113-2 Embodied Vision

Diffusion Models and Flow Matching

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Learning Resources for Diffusion Models

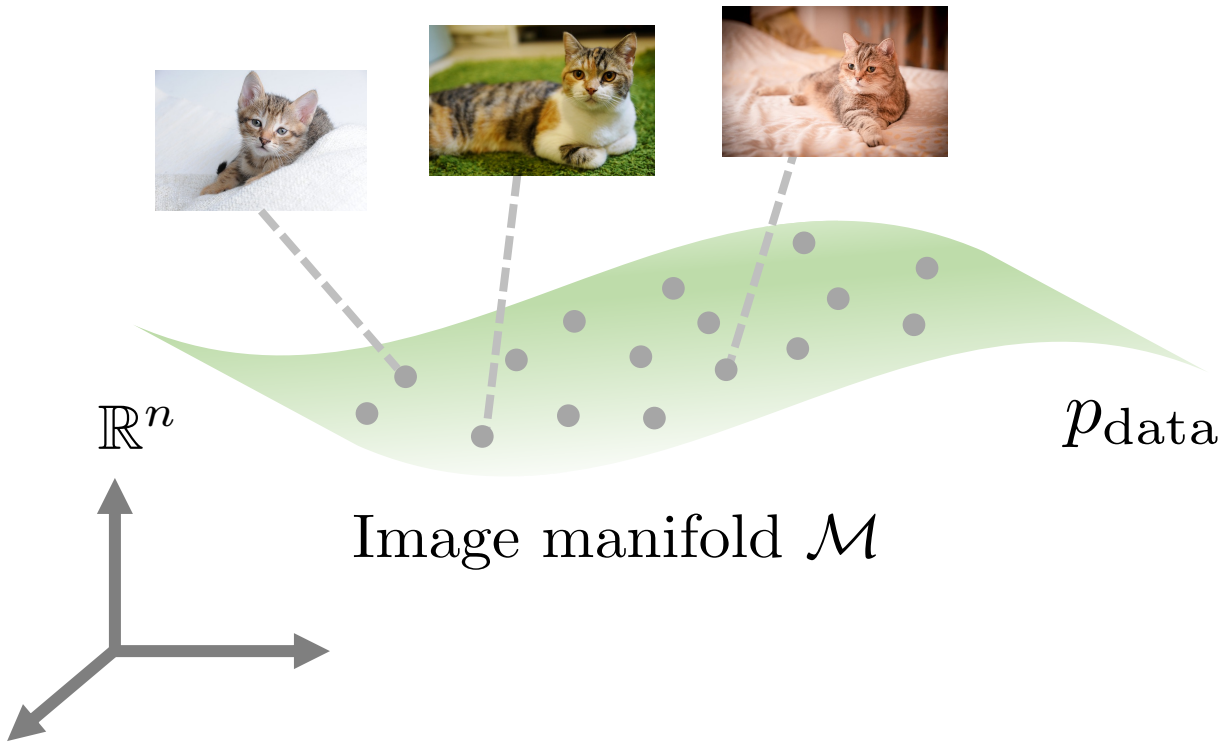
- 【漫士科普】人工智慧博士生告訴你 SORA 擴散模型究竟是怎麼產生影片的？
- Hung-Yi Lee YouTube
- Jia-Bin Huang YouTube
- Diffusion and Score-Based Generative Models (Yang Song)
- Evolution of Diffusion Models: From Birth to Enhanced Efficiency and Controllability (Jesse)
- Lil'Log What are Diffusion Models?
- 生成擴散模型漫談 (蘇劍林)

Outline

- Theoretical Foundations (ODE/SDE, Score Function)
- Training and Sampling
- Advanced Variants (DDIM, CM, CTM, Flow Matching, Rectified Flow)
- Controllability and Applications (CG, CFG, ControlNet)

What is Generative Model Learning?

Data Manifold Assumption
Natural high-dimensional data concentrate close to a non-linear low-dimensional manifold



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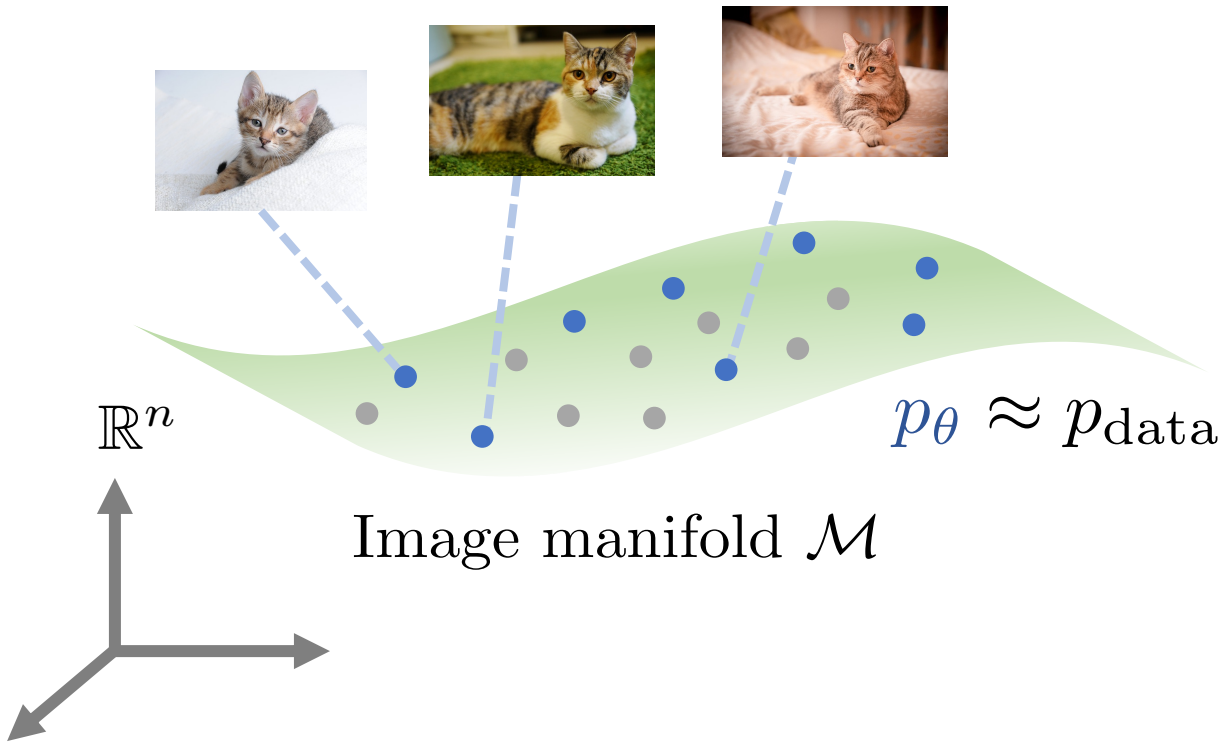

