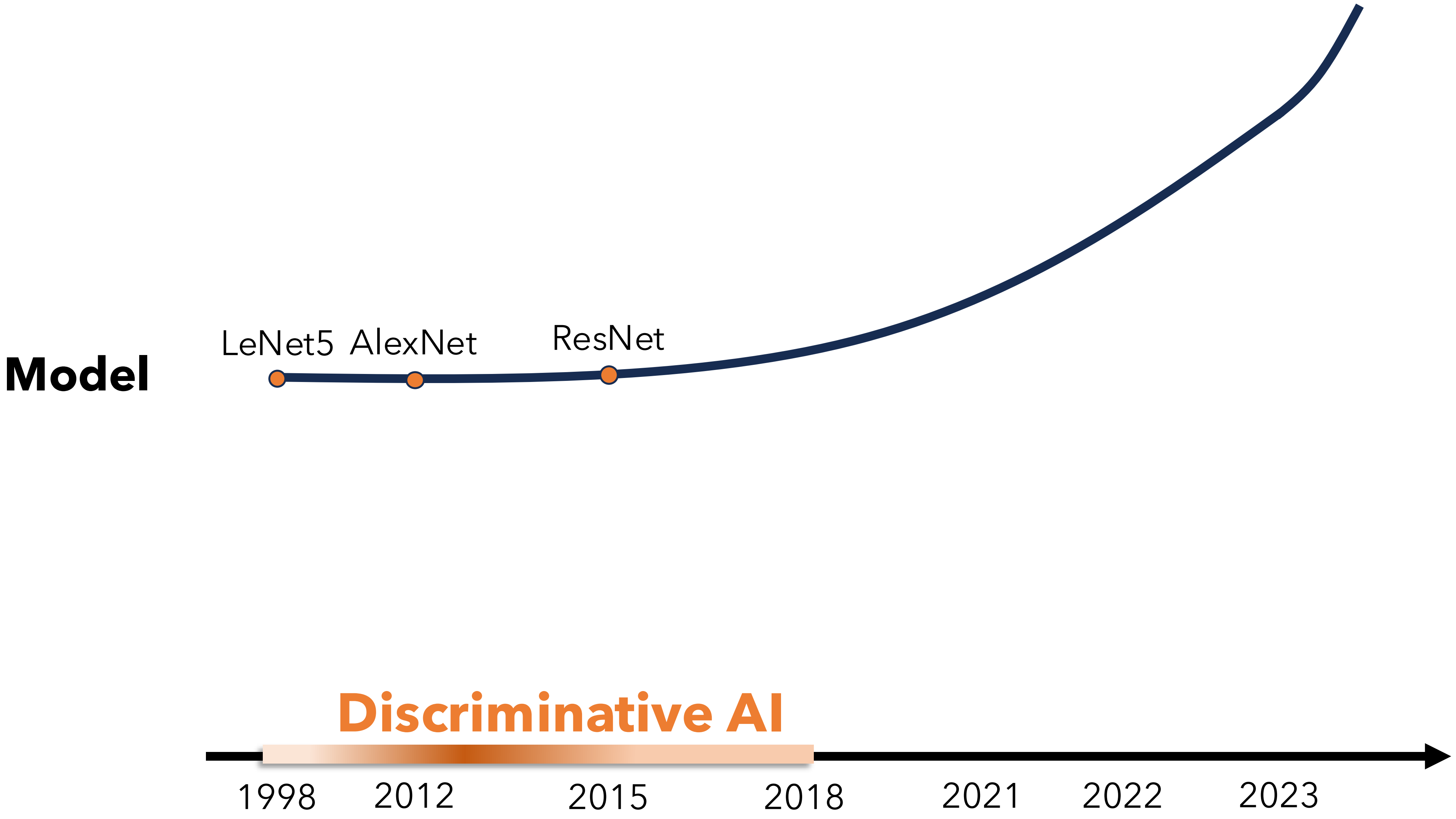
AI Comes to The Nobels





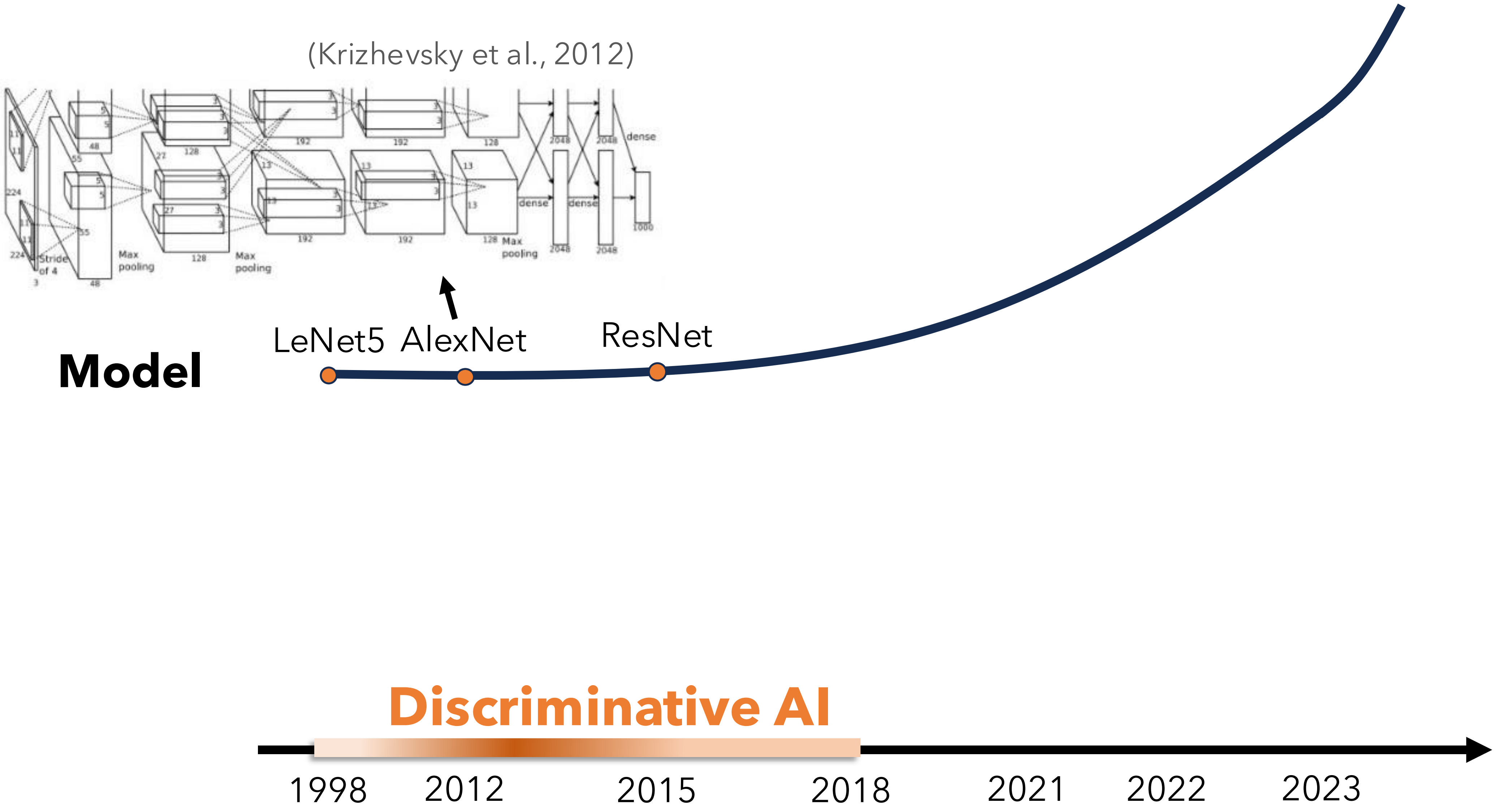
"For me, this story highlights how far **AI** has come and how much more potential there is to explore."

Millennium Growth of AI



-- Thanks to blogs by Rockwell Anyoha , Toloka Team and Rick Merritt

Millennium Growth of AI



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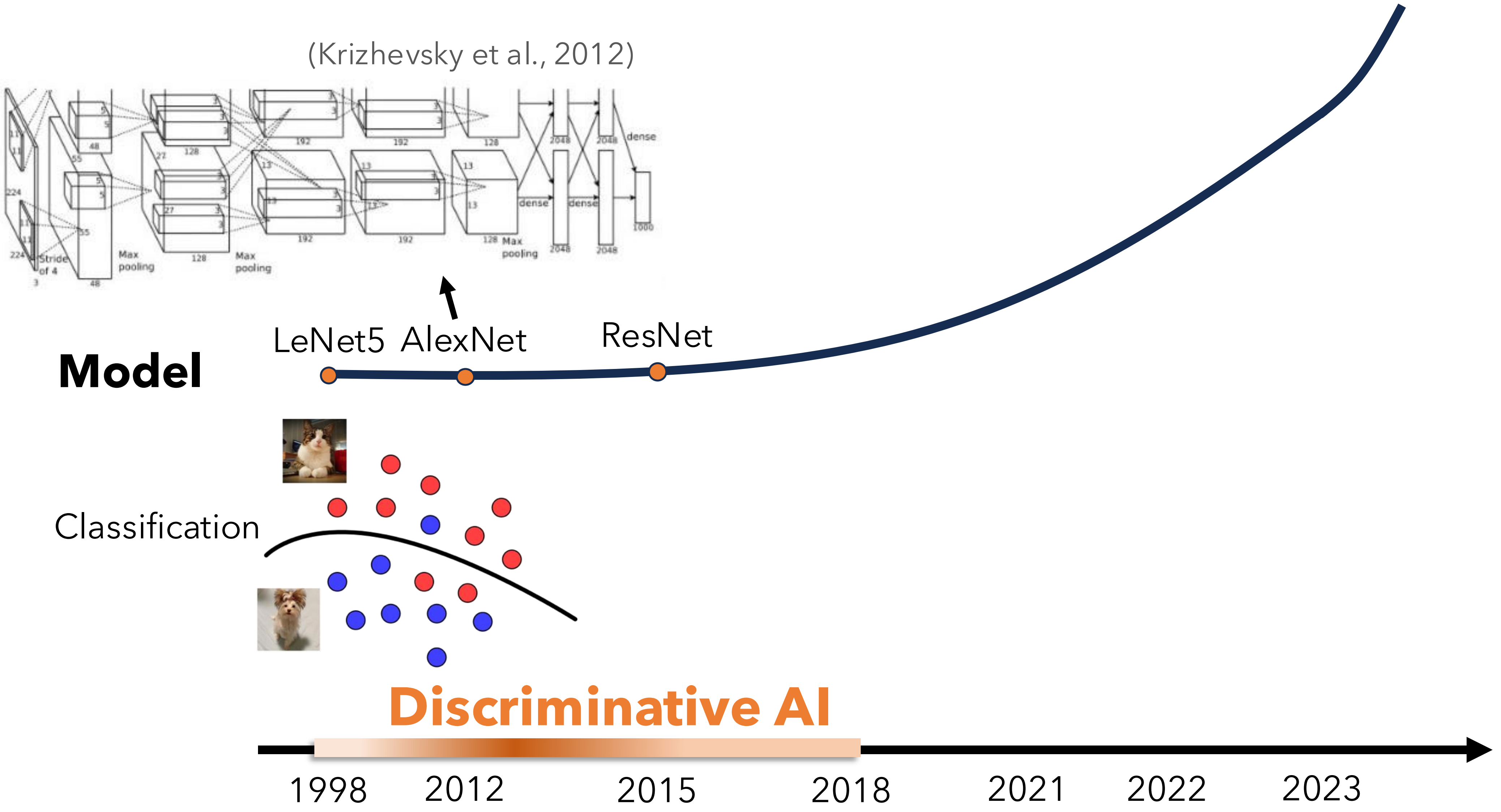

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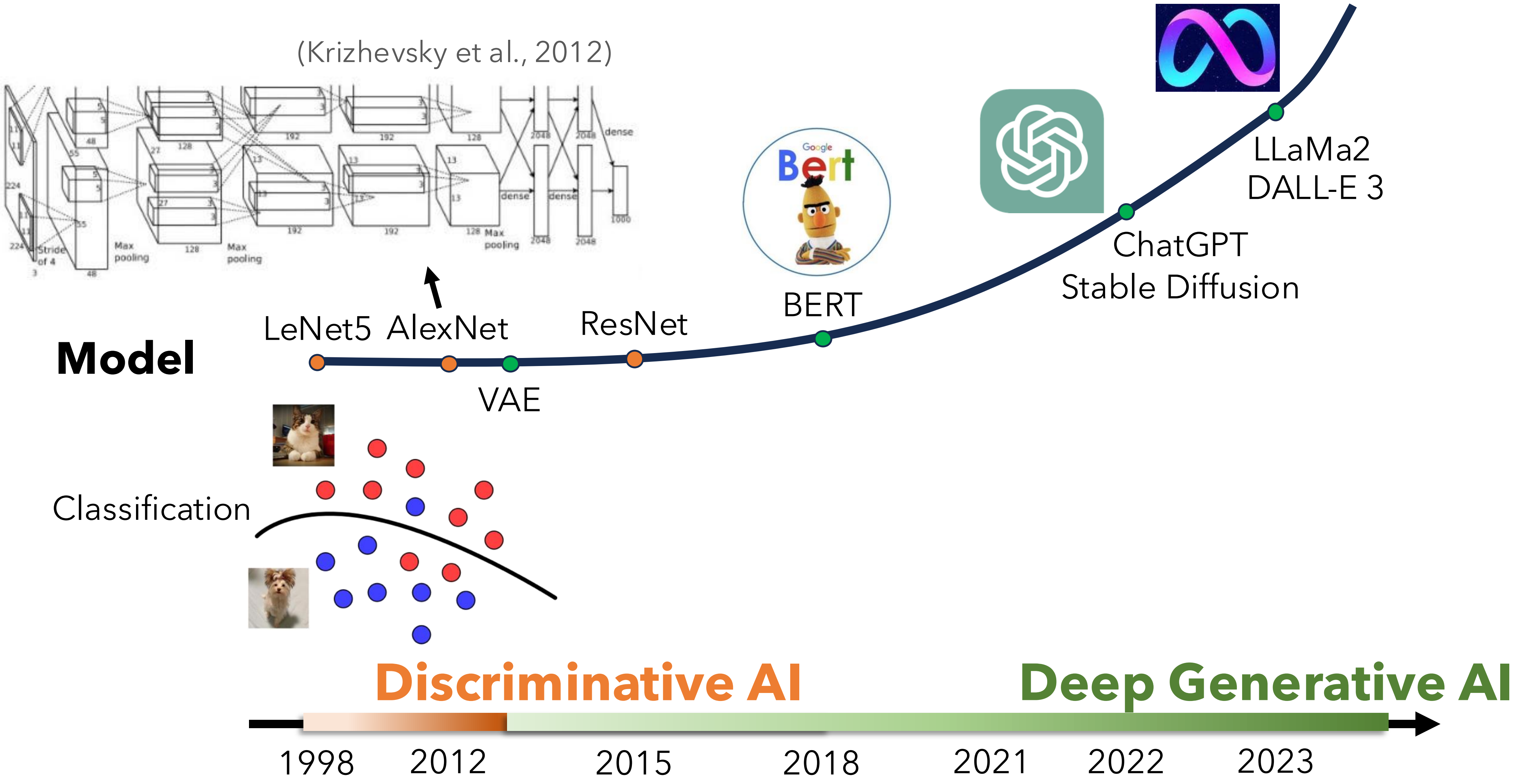

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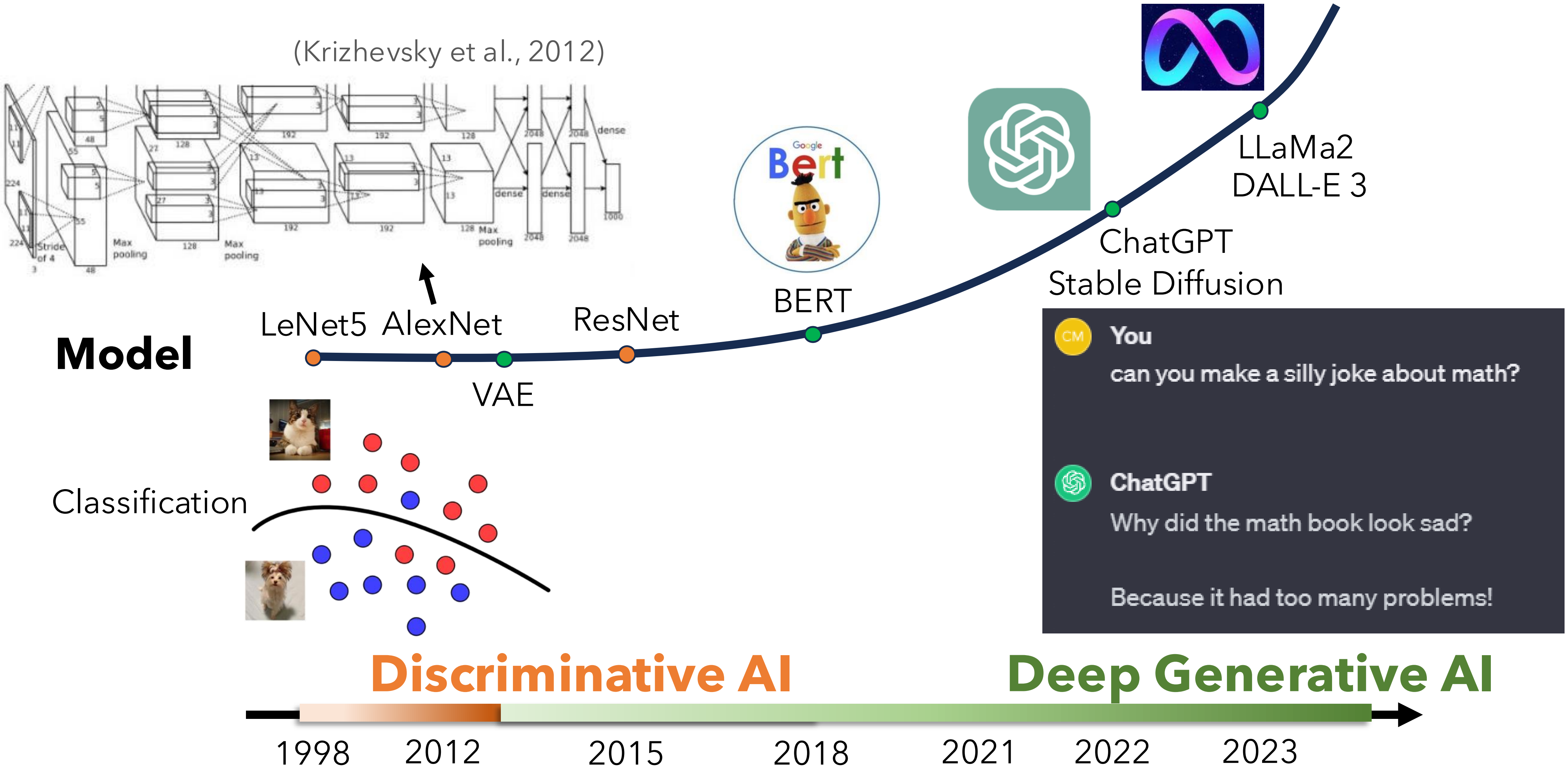

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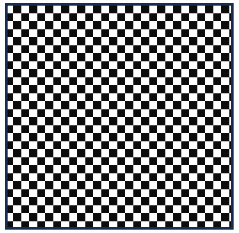
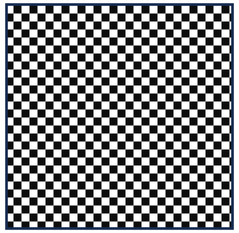
Transformative Power of Deep Generative AI

Noise   **Generative AI**

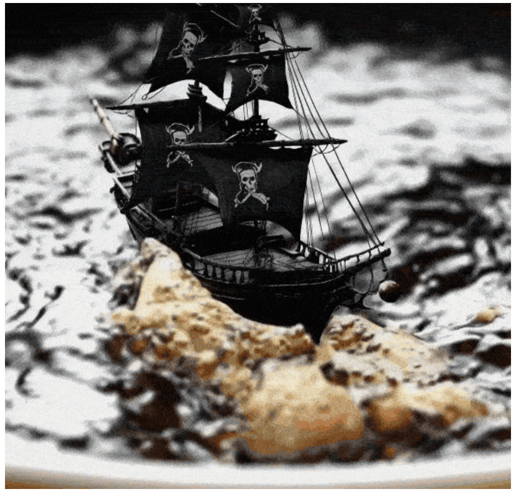
Transformative Power of Deep Generative AI

Noise   **Generative AI**

ChatGPT

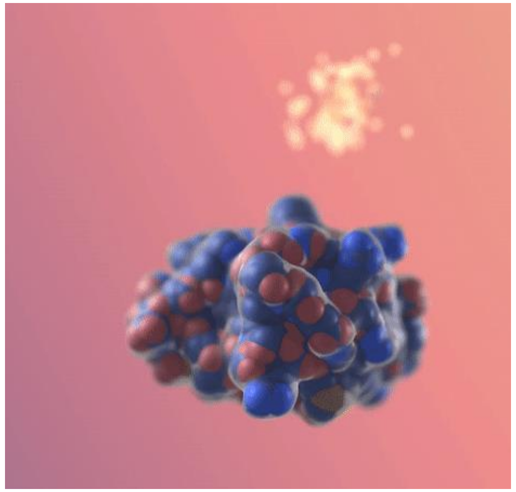
Language

Sora



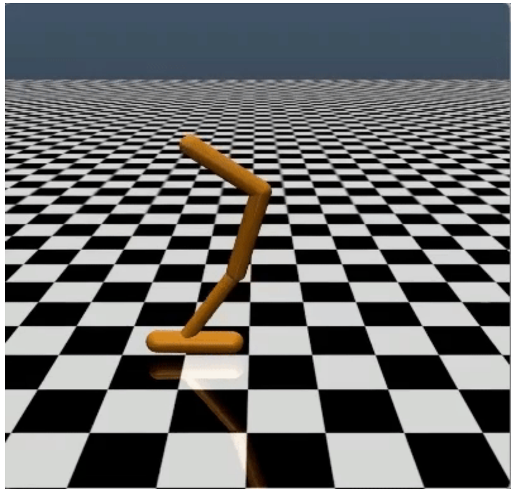
Video

RFDiffusion



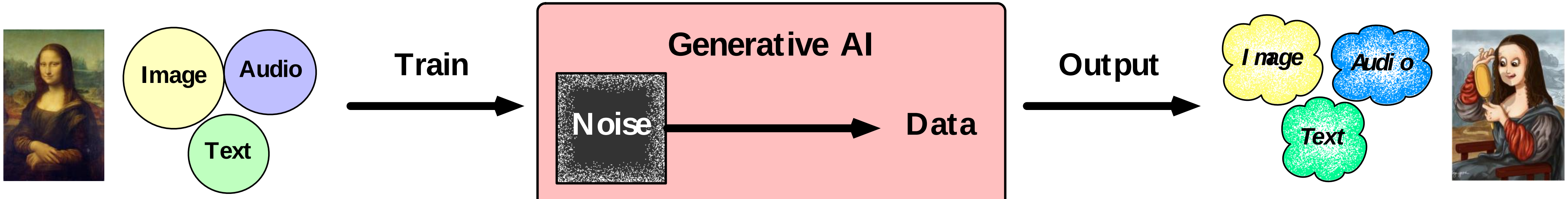
Biology

Decision Diffuser

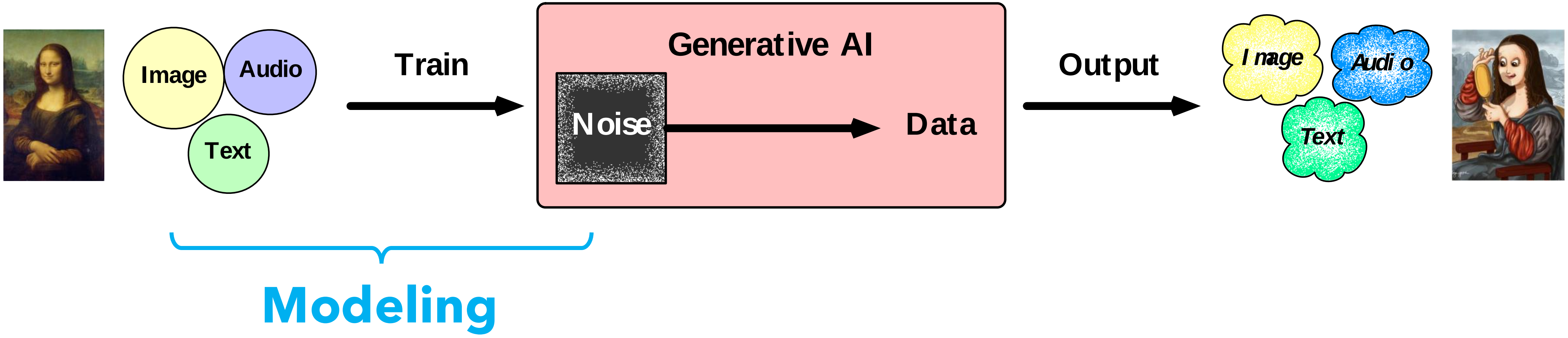


RL/control

Constitution of Deep Generative AI

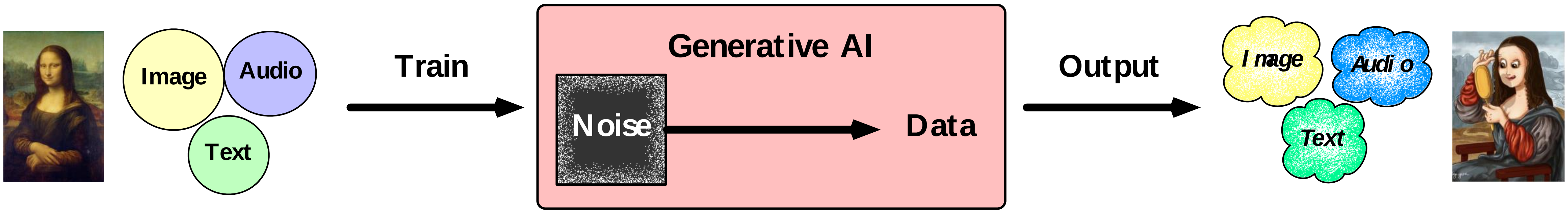


Constitution of Deep Generative AI



$$P(\cdot), P(\cdot|y)$$

Constitution of Deep Generative AI



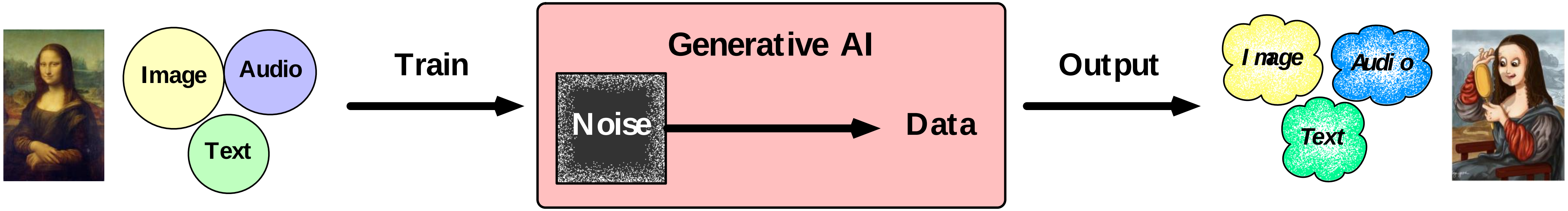
Modeling

$$P(\cdot), P(\cdot|y)$$

Sampling

$$x \sim P(\cdot), P(\cdot|y)$$

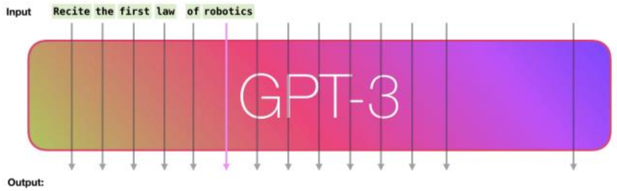
Constitution of Deep Generative AI



Modeling

$$P(\cdot), P(\cdot|y)$$

Autoregressive

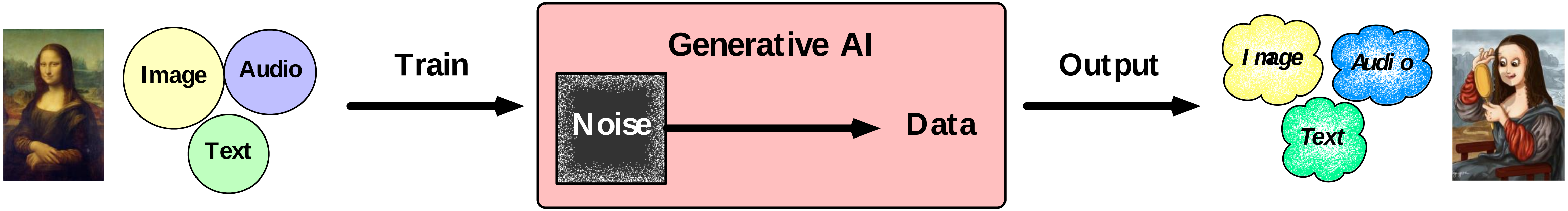


Sampling

$$x \sim P(\cdot), P(\cdot|y)$$

Autoregressive

Constitution of Deep Generative AI



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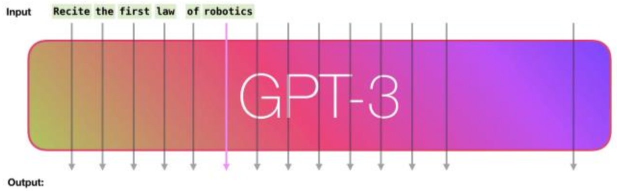
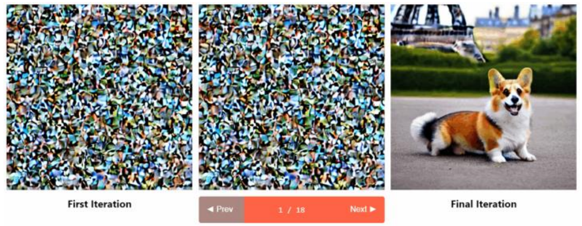


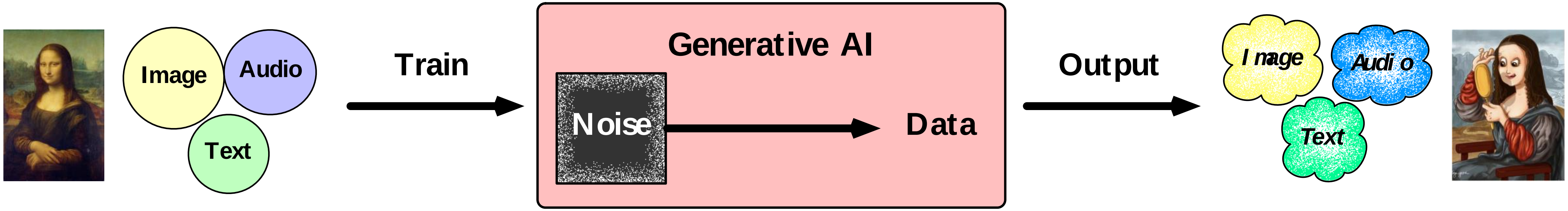
Autoregressive

Diffusion



Denoising

Constitution of Deep Generative AI



Modeling

$$P(\cdot), P(\cdot|y)$$

Sampling

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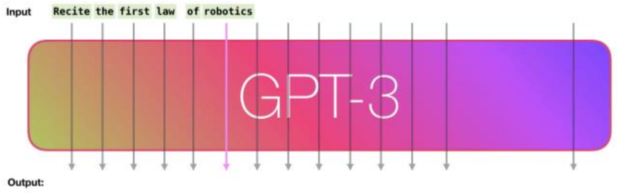
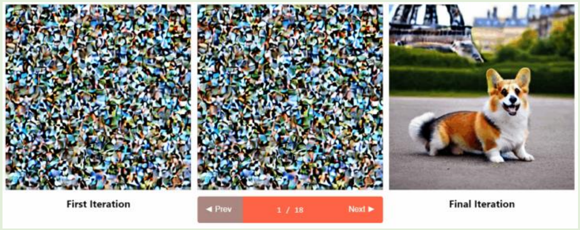
Autoregressive



Autoregressive

Diffusion



Denoising

New Promises of Diffusion Models

New Promises of Diffusion Models

Diffusion Models Beat GANs on Image Synthesis

Prafulla Dhariwal*
OpenAI
prafulla@openai.com

Alex Nichol*
OpenAI
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Score-Based Generative Modeling through Stochastic Differential Equations

Yang Song*

durk@google.com

abhishk@google.com

Stefano Ermon
Stanford University
ermon@cs.stanford.edu

Ben Poole
Google Brain
pooleb@google.com

colorization. Combined with multiple architectural improvements, we achieve $\boxed{\text{record-breaking performance}}$ for unconditional image generation on CIFAR-10 with an Inception score of 9.89 and FID of 2.20, a competitive likelihood of 2.99

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Diffusion Models Beat GANs on Image Synthesis

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SCORE-BASED GENERATIVE MODELING THROUGH STOCHASTIC DIFFERENTIAL EQUATIONS

Yang Song* Stanford Uni…

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Stefano Ermon Stanford University ermon@cs.stanford.edu

Ben Poole Google Brain pooleb@google.com

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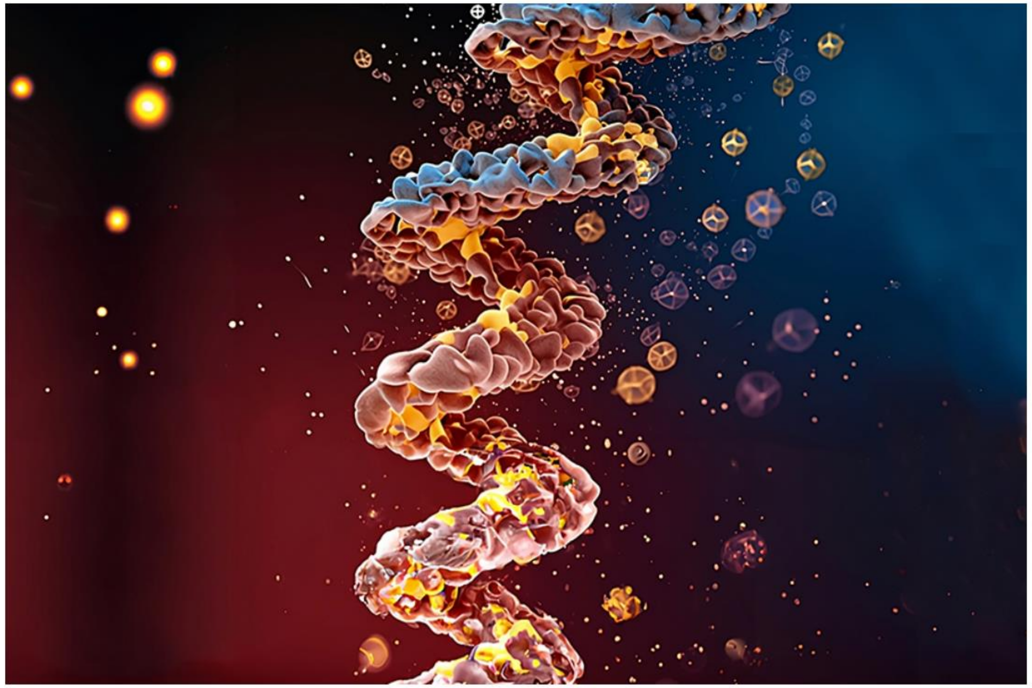
New Promises of Diffusion Models

Generative AI imagines new protein structures

"FrameDiff" is a computational tool that uses generative AI to craft new protein structures, with the aim of accelerating drug development and improving gene therapy.

Rachel Gordon | MIT CSAIL
July 12, 2023



Biology is a wondrous yet delicate tapestry. At the heart is DNA, the master weaver that encodes proteins, responsible for orchestrating the many biological functions that sustain life within the human body. However, our body is akin to a finely tuned instrument, susceptible to losing its harmony. After all, we're faced with an ever-changing and relentless natural world: pathogens, viruses, diseases, and cancer.

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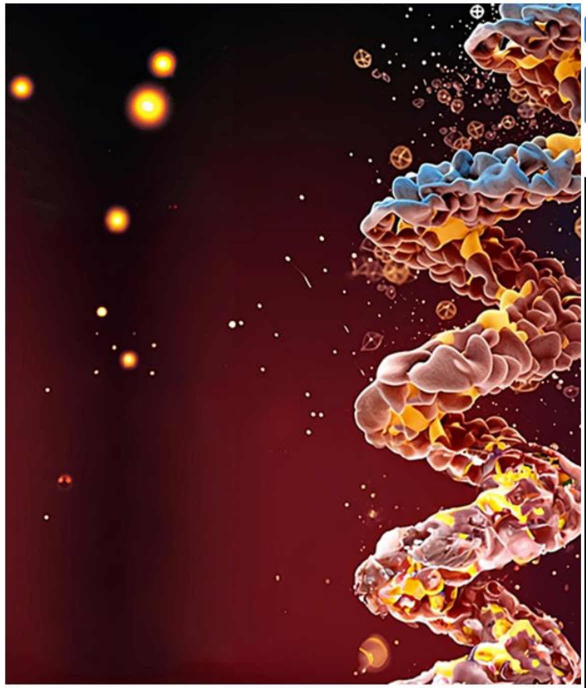

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Diffusion models are now turbocharging reinforcement learning systems

By **Ben Dickson** - March 4, 2024

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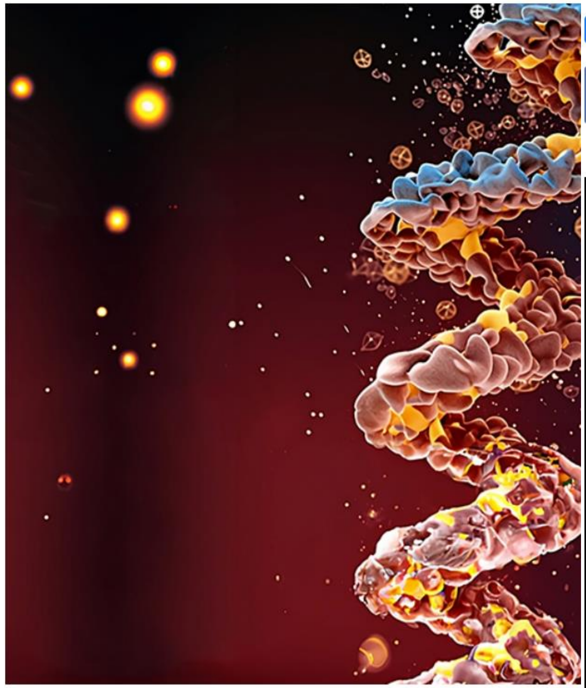

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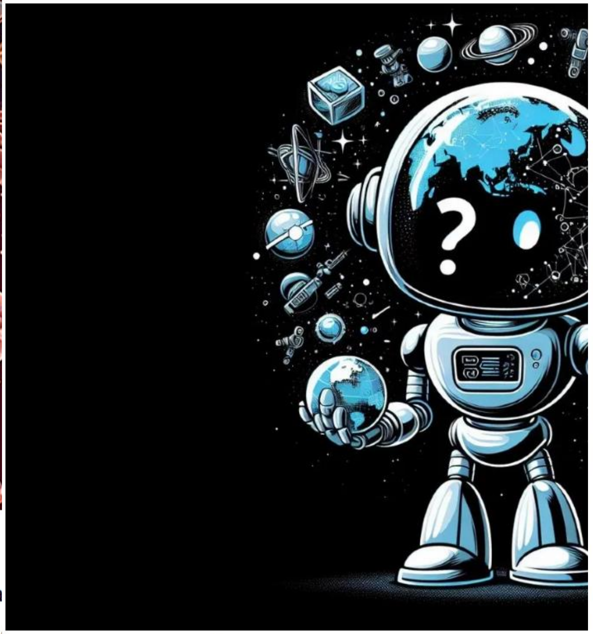

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ARTIFICIAL INTELLIGENCE

AniPortrait: Audio-Driven Synthesis of Photorealistic Portrait Animation

Published 3 days ago on May 3, 2024
By **Kunal Kejriwal**

Over the years, the creation of realistic and expressive portraits animations from static images and audio has found a range of applications including gaming, digital media, virtual reality, and a lot more. Despite its potential application, it is still difficult for developers to create frameworks capable of generating high-quality animations that maintain temporal consistency and are visually captivating. A major cause for the complexity is the need for intricate coordination of lip movements, head positions, and facial expressions to craft a visually compelling effect.