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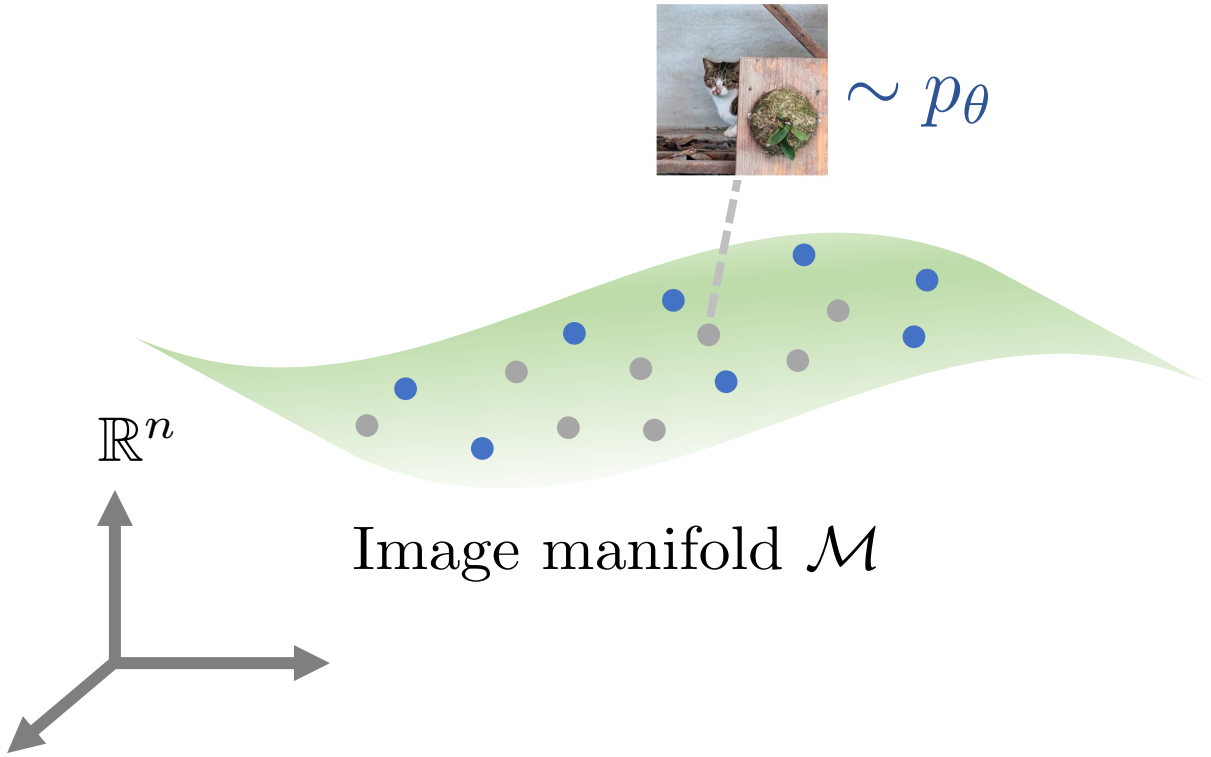
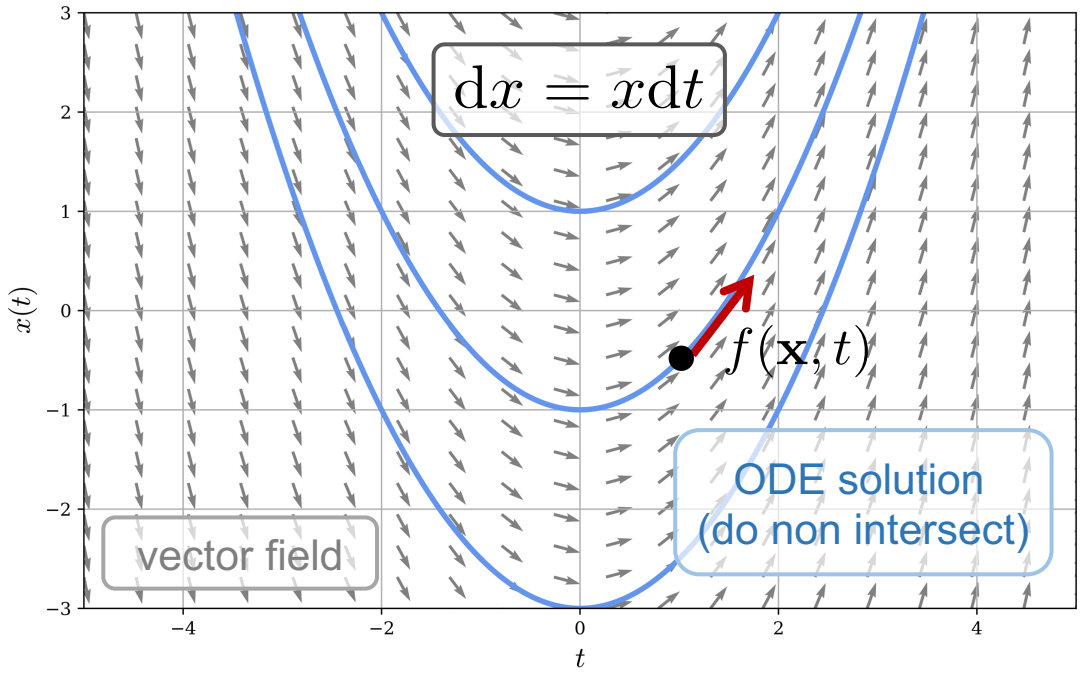
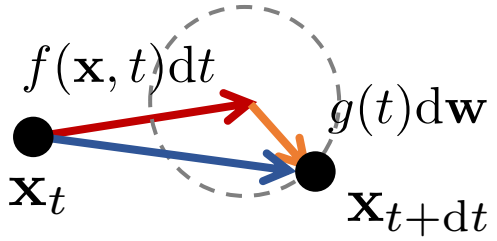


Recap ODE and SDE

$$\mathrm{d}\mathbf{x} = f(\mathbf{x}, t)\mathrm{d}t \quad \text{or} \quad \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = f(\mathbf{x}, t)$$

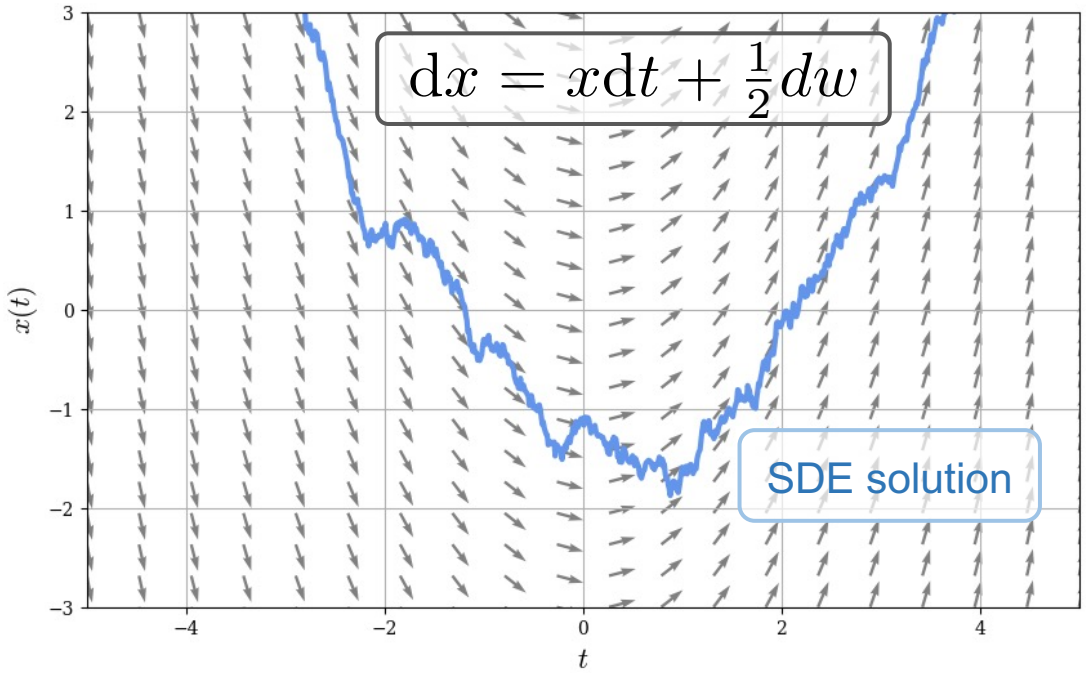


The arrow indicates the direction of movement at the moment of downward shift

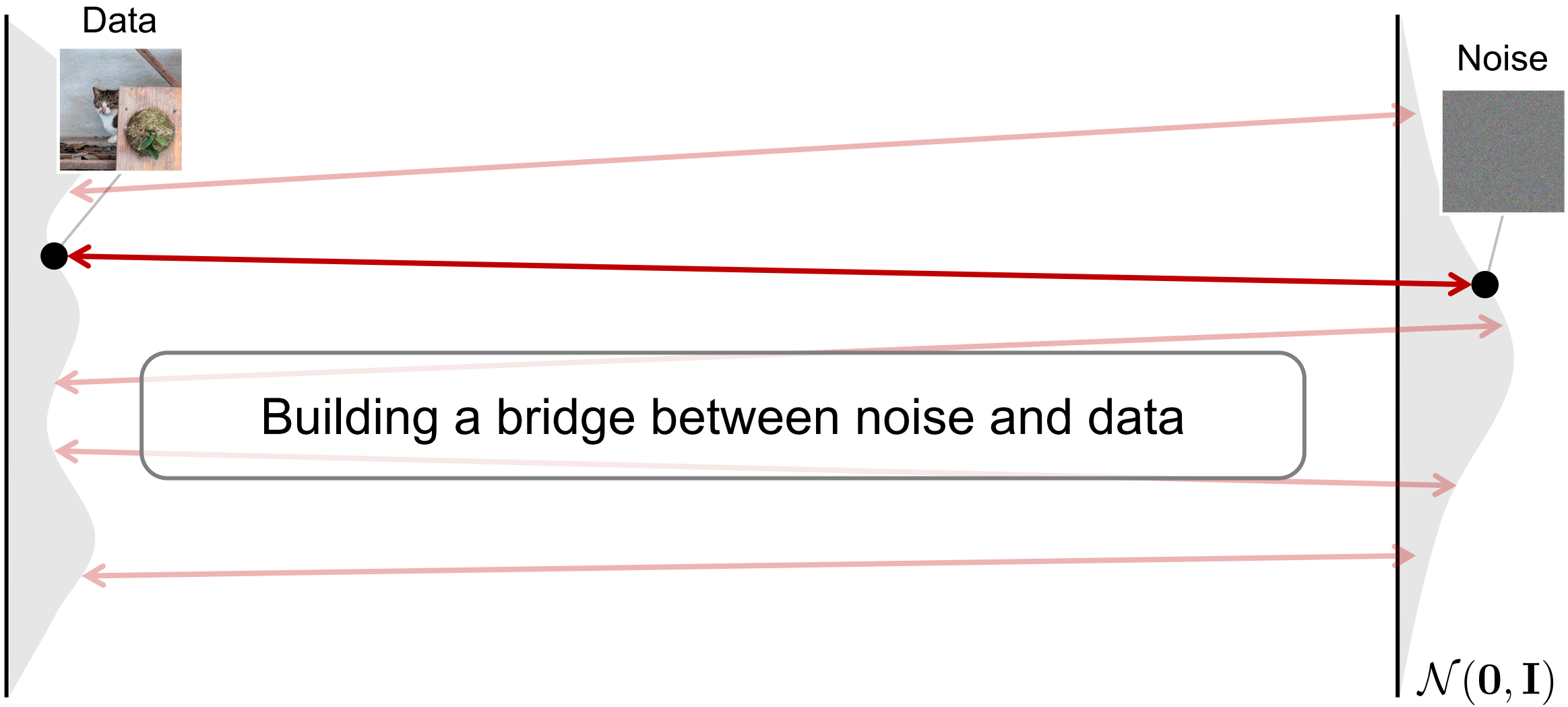


$$\mathrm{d}\mathbf{x} = f(\mathbf{x}, t)\mathrm{d}t + g(t)\mathrm{d}\mathbf{w}$$