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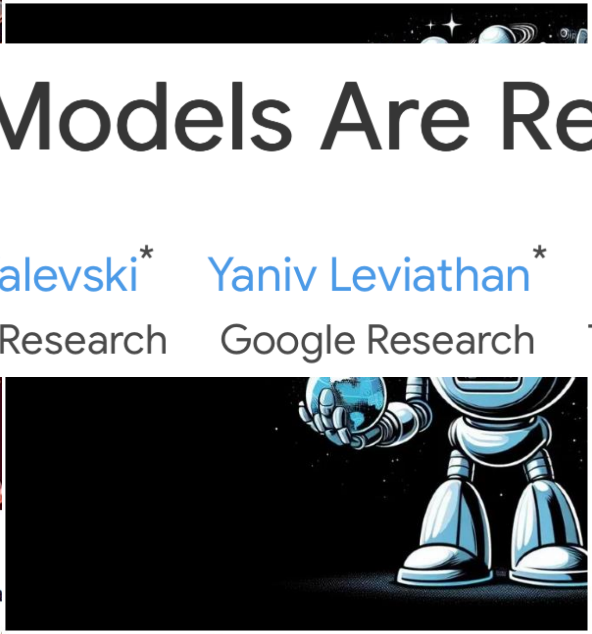

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Diffusion Models Are Real-Time Game Engines

Dani Valevski* Yaniv Leviathan* Moab Arar*† Shlomi Fruchter*
Google Research Google Research Tel Aviv University Google DeepMind

Outline

- A probabilistic foundation for diffusion models
- How diffusion models capture diverse data
- How to leverage diffusion models
- Inspirations and future directions

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Chen et al., “Challenges and Opportunities of Diffusion Models for Generative AI”, NSR 2024

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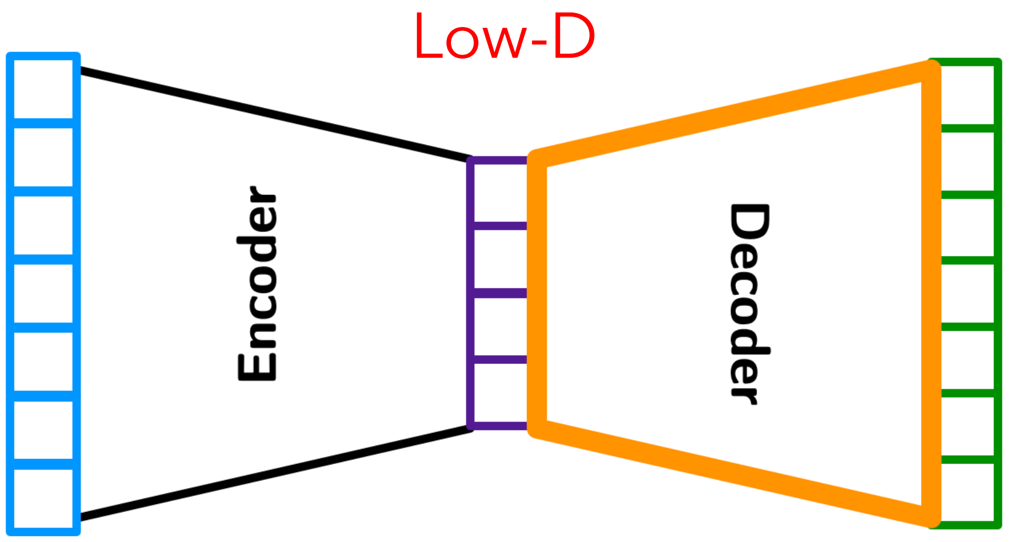
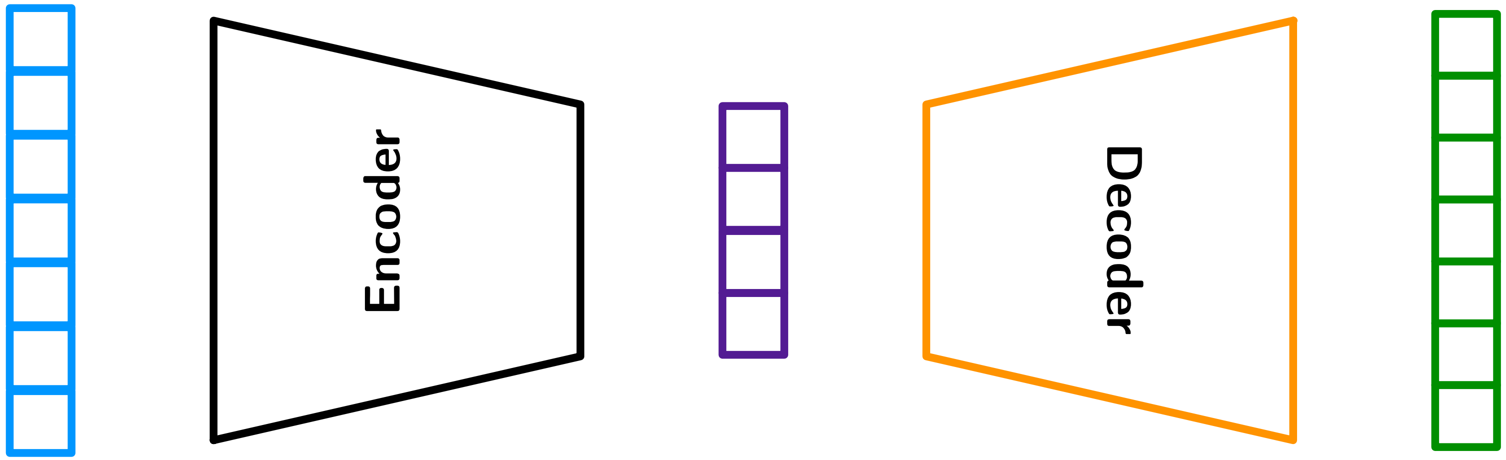
Foundation of Diffusion Models

Early Model of Deep Generative AI



VAE (Kingma & Welling, 2013)

Dissemble VAE



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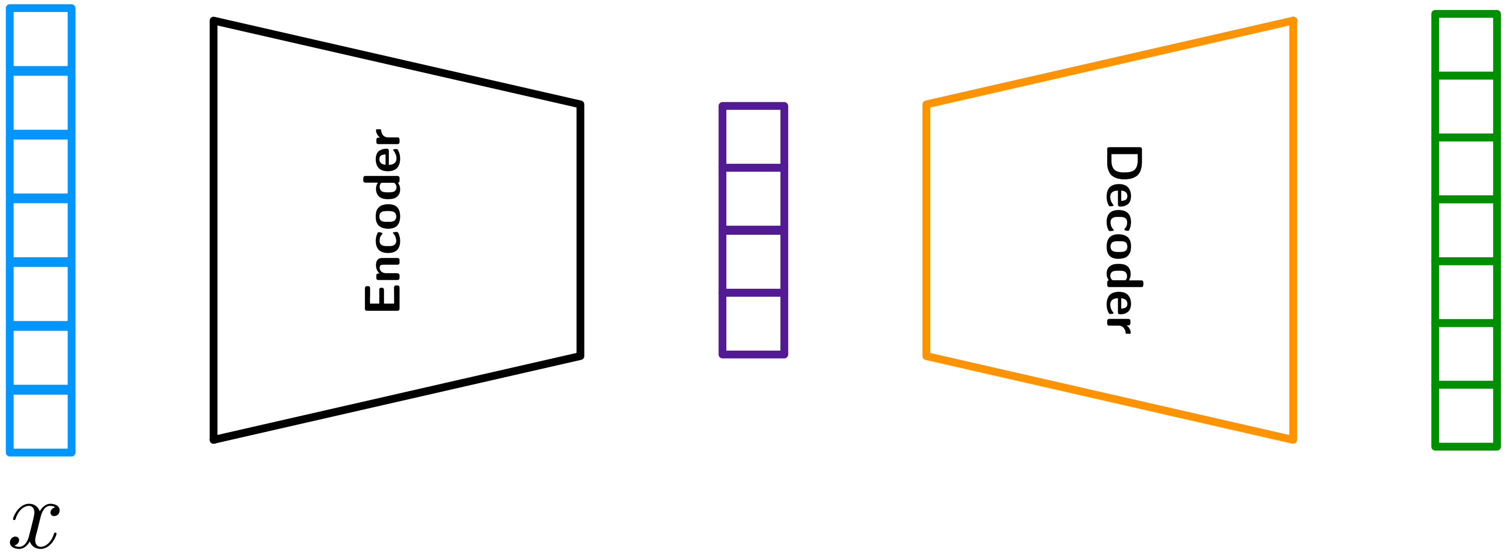

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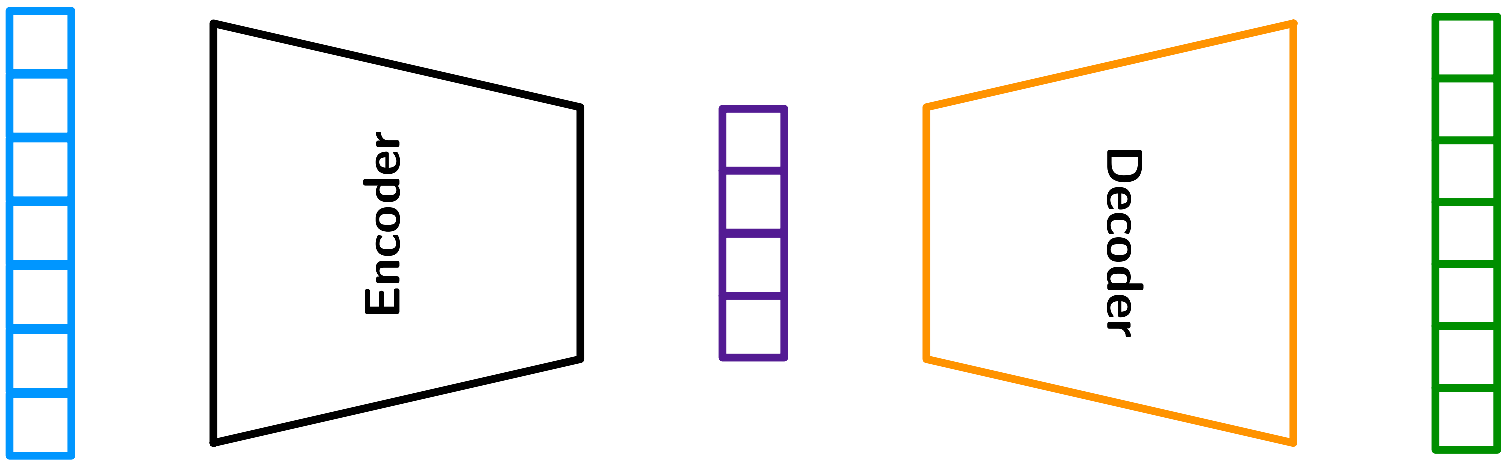
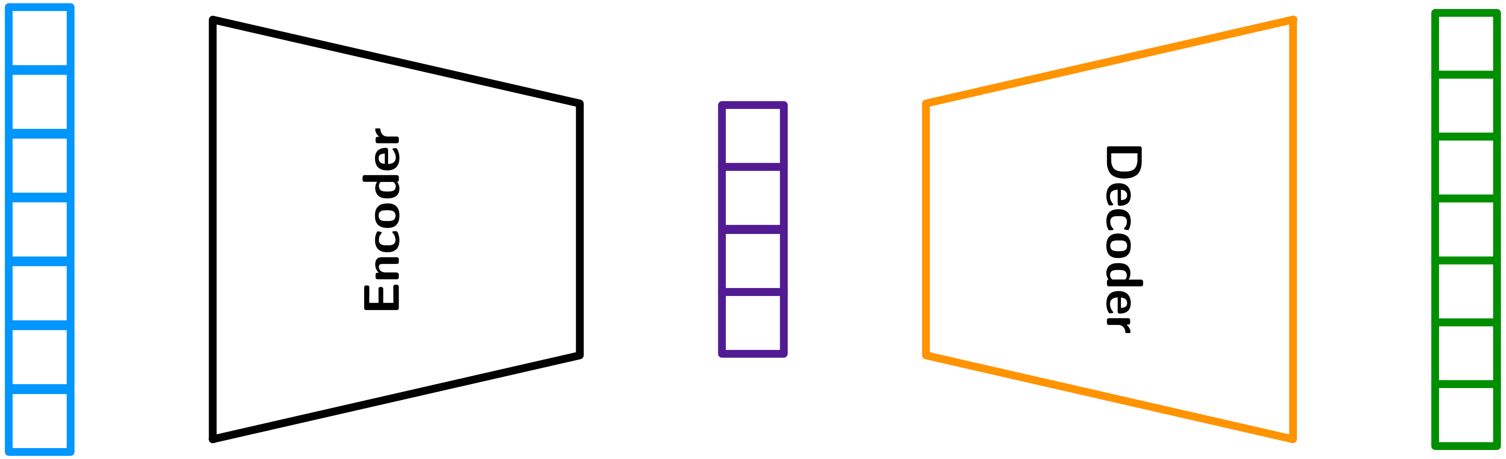


$$x \longrightarrow p(z|x) \longrightarrow z$$

Dissemble VAE

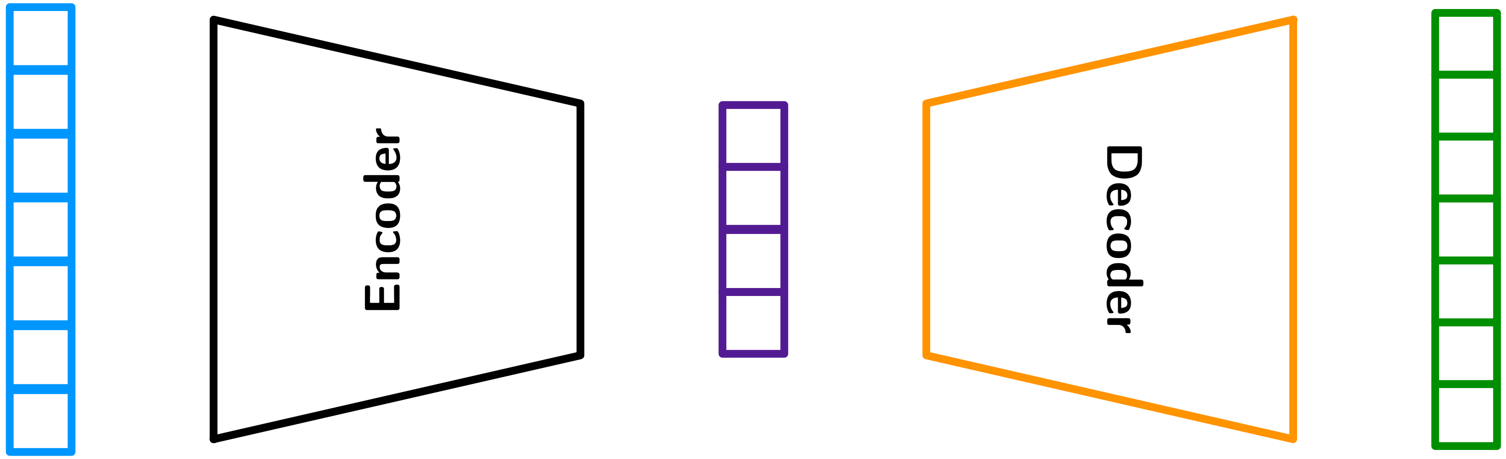


$x \longrightarrow p(z|x) \longrightarrow z$

$\wr$

$\mathrm{N}(0, I)$

Dissemble VAE

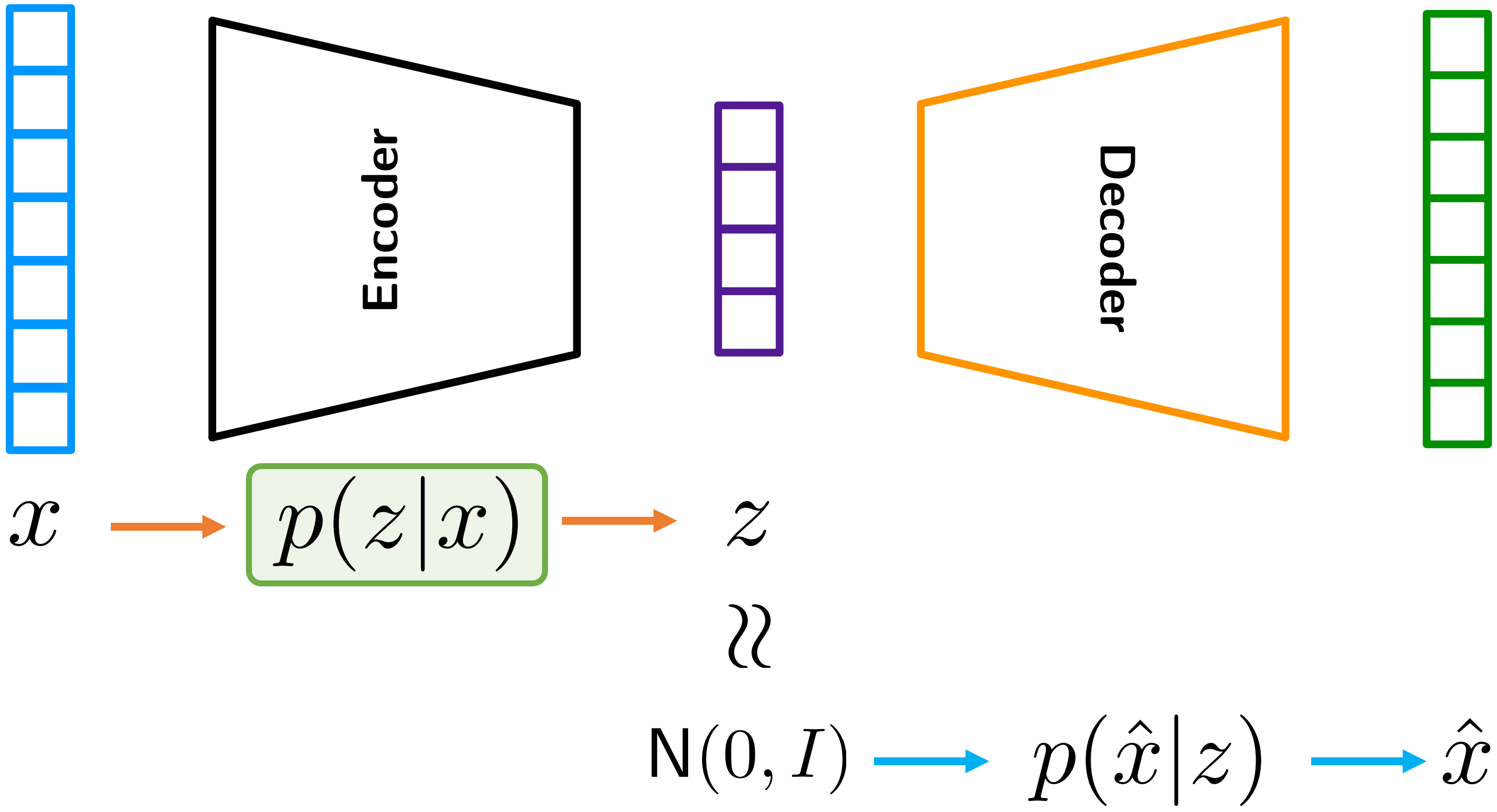


$$x \longrightarrow p(z|x) \longrightarrow z$$

$$\wr\wr$$

$$\mathrm{N}(0, I) \longrightarrow p(\hat{x}|z) \longrightarrow \hat{x}$$

Dissemble VAE



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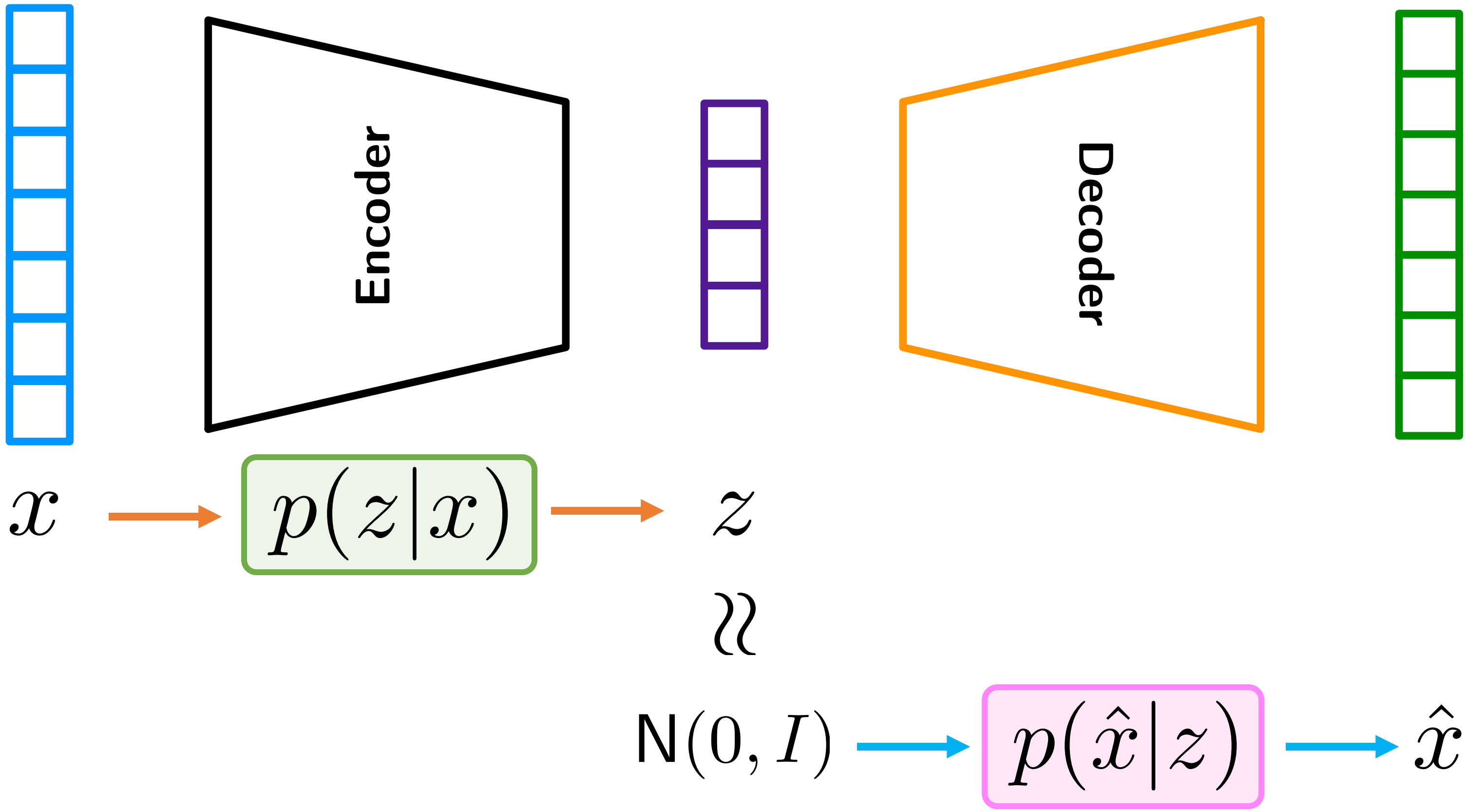

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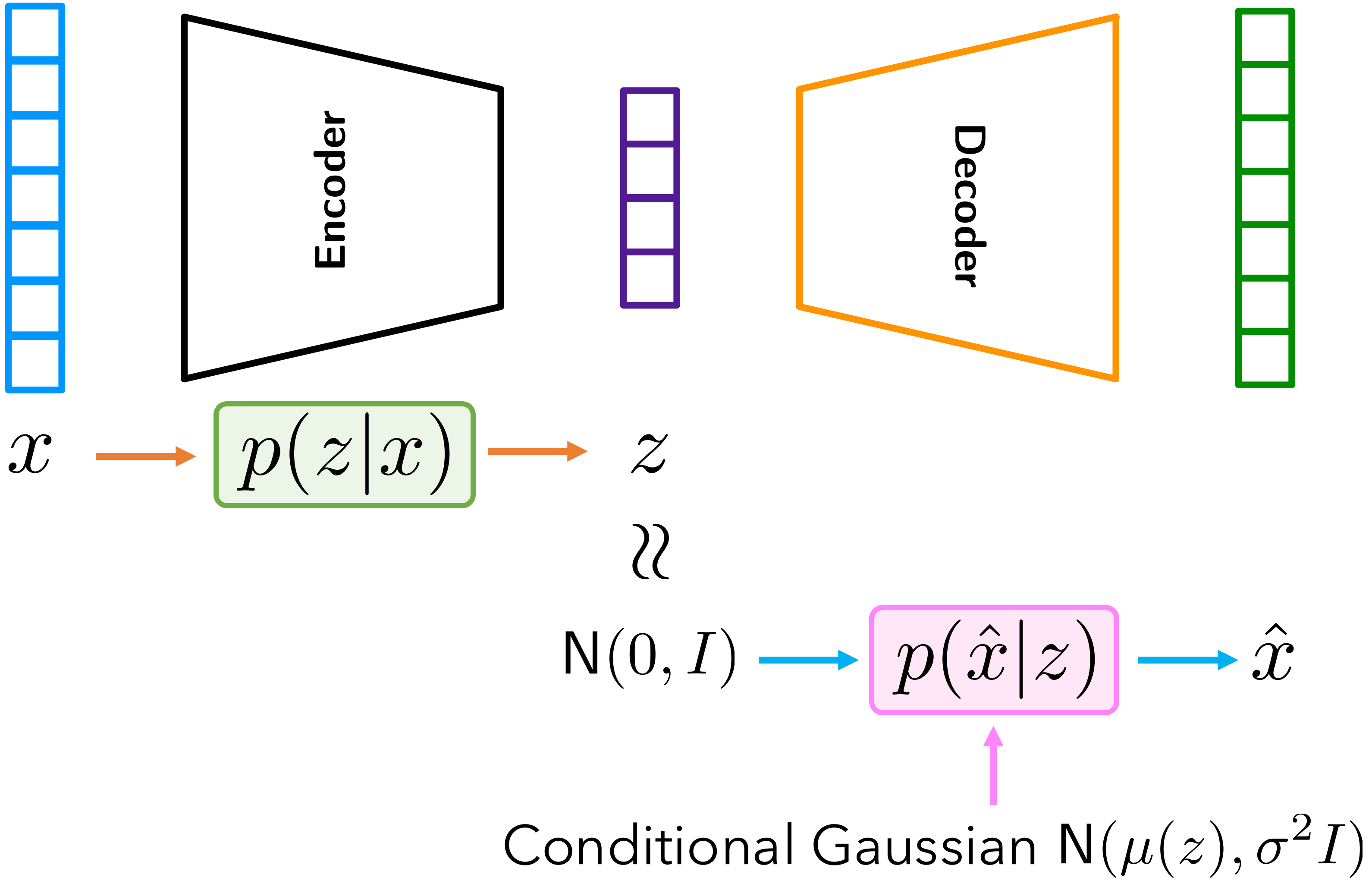

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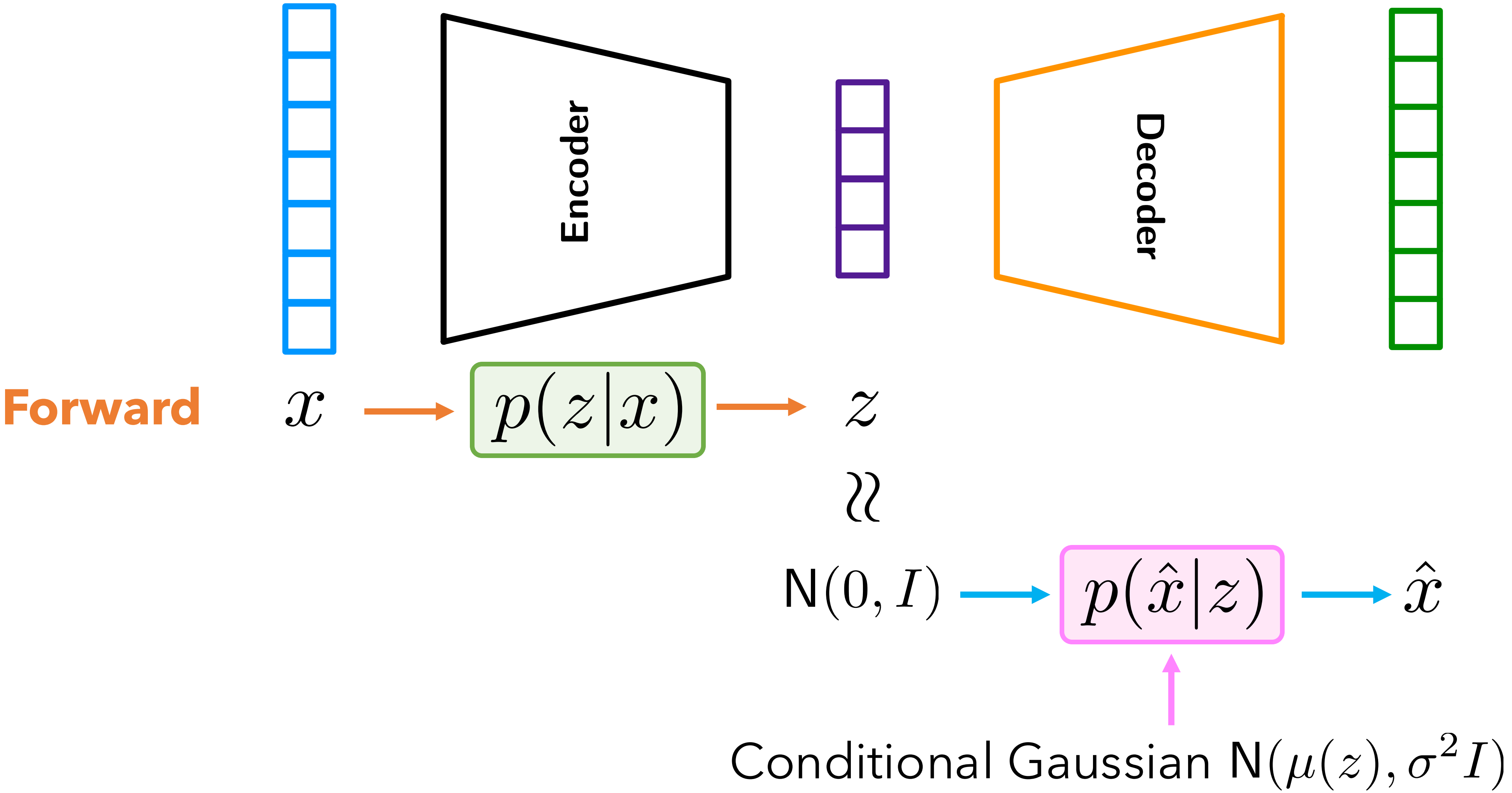

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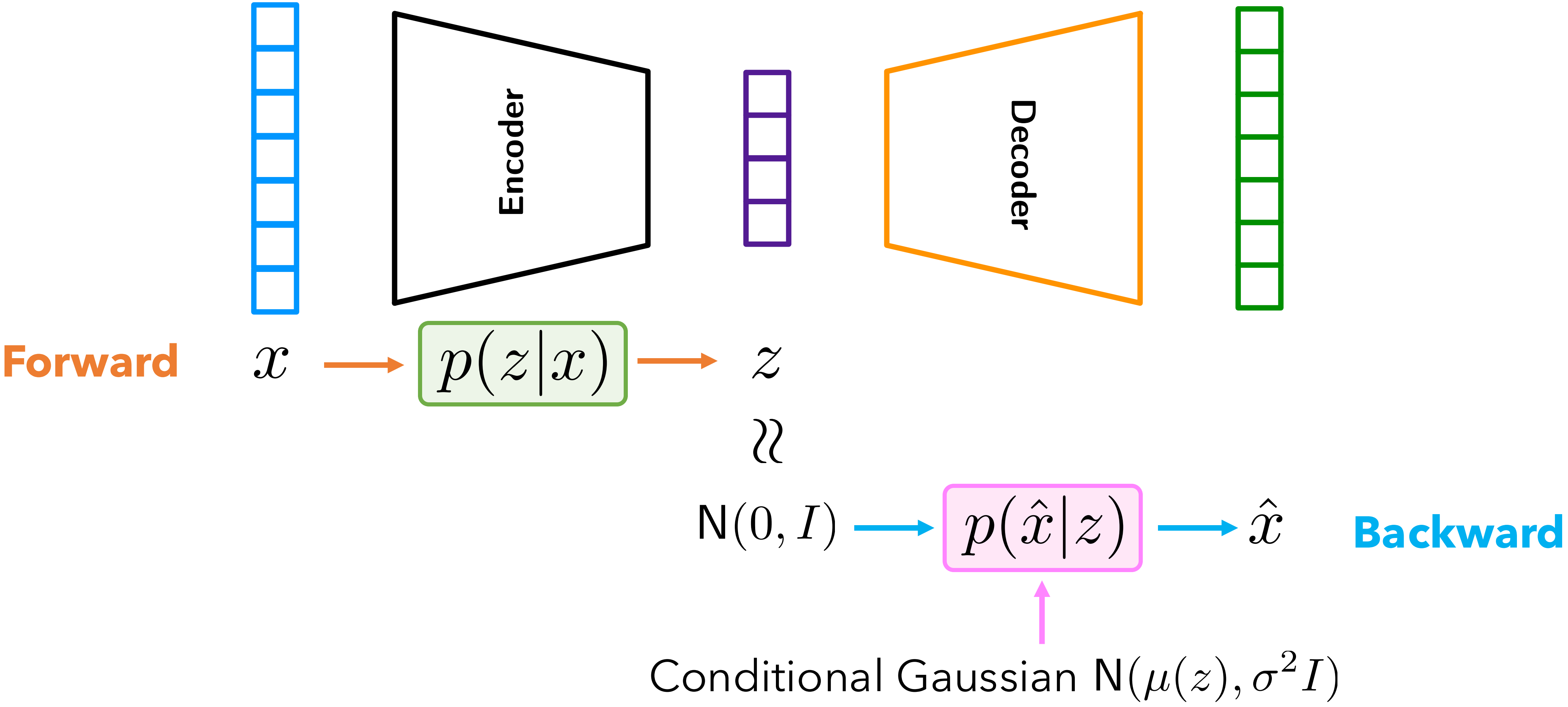

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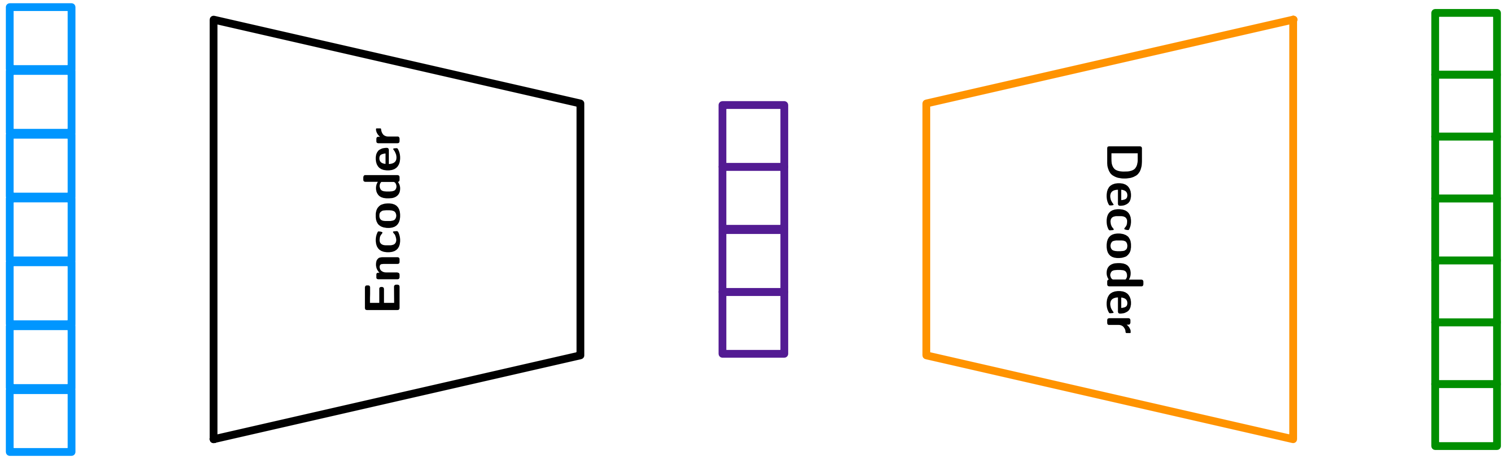


Forward $x \rightarrow \boxed{p(z|x)} \rightarrow z$

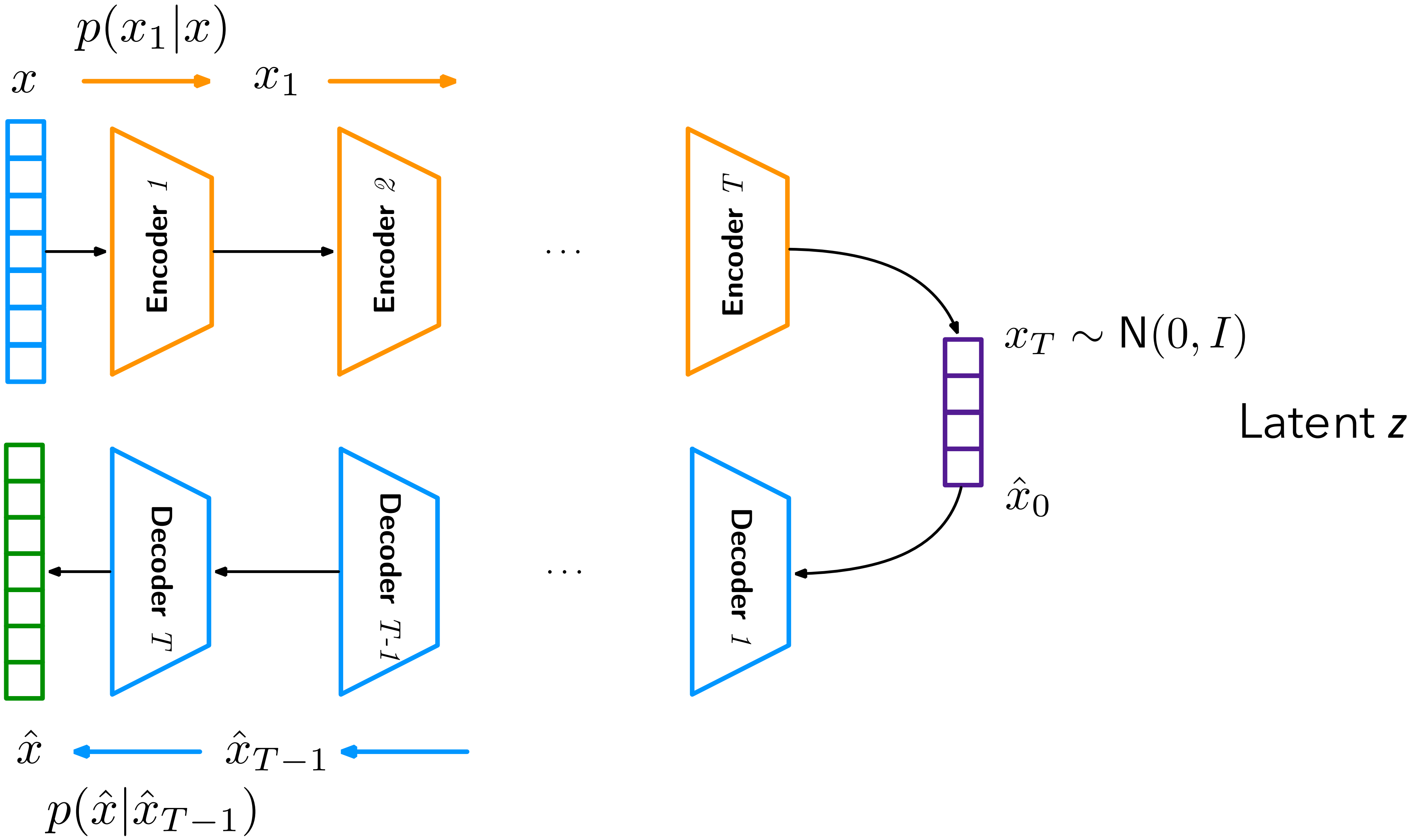
$\wr$

$\mathrm{N}(0, I) \rightarrow \boxed{p(\hat{x}|z)} \rightarrow \hat{x}$ **Backward**

One-step transformation?

Conditional Gaussian $\mathrm{N}(\mu(z), \sigma^2 I)$

Let's Insert Some Intermediate Layers



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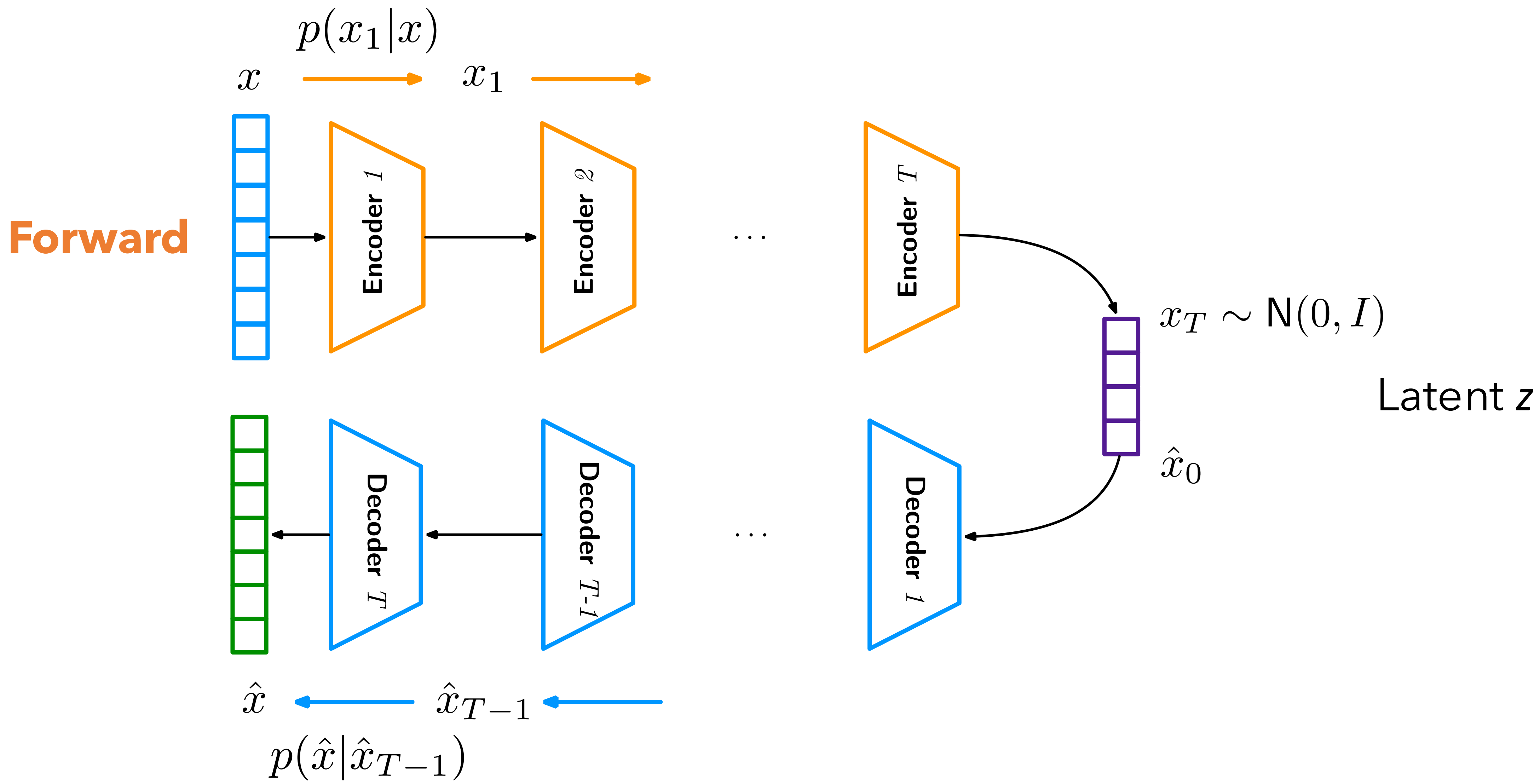

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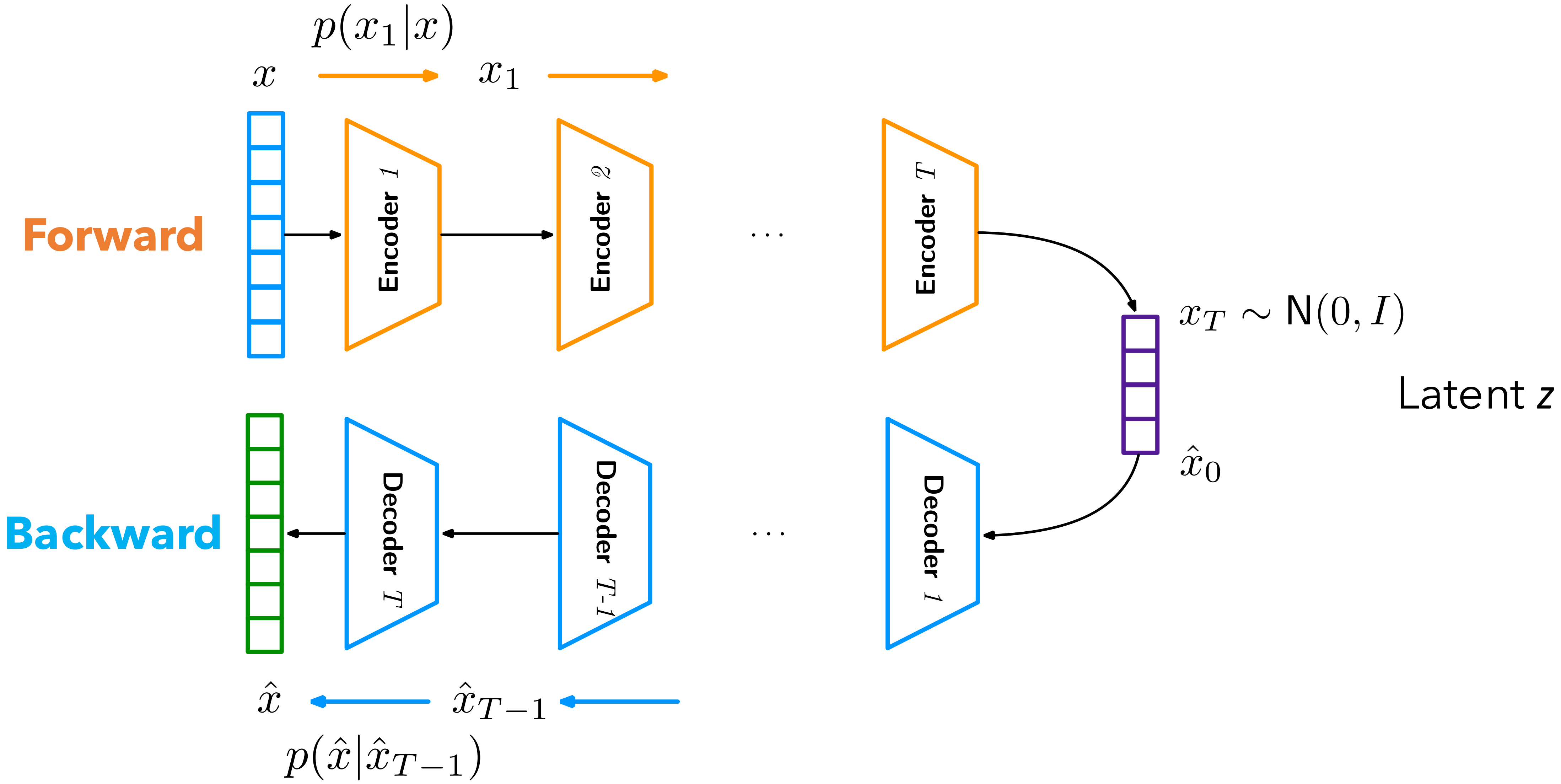

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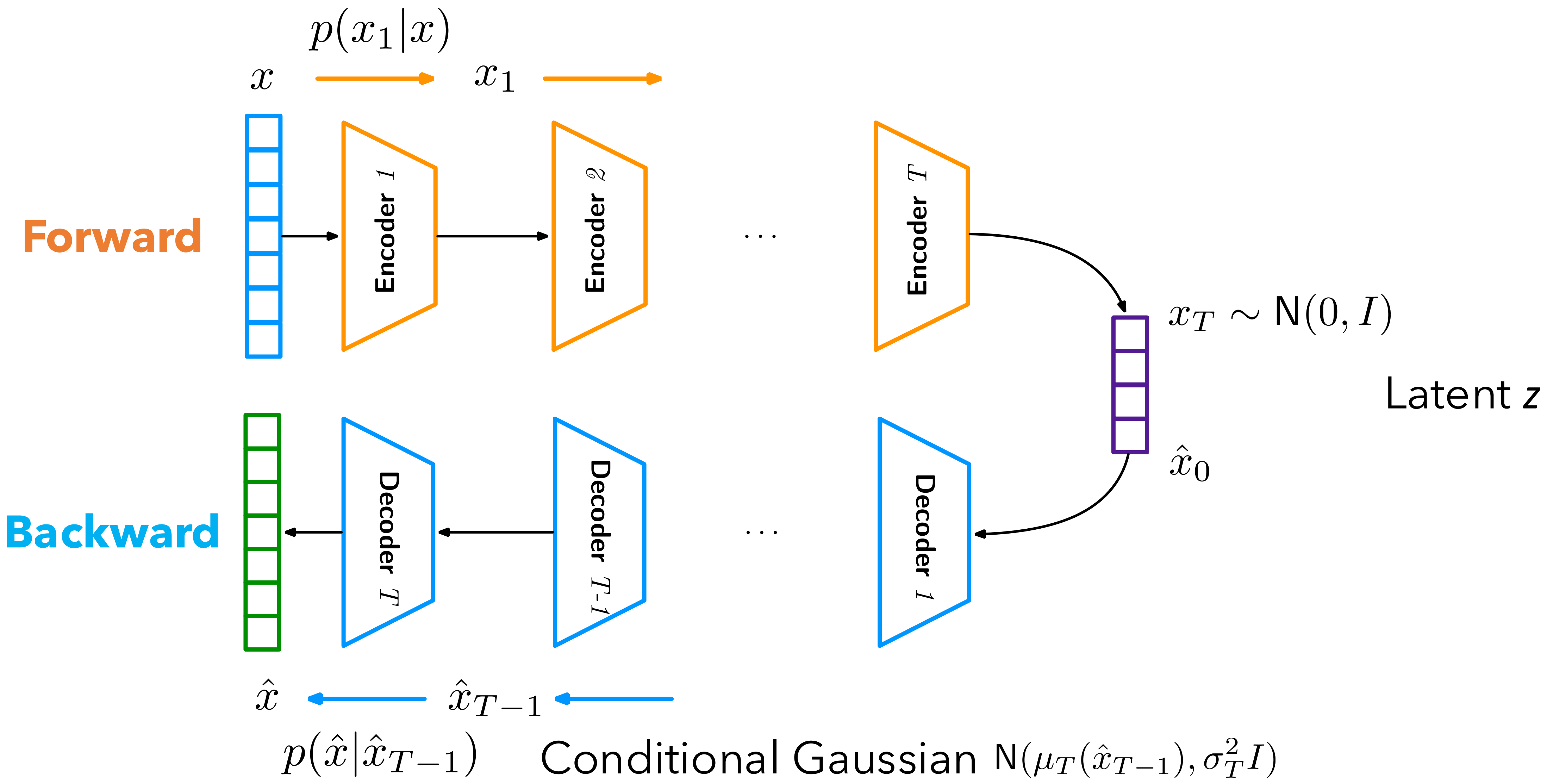

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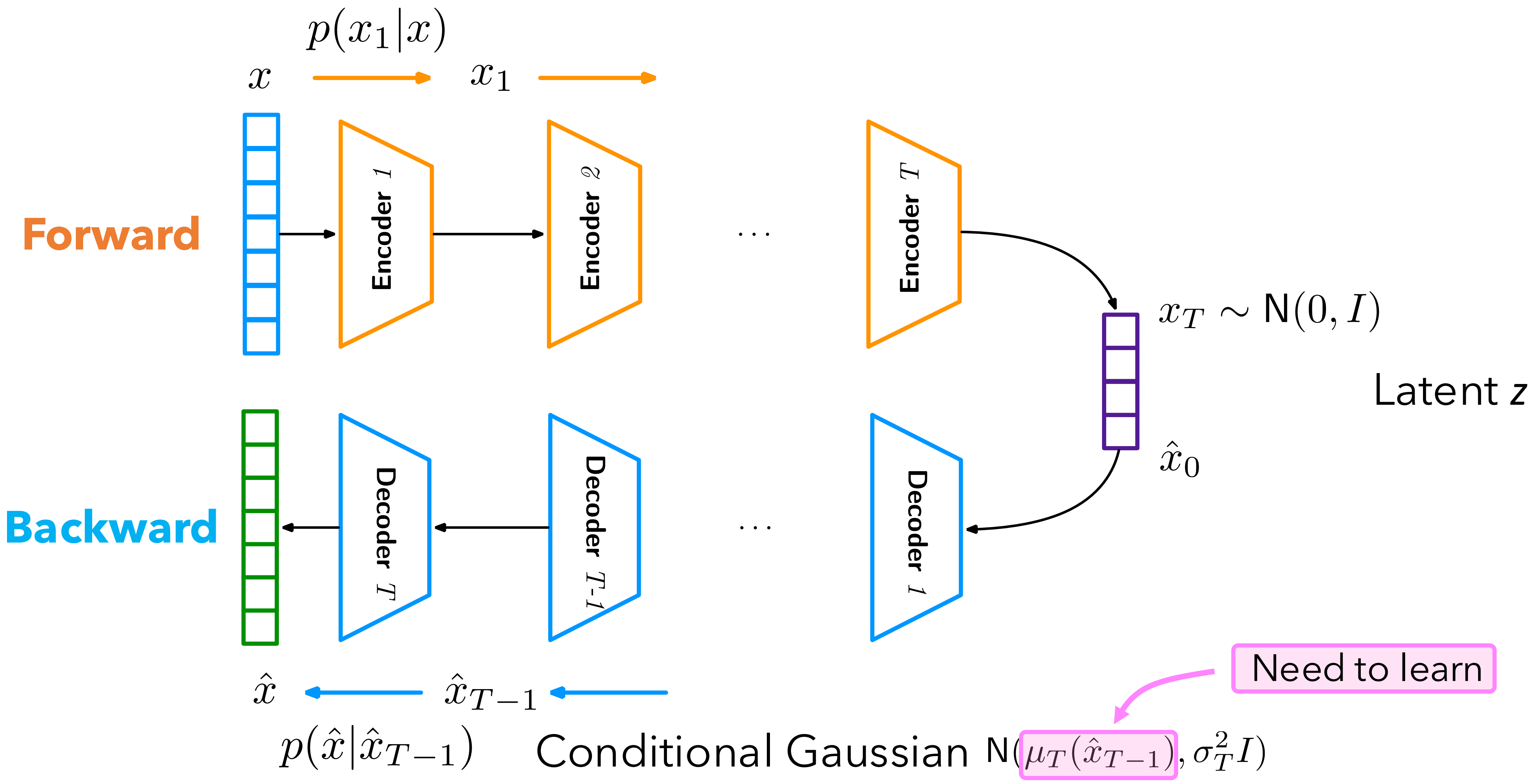

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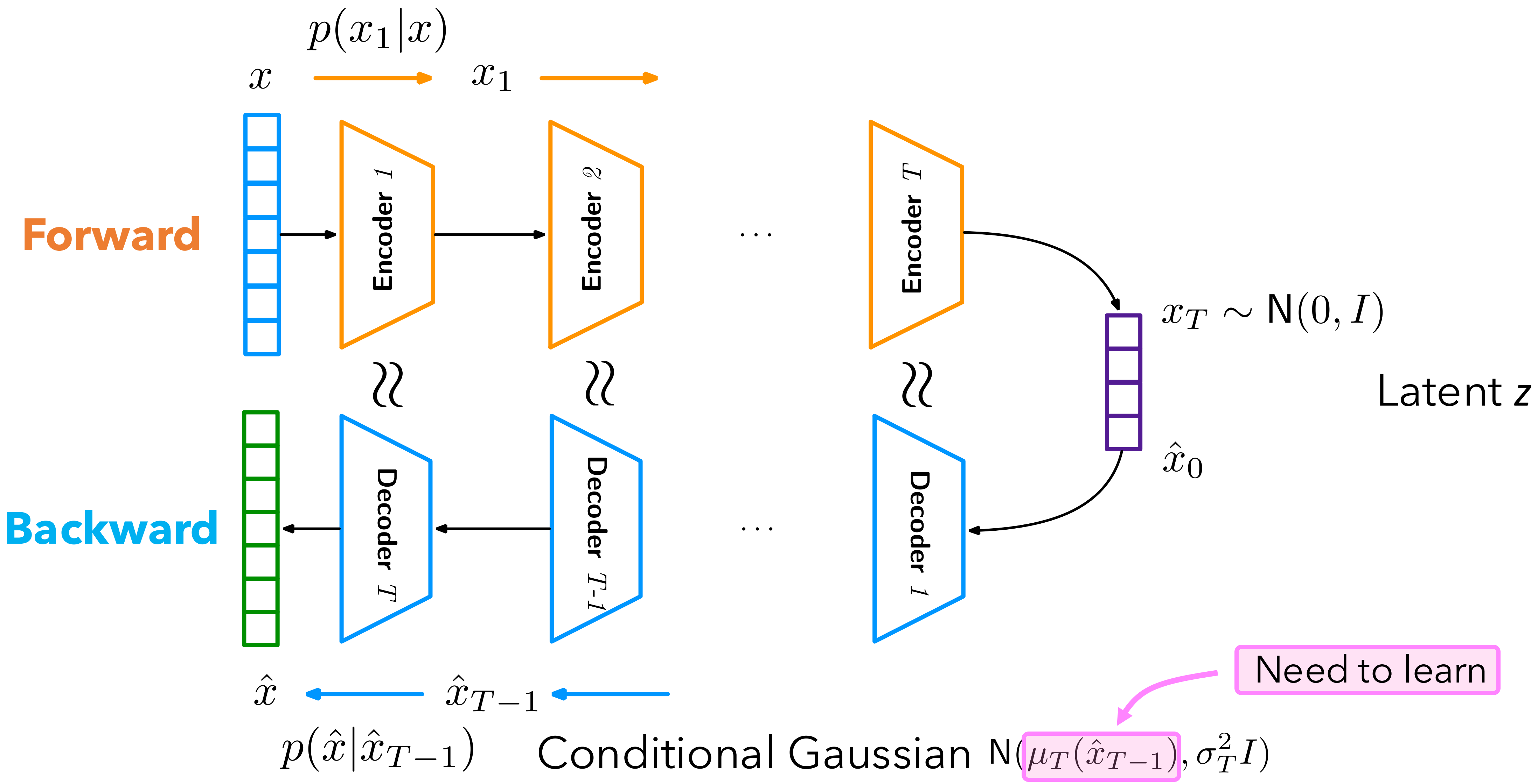
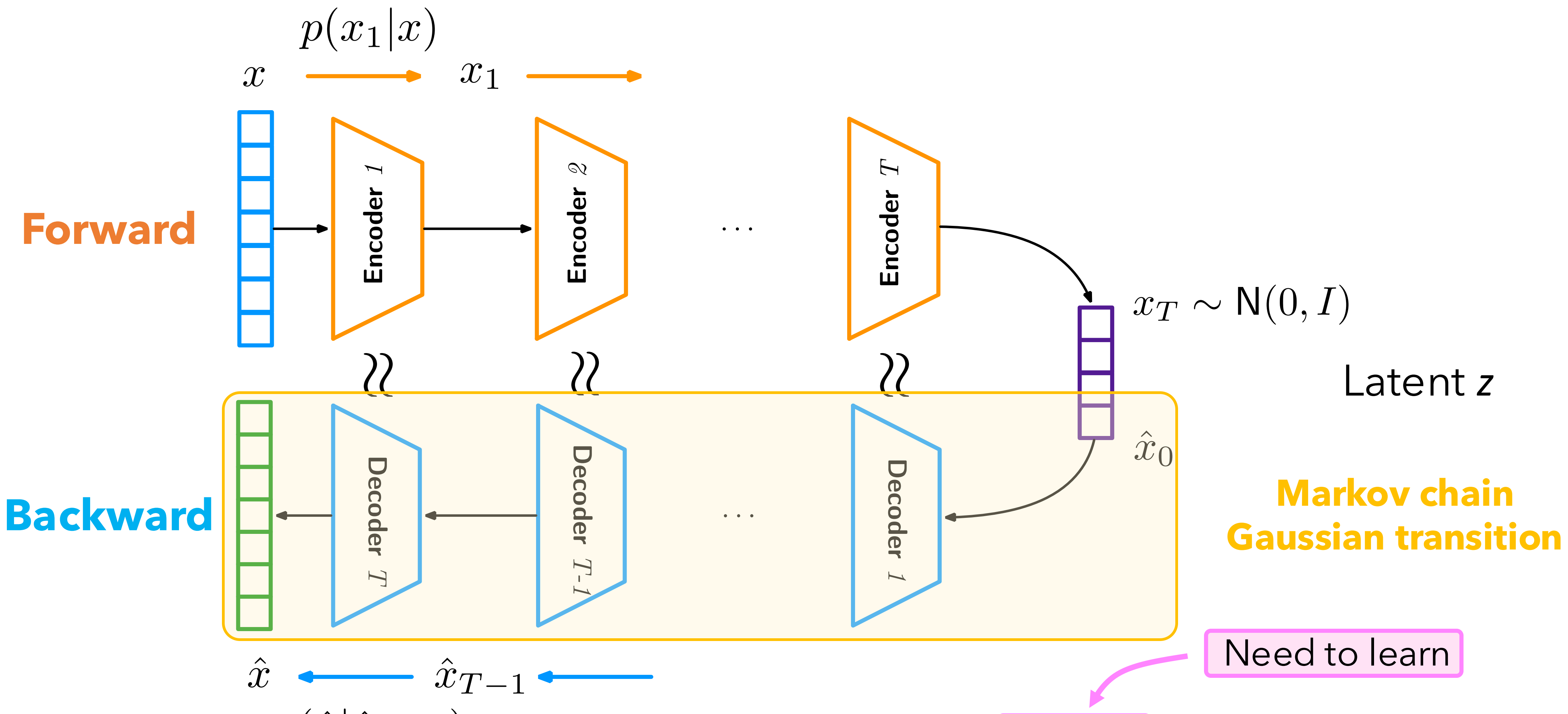


Need to learn

Conditional Gaussian $\mathrm{N}(\boxed{\mu_T(\hat{x}_{T-1})}, \sigma_T^2 I)$

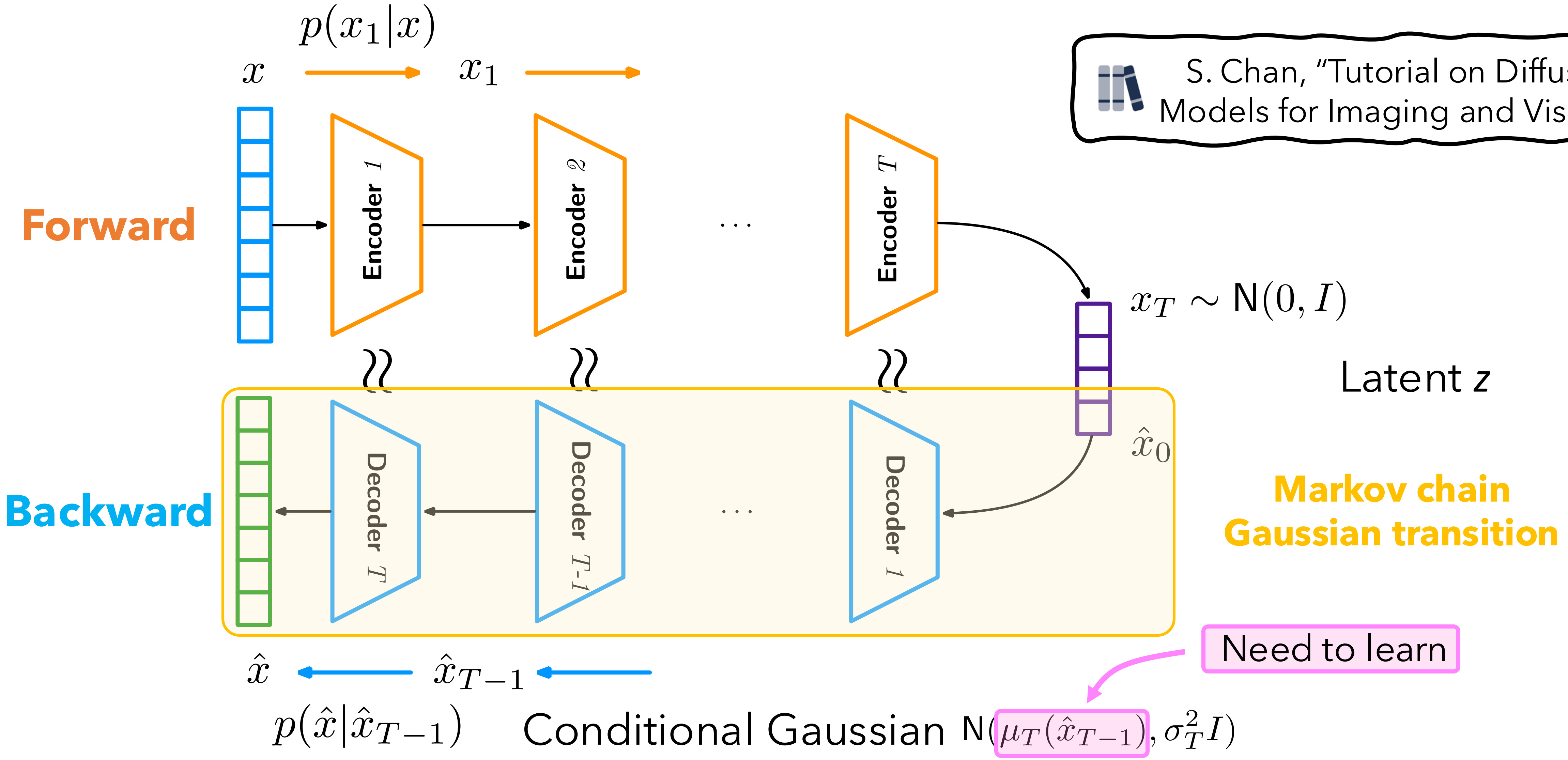
Let's Insert Some Intermediate Layers



$p(\hat{x}|\hat{x}_{T-1})$ Conditional Gaussian $\mathrm{N}(\boxed{\mu_T(\hat{x}_{T-1})}, \sigma_T^2 I)$

Let's Insert Some Intermediate Layers

S. Chan, "Tutorial on Diffusion Models for Imaging and Vision"



Conditional Gaussian $\mathrm{N}(\boxed{\mu_T(\hat{x}_{T-1})}, \sigma_T^2 I)$

Need to learn

A Revolution – Diffusion Model

- Sequential transformation in high-D

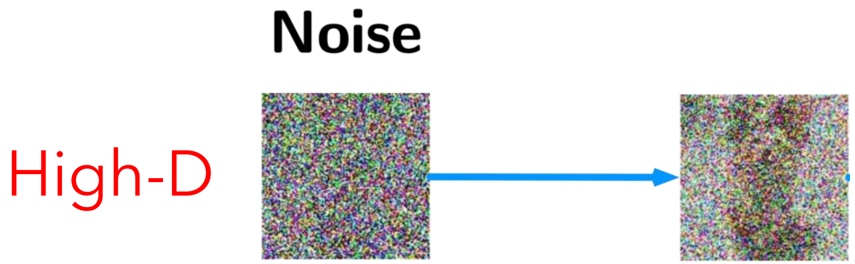
Noise

High-D

(Sohl-Dickstein et al., 2015)
(Song and Ermon, 2019)
(Ho et al., 2020)

A Revolution – Diffusion Model

- Sequential transformation in high-D



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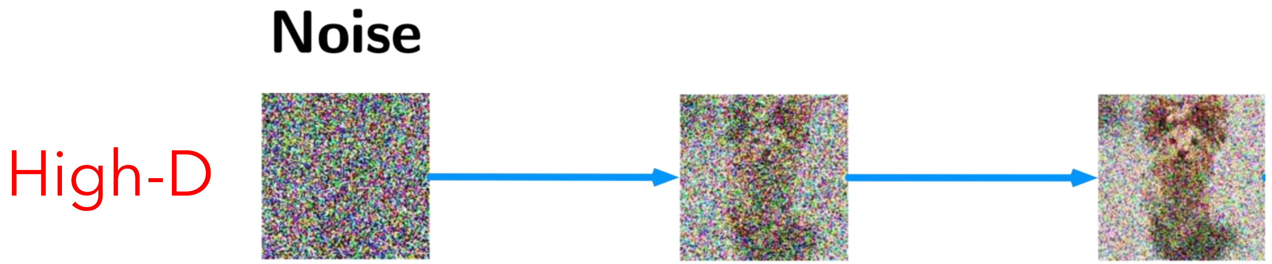
A Revolution – Diffusion Model

- Sequential transformation in high-D



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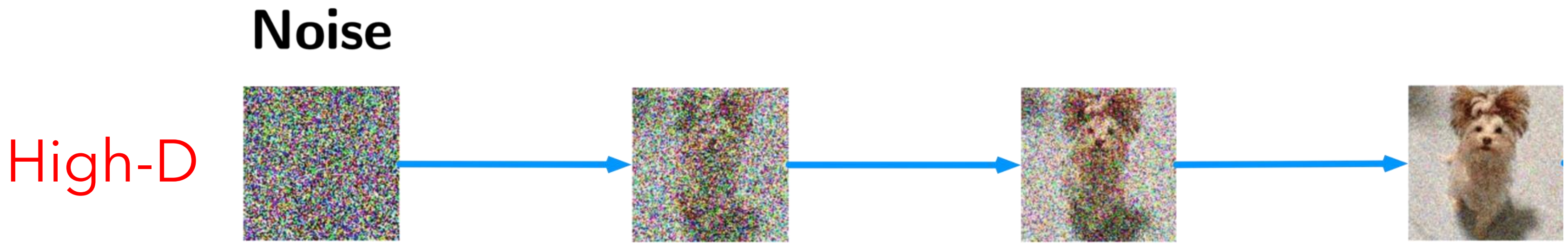
- Sequential transformation in high-D



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A Revolution – Diffusion Model

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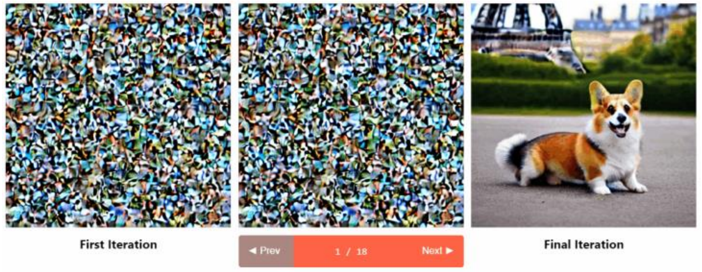

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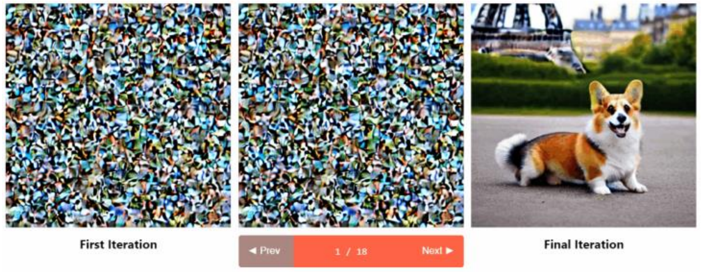
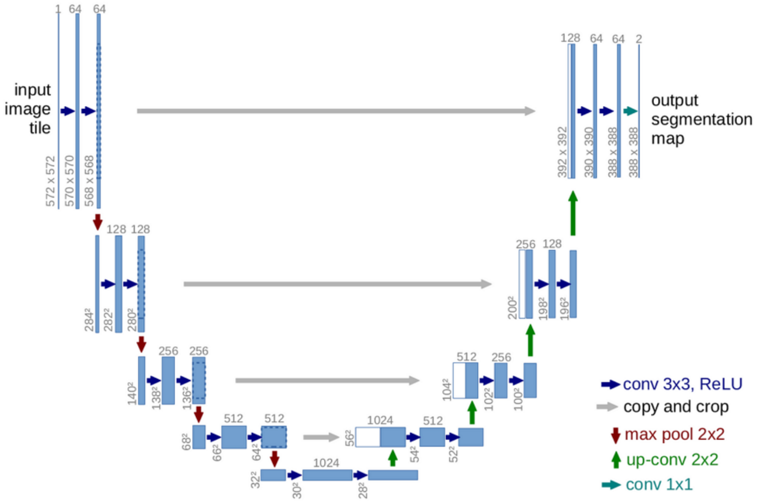
A Revolution – Diffusion Model



- Sequential transformation in high-D

Noise **Data**

High-D



> 890M parameters
(Stable Diffusion)

(Sohl-Dickstein et al., 2015)
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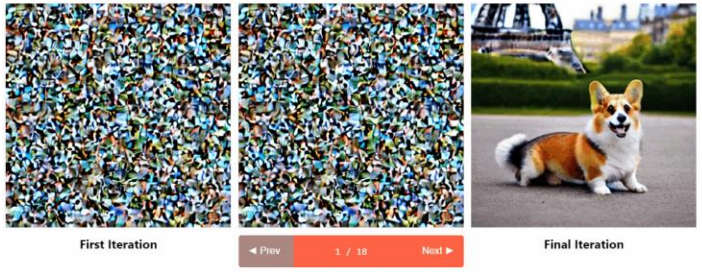
A Revolution – Diffusion Model

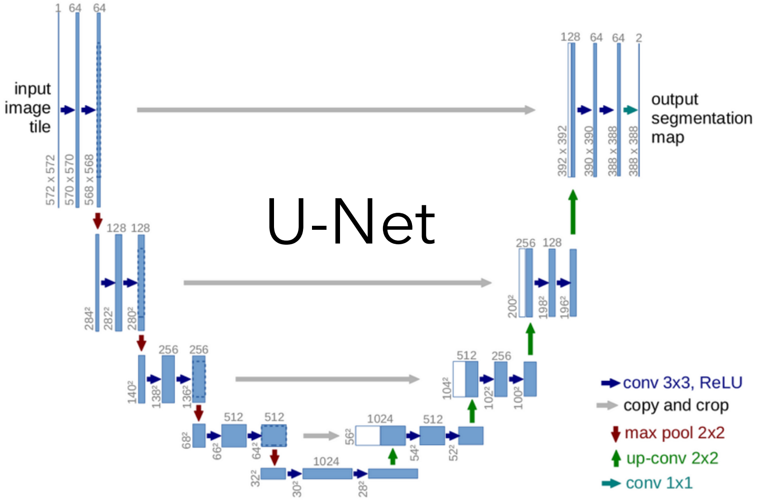


- Sequential transformation in high-D

Noise

Data

High-D



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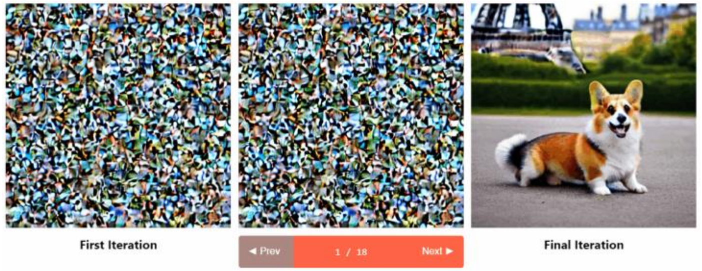
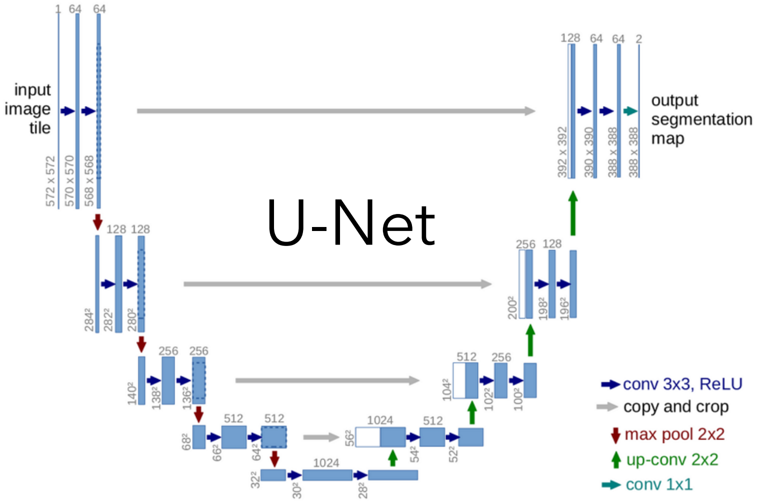
A Revolution – Diffusion Model



- Sequential transformation in high-D

Noise **Data**

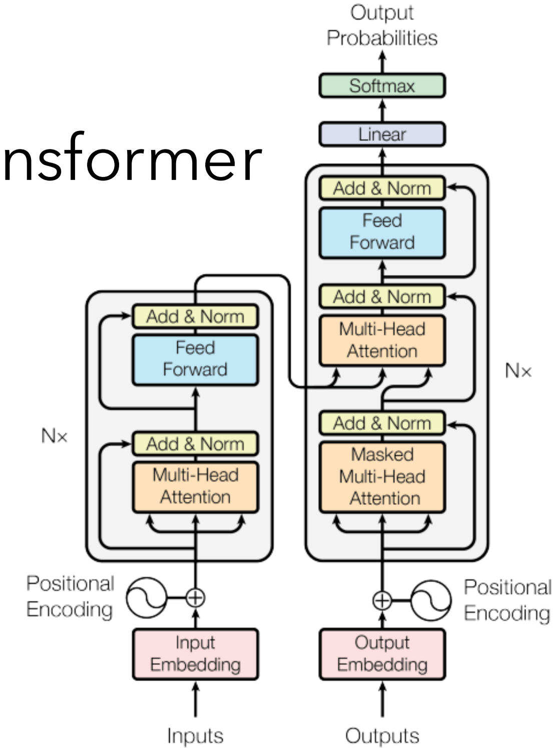
High-D



U-Net

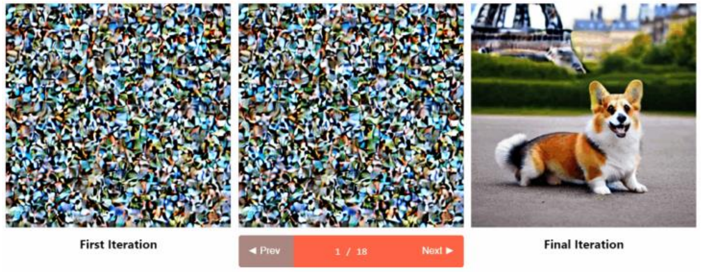
> 890M parameters
(Stable Diffusion)

Transformer



2015)
2019)
2020)