drift diffusion



The Goal of Diffusion Models



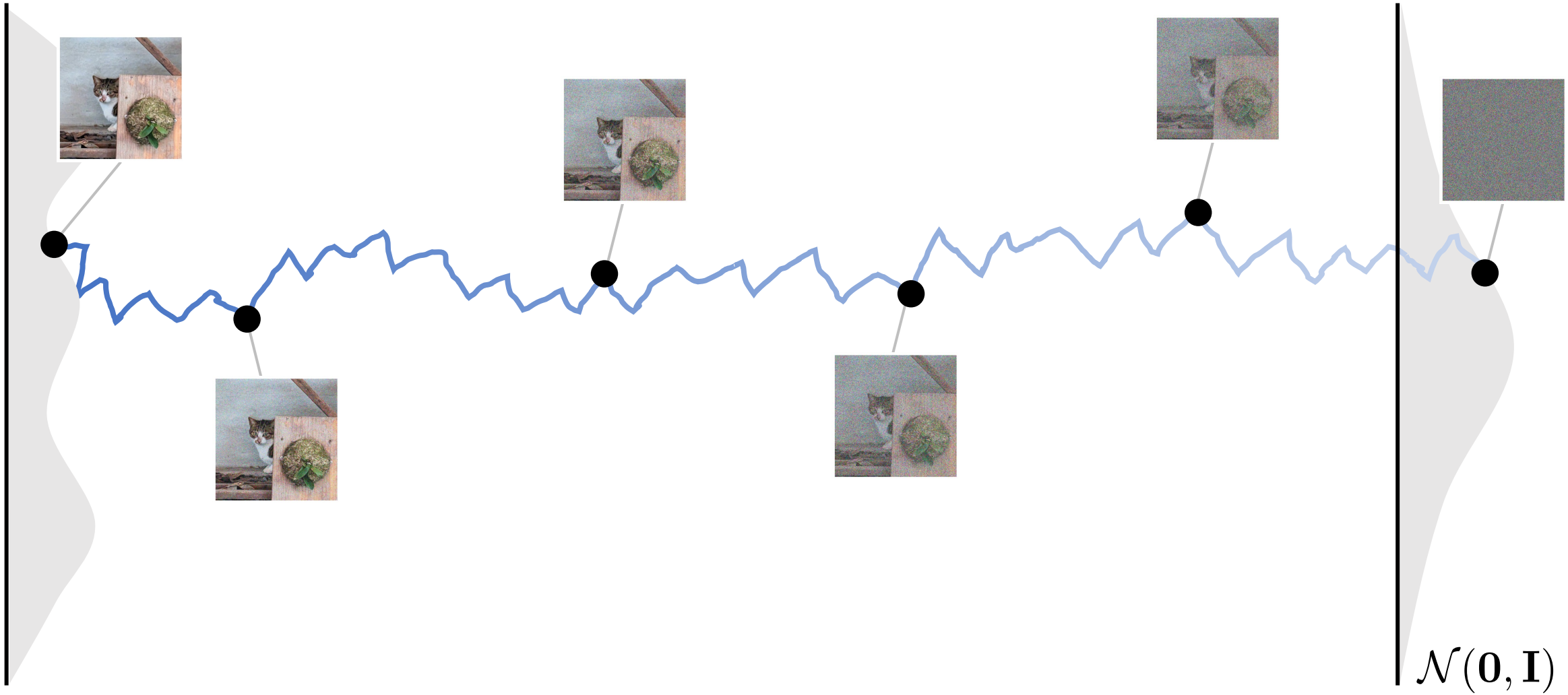
What is Diffusion Model?

Forward Process: add noise step by step, from data to pure noise

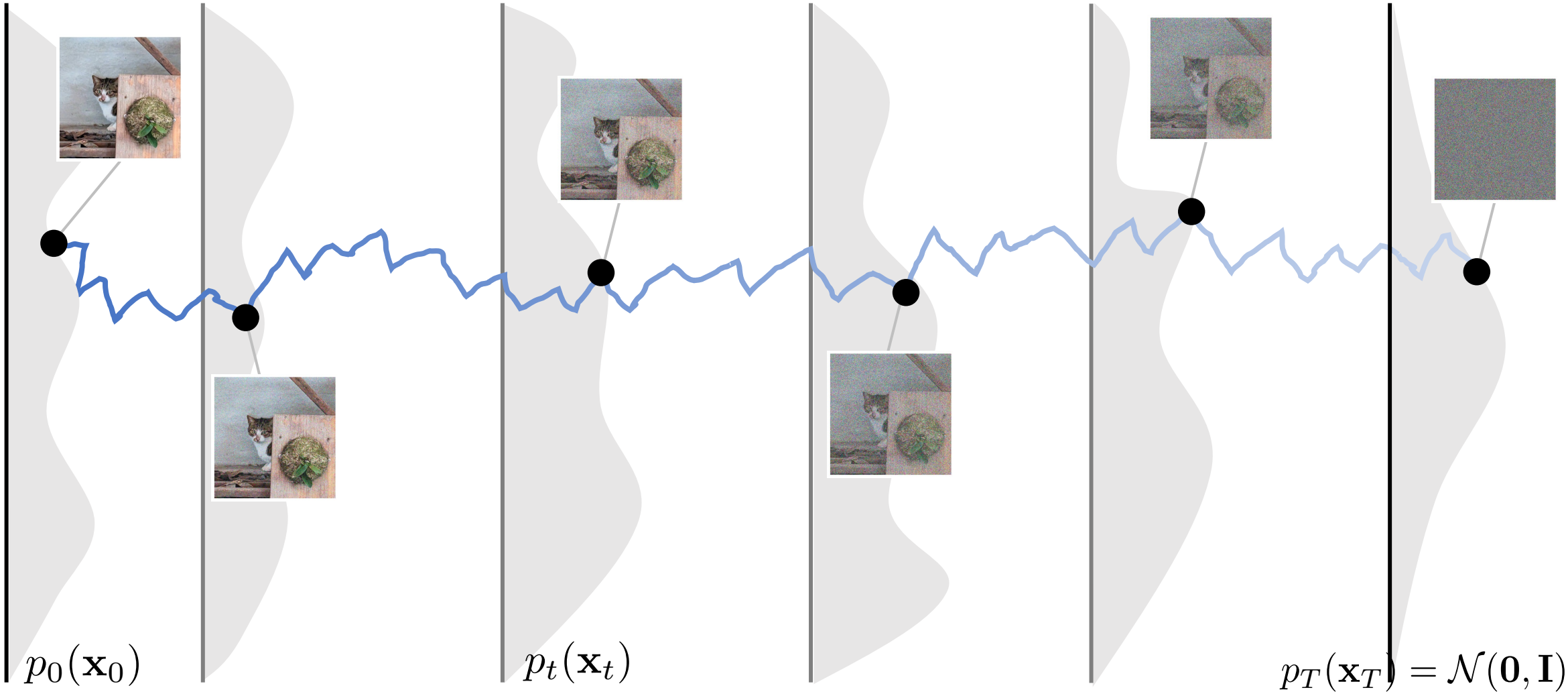
Reverse Process: generate data from pure noise by denoising

Creating noise from data is easy; creating data from noise is generative modeling – *Yang Song*