A Revolution – Diffusion Model

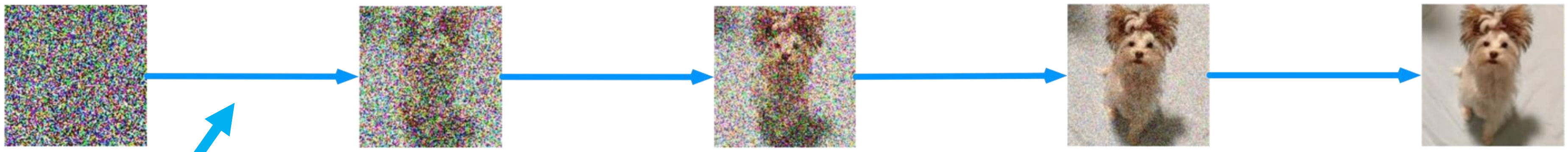


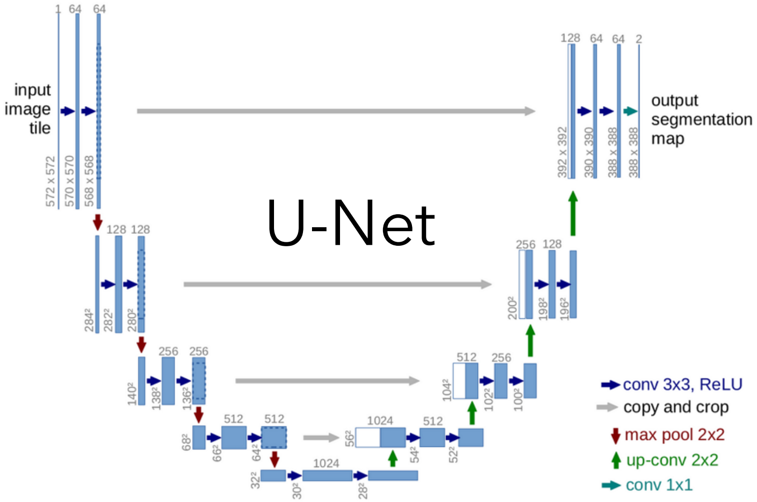
- Sequential transformation in high-D

Noise

Data

High-D

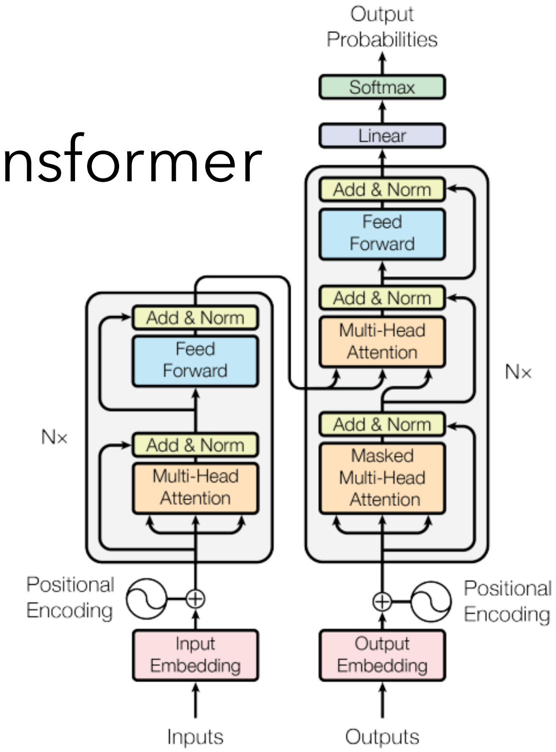




U-Net

$\mu_t(\cdot)$

Transformer



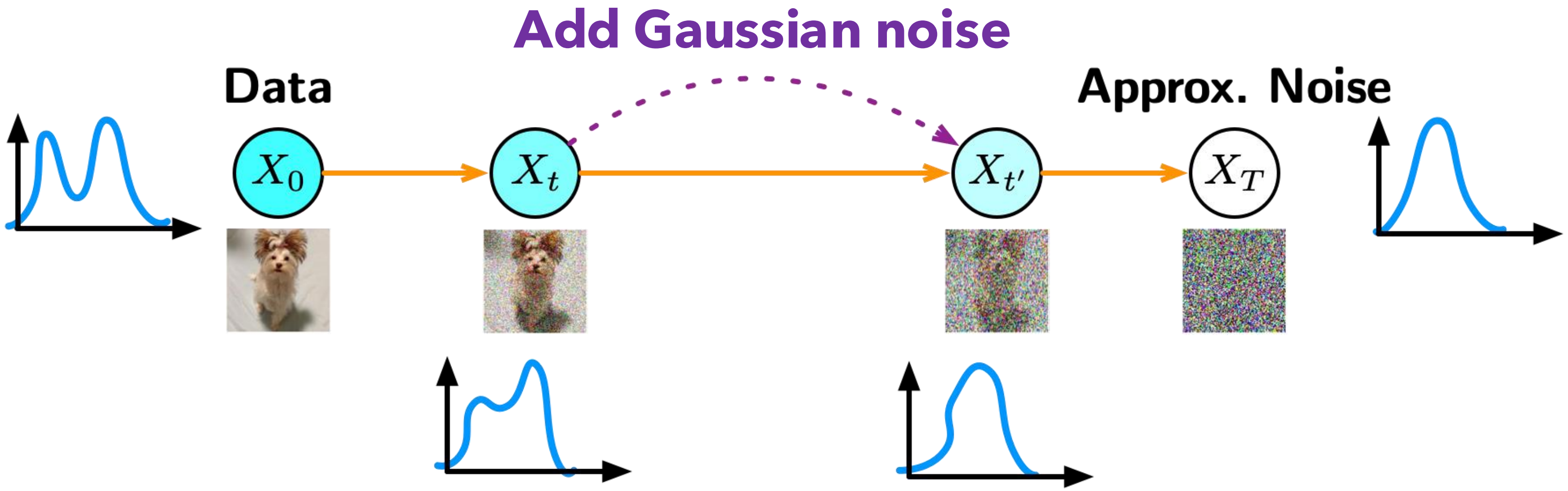
2015)
2019)
2020)

> 890M parameters
(Stable Diffusion)

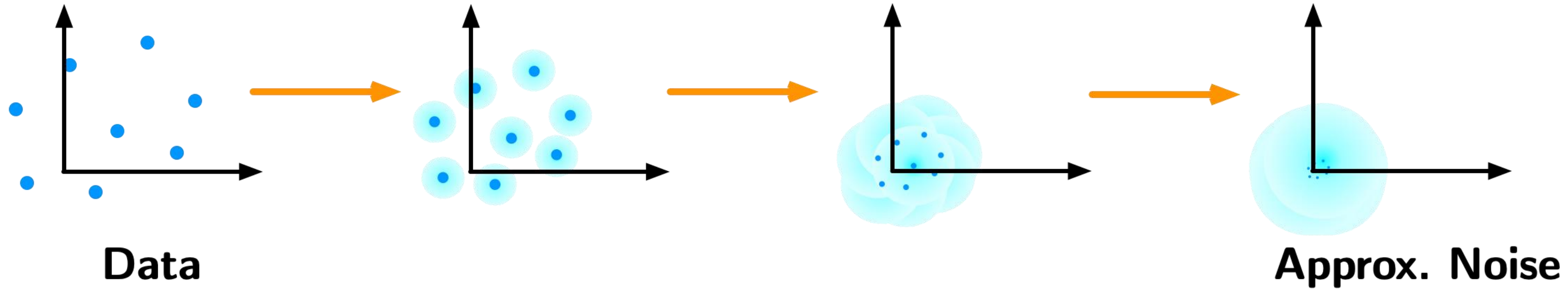
Forward Process – Noise Corruption

Insert infinitely many intermediate layers!

- Noise corruption process $\mathrm{d}X_t = -\frac{1}{2}X_t\mathrm{d}t + \mathrm{d}W_t$

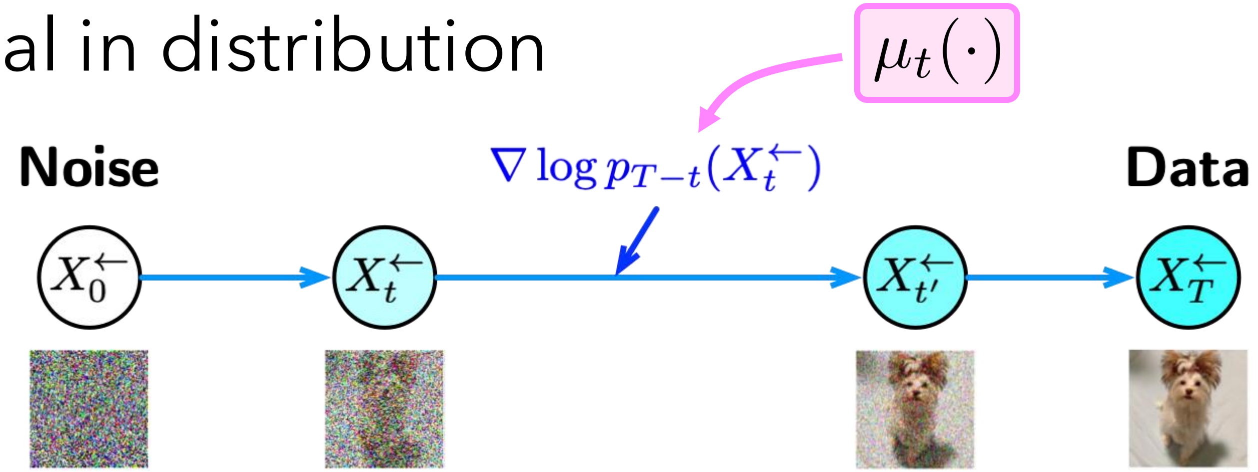


- The noise corruption



Backward Process – Sample Generation

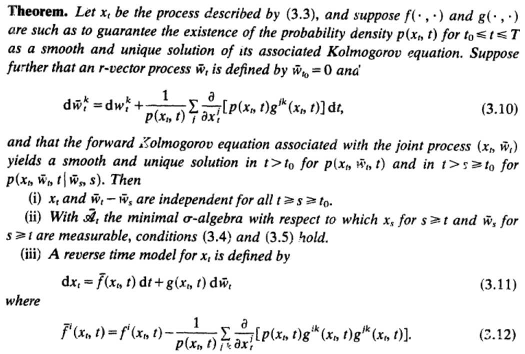
- Time reversal in distribution



- The math (Anderson, 1982; Haussmann and Pardoux, 1986)

Forward $$\mathrm{d}X_t = -\frac{1}{2}X_t \mathrm{d}t + \mathrm{d}W_t$$

Backward $$\mathrm{d}X_t^{\leftarrow} = \Big[\frac{1}{2}X_t^{\leftarrow} + \underbrace{\nabla \log p_{T-t}(X_t^{\leftarrow})}_{\text{Score Function}}\Big]\mathrm{d}t + \underbrace{\mathrm{d}\overline{W}_t}_{\text{Brownian}}$$



Theorem. *Let x_t be the process described by (3.3), and suppose $f(\cdot,\cdot)$ and $g(\cdot,\cdot)$ are such as to guarantee the existence of the probability density $p(x_t, t)$ for $t_0 \leqslant t \leqslant T$ as a smooth and unique solution of its associated Kolmogorov equation. Suppose further that an r-vector process $\bar{w}_t$ is defined by $\bar{w}_{t_0} = 0$ and*

$$\mathrm{d}\bar{w}_t^k = \mathrm{d}w_t^k + \frac{1}{p(x_t, t)} \sum_j \frac{\partial}{\partial x_t^j}[p(x_t, t) g^{jk}(x_t, t)]\,\mathrm{d}t, \tag{3.10}$$

and that the forward Kolmogorov equation associated with the joint process $(x_t, \bar{w}_t)$ yields a smooth and unique solution in $t > t_0$ for $p(x_t, \bar{w}_t, t)$ and in $t > s \geqslant t_0$ for $p(x_t, \bar{w}_t, t \mid \bar{w}_s, s)$. Then

(i) *x_t and $\bar{w}_t - \bar{w}_s$ are independent for all $t \geqslant s \geqslant t_0$.*

(ii) *With $\bar{\mathscr{A}}_t$ the minimal σ-algebra with respect to which x_s for $s \geqslant t$ and $\bar{w}_s$ for $s \geqslant t$ are measurable, conditions (3.4) and (3.5) hold.*

(iii) *A reverse time model for x_t is defined by*

$$\mathrm{d}x_t = \bar{f}(x_t, t)\,\mathrm{d}t + g(x_t, t)\,\mathrm{d}\bar{w}_t \tag{3.11}$$

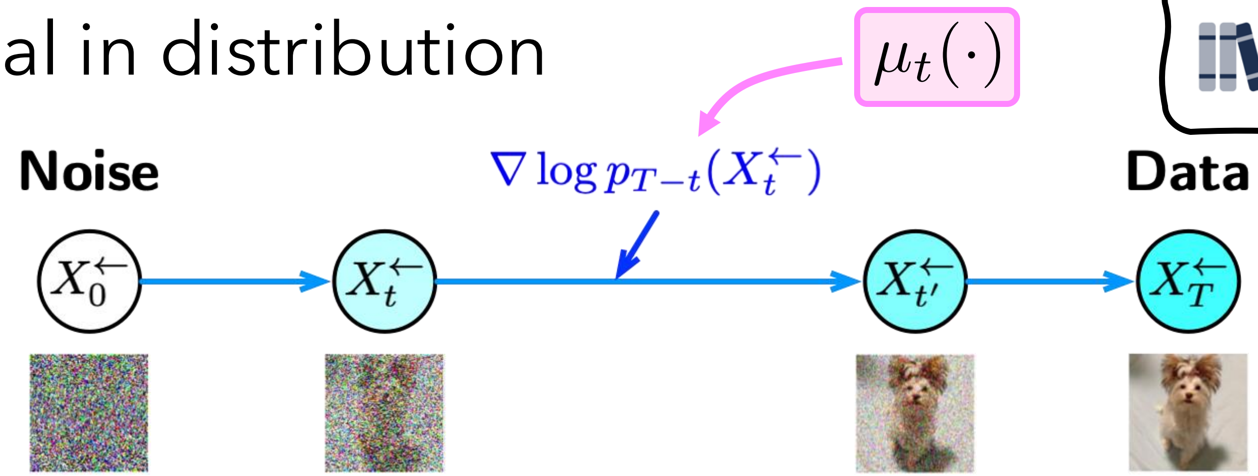
where

$$\bar{f}^i(x_t, t) = f^i(x_t, t) - \frac{1}{p(x_t, t)} \sum_{j,k} \frac{\partial}{\partial x_t^j}[p(x_t, t) g^{ik}(x_t, t) g^{jk}(x_t, t)]. \tag{3.12}$$

Backward Process – Sample Generation

> Tang & Zhao, “Score-based Diffusion Models via SDE”

- Time reversal in distribution



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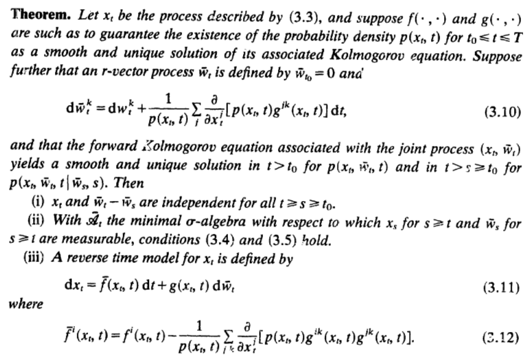

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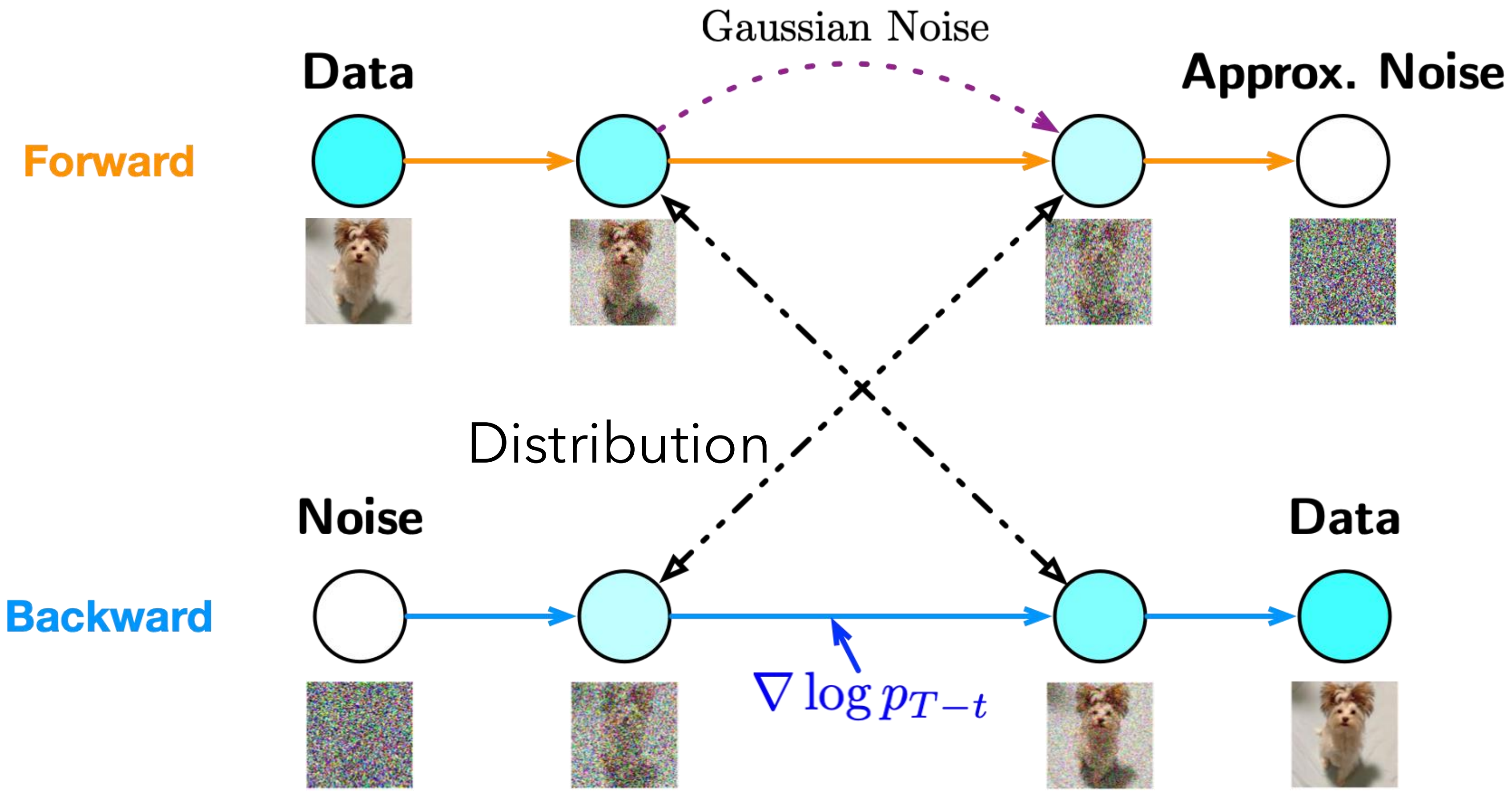
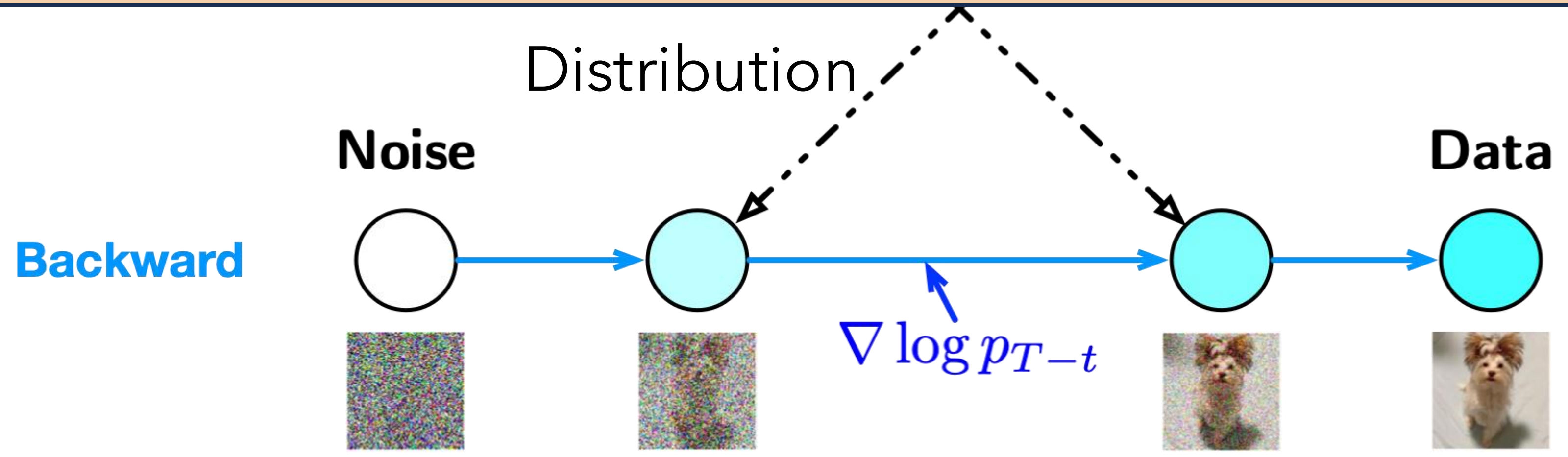
Forward and Backward Coupling



Forward and Backward Coupling

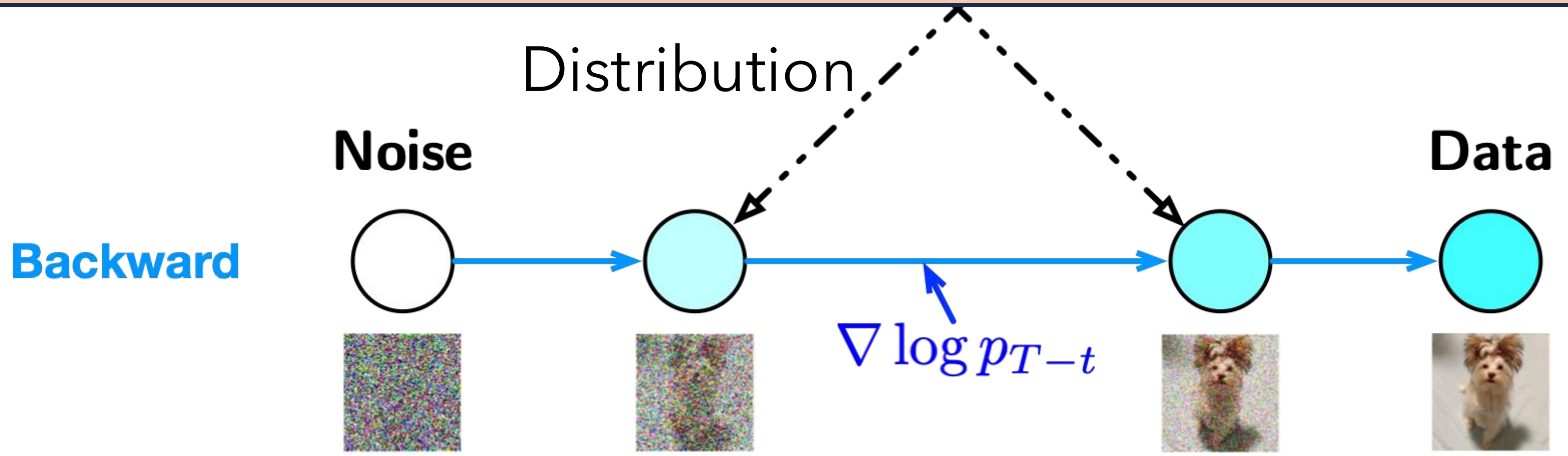
Training $\int_0^T \mathbb{E}_{x_t}\left[\|\nabla \log p_t(x_t) - s(x_t, t)\|_2^2\right] \mathrm{d}t$



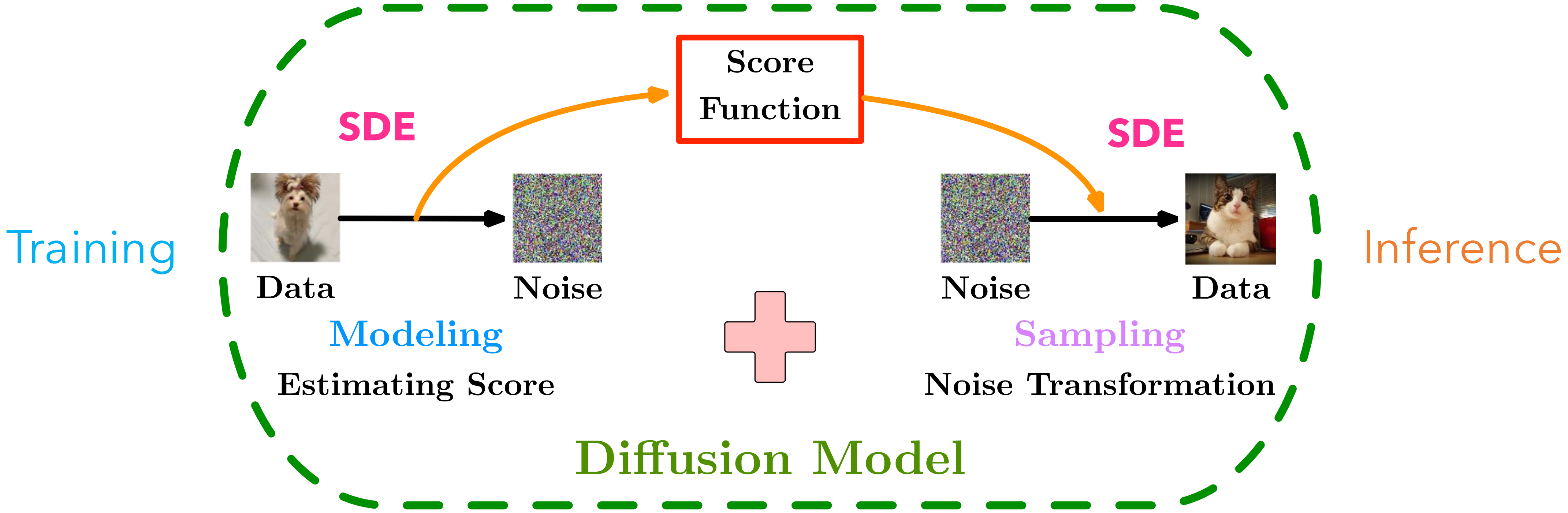
Forward and Backward Coupling

Training $\int_0^T \mathbb{E}_{x_t}\left[\|\nabla \log p_t(x_t) - s(x_t, t)\|_2^2\right] \mathrm{d}t$

Unsupervised learning → **Regression!**



Decomposition of Diffusion Models



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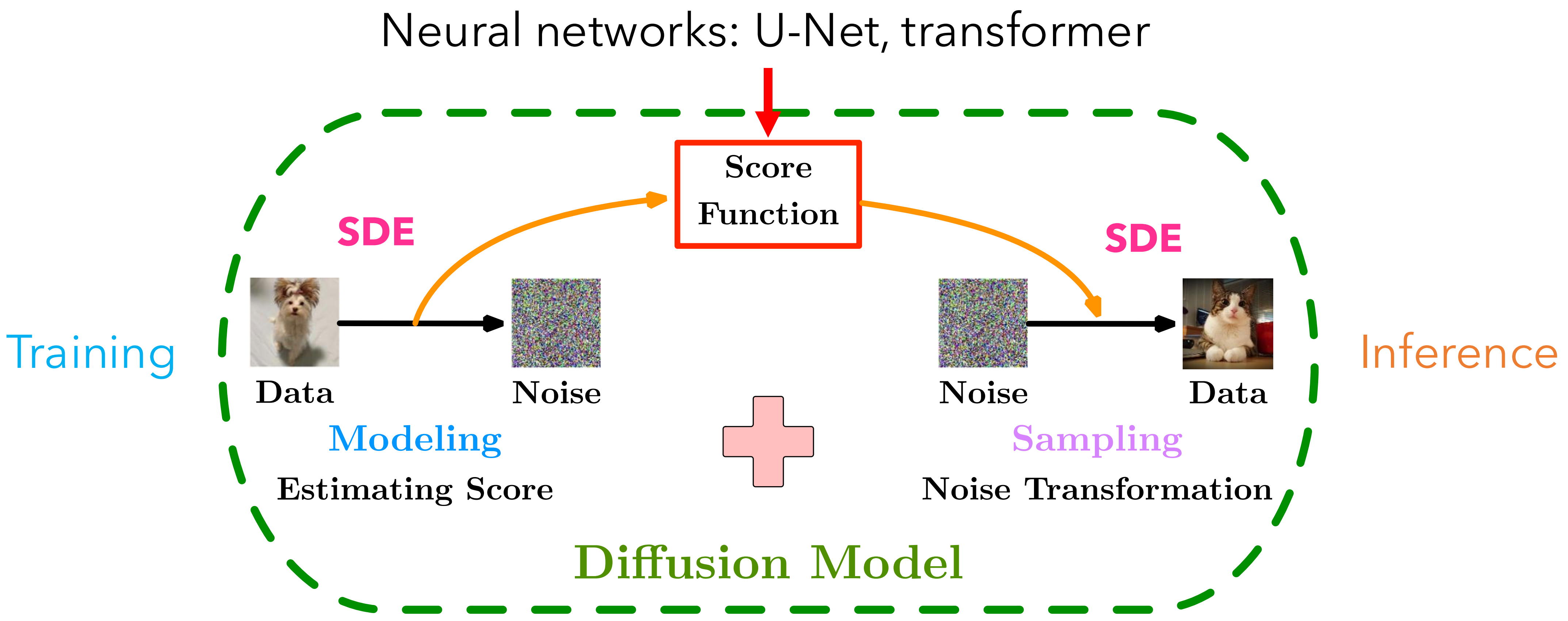

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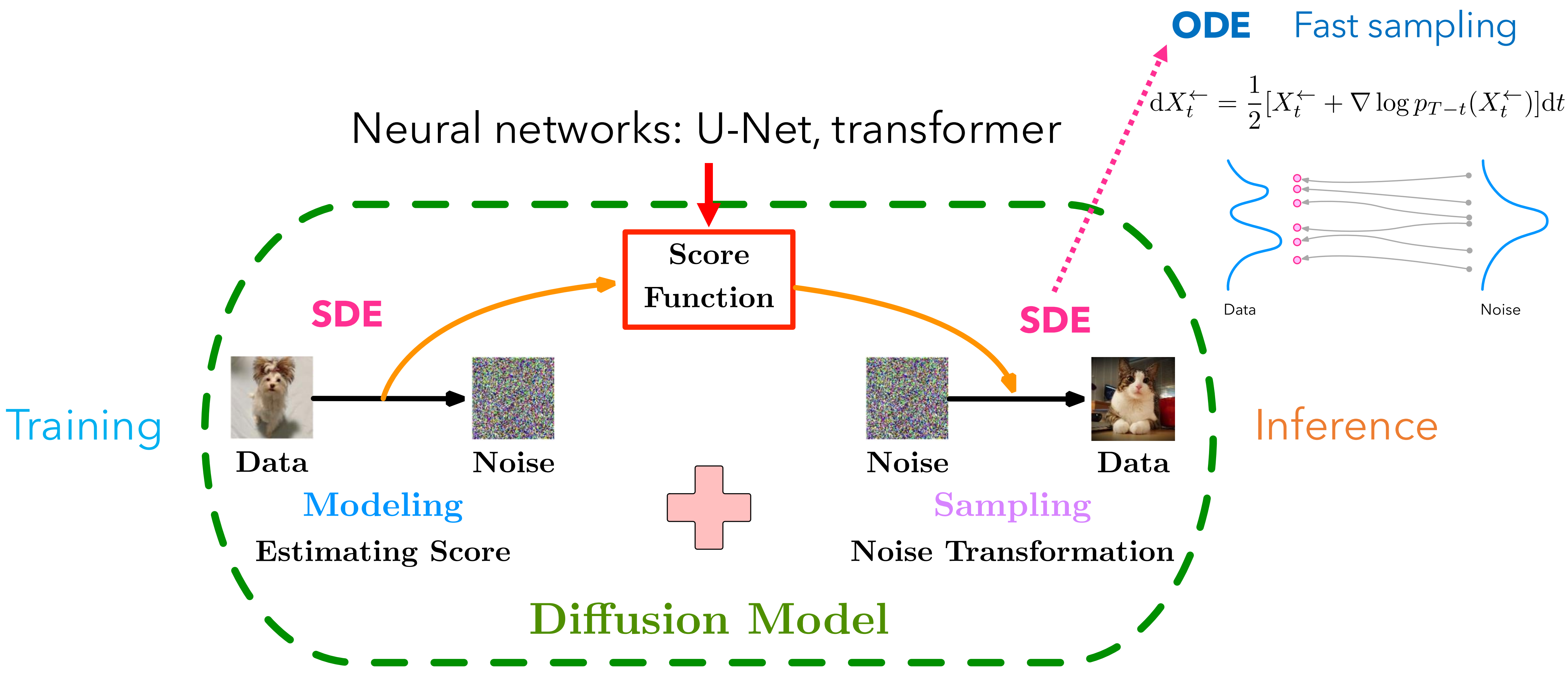

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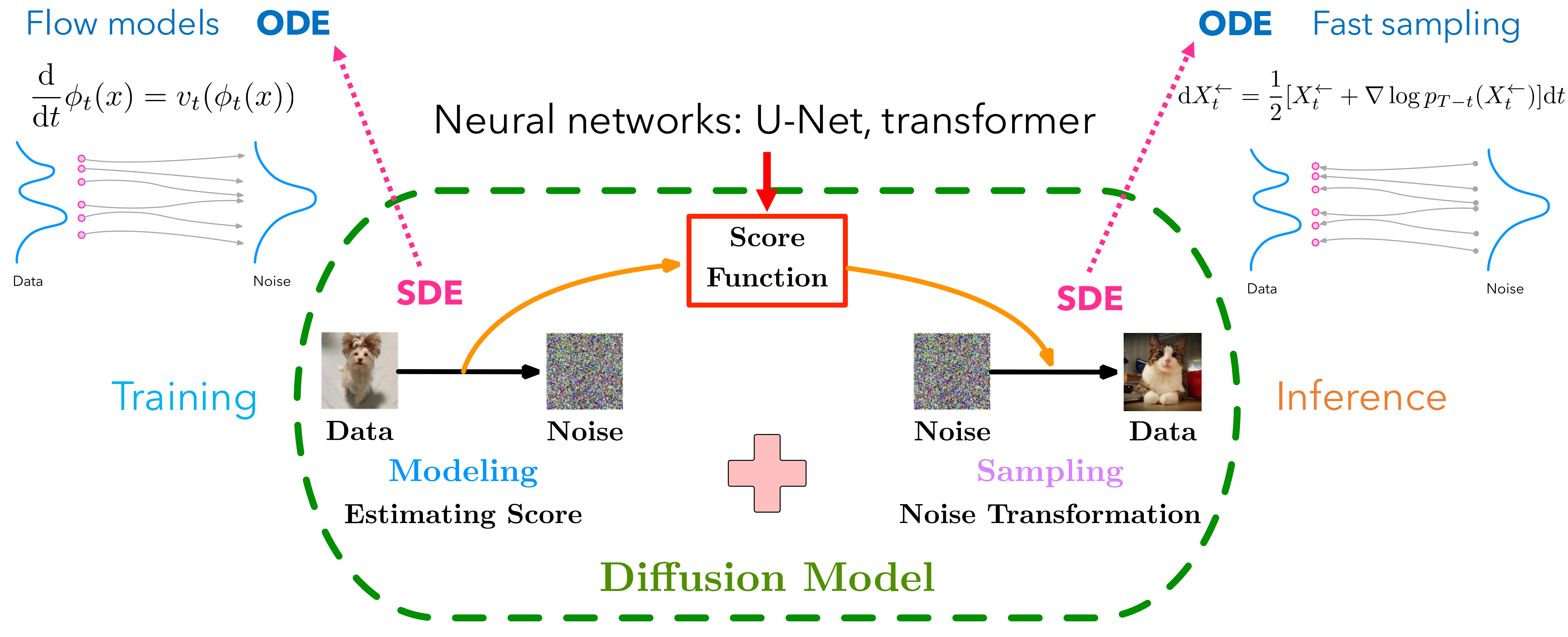
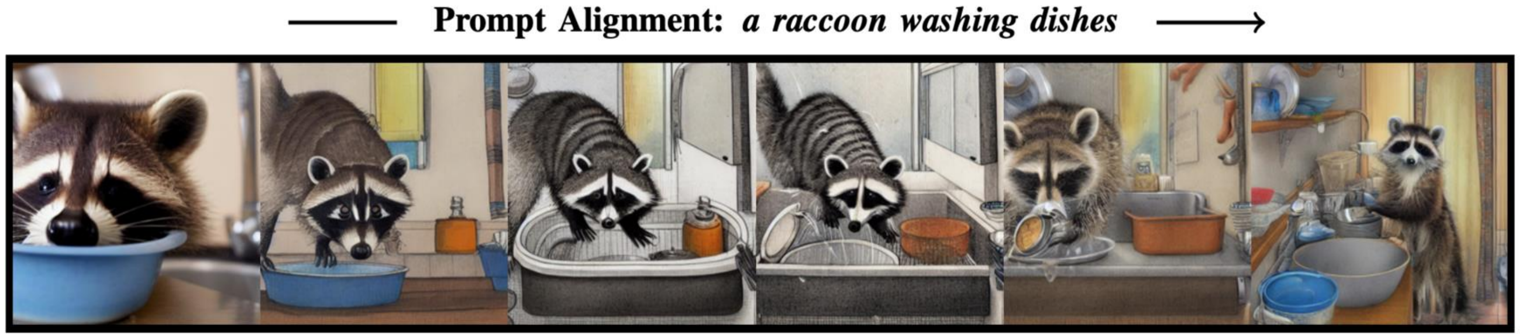
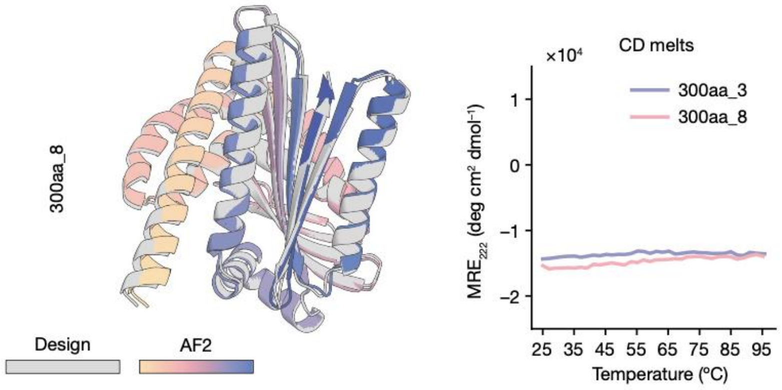


From $P(x)$ to $P(x|y)$

- Text-to-image generation (Black et al., 2023)



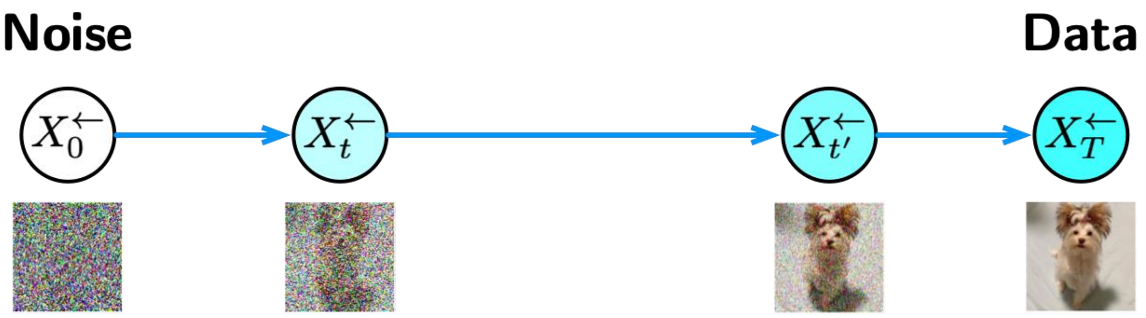
- Protein generation with biochemical properties (Watson et al., 2023; Gruver et al., 2023)