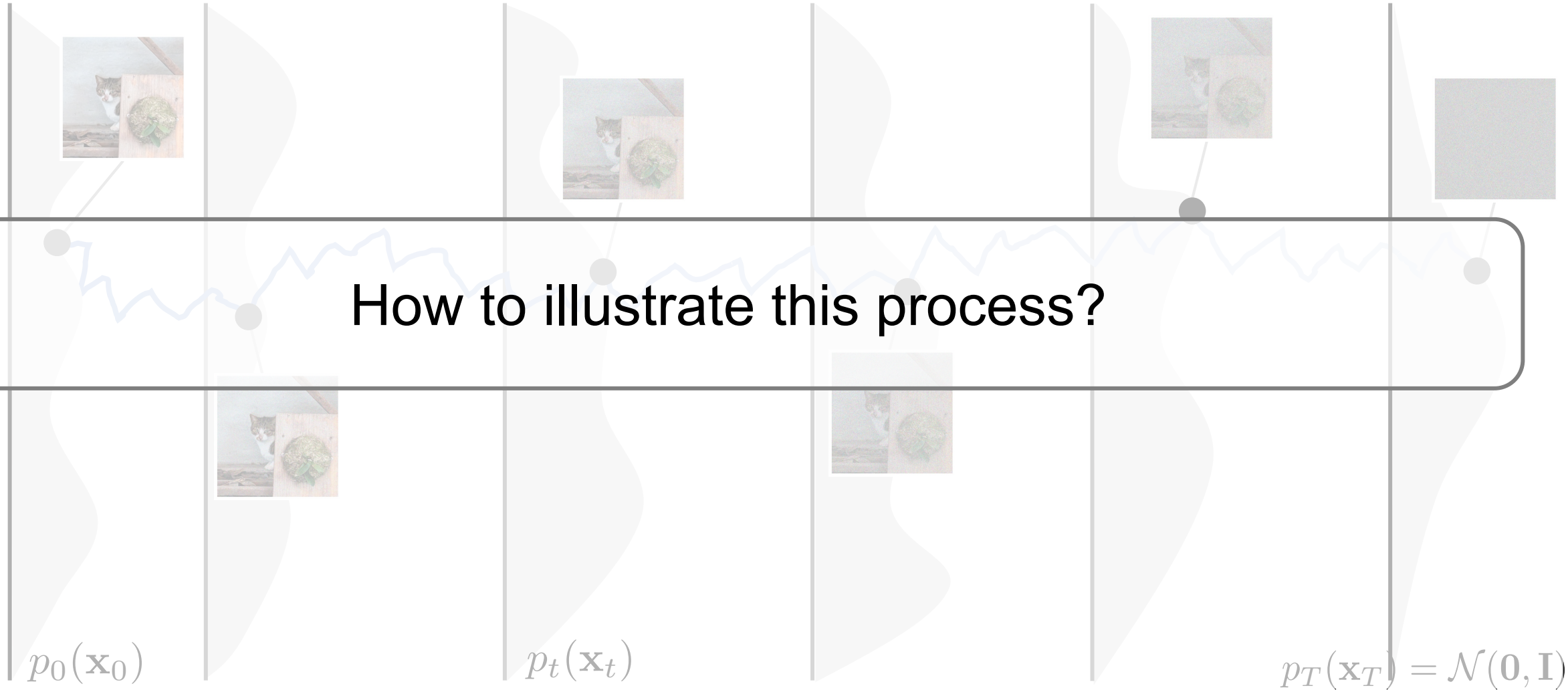
Diffusion Models



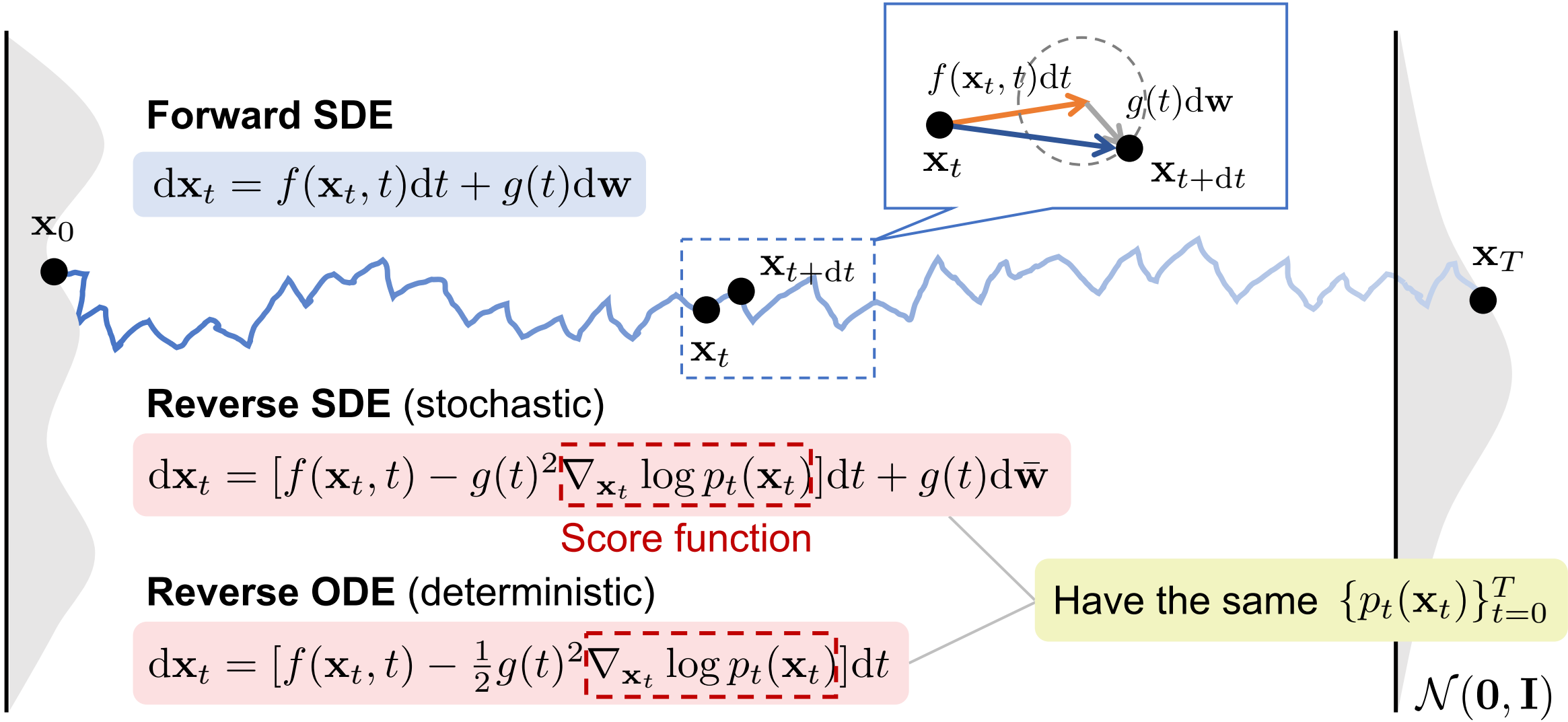
Diffusion Models



Diffusion Models



Score-based Diffusion Models [Song+ ICLR'21]



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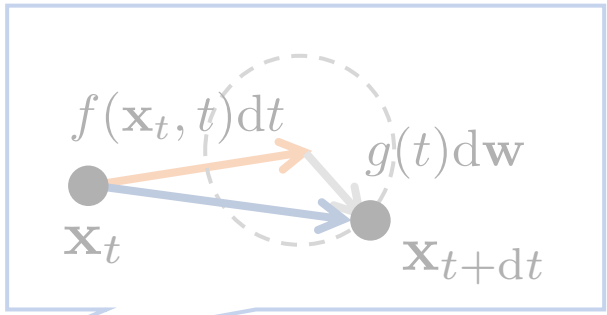


Forward SDE

$$\mathrm{d}\mathbf{x}_t = f(\mathbf{x}_t, t)\mathrm{d}t + g(t)\mathrm{d}\mathbf{w}$$

$\mathbf{x}_0$ $\mathbf{x}_{t-\mathrm{d}t}$ $\mathbf{x}_{t+\mathrm{d}t}$ $\mathbf{x}_t$ $\mathbf{x}_T$

What is intuition of score function?

Reverse SDE (stochastic)

$$\mathrm{d}\mathbf{x}_t = [f(\mathbf{x}_t, t) - g(t)^2 \nabla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t)]\mathrm{d}t + g(t)\mathrm{d}\bar{\mathbf{w}}$$

Score function

Reverse ODE (deterministic)

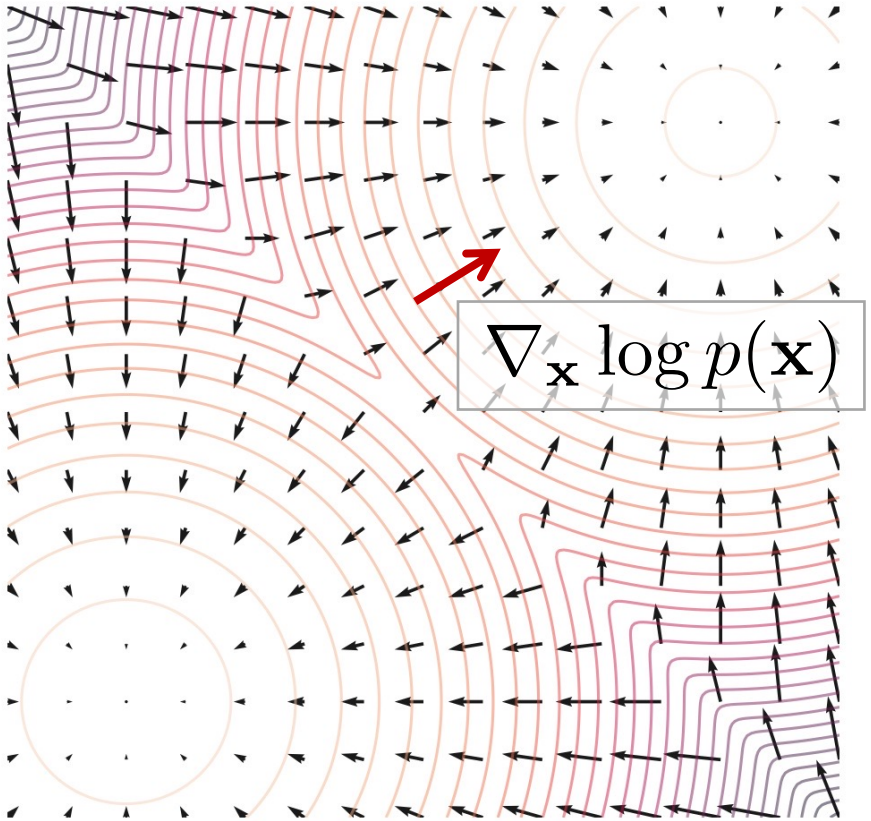
$$\mathrm{d}\mathbf{x}_t = [f(\mathbf{x}_t, t) - \tfrac{1}{2} g(t)^2 \nabla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t)]\mathrm{d}t$$

Have the same $\{p_t(\mathbf{x}_t)\}_{t=0}^{T}$

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

Score Function

Probability Density Function $p(\mathbf{x})$



Score Function: The direction in which the probability density increases most rapidly

Score-based Diffusion Models [Song+ ICLR'21]

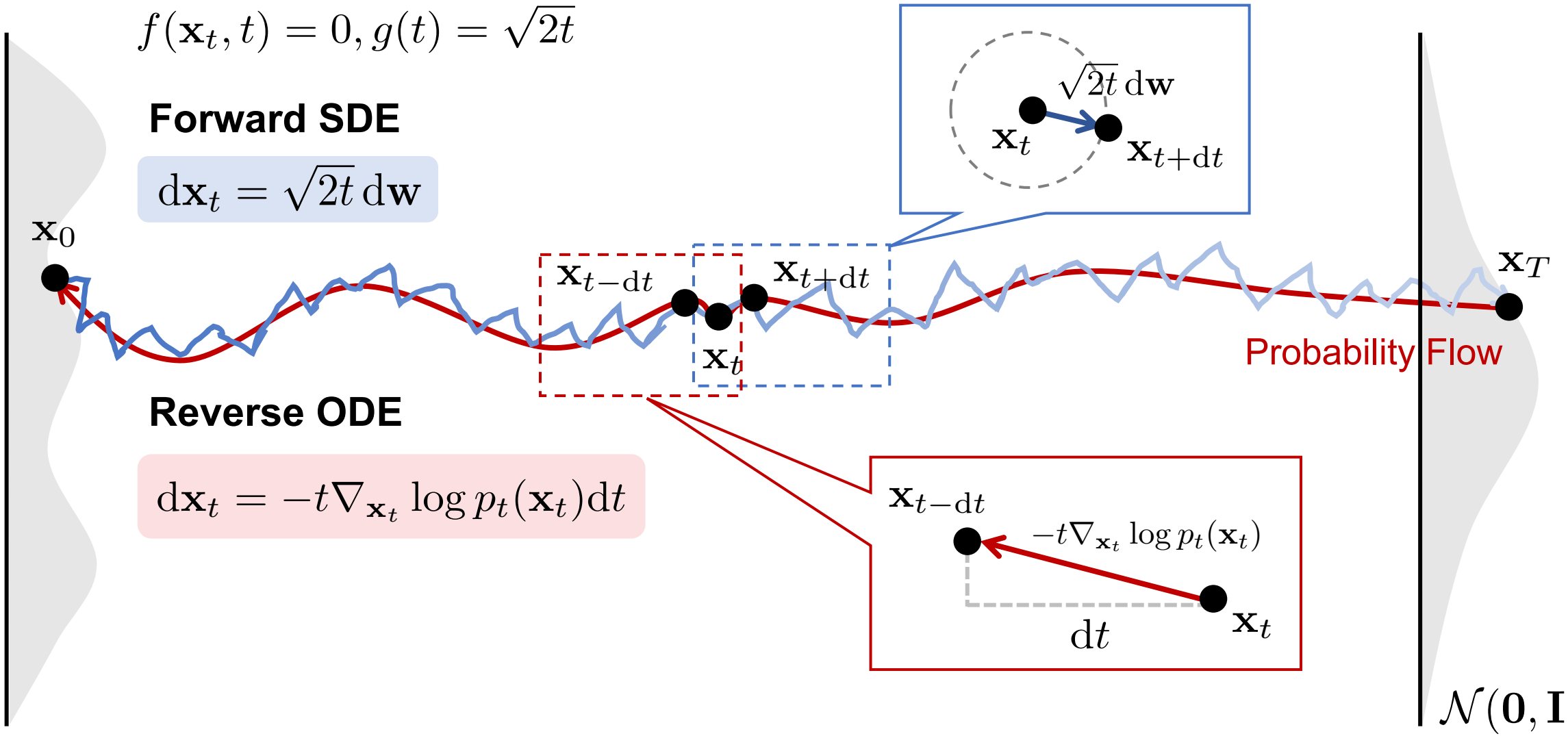
$$f(\mathbf{x}_t, t) = 0, g(t) = \sqrt{2t}$$

Forward SDE

$$\mathrm{d}\mathbf{x}_t = \sqrt{2t}\,\mathrm{d}\mathbf{w}$$

Reverse ODE

$$\mathrm{d}\mathbf{x}_t = -t\nabla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t)\mathrm{d}t$$



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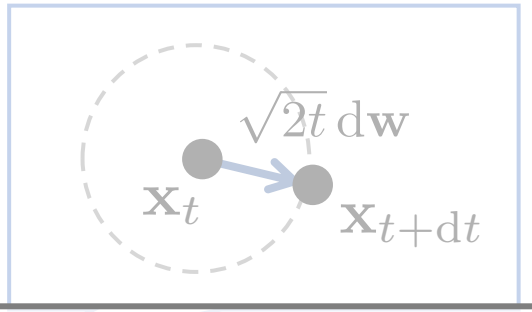
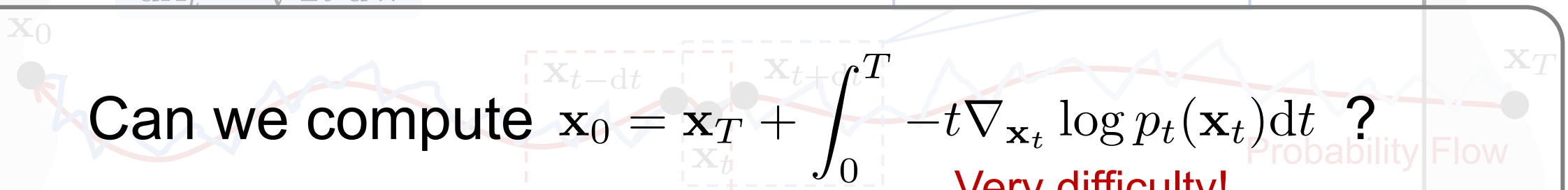


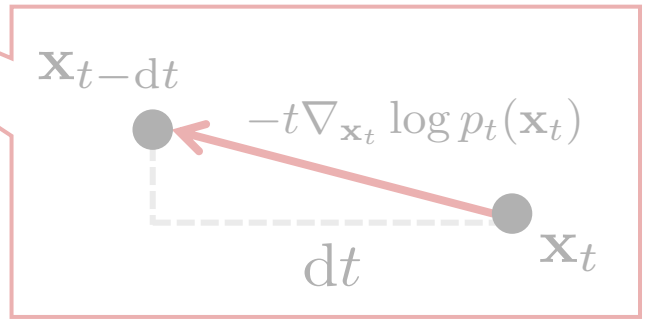


Can we compute $\mathbf{x}_0 = \mathbf{x}_T + \int_0^T -t\nabla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t)\mathrm{d}t$?

Very difficulty!

Reverse ODE

$$\mathrm{d}\mathbf{x}_t = -t\nabla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t)\mathrm{d}t$$



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

Score-based Diffusion Models [Song+ ICLR'21]

$f(\mathbf{x}_t, t) = 0, g(t) = \sqrt{2t}$

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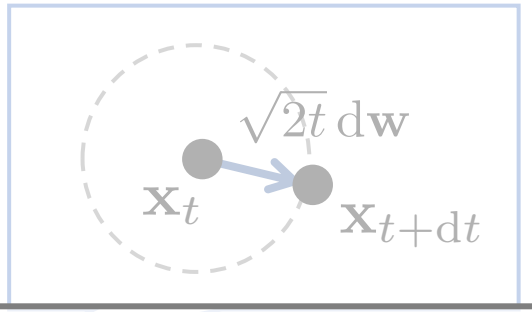
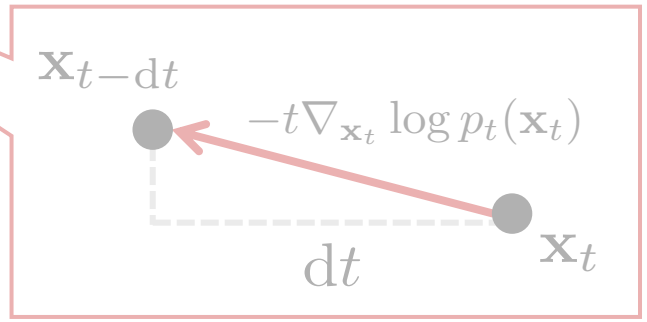


1. How do we obtain the score function during sampling?
2. How to solve the reverse ODE?

Reverse ODE

$$\mathrm{d}\mathbf{x}_t = -t\nabla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t)\mathrm{d}t$$



$\mathbf{x}_0$ $\mathbf{x}_T$ Probability Flow $\mathcal{N}(\mathbf{0}, \mathbf{I})$

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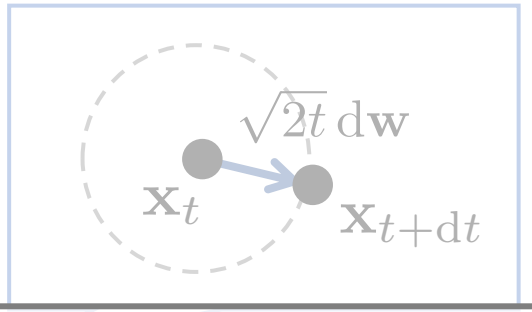