Adding Guidance to Diffusion Models

- Conditioned sample generation

$y = \mathrm{dog}$

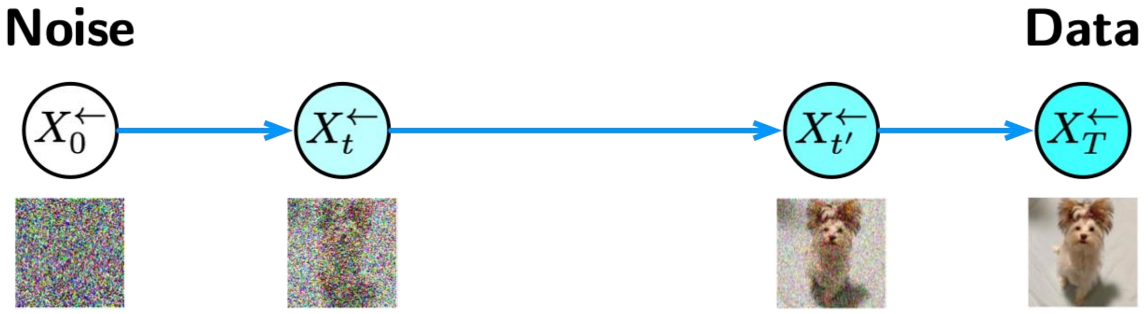


$$\mathrm{d}X_t^{\leftarrow} = \left[\frac{1}{2}X_t^{\leftarrow} + \boxed{\nabla \log p_{T-t}(X_t^{\leftarrow} \mid y)}\right]\mathrm{d}t + \mathrm{d}\overline{W}_t$$

Conditional Score **Brownian**

Adding Guidance to Diffusion Models

- Conditioned sample generation



$y = \text{dog}$

Guidance

$$\mathrm{d}X_t^{\leftarrow} = \left[\frac{1}{2}X_t^{\leftarrow} + \boxed{\nabla \log p_{T-t}(X_t^{\leftarrow} \mid y)}\right]\mathrm{d}t + \mathrm{d}\overline{W}_t$$

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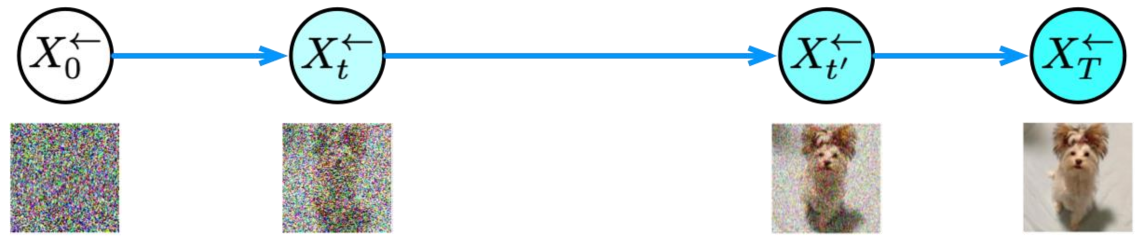

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Conditional Score **Brownian**

Classifier guidance (Dhariwal & Nichol, 2021)
Classifier-free guidance (Ho & Salimans, 2022)

The Bayes Rule – Classifier Guidance

- Discrete label

External Classifier

$$\nabla \log p_t(x_t \mid y) = \nabla \log p_t(x_t) + \nabla \log c_t(y \mid x_t)$$

Unconditioned Logit

The Bayes Rule – Classifier Guidance

- Discrete label

External Classifier

$$\nabla \log p_t(x_t \mid y) = \nabla \log p_t(x_t) + \nabla \log c_t(y \mid x_t)$$

Unconditioned Logit

- The magic in practical implementation

$$s_{\text{practice}}(x_t, y, t) = \nabla \log p_t(x_t) + \eta \nabla \log c_t(y \mid x_t)$$

The Bayes Rule – Classifier Guidance

- Discrete label

External Classifier

$$\nabla \log p_t(x_t \mid y) = \underbrace{\nabla \log p_t(x_t)}_{\text{Unconditioned}} + \underbrace{\nabla \log c_t(y \mid x_t)}_{\text{Logit}}$$

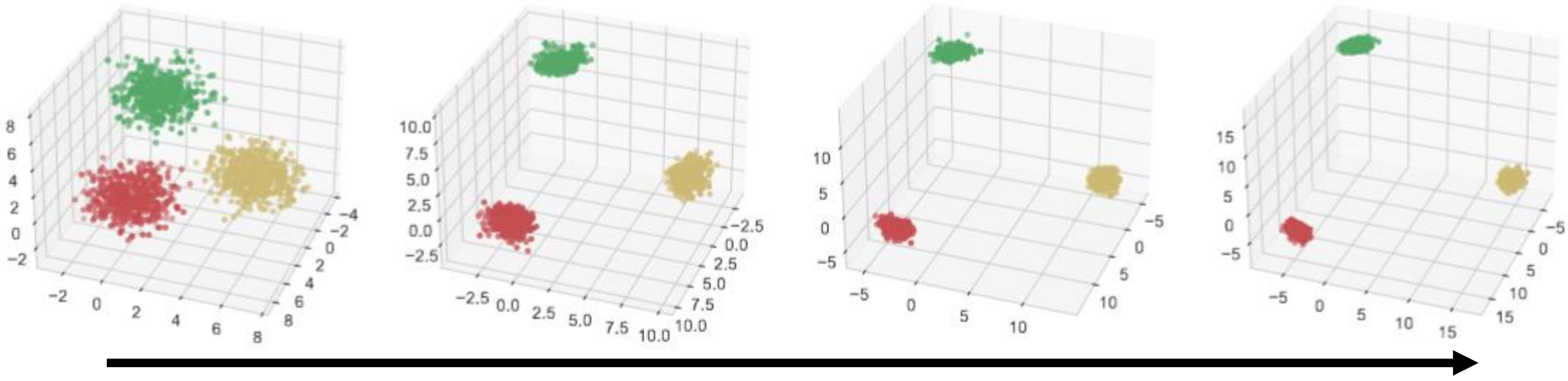
- The magic in practical implementation

$$s_{\text{practice}}(x_t, y, t) = \nabla \log p_t(x_t) + \eta \nabla \log c_t(y \mid x_t)$$

🤔

A Glimpse of Influence in 3D Gaussian Mixture

$\eta = 1$ $\eta = 10$ $\eta = 50$ $\eta = 100$



Class alignment increase

Diversity decrease

-- Y. Wu, M. Chen, Z. Li, M. Wang, Y. Wei. "Theoretical Insights for Diffusion Guidance: A Case Study for Gaussian Mixture Models", ICML 2024.

Classifier-Free Guidance

- Limitations of classifier guidance

Discrete label and external training

Classifier-Free Guidance

- Limitations of classifier guidance

Discrete label and external training

- Classifier-free guidance introduces a mask signal

$$\tau \in \{\emptyset, \mathrm{id}\}$$

Classifier-Free Guidance

- Limitations of classifier guidance

Discrete label and external training

- Classifier-free guidance introduces a mask signal

$$\tau \in \{\emptyset, \mathrm{id}\} \xrightarrow{\tau = \emptyset} s_1(x, \emptyset, t)$$

Classifier-Free Guidance

- Limitations of classifier guidance

Discrete label and external training

- Classifier-free guidance introduces a mask signal

$$
\begin{tikzcd}
 & s_1(x, \emptyset, t) \\
\tau \in \{\emptyset, \mathrm{id}\} \arrow[ur, "\tau = \emptyset"] \arrow[dr, "\tau = \mathrm{id}"'] & \\
 & s_2(x, y, t)
\end{tikzcd}
$$

Classifier-Free Guidance

- Limitations of classifier guidance

Discrete label and external training

- Classifier-free guidance introduces a mask signal

$$\tau \in \{\emptyset, \mathrm{id}\} \quad \xrightarrow{\tau = \emptyset} \; s_1(x, \emptyset, t)$$

Ignore label to extract common features

$$\tau \in \{\emptyset, \mathrm{id}\} \quad \xrightarrow{\tau = \mathrm{id}} \; s_2(x, y, t)$$

Classifier-Free Guidance

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\begin{tikzcd}
 & s_1(x, \emptyset, t) \\
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 & s_2(x, y, t)
\end{tikzcd}
$$

$s_1(x, \emptyset, t)$ Ignore label to extract common features

$s_2(x, y, t)$ Respect label to find specific information

Classifier-Free Guidance

- Limitations of classifier guidance

Discrete label and external training

- Classifier-free guidance introduces a mask signal

$$\tau \in \{\emptyset, \mathrm{id}\} \quad \begin{cases} \xrightarrow{\tau = \emptyset} s_1(x, \emptyset, t) & \text{Ignore label to extract common features} \\ \xrightarrow{\tau = \mathrm{id}} s_2(x, y, t) & \text{Respect label to find specific information} \end{cases}$$

Trained together
Share parameters

Modeling Diverse Data

Practical Data Is High-D And Complex

- ImageNet resolution: $D = 224 \times 224 \times 3$

Practical Data Is High-D And Complex

- ImageNet resolution: $D = 224 \times 224 \times 3$

Curse of Dimensionality

Practical Data Is High-D And Complex

- ImageNet resolution: $D = 224 \times 224 \times 3$

Curse of Dimensionality

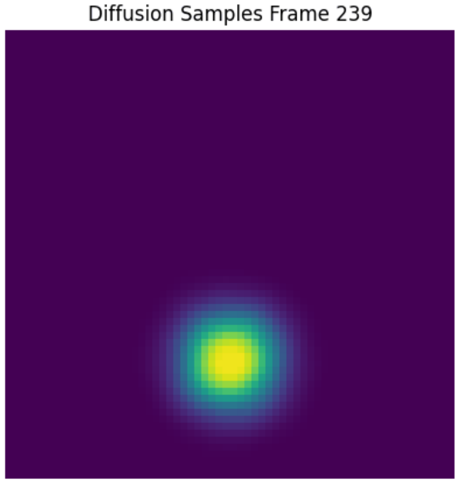
- Sequential data enlarges the dimension heavily

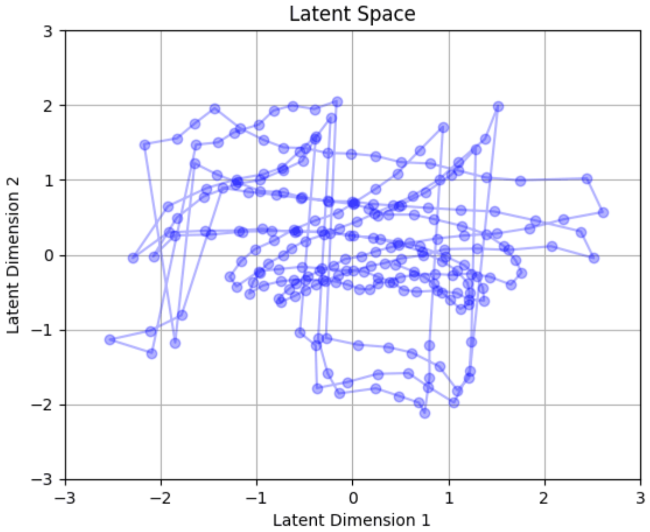
Practical Data Is High-D And Complex

- ImageNet resolution: $D = 224 \times 224 \times 3$

Curse of Dimensionality 😰

- Sequential data enlarges the dimension heavily





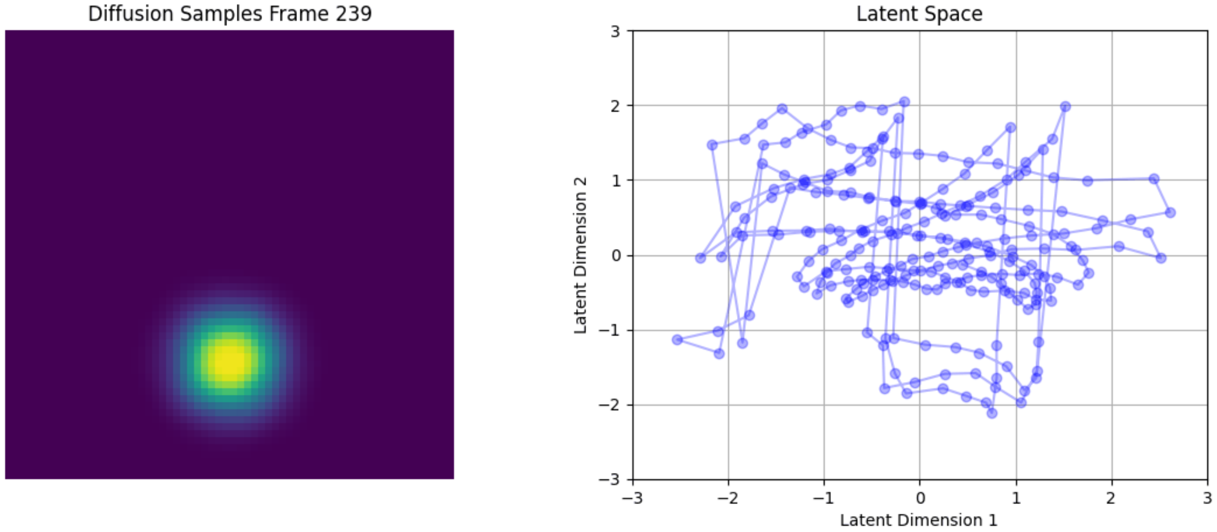
2D bouncing ball

Practical Data Is High-D And Complex

- ImageNet resolution: $D = 224 \times 224 \times 3$

Curse of Dimensionality

- Sequential data enlarges the dimension heavily
- also introduces **spatial-temporal dependencies**



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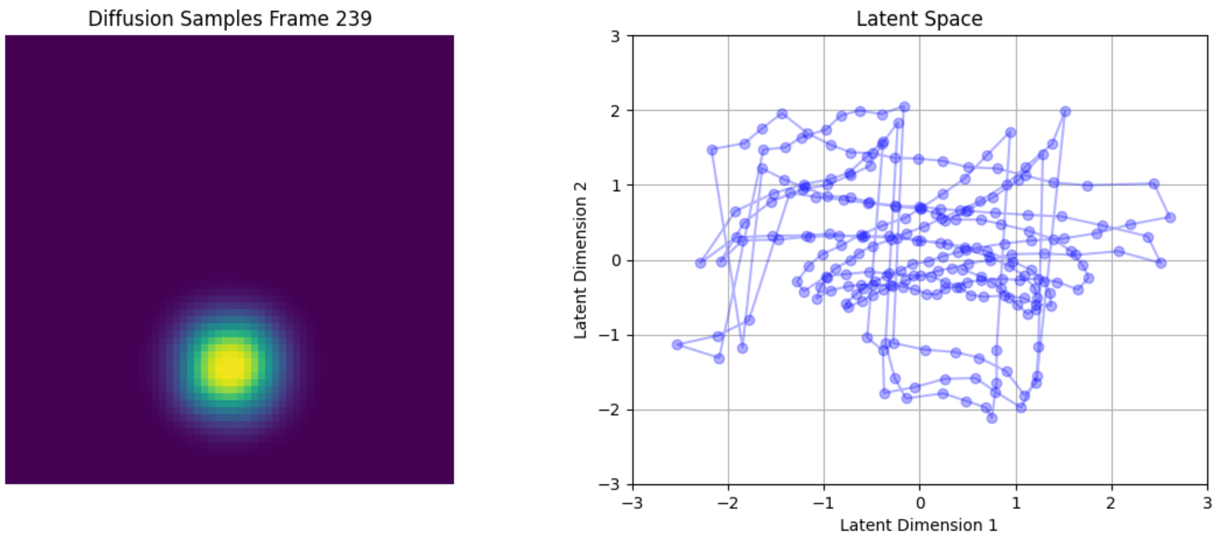

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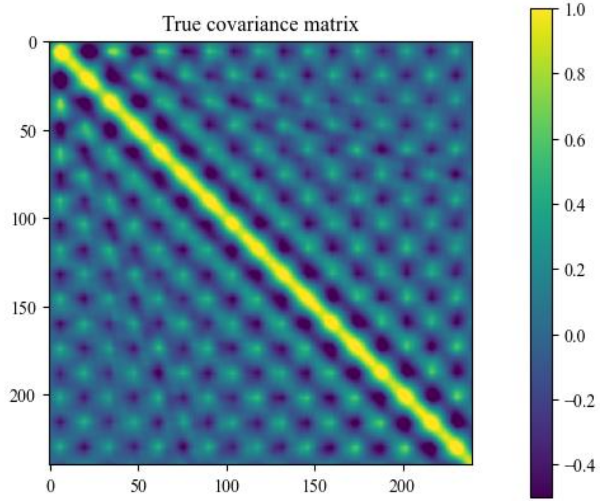
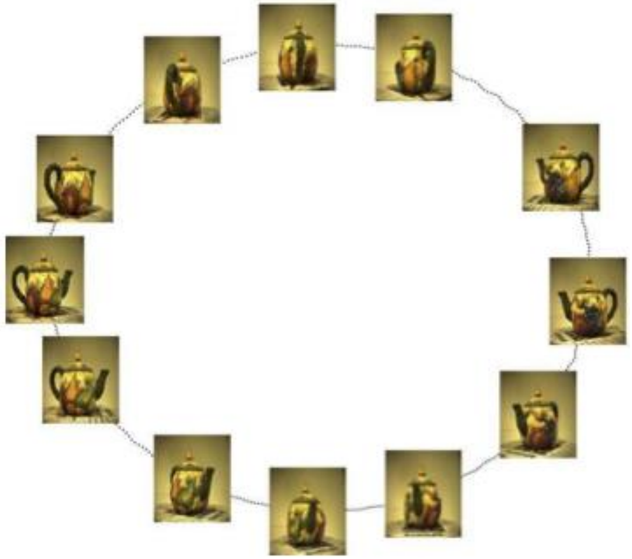


Correlation between frames

Practical High-D Data Is Low-Dimensional



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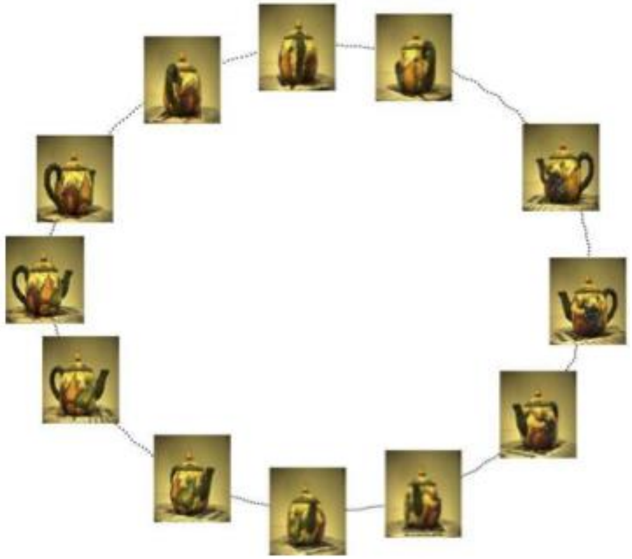

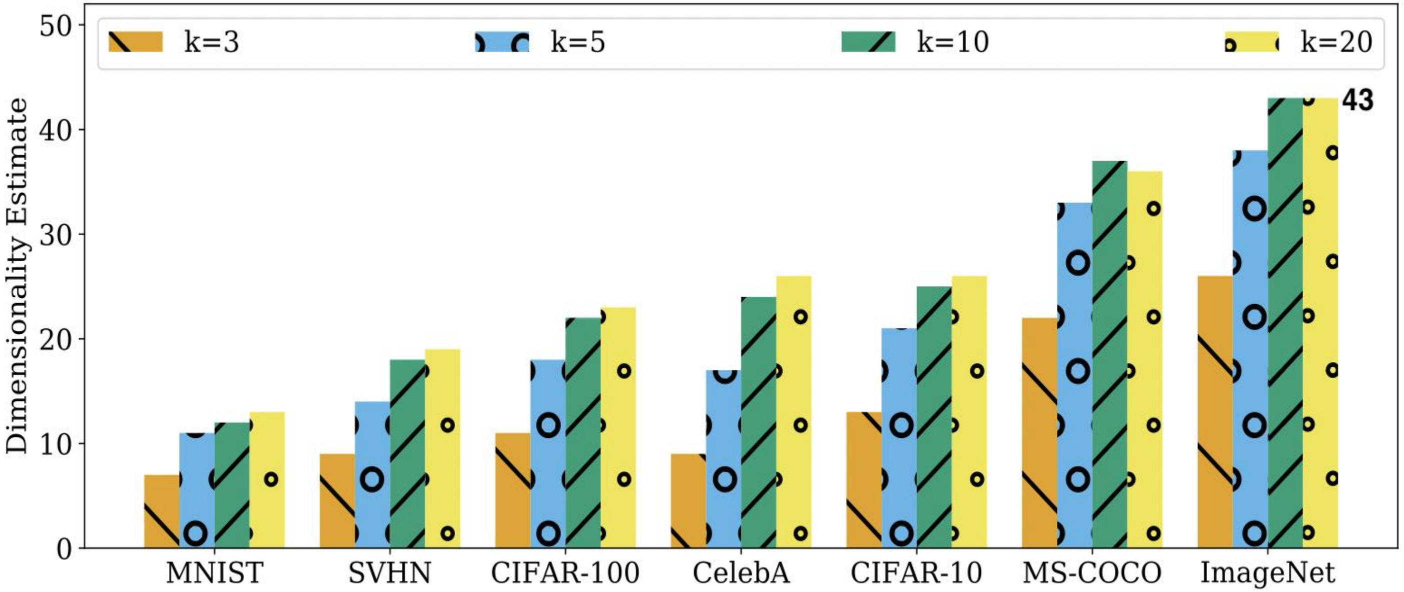

$$224 \times 224 \times 3 \qquad \text{v.s.} \qquad \leq 43$$

-- Figure credit: (Weinberger & Saul, 2006; P. Pope et al., 2021)

How Diffusion Model Finds Structures?

- Dynamic evolution

Backward $$\mathrm{d}X_t^{\leftarrow} = \left[\frac{1}{2}X_t^{\leftarrow} + \boxed{\nabla \log p_{T-t}(X_t^{\leftarrow})}\right]\mathrm{d}t + \mathrm{d}\overline{W}_t$$

Score Function **Brownian**

How Diffusion Model Finds Structures?

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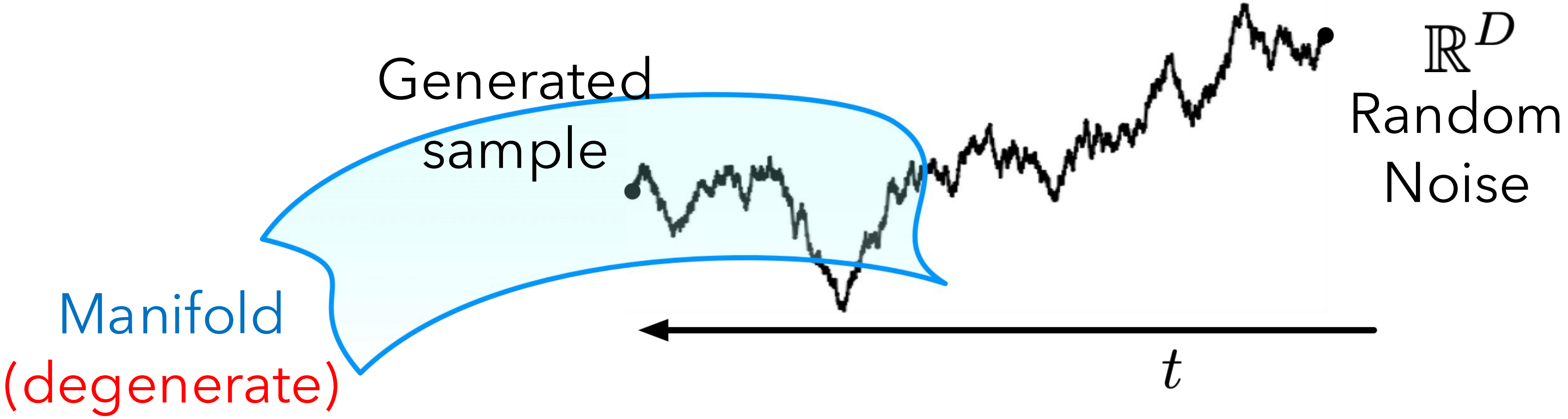
Backward

$$\mathrm{d}X_t^{\leftarrow} = \left[\frac{1}{2}X_t^{\leftarrow} + \underbrace{\boxed{\nabla \log p_{T-t}(X_t^{\leftarrow})}}_{\text{Score Function}}\right]\mathrm{d}t + \underbrace{\mathrm{d}\overline{W}_t}_{\text{Brownian}}$$

- Start from high-D but land in a manifold?



Score Function Adapts to Data Structures

- Linear subspace data

$$x = Az \quad \text{with} \quad z \sim P_z \quad z \in \mathbb{R}^d$$

- Score decomposition

$$\nabla \log p_t(x) = \boxed{A \nabla \log p_t^z(A^\top x)} - \boxed{\frac{1}{1 - e^{-t}} \left(I_D - AA^\top\right) x}$$

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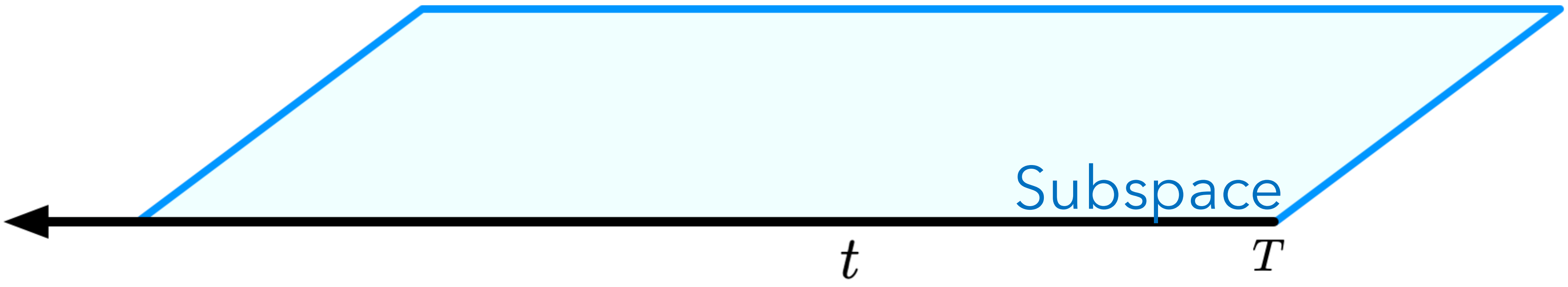

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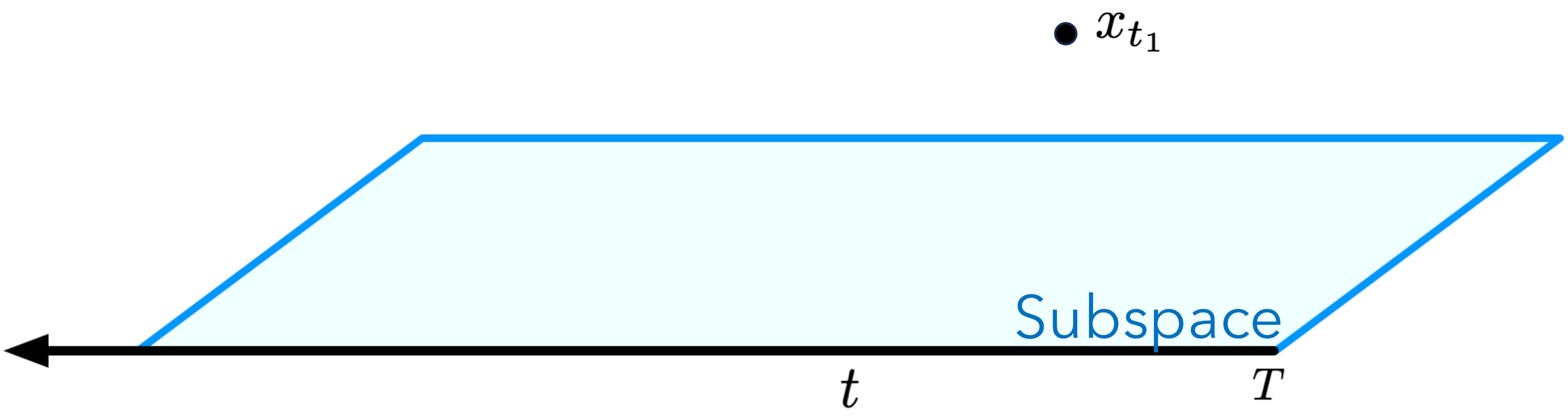

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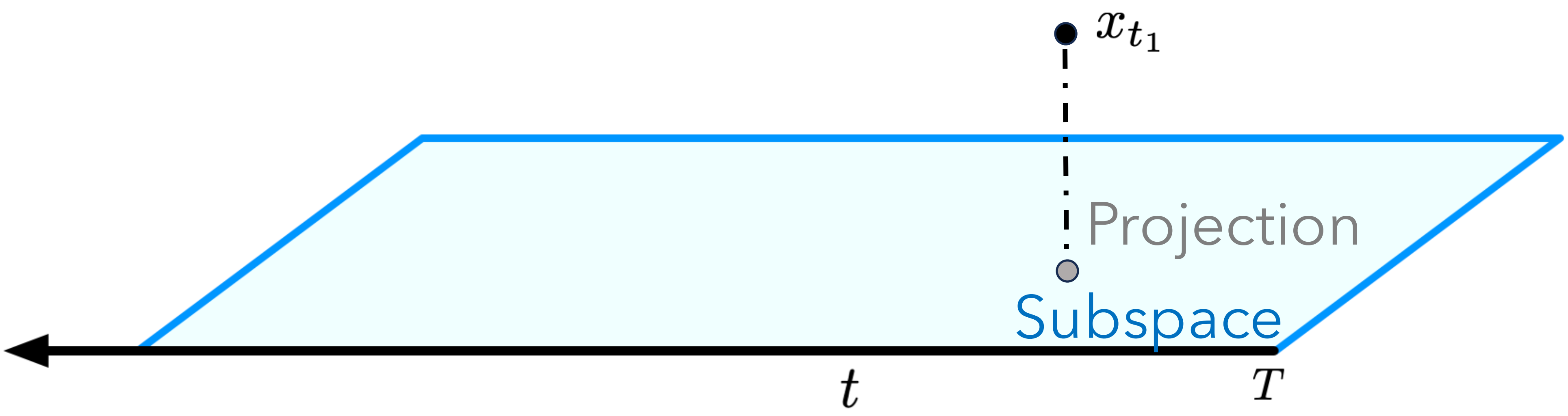

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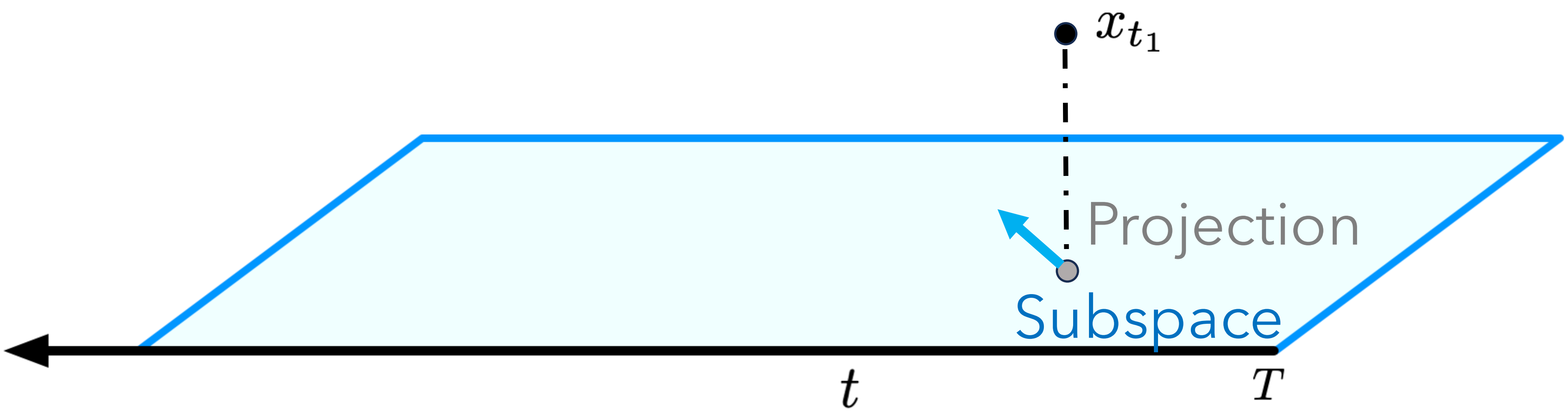

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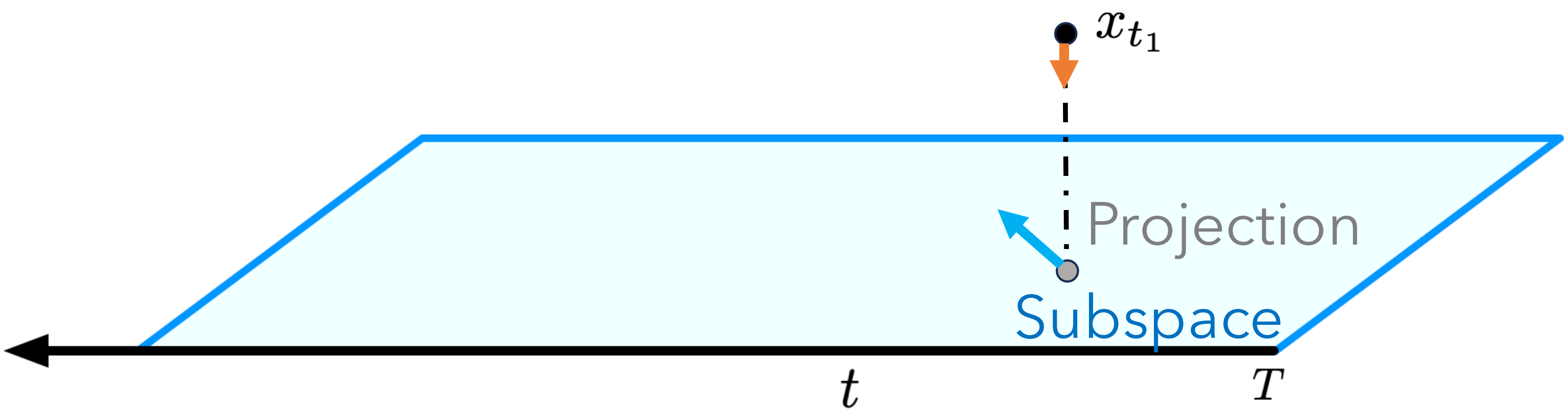

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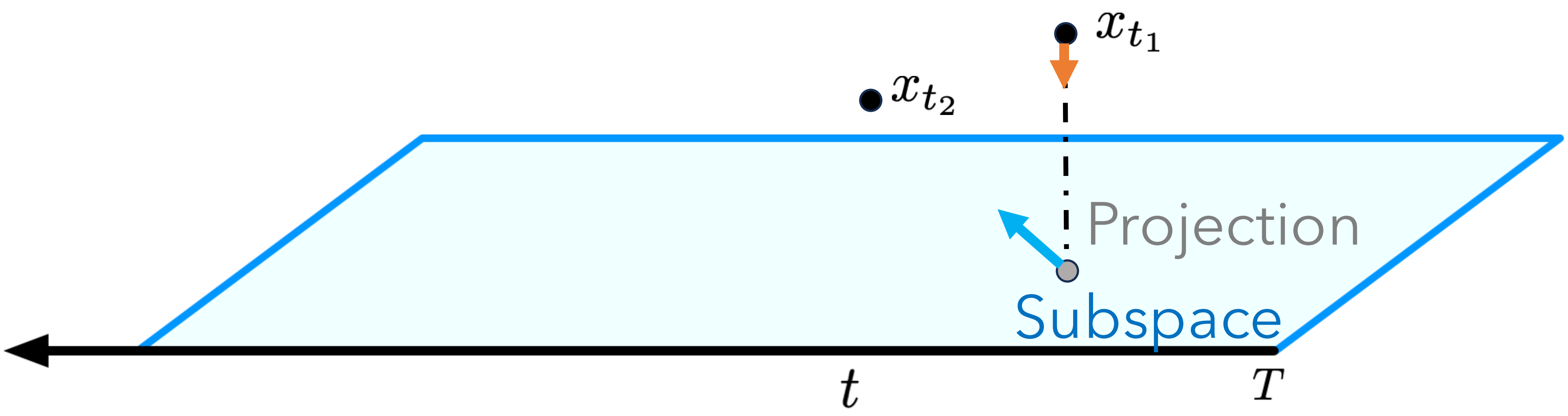

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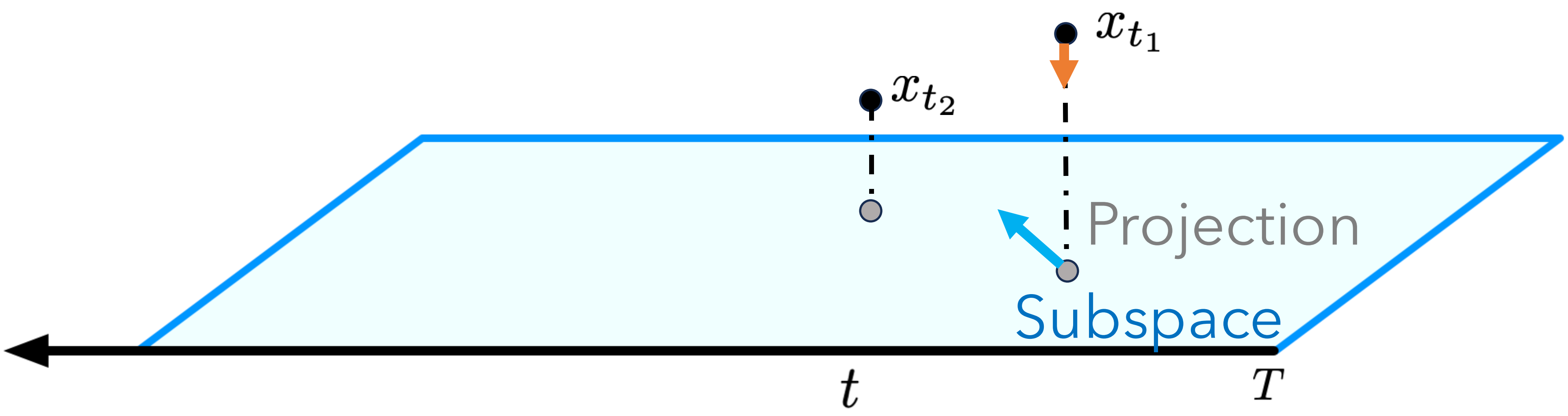

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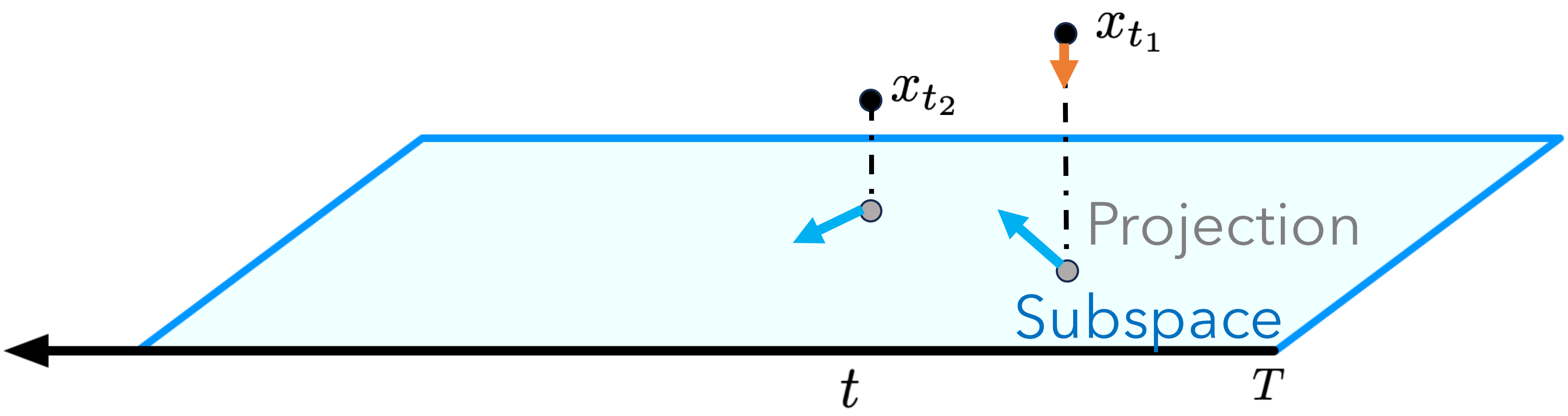