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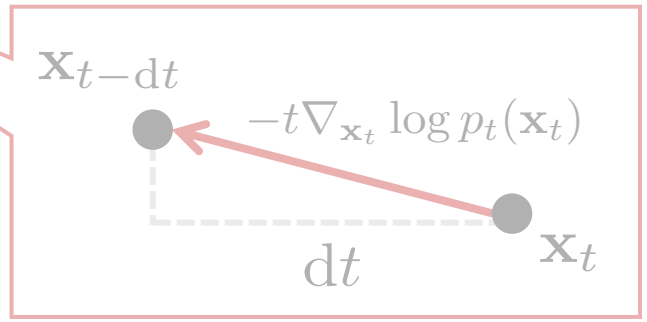


$\mathbf{x}_0$ $\mathbf{x}_T$ Probability Flow $\mathcal{N}(\mathbf{0}, \mathbf{I})$

Training Score-based Diffusion Models

We train the model to approximate the score function

$$\mathbf{s}_\theta(\mathbf{x}_t, t) \approx \nabla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t)$$

During sampling, we use the model to predict the score and plug it into SDE/ODE

$$\mathrm{d}\mathbf{x}_t = [f(\mathbf{x}_t, t) - g(t)^2 \mathbf{s}_\theta(\mathbf{x}_t, t)]\mathrm{d}t + g(t)\mathrm{d}\bar{\mathbf{w}}$$

The training objective can be expressed as

$$\mathcal{L}_{\mathrm{SM}}(\mathbf{x}_0; \theta) = \mathbb{E}_{\mathbf{x}_t|\mathbf{x}_0} \|\mathbf{s}_\theta(\mathbf{x}_t, t) - \nabla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t)\|_2^2 \quad \text{(Score Matching)}$$

Training Score-based Diffusion Models

We train the model to approximate the score function

$$\mathbf{s}_\theta(\mathbf{x}_t, t) \approx \nabla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t)$$

During sampling, we use the model to predict the score and plug it into SDE (ODE)

$$\mathrm{d}\mathbf{x}_t = [f(\mathbf{x}_t, t) - g(t)^2 \mathbf{s}_\theta(\mathbf{x}_t, t)]\mathrm{d}t + g(t)\mathrm{d}\bar{\mathbf{w}}$$

Can we easily compute the score function during training?

The training objective can be expressed as

$$\mathcal{L}_{\mathrm{SM}}(\mathbf{x}_0; \theta) = \mathbb{E}_{\mathbf{x}_t|\mathbf{x}_0} \|\mathbf{s}_\theta(\mathbf{x}_t, t) - \nabla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t)\|_2^2 \quad \text{(Score Matching)}$$

Training Score-based Diffusion Models

Score Matching (SM) [Hyvarinen JMLR'05]:

$$\mathcal{L}_{\mathrm{SM}}(\mathbf{x}_0;\theta) = \mathbb{E}_{\mathbf{x}_t|\mathbf{x}_0} \left\| \mathbf{s}_\theta(\mathbf{x}_t, t) - \nabla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t) \right\|_2^2$$

Denoising Score Matching (DSM) [Vincent Neural Comput.'11]:

$$\mathcal{L}_{\mathrm{DSM}}(\mathbf{x}_0;\theta) = \mathbb{E}_{\mathbf{x}_t|\mathbf{x}_0} \left\| \mathbf{s}_\theta(\mathbf{x}_t, t) - \nabla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t|\mathbf{x}_0) \right\|_2^2$$

$$\| \quad \frac{\mathbf{x}_0 - \mathbf{x}_t}{\sigma_t^2}$$

noise level

$+\epsilon_t \sim \mathcal{N}(\mathbf{0}, \sigma_t^2 \mathbf{I})$

$p_t(\mathbf{x}_t|\mathbf{x}_0)$

$\mathbf{x}_0 \sim p_{\mathrm{data}}$

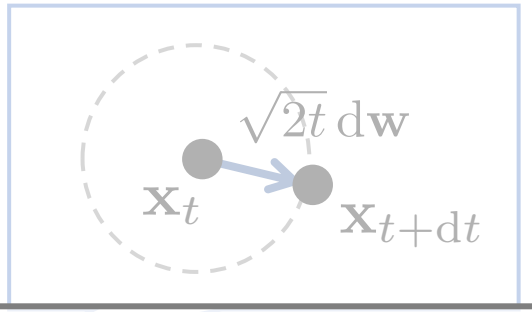
$\mathbf{x}_t$

Score-based Diffusion Models [Song+ ICLR'21]

$f(\mathbf{x}_t, t) = 0, g(t) = \sqrt{2t}$

Forward SDE

$$\mathrm{d}\mathbf{x}_t = \sqrt{2t}\,\mathrm{d}\mathbf{w}$$



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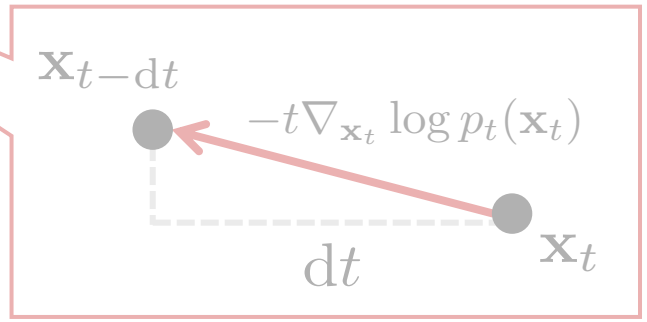
2. How to solve the reverse ODE?

Reverse ODE

$$\mathrm{d}\mathbf{x}_t = -t\nabla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t)\mathrm{d}t$$



$\mathbf{x}_0$ $\mathbf{x}_T$ Probability Flow $\mathcal{N}(\mathbf{0}, \mathbf{I})$

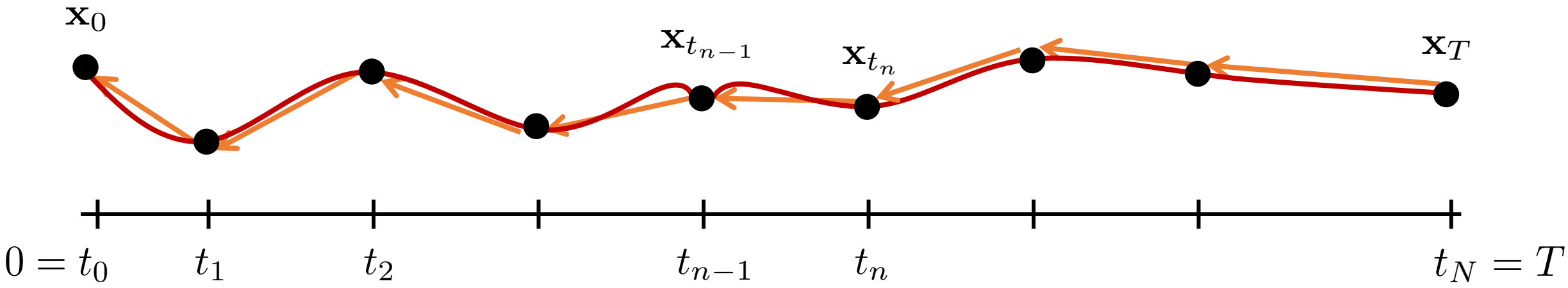
How to Solve the Reverse ODE?

Euler's Method (1st order):

$$\frac{\mathrm{d}\mathbf{x}_t}{\mathrm{d}t} = -t\mathbf{s}_\theta(\mathbf{x}_t, t)$$