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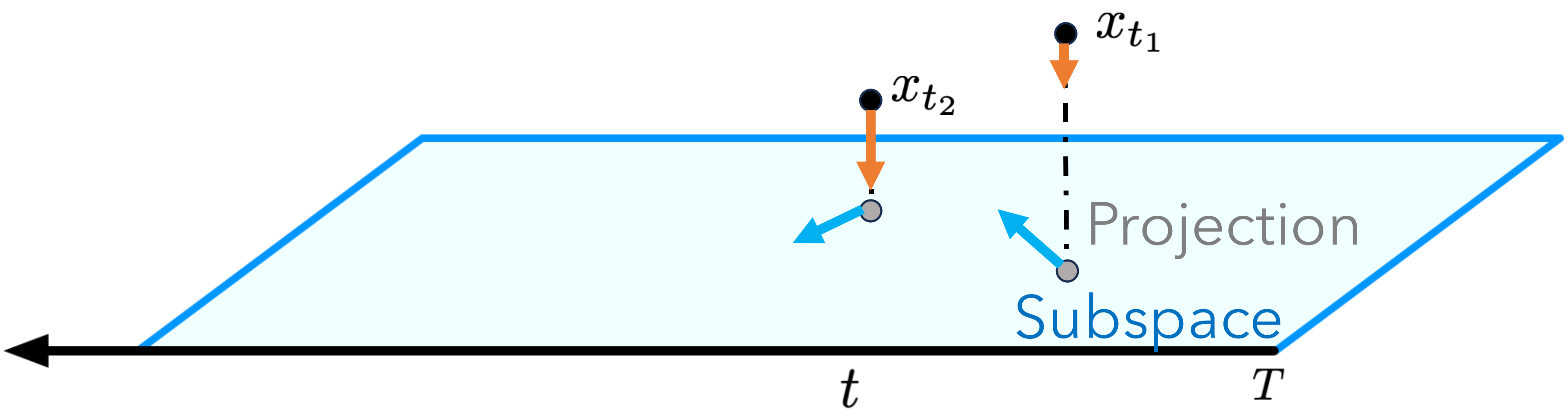

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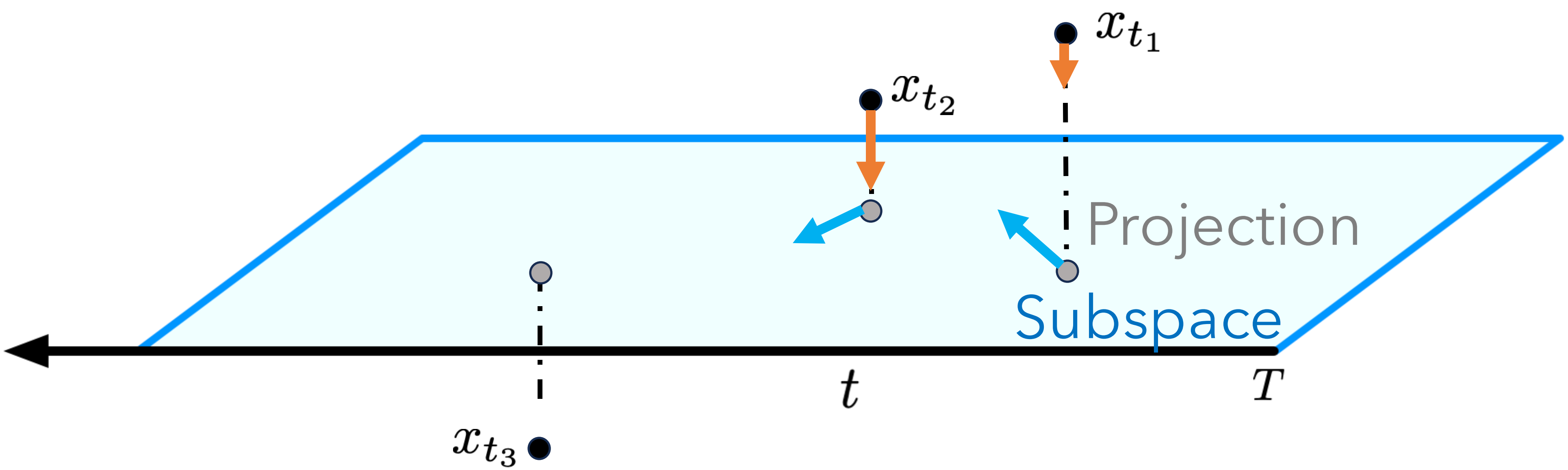

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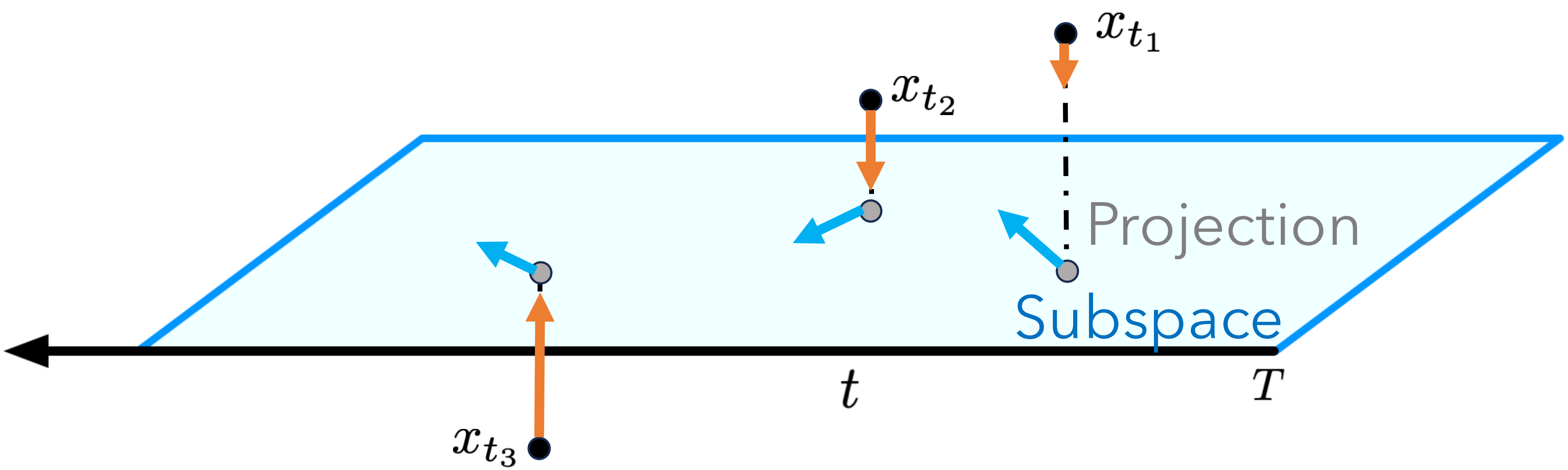

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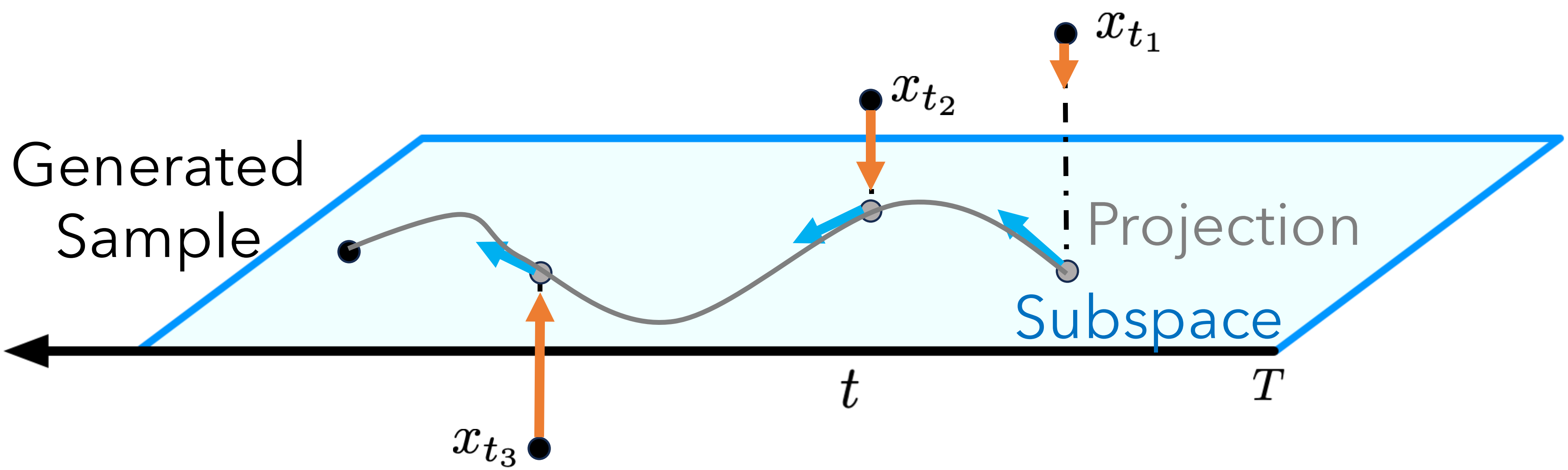

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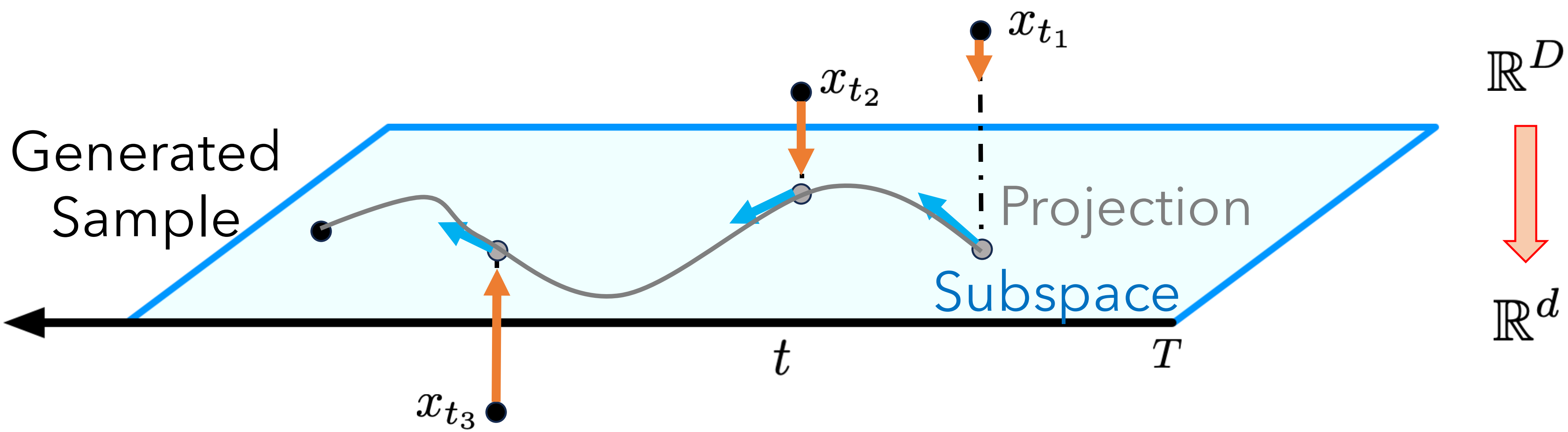

Diffusion Model Efficiently Learns Low-D Data

Theorem

✓ Score function can be learned efficiently at the rate

$$\tilde{\mathcal{O}}\left(n^{-\frac{1}{2(d+5)}}\right)$$

✓ Underlying distribution is learned at the same rate.

-- M. Chen, K. Huang, T. Zhao, M. Wang. "Score Approximation, Estimation and Distribution Recovery of Diffusion Models on Low-Dimensional Data", ICML 2023

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Take-home message:

✓ **Accurate** in learning data distributions

✓ **Efficient**: no curse of dimensionality

✓ **Generalizable** to manifold data (Tang and Yang, 2024)

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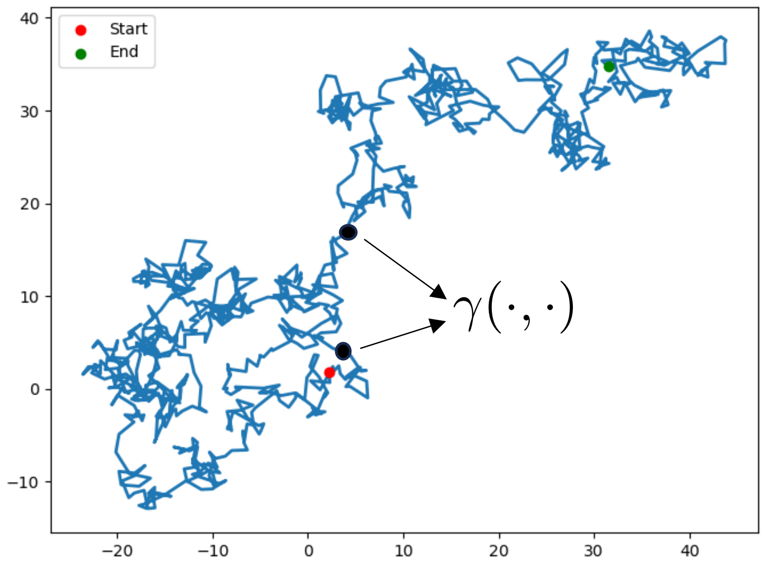
Sequence Data with Dependencies

- We consider

$$X_1, \ldots, X_{h_N} \sim \mathcal{GP}(\mu(\cdot), \gamma(\cdot,\cdot), \Lambda) \in \mathbb{R}^D$$

  - $0 = h_1 < \cdots < h_N = H$ sampling times
  - $\mu(\cdot)$ time varying mean function
  - $\gamma(\cdot,\cdot)$ covariance function (kernel)
  - $\Lambda = \mathrm{Cov}[X_h]$ marginal covariance matrix



2D Brownian motion

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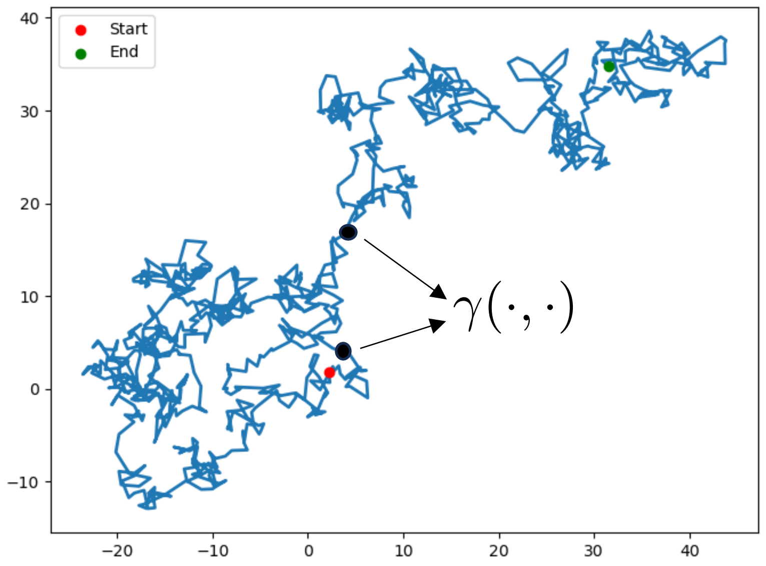


2D Brownian motion

Simplification

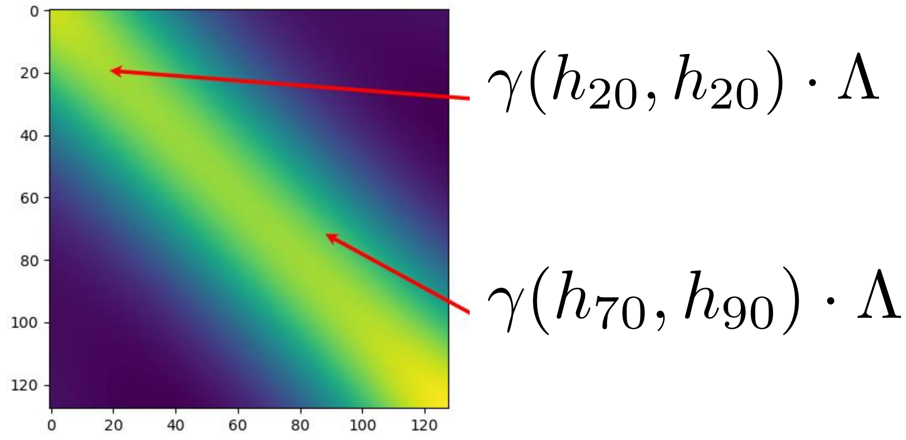
✓ $\gamma(\cdot,\cdot)$ only depends on time gaps, i.e.,

$$\gamma(t_1, t_2) = g(|t_1 - t_2|)$$

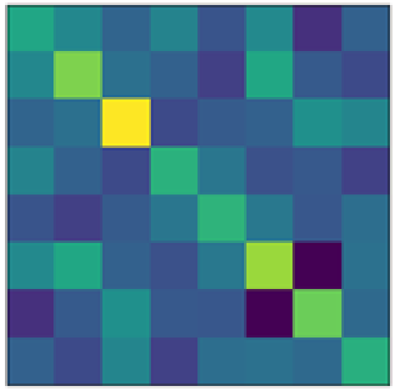
Description of Spatial-Temporal Dependencies

- We stack data together as a vector in $\mathbb{R}^{DN}$, whose distribution is Gaussian

$$\mathrm{N}\left(\begin{bmatrix}\mu(h_1)\\ \vdots \\ \mu(h_N)\end{bmatrix}, \Gamma\otimes\Lambda = \begin{bmatrix}\gamma(h_1,h_1)\Lambda,\ldots,\gamma(h_1,h_N)\Lambda\\ \vdots \\ \gamma(h_N,h_1)\Lambda,\ldots,\gamma(h_N,h_N)\Lambda\end{bmatrix}\right)$$



Temporal dependencies



Spatial dependencies

Description of Spatial-Temporal Dependencies

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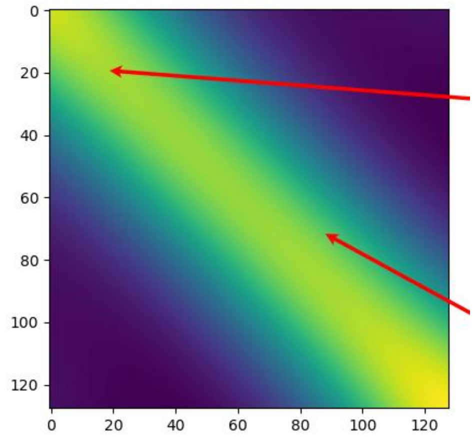
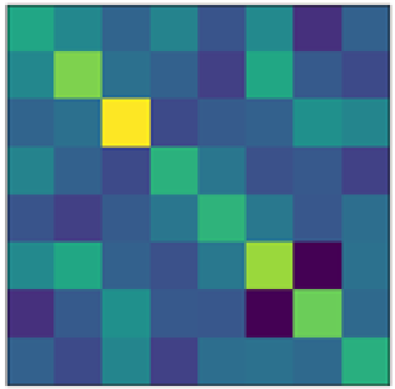
Huge dimension?

$$\mathrm{N}\left(\begin{bmatrix}\mu(h_1)\\ \vdots \\ \mu(h_N)\end{bmatrix}, \Gamma\otimes\Lambda=\begin{bmatrix}\gamma(h_1,h_1)\Lambda,\ldots,\gamma(h_1,h_N)\Lambda\\ \vdots\\ \gamma(h_N,h_1)\Lambda,\ldots,\gamma(h_N,h_N)\Lambda\end{bmatrix}\right)$$



$\gamma(h_{20},h_{20})\cdot\Lambda$

$\gamma(h_{70},h_{90})\cdot\Lambda$

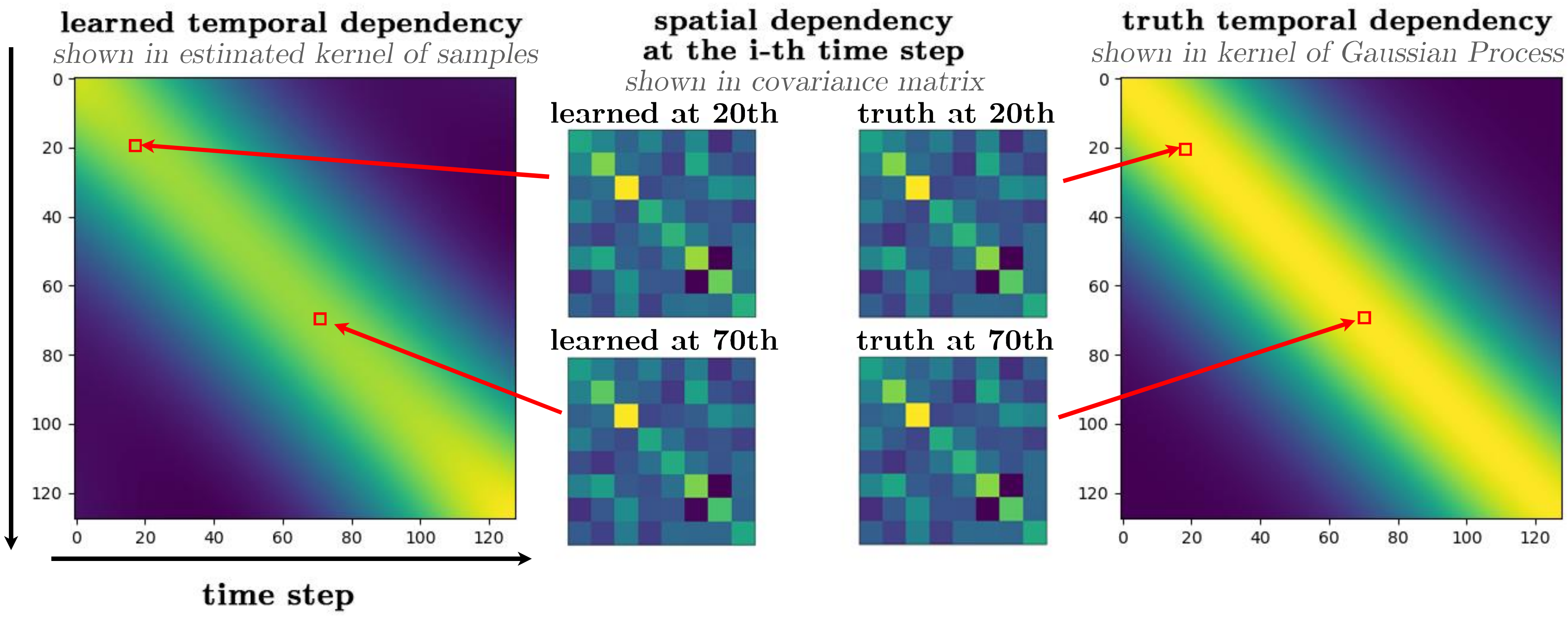


Temporal dependencies

Spatial dependencies

Proper Score Network Learns Dependencies

- We simulate a Gaussian process with 128 length
- Diffusion model with transformer learns very well!



Represent Score via Algorithm Unrolling

Score Function

$$\boxed{\nabla \log p_t(\mathbf{v}_t)} = \arg\min_{\mathbf{s} \in \mathbb{R}^{dN}} L_t(\mathbf{s}) = \frac{1}{2}\mathbf{s}^\top \left(\alpha_t^2 (\Gamma \otimes \mathbf{I}) + \sigma_t^2 \mathbf{I} \right) \mathbf{s} - (\mathbf{v}_t - \alpha_t \mu)^\top \mathbf{s}$$

Represent Score via Algorithm Unrolling

Score Function

Gradient Descent

$$\boxed{\nabla \log p_t(\mathrm{v}_t)} = \arg\min_{\mathrm{s} \in \mathbb{R}^{dN}} L_t(\mathrm{s}) = \frac{1}{2}\mathrm{s}^\top \left(\alpha_t^2(\Gamma \otimes \mathrm{I}) + \sigma_t^2 \mathrm{I}\right)\mathrm{s} - (\mathrm{v}_t - \alpha_t \mu)^\top \mathrm{s}$$

$$\mathrm{s}_i^{(0)} \longrightarrow \boxed{\Gamma} \xrightarrow{-\eta_t \nabla L_t(\mathrm{s}_i^{(0)})} \mathrm{s}_i^{(1)} \longrightarrow \cdots \longrightarrow \mathrm{s}_i^{(K)}$$

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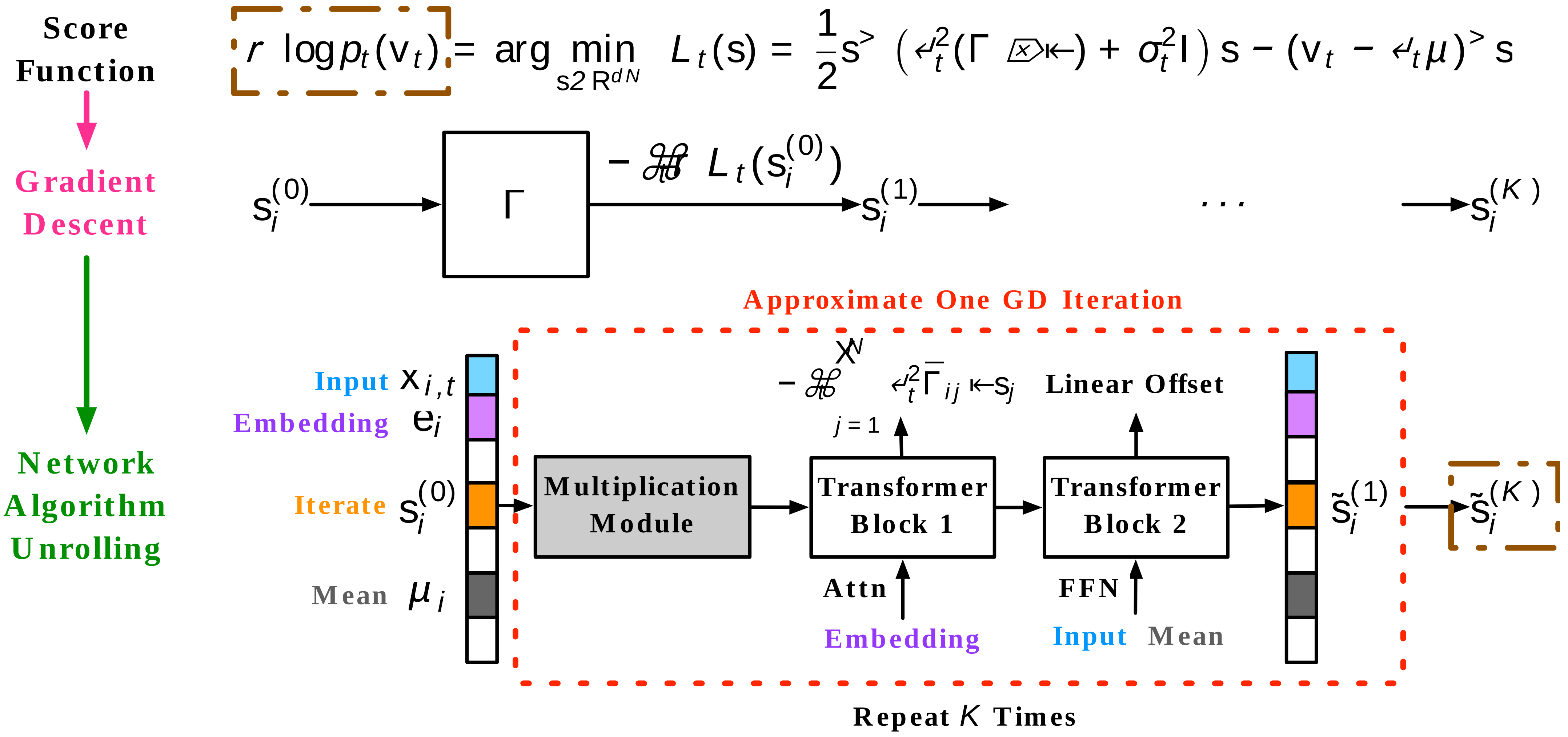

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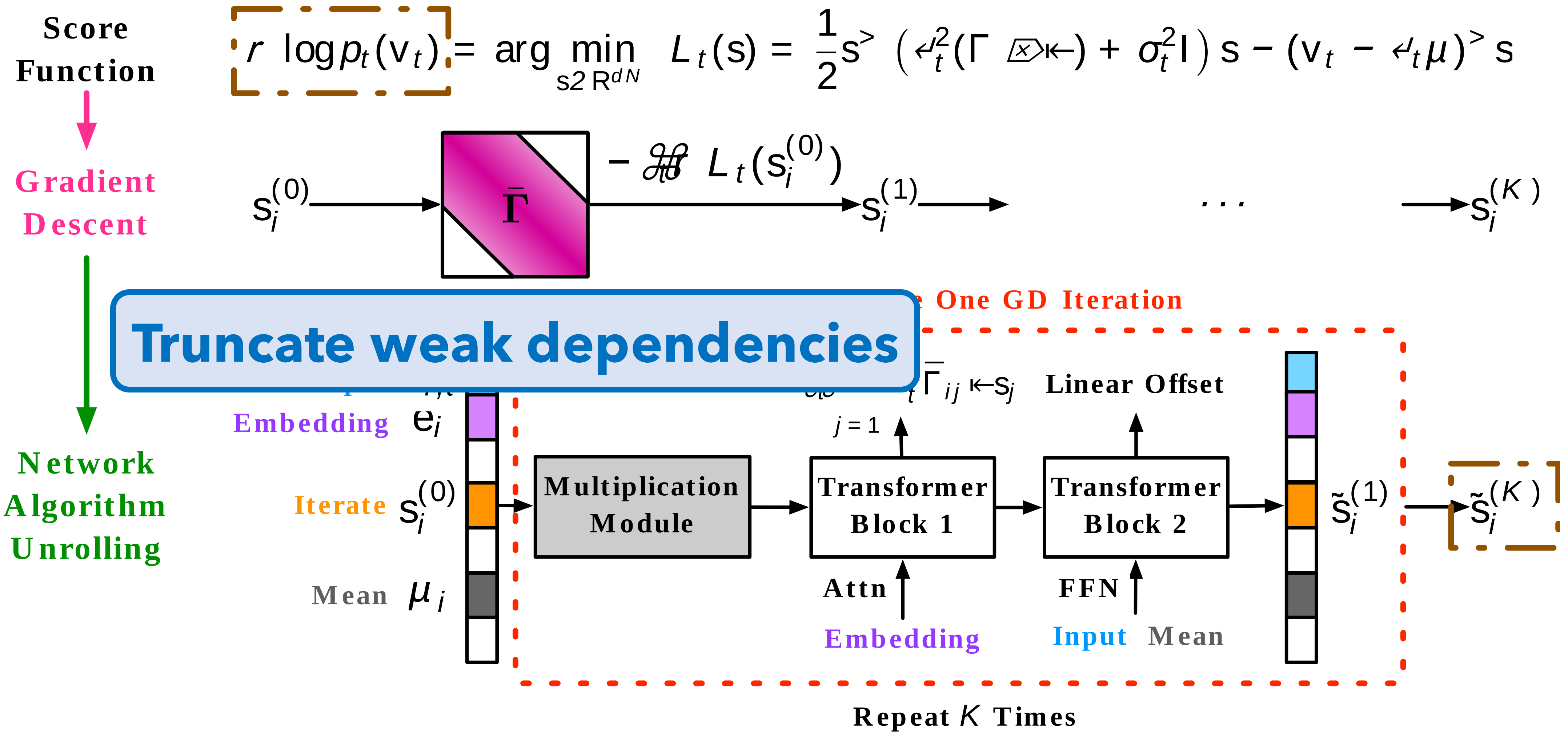

Diffusion Model Learns Gaussian Process

Theorem

- ✓ Score function can be learned efficiently at the rate

$$\tilde{O}\left(\sqrt{\frac{\text{dependency-decay} \cdot \texttt{sequence-length} \cdot D^3}{n}}\right)$$

- ✓ Gaussian process distribution is learned at the same rate.

-- H. Fu, Z. Dou, J. Guo, M. Wang, M. Chen. “Diffusion Transformer Captures Spatial-Temporal Dependencies: A Theory for Gaussian Process Data”, 2024

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Take-home message:

✓ **Weak** dependence on the length of sequence

✓ **Adaptive** to spatial-temporal dependencies

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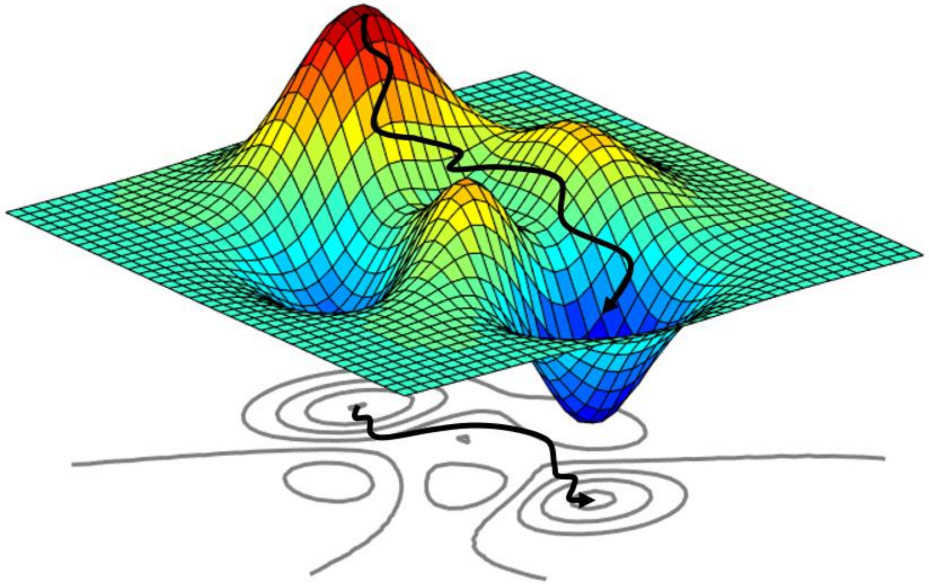
Leverage Diffusion Models

Rethinking Optimization

$$x \in \arg\max \;\; f^*(\cdot)$$



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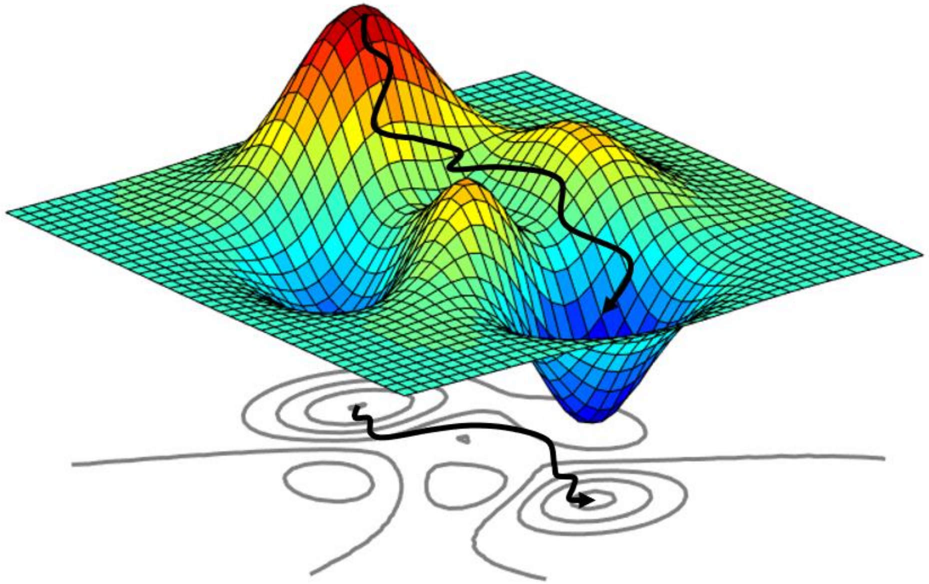

High-D

Nonconvex

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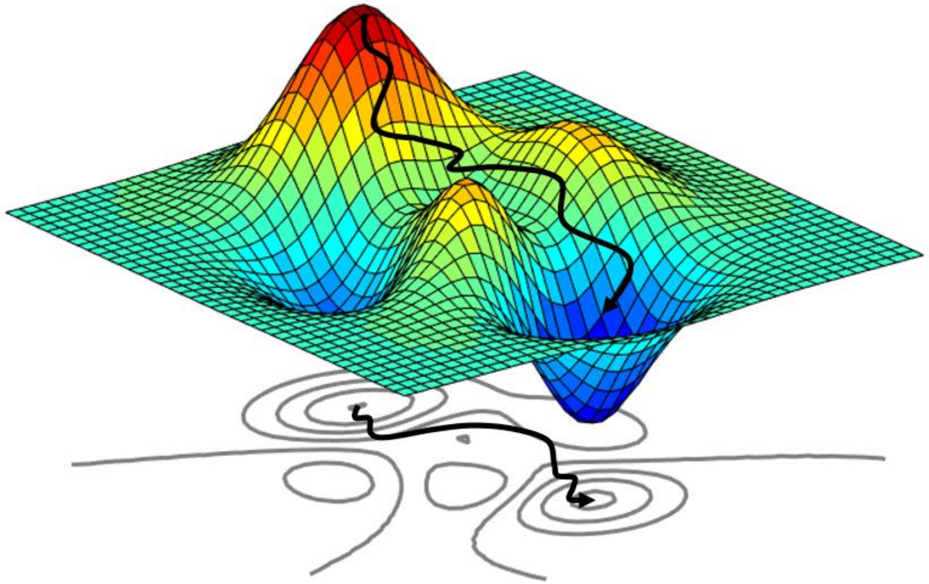

High-D

Nonconvex

Generate solution

$$x \sim \mathbb{P}(\cdot|\ f^*(\cdot) \geq a)$$

Rethinking Optimization

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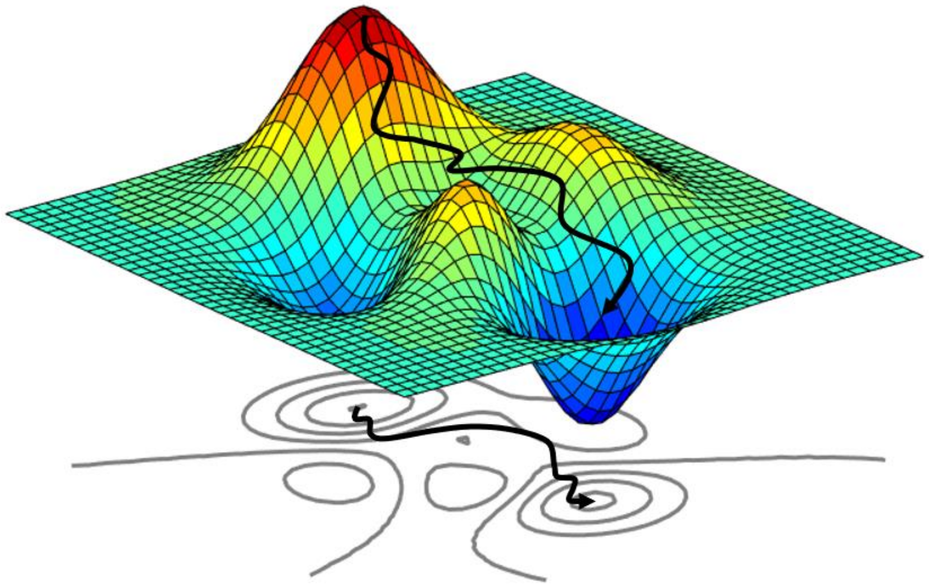

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Rethinking Optimization

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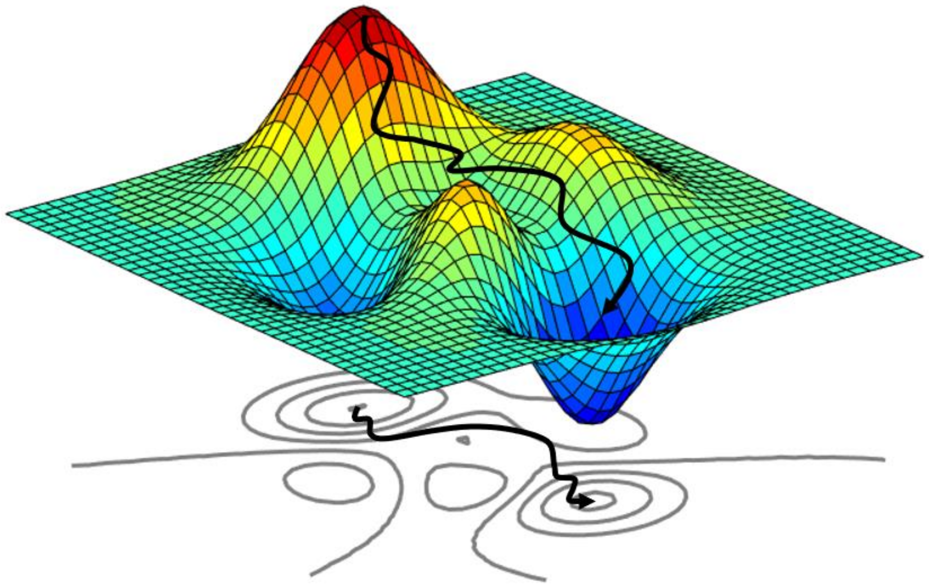

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High-D

Conditional distribution

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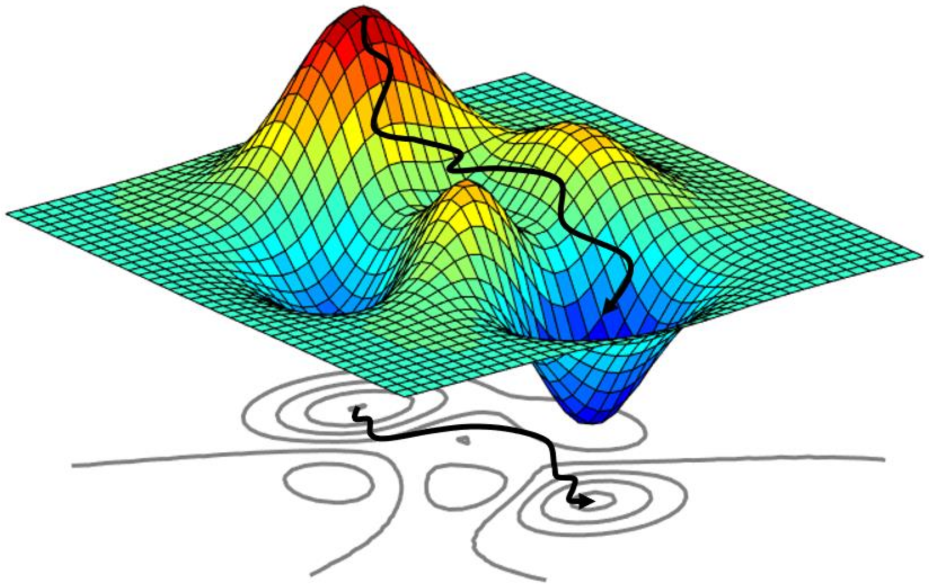

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Guidance

High-D

High-D

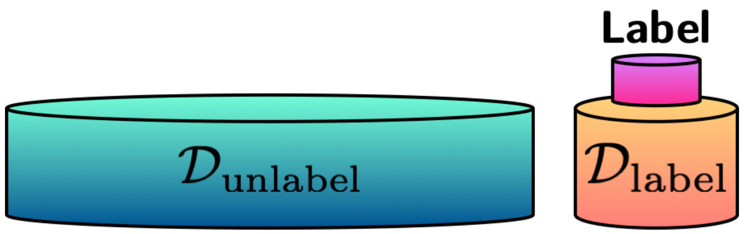
Nonconvex

Conditional distribution

Problem Setup: Offline Reward Maximization

- Given a training data set, generate new x
- Training data set

$$\mathcal{D}_{\text{unlabel}} = \{x_j\}_{j=1}^{n_{\text{unlabel}}}$$
$$\mathcal{D}_{\text{label}} = \{x_i, y_i = f^*(x_i) + \epsilon_i\}_{i=1}^{n_{\text{label}}}$$



  - ϵ_i is observation noise
  - f^* is reward function

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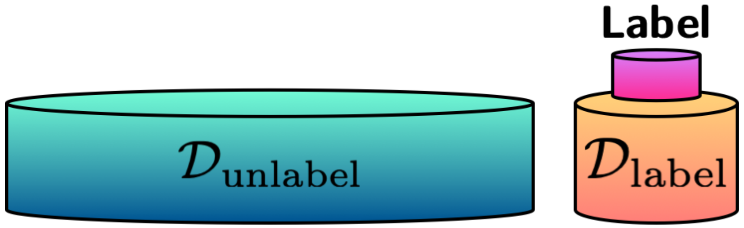


  - ϵ_i is observation noise
  - f^* is reward function

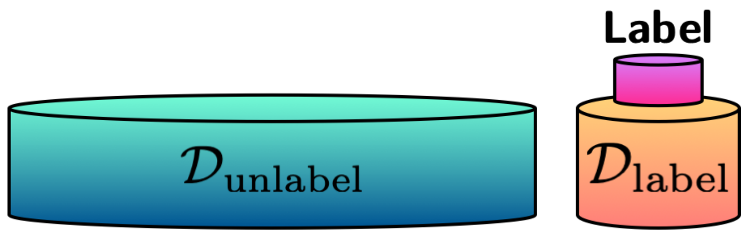
❑ Example: a large collection of unlabeled protein structures; only a few has measured properties.

Problem Setup: Offline Reward Maximization

- Given a training data set, generate new x
- Training data set

$$\mathcal{D}_{\text{unlabel}} = \{x_j\}_{j=1}^{n_{\text{unlabel}}}$$

$$\mathcal{D}_{\text{label}} = \{x_i, y_i = f^*(x_i) + \epsilon_i\}_{i=1}^{n_{\text{label}}}$$

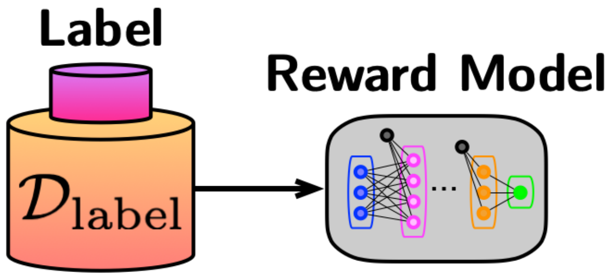


  - ➢ ϵ_i is observation noise
  - ➢ f^* is reward function

Off-policy bandit problem
(Jin et al., 2021; Nguyen-Tang et al., 2021)

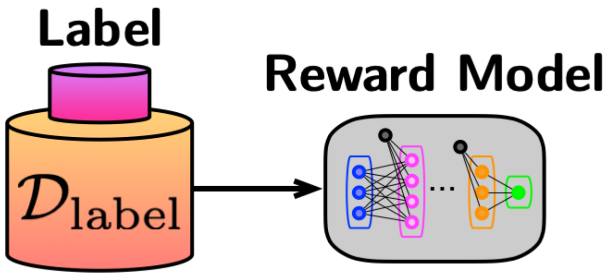
❑ Example: a large collection of unlabeled protein structures; only a few has measured properties.

Meta Algorithm



Step 1: Reward Learning

Meta Algorithm



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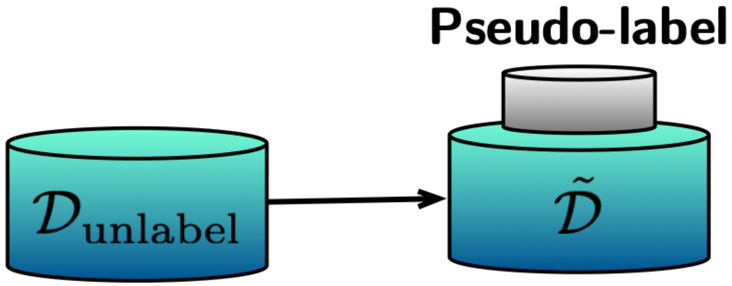
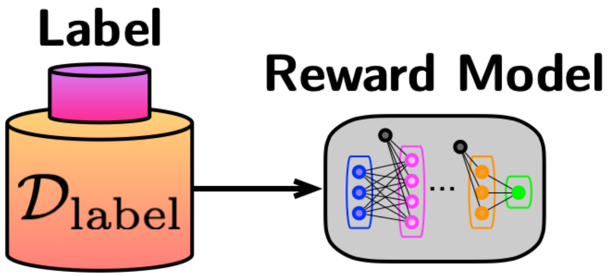


Step 2: Pseudo Labeling

Meta Algorithm



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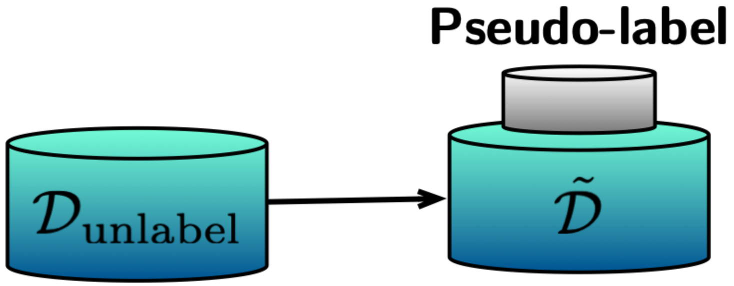

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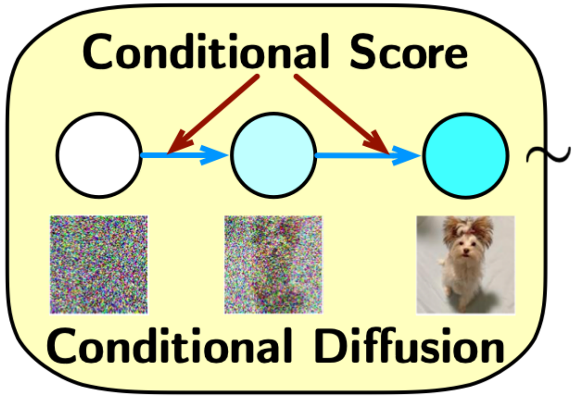
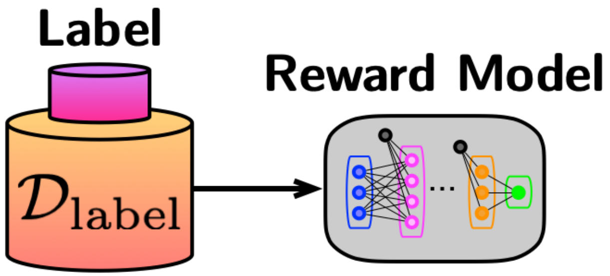


$$\sim \hat{\mathbb{P}}(\cdot \mid \text{reward})$$

Step 3: Conditional Diffusion Training

Meta Algorithm



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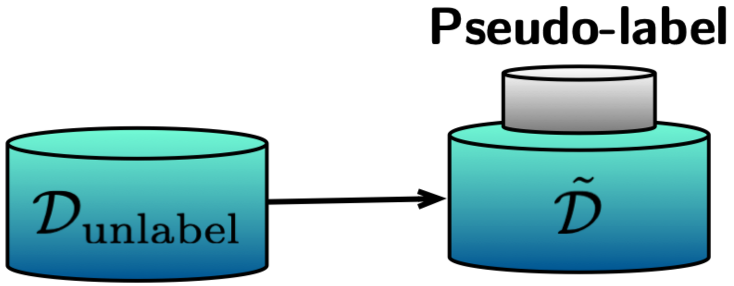

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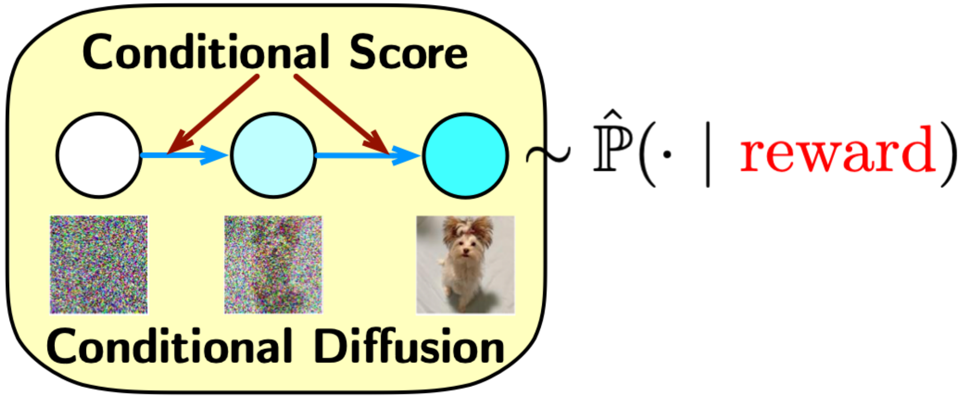

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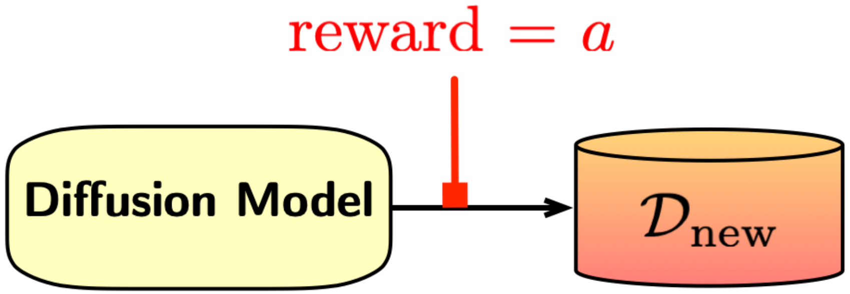

Step 4: Guided Generation

How Far Are We from The Targeted Reward

- Let a be the target reward of generation

$$\texttt{SubOpt}(a) = a - \texttt{Generated Average Reward}$$

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(Reward estimation error)

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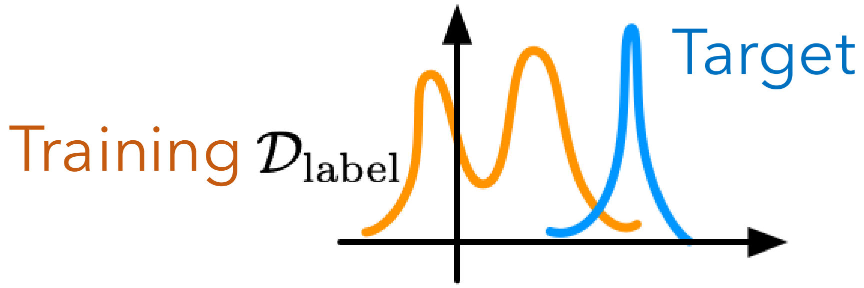
(Reward estimation error) $\circ$ (Reward distribution shift)



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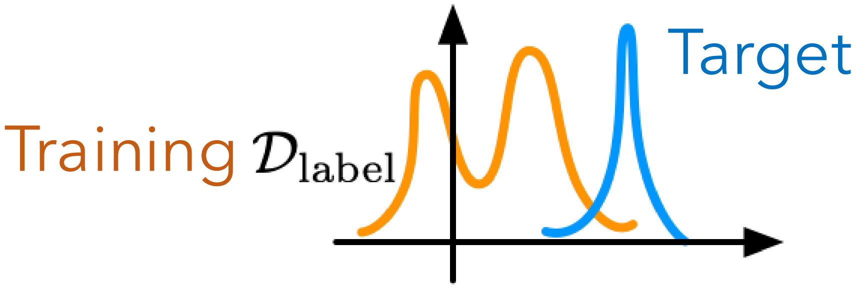
(Reward estimation error) ∘ (Reward distribution shift)

(Conditional diffusion error)



How Far Are We from The Targeted Reward

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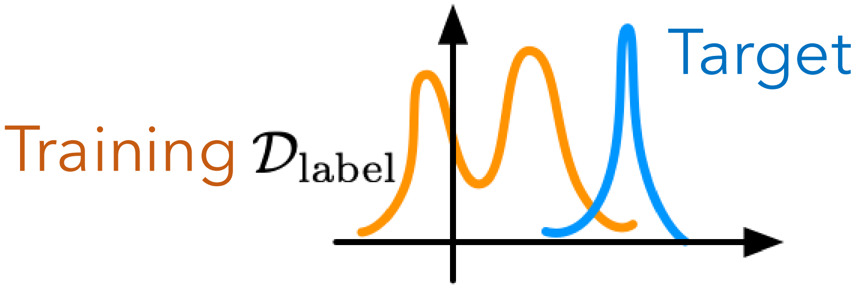
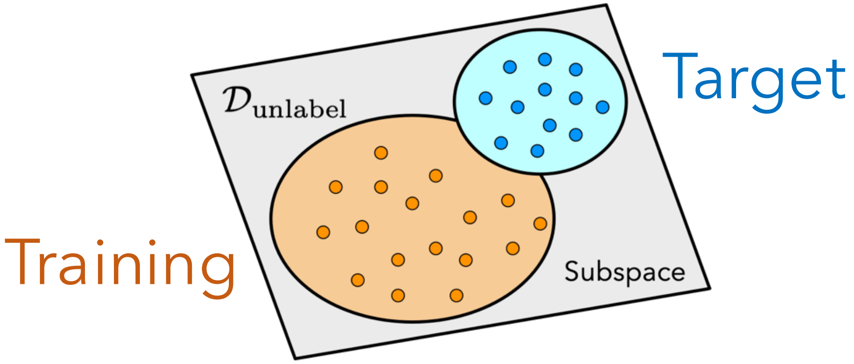
(Reward estimation error) $\circ$ (Reward distribution shift)

(Conditional diffusion error) $\circ$ (Diffusion distribution shift)





Case Study: Subspace Data + Linear Reward

Theorem

✓ The sub-optimality satisfies

$$\texttt{SubOpt}(a) = \tilde{\mathcal{O}}\left(\sqrt{\mathrm{Trace}\left(\hat{\Sigma}_\lambda^{-1}\Sigma_a\right)} \cdot \sqrt{\frac{d\log(n_{\mathrm{label}})}{n_{\mathrm{label}}}} + \min\{a, d\} \cdot \frac{a \cdot \mathrm{poly}(D, d)}{n_{\mathrm{unlabel}}^{1/6}}\right)$$

where $\hat{\Sigma}_\lambda = (X^\top X + \lambda I)/n_{\mathrm{label}}$ for X the data matrix, $\lambda > 0$, and Σ_a is the covariance matrix of $P_a(\cdot \mid \mathrm{reward} = a)$.

-- H. Yuan, K. Huang, C. Ni, Y. Ye, M. Chen, M. Wang. "Diffusion Model for Data-Driven Black-Box Optimization", NeurIPS 2023

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❖ Match optimal off-policy bandit learning with representation learning (Jin et al., 2021; Nguyen-Tang et al., 2021)

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Advantages of Generative Optimization

✓ Meta algorithm provably generates samples of high reward and fidelity, in nonparametric settings.

$$\texttt{SubOpt}(a) = \tilde{O}\left(\kappa_1(a) \cdot n_{\text{label}}^{-\frac{\alpha}{d+2\alpha}} + \kappa_2(a) \cdot n_{\text{unlabel}}^{-\frac{2}{3(d+6)}}\right)$$

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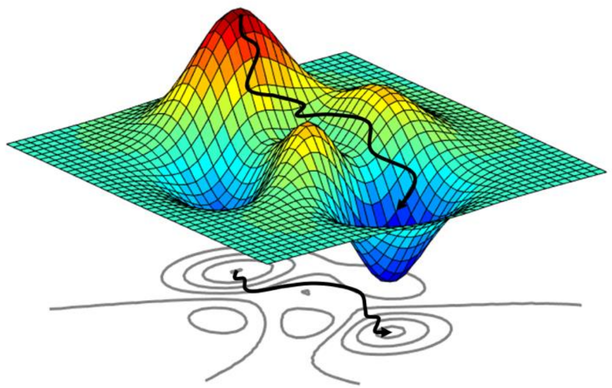
Generative optimization in offline:

✓ **Off-policy bandit optimality**

✓ **High-fidelity** to intrinsic structures

✓ **Efficiency**: no curse of dimensionality

✓ **Generalizable** to human preferences



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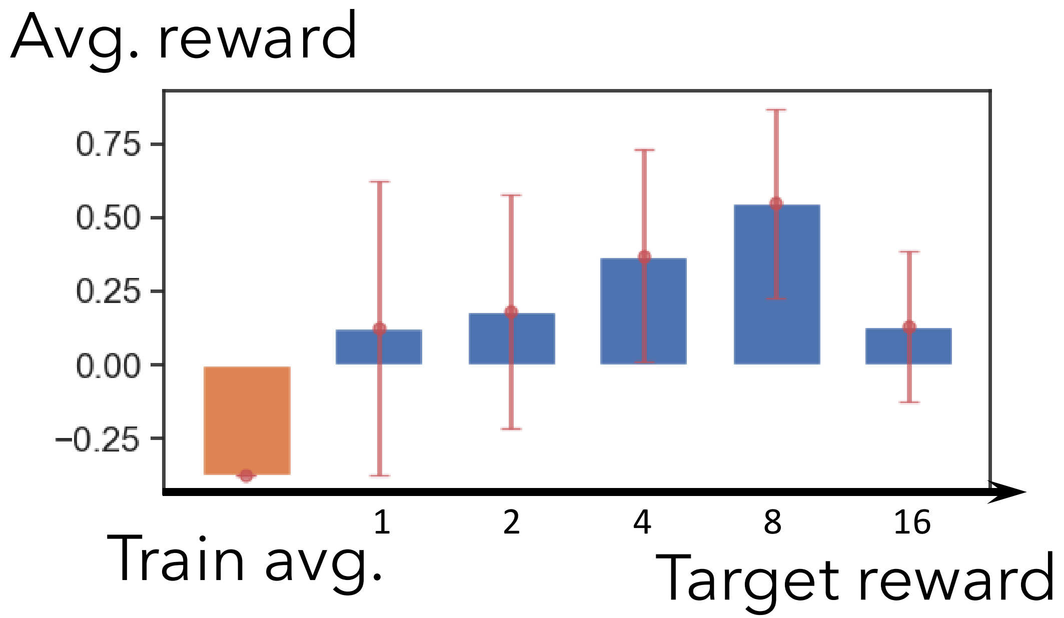
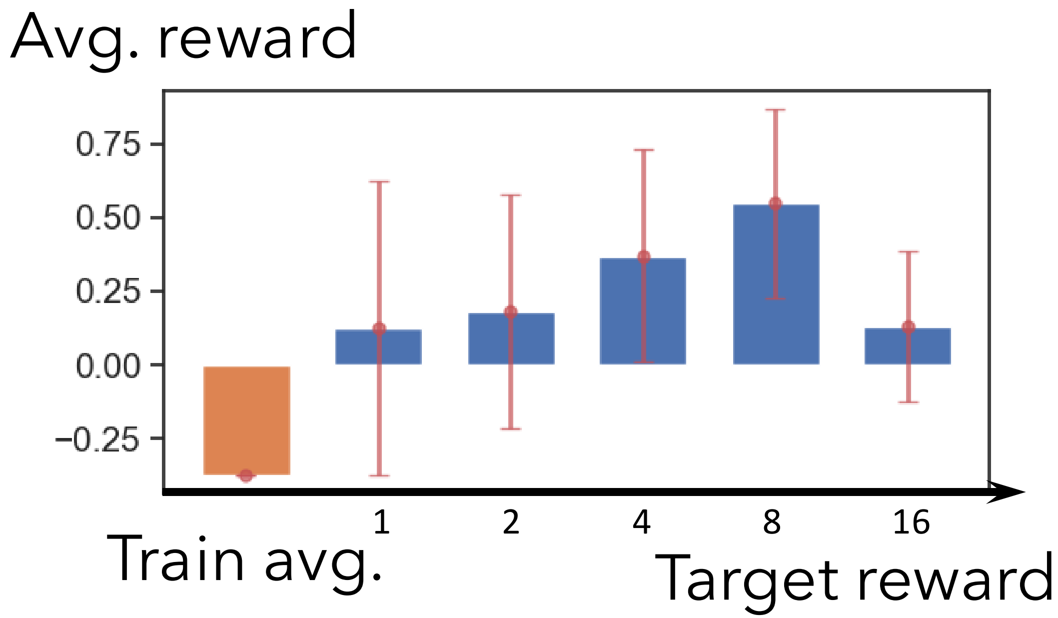
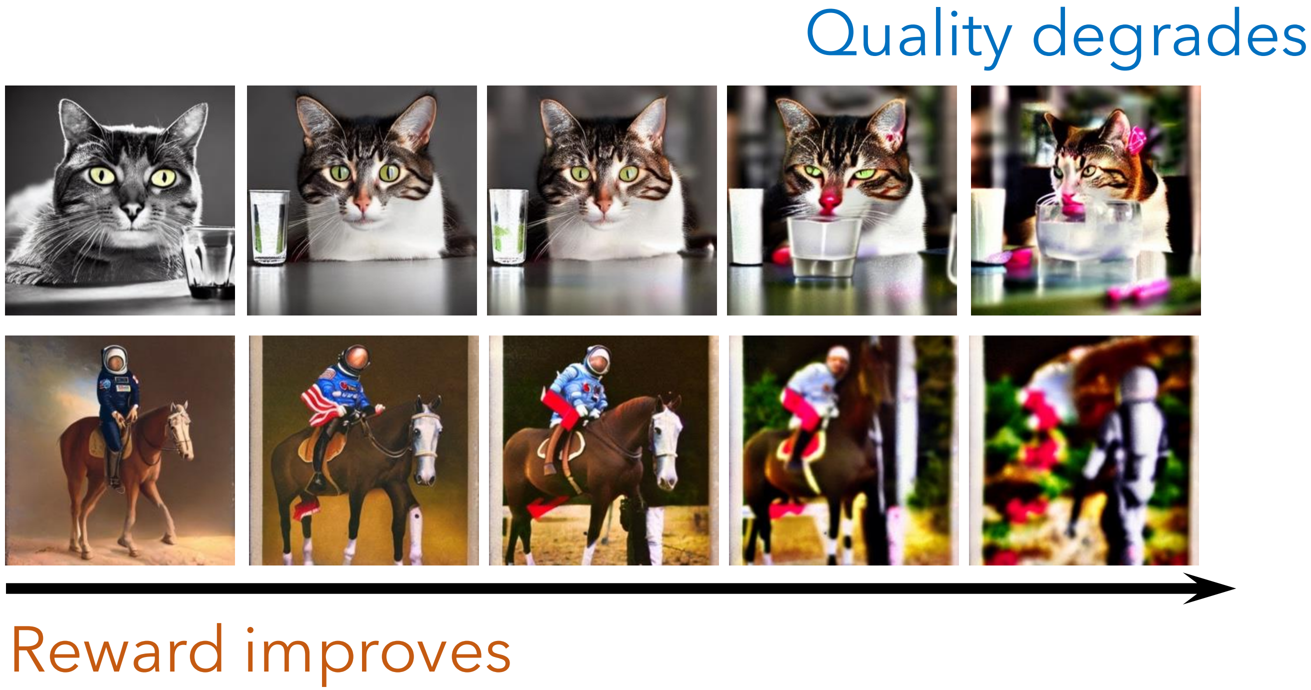
Application 1: CIFAR Reward Optimization



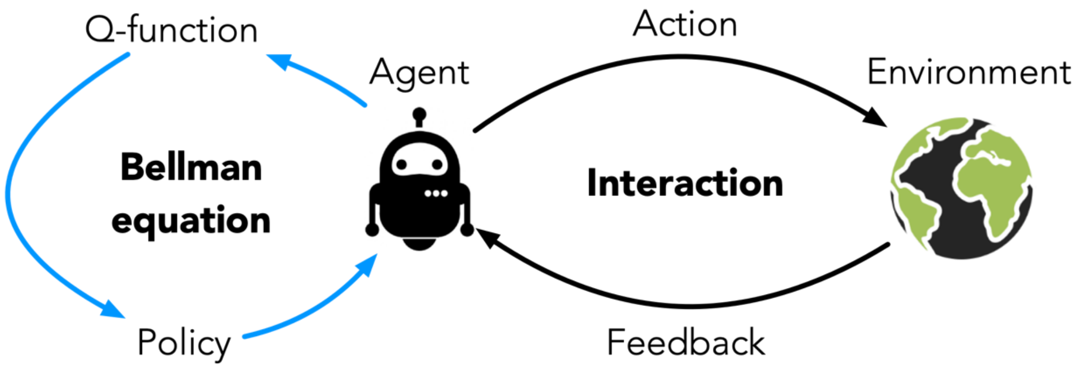
Application 1: CIFAR Reward Optimization





Application 2: Generative Optimization in RL

- Reinforcement learning



Application 2: Generative Optimization in RL

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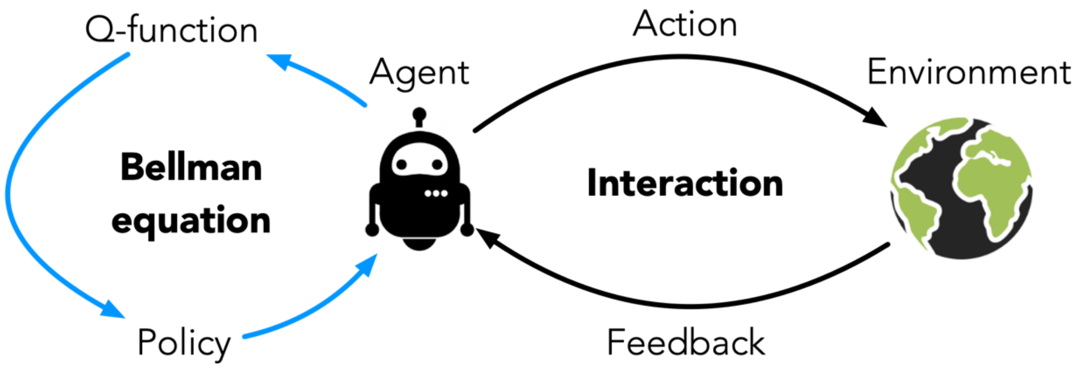
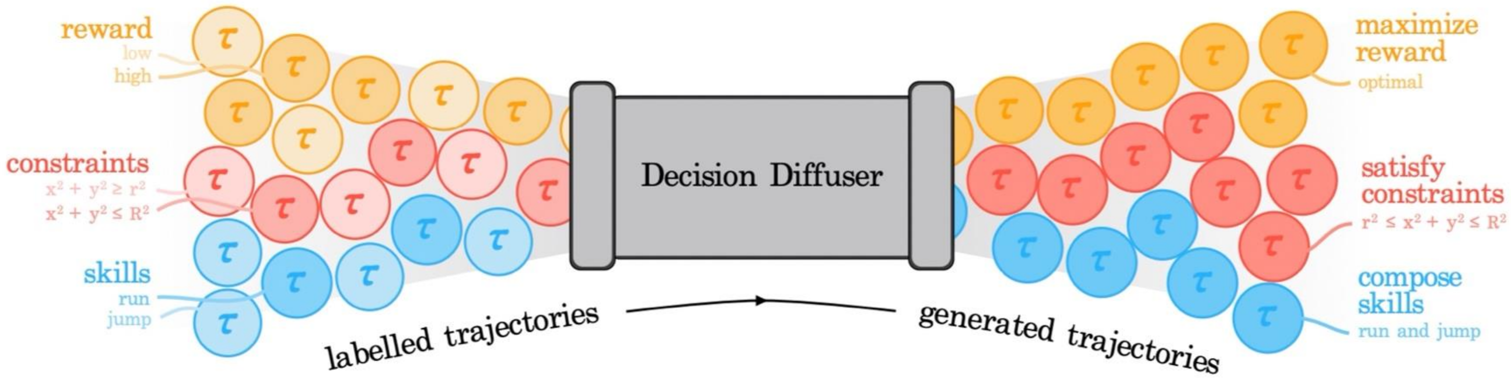
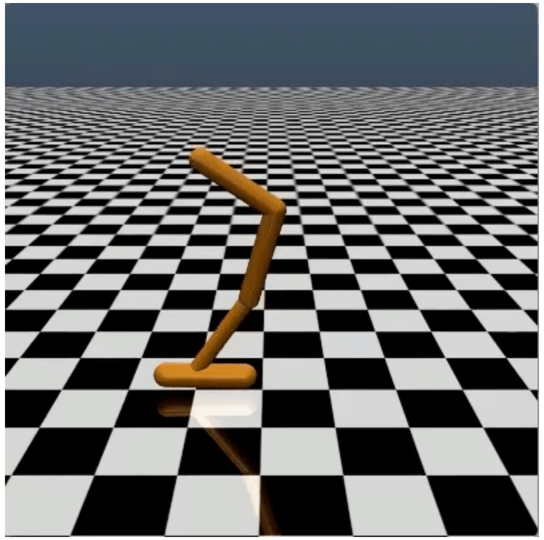
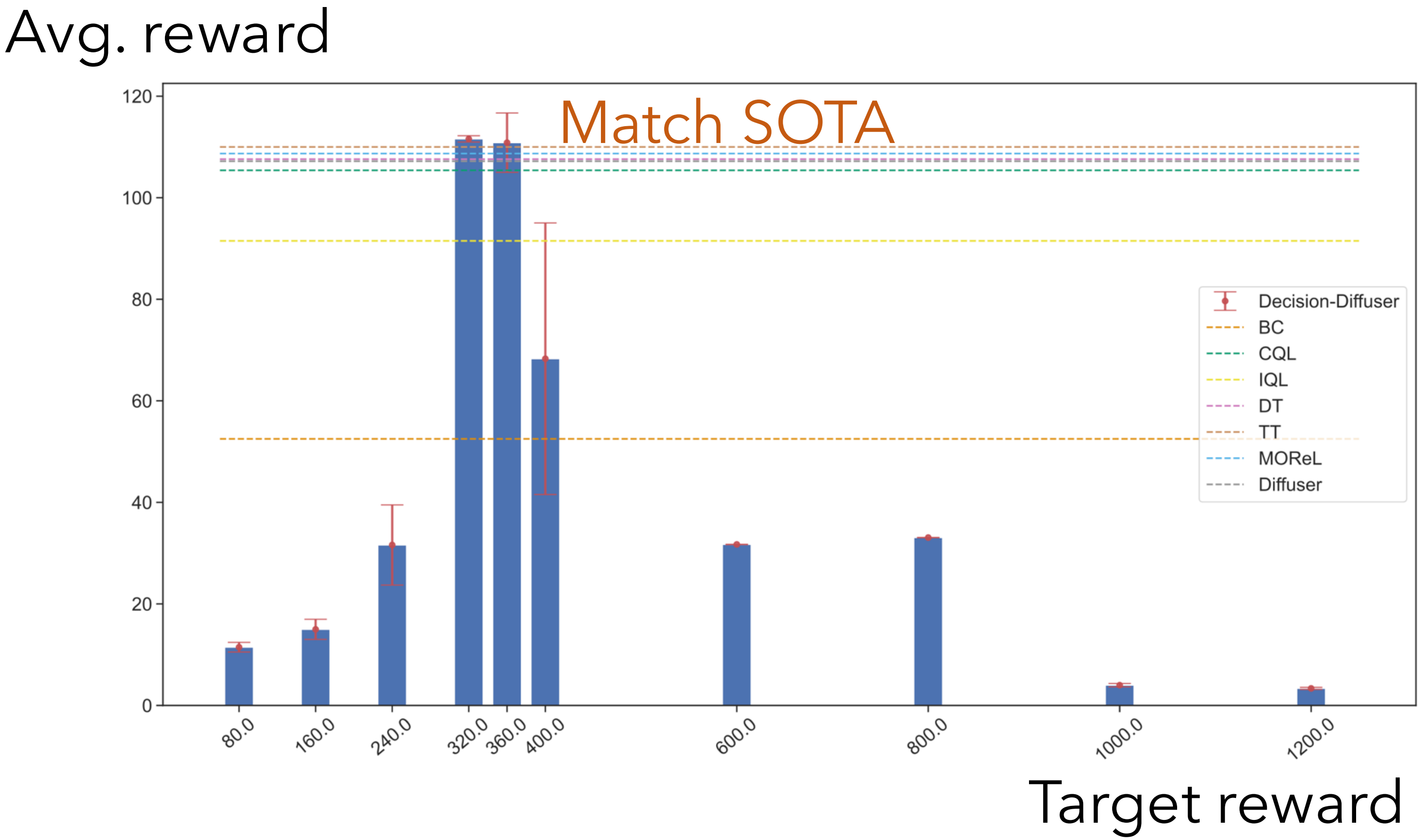


- Generative optimization (Decision diffuser, Ajay et al., 2023)



Hopper Control

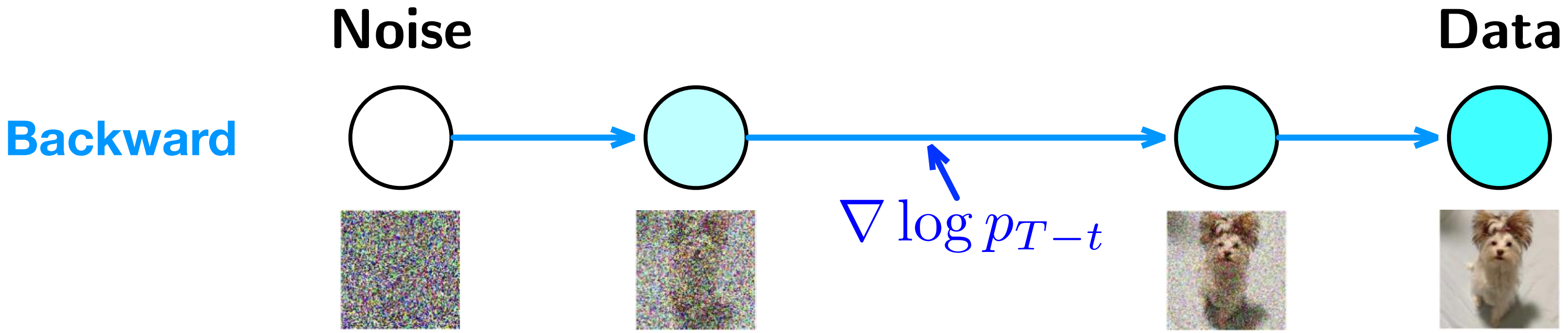




Inspirations and Future Directions

Control/RL Perspective on Diffusion Model

- We design backward process to be Markovian



Control/RL Perspective on Diffusion Model

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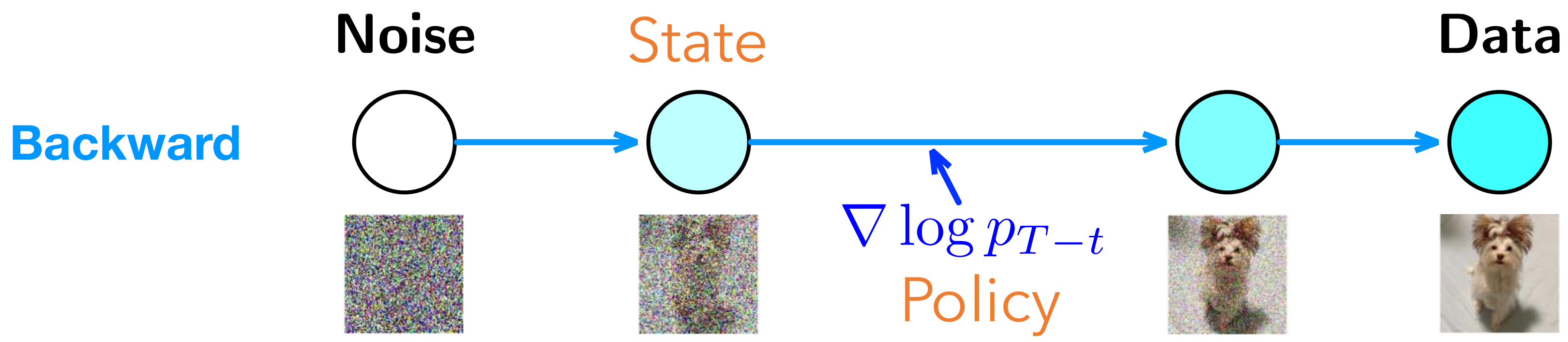

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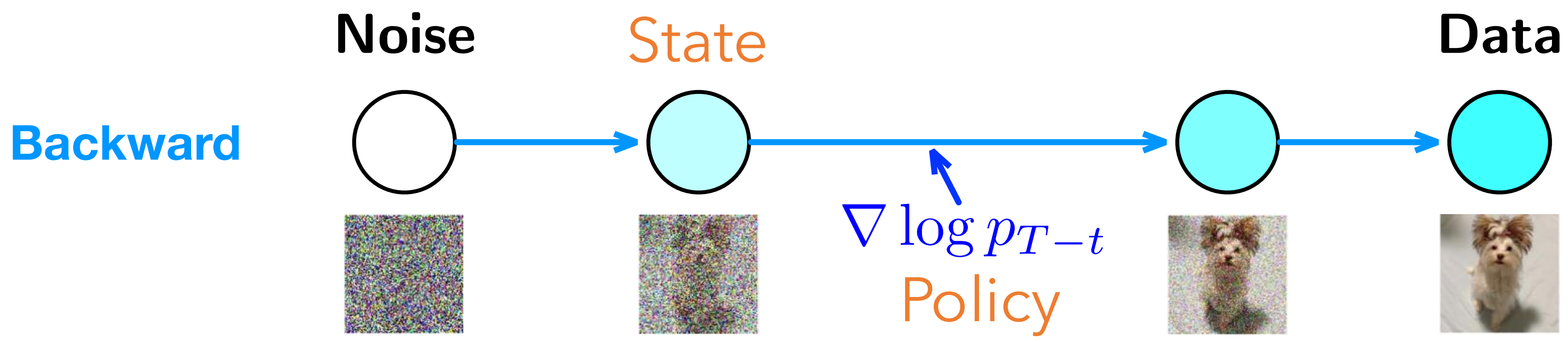
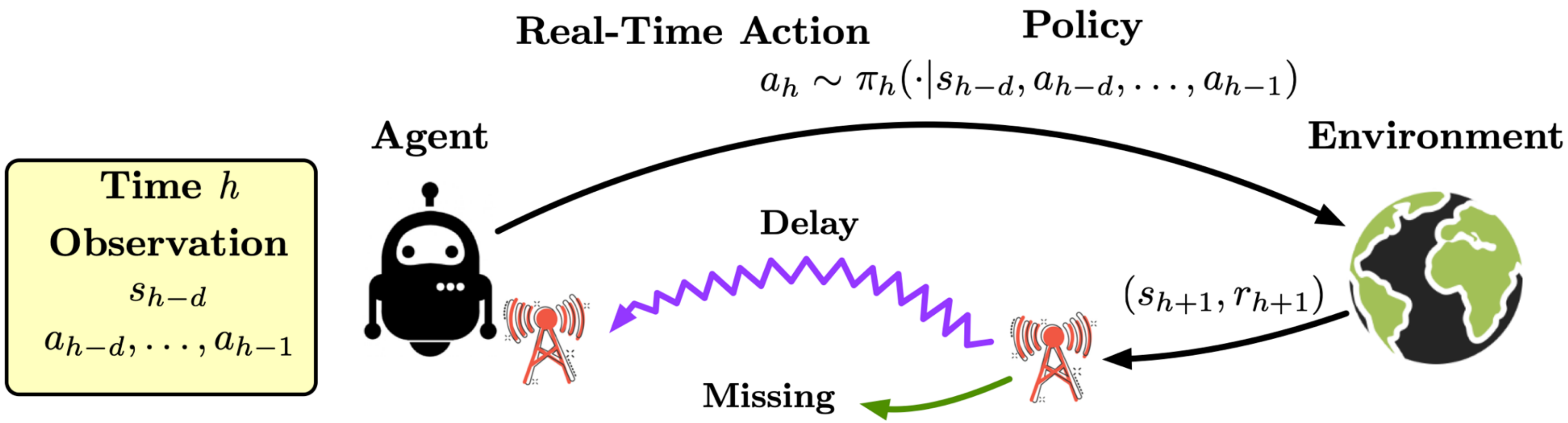


- Reward choice is task dependent
  - ➢ Fidelity metric for image generation
  - ➢ Satisfactory level for product design
  - ➢ Biochemical property for protein synthesis
  - ➢ Etc.