$$\wr$$

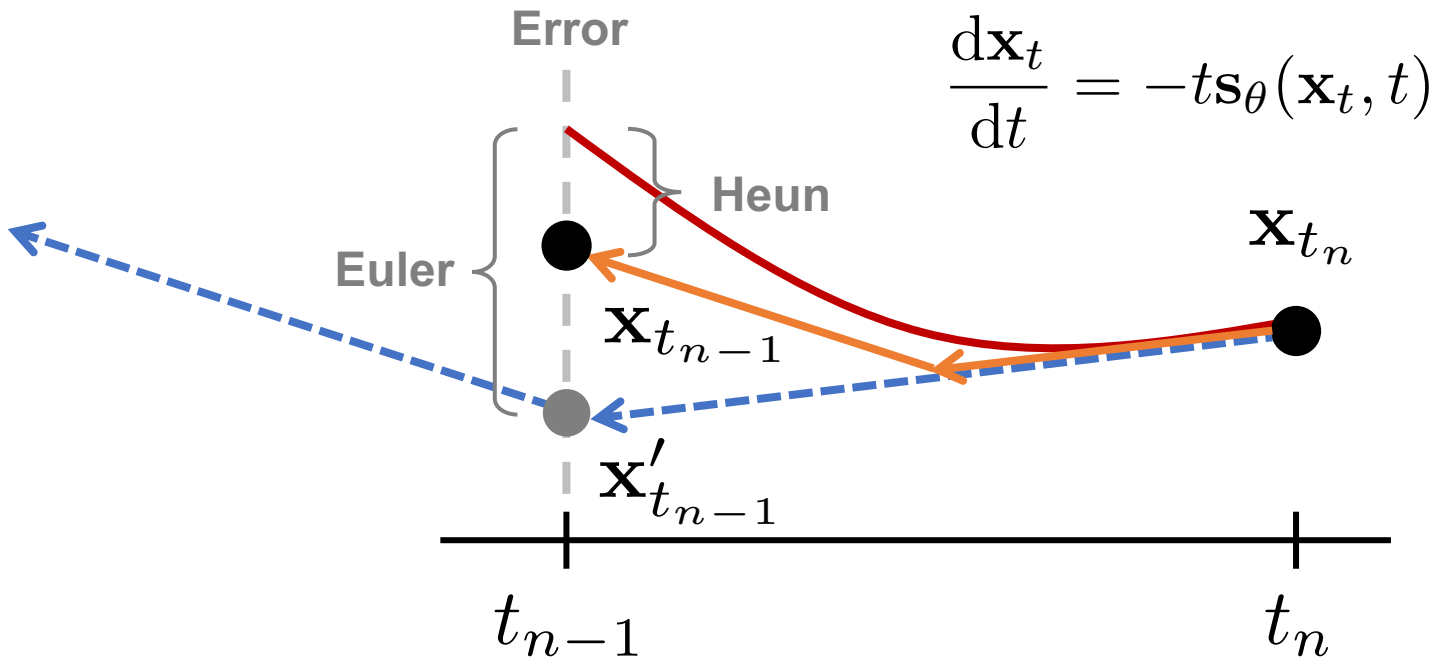
$$\frac{\mathbf{x}_{t_{n-1}} - \mathbf{x}_{t_n}}{t_{n-1} - t_n} + O(n)$$



$$\mathbf{x}_{t_{n-1}} = \mathbf{x}_{t_n} - (t_{n-1} - t_n)t_n\mathbf{s}_\theta(\mathbf{x}_{t_n}, t_n)$$

How to Solve the Reverse ODE?

Heun's Method (2nd order):

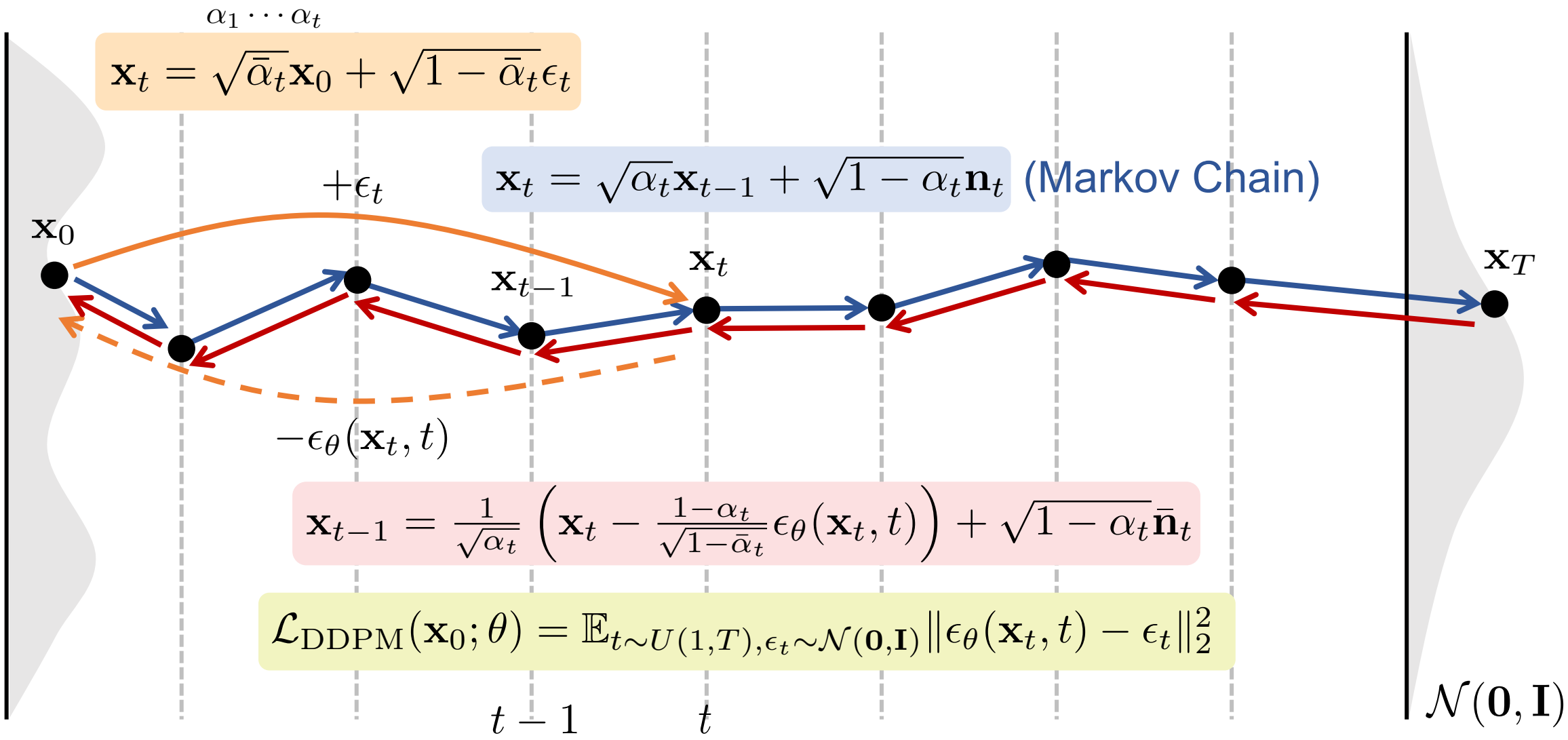


$$\frac{\mathrm{d}\mathbf{x}_t}{\mathrm{d}t} = -t\mathbf{s}_\theta(\mathbf{x}_t, t)$$

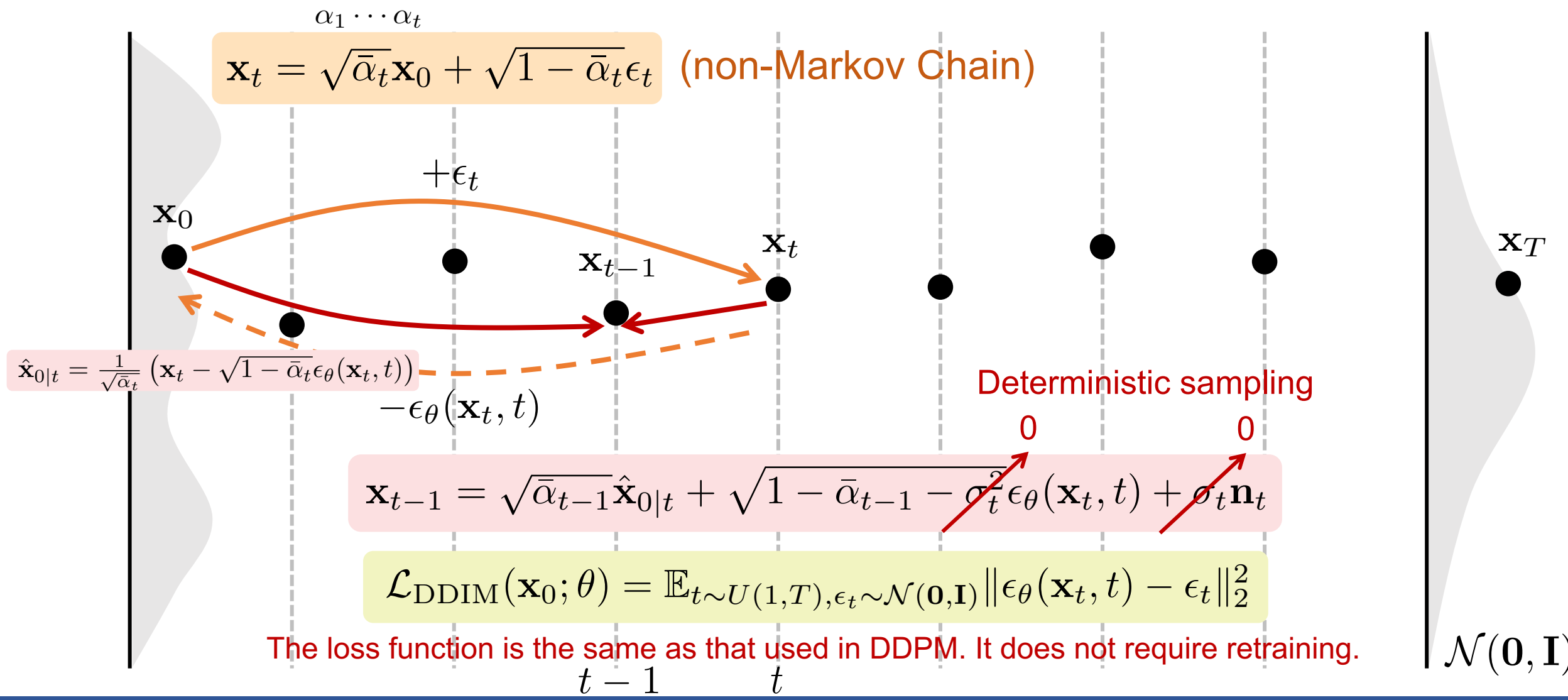
$$\mathbf{x}'_{t_{n-1}} = \mathbf{x}_{t_n} - (t_{n-1} - t_n)t_n\mathbf{s}_\theta(\mathbf{x}_{t_n}, t_n)$$

$$\mathbf{x}_{t_{n-1}} = \mathbf{x}_{t_n} - \tfrac{1}{2}(t_{n-1} - t_n)[t_n\mathbf{s}_\theta(\mathbf{x}_{t_n}, t_n) + t_{n-1}\mathbf{s}_\theta(\mathbf{x}'_{t_{n-1}}, t_{n-1})]$$