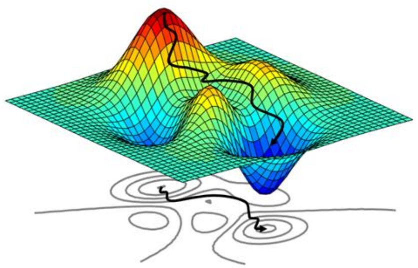
Diffusion Model for Control/RL

- Conditional diffusion models as a rich class for parameterizing **policies** and **transition kernels**

- Diffusion for practical RL with impaired observability (Chen et al., 2023)



Diffusion Model for Generative Optimization



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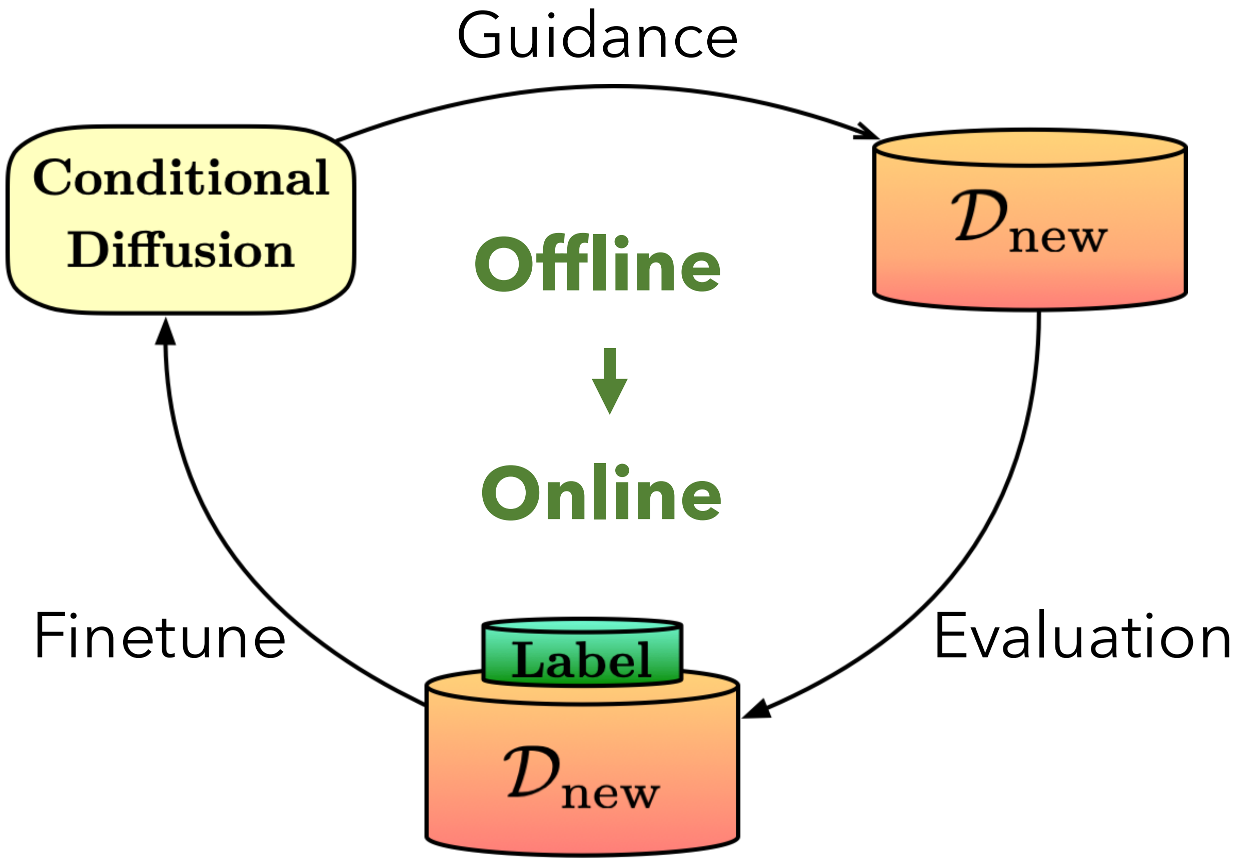

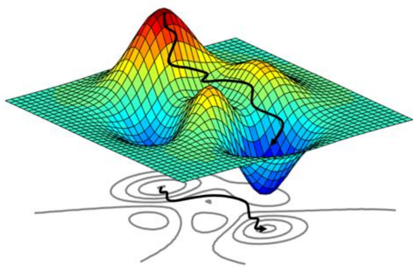

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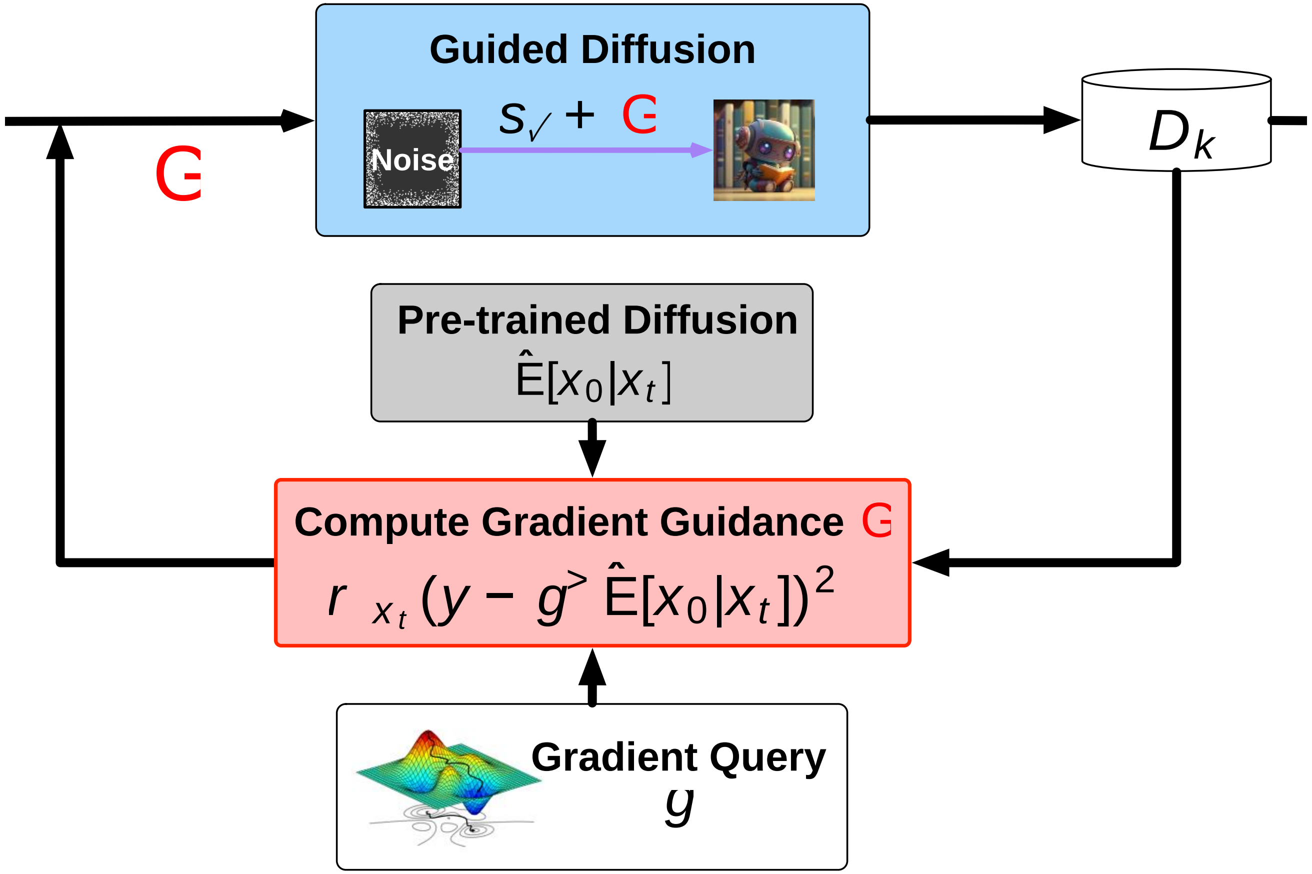

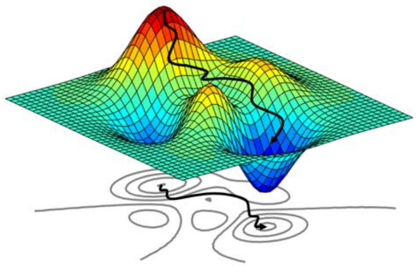

-- Y. Guo, H. Yuan, Y. Yang, M. Chen, M. Wang. "Gradient Guidance for Diffusion Models: An Optimization Perspective", NeurIPS 2024

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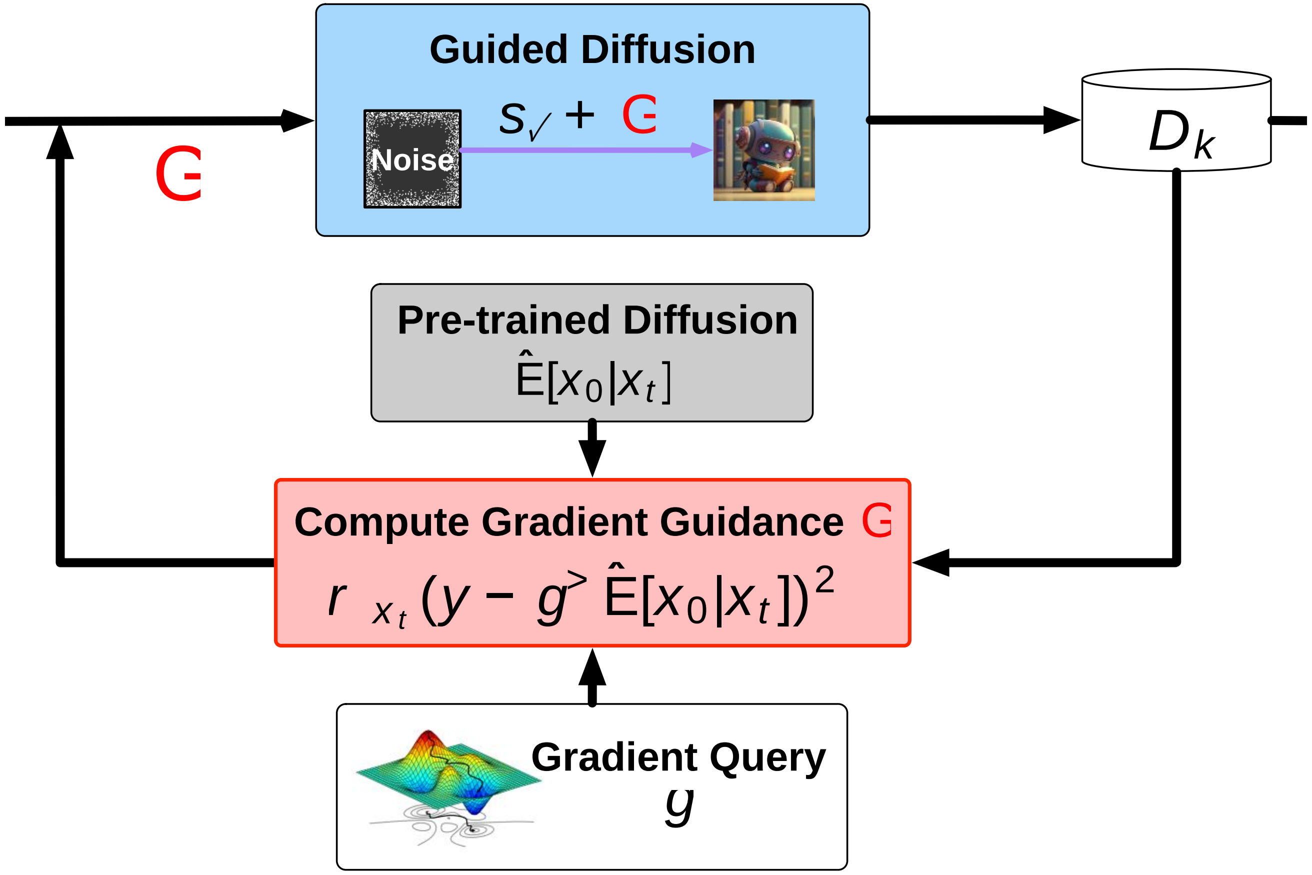

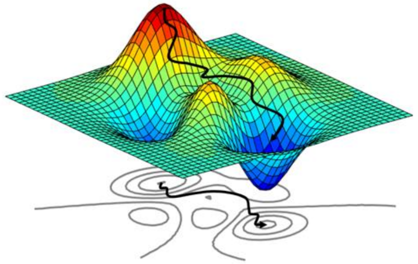

✓ High-D data

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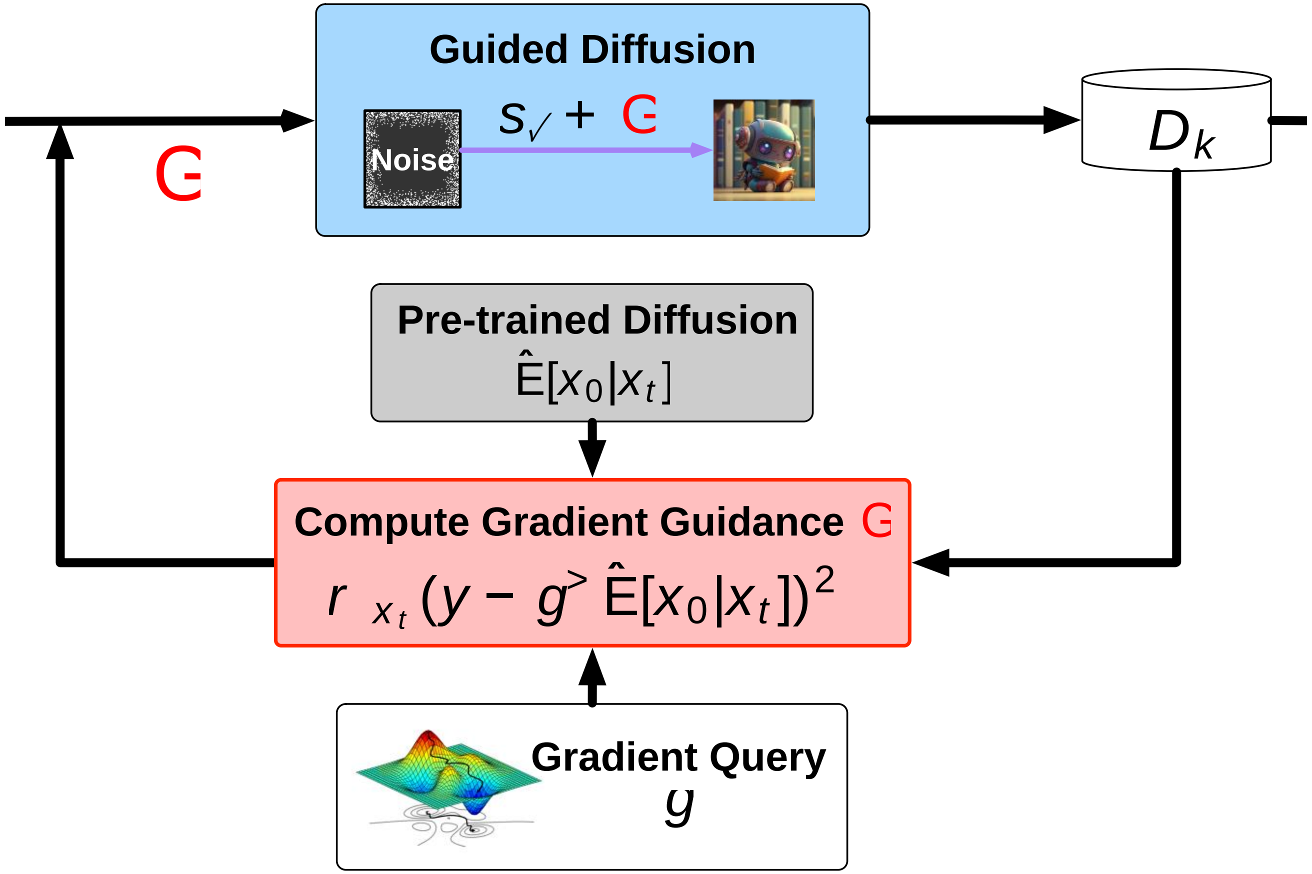

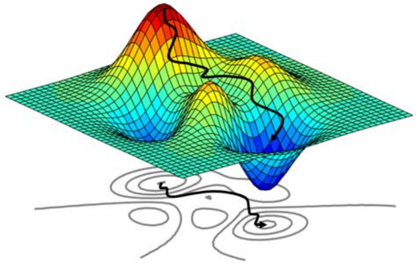

- ✓ High-D data
- ✓ Efficient adaptation

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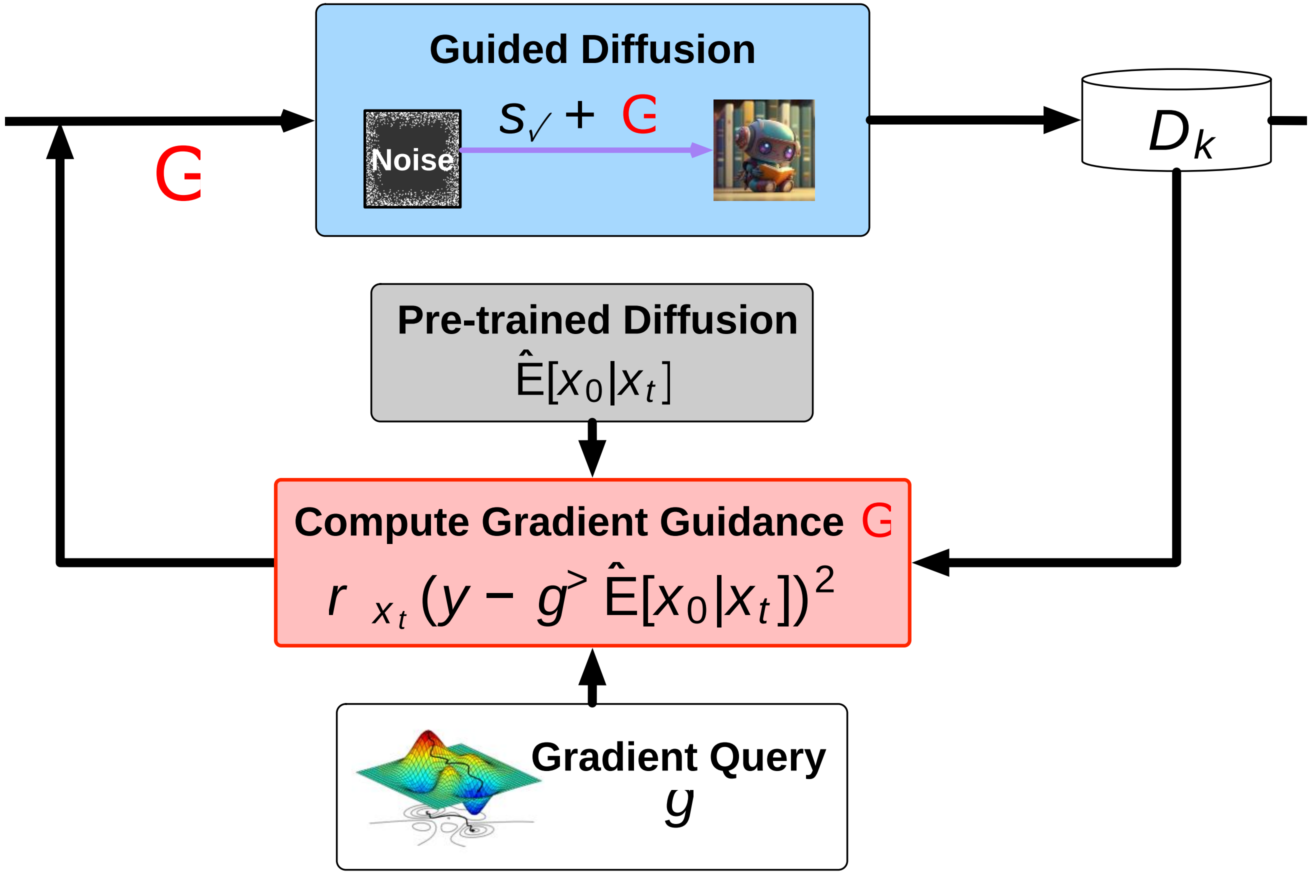

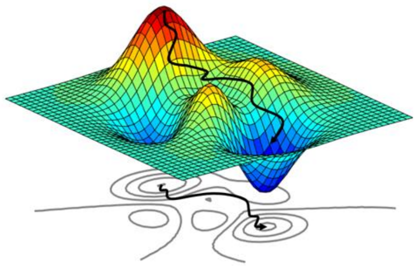

- ✓ High-D data
- ✓ Efficient adaptation
- ✓ Escape from bad local optima and saddle points

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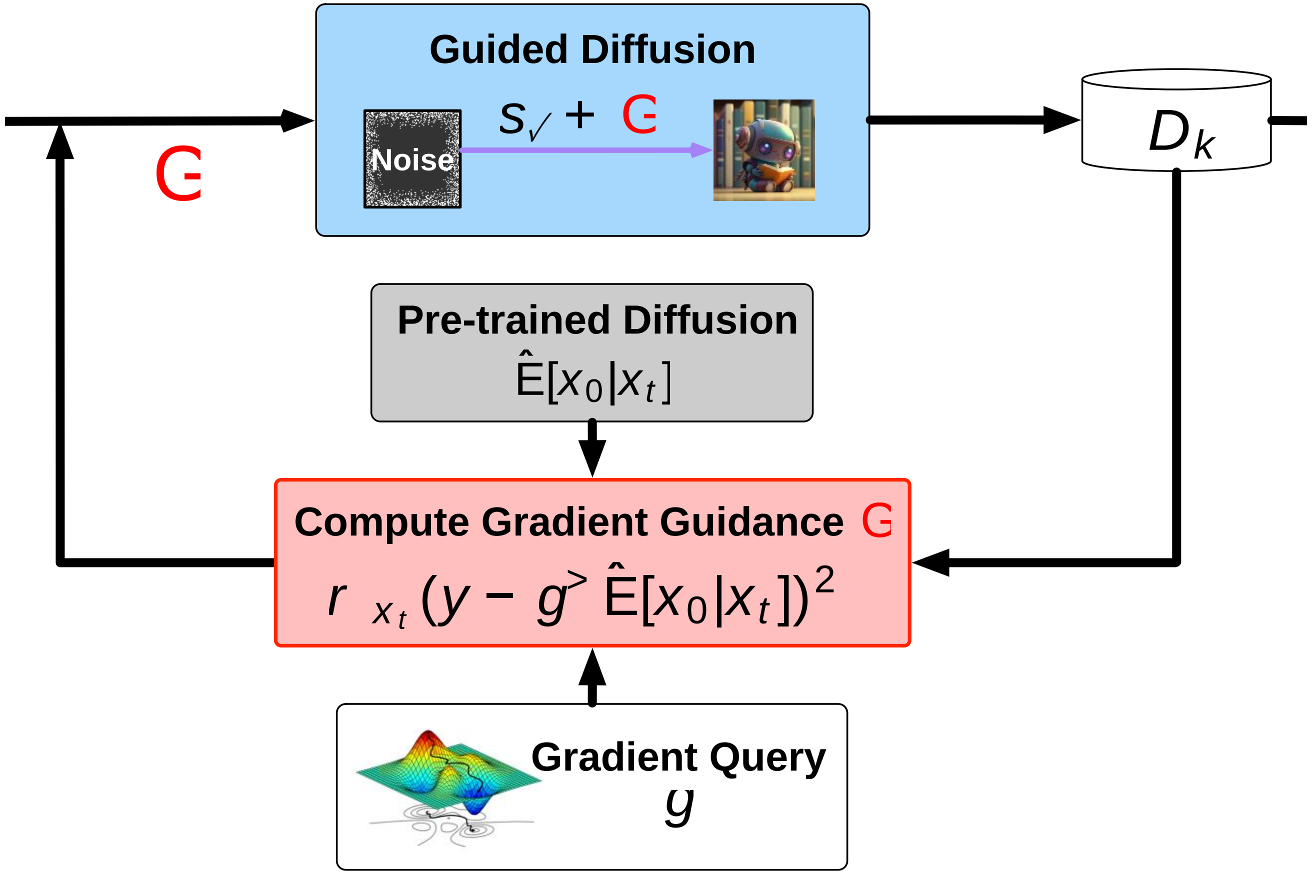
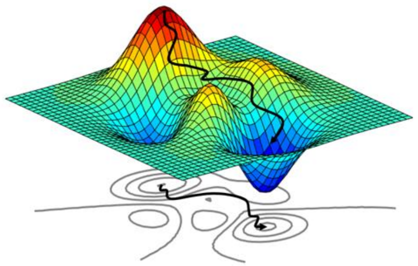
Diffusion Model for Generative Optimization





- ✓ High-D data
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- ✓ Connecting to DRO

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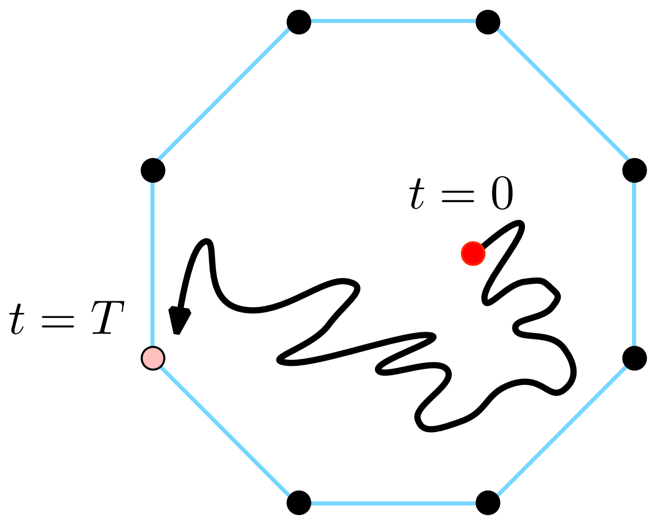
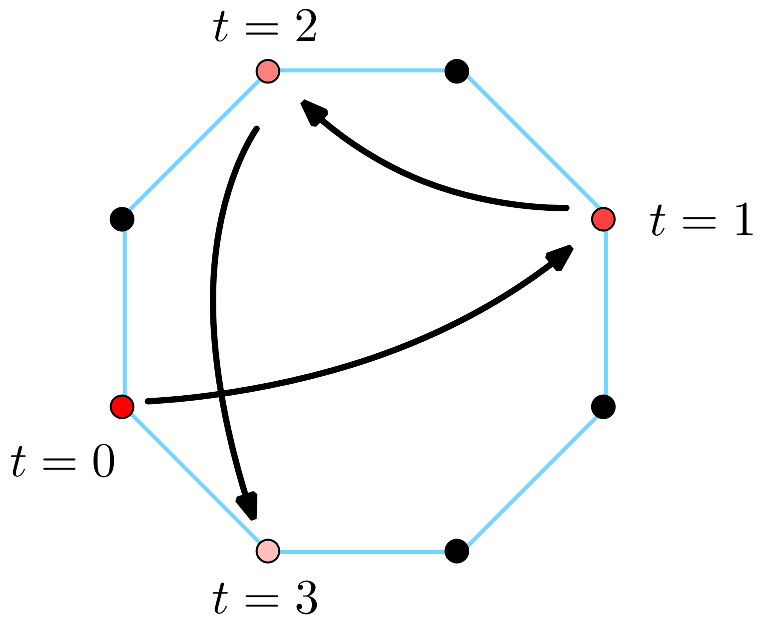
Diffusion Model for Discrete Data

- Gaussian noise may not be suitable for discrete data





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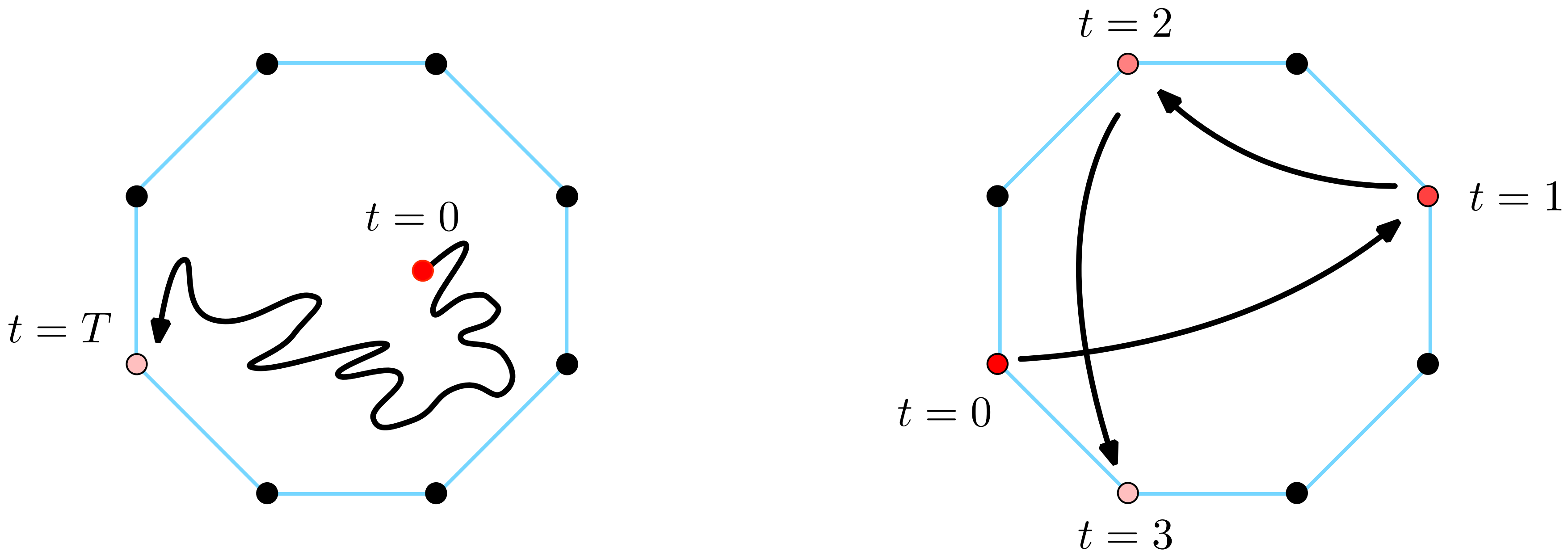

- Discrete diffusion jumps inside data support as "corruption"

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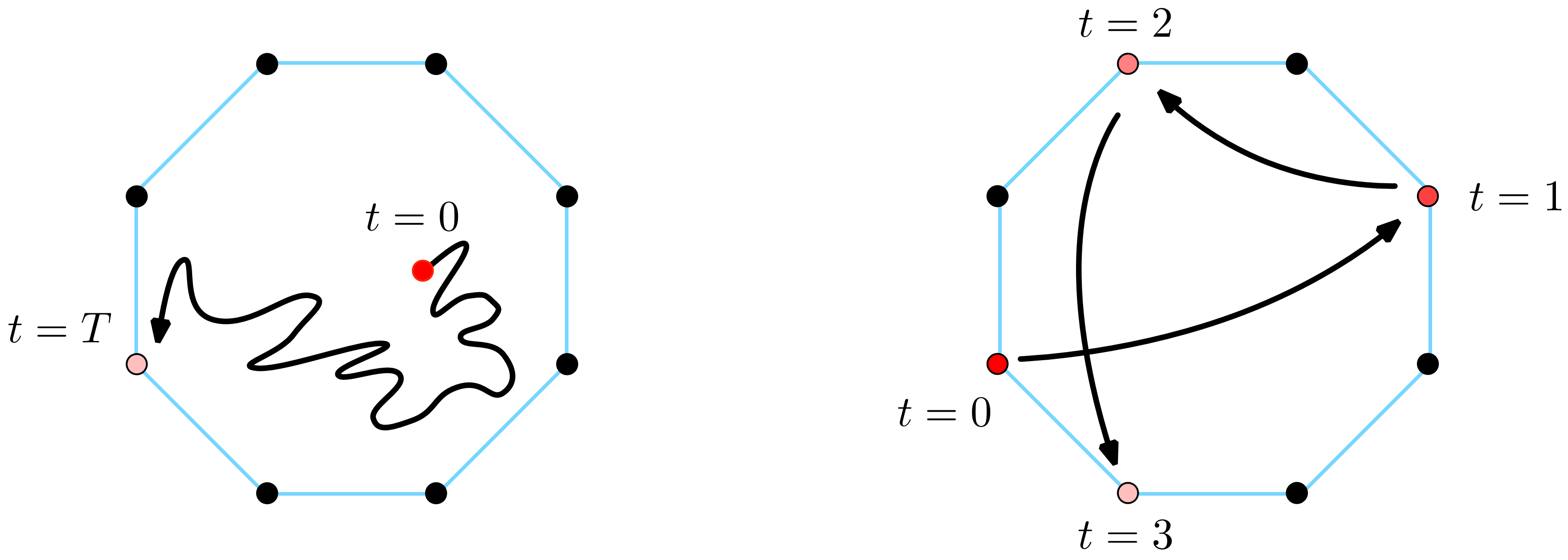

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  - ➢ Integer optimization

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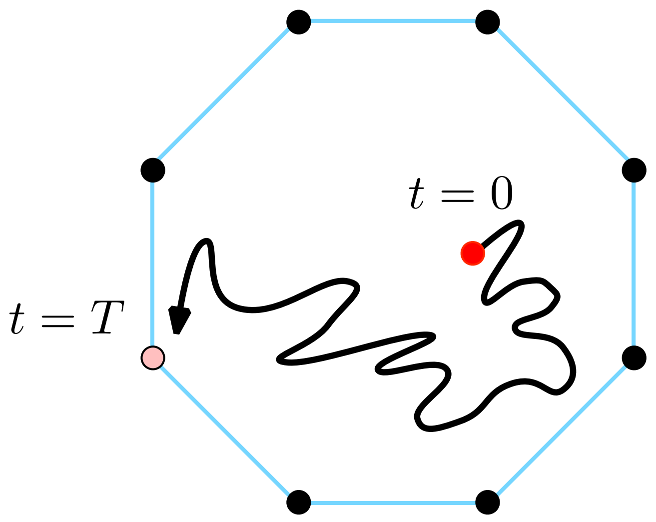

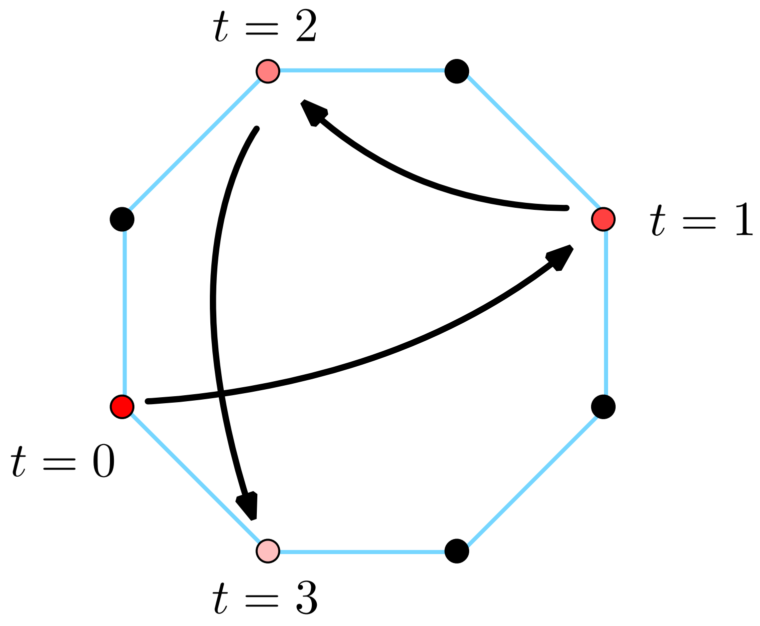

- Discrete diffusion jumps inside data support as "corruption"
  - ➢ Integer optimization
  - ➢ Protein generation

Thank You!