Denoising Diffusion Probabilistic Models (DDPM) [Ho+ NeurIPS'20]

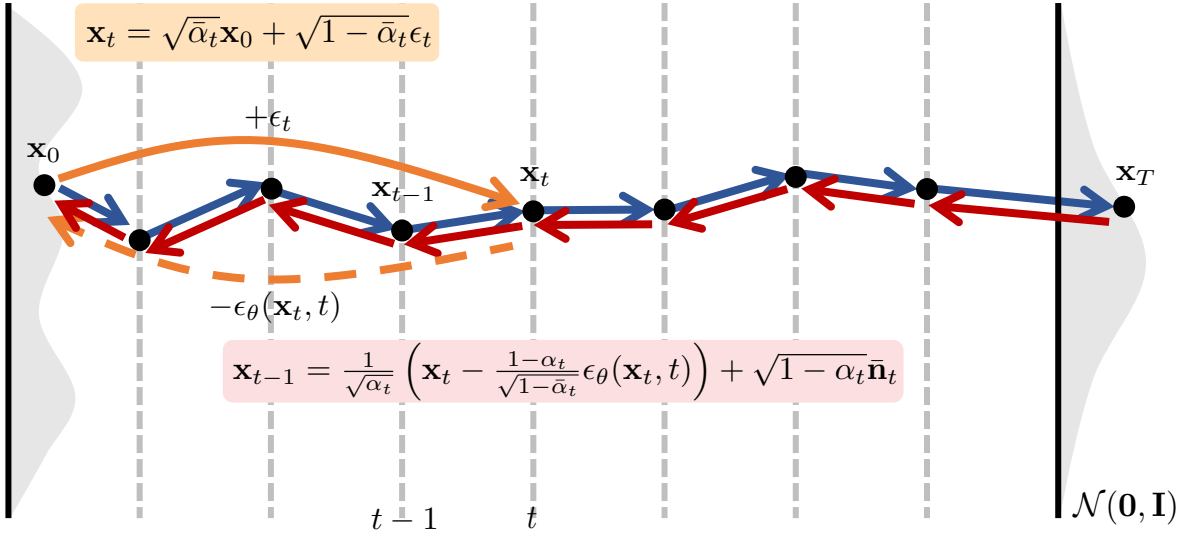


Denoising Diffusion Implicit Models (DDIM) [Song+ ICLR'21]



Summary: Discreate vs Continuous

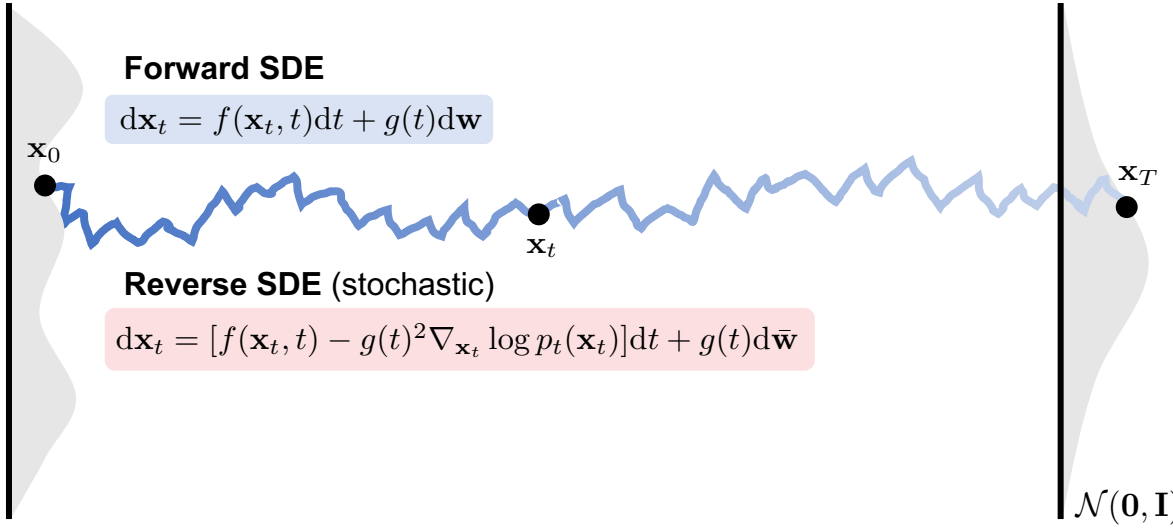
DDPM



$$\mathcal{L}_{\text{DDPM}}(\mathbf{x}_0;\theta) = \mathbb{E}_{t\sim U(1,T),\epsilon_t\sim\mathcal{N}(\mathbf{0},\mathbf{I})}\|\epsilon_\theta(\mathbf{x}_t,t) - \epsilon_t\|_2^2$$

Discretized in the training phase

Score-based SDE

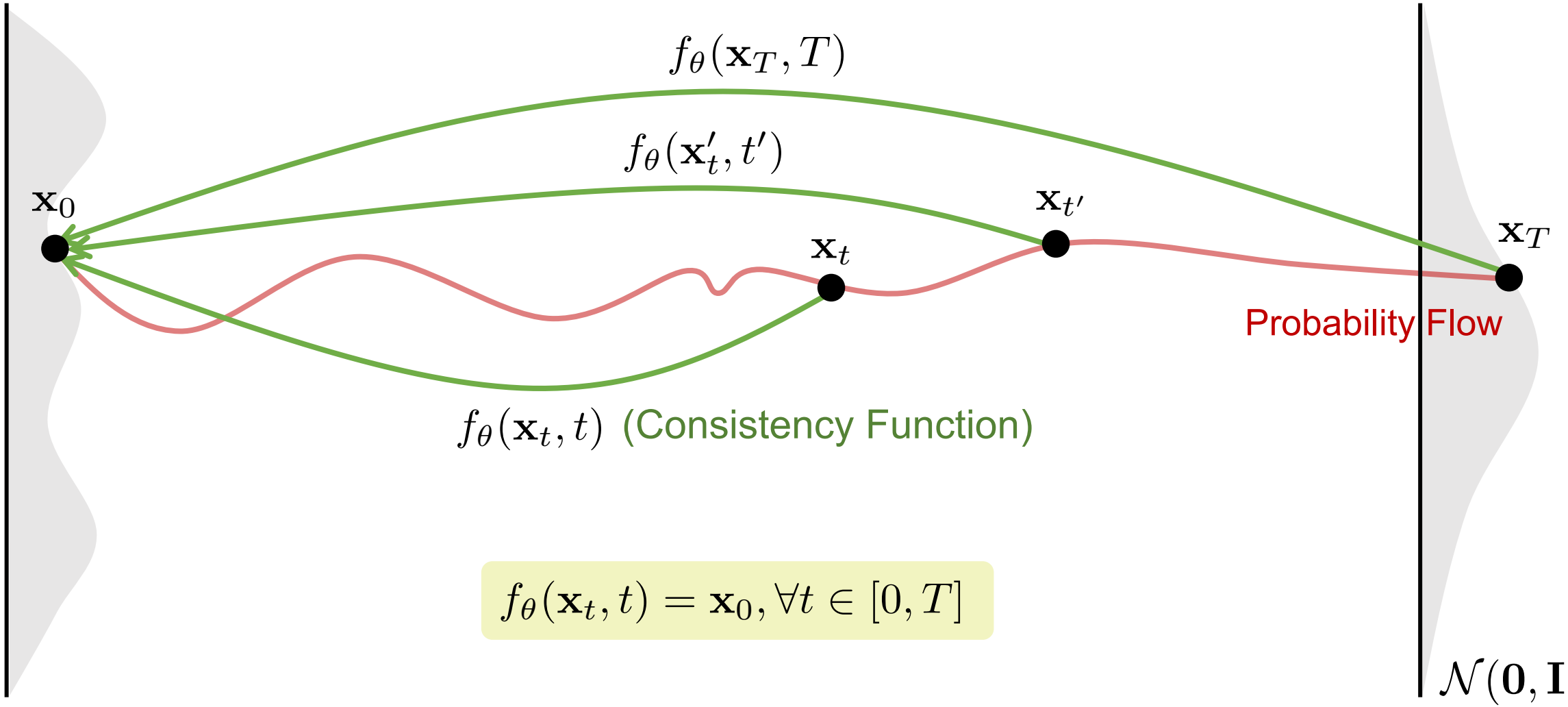


$$\mathcal{L}_{\text{DSM}}(\mathbf{x}_0;\theta) = \mathbb{E}_{\mathbf{x}_t|\mathbf{x}_0}\|\mathbf{s}_\theta(\mathbf{x}_t,t) - \nabla_{\mathbf{x}_t}\log p_t(\mathbf{x}_t|\mathbf{x}_0)\|_2^2$$

Discretized during sampling
The error is only affected by the order of the solver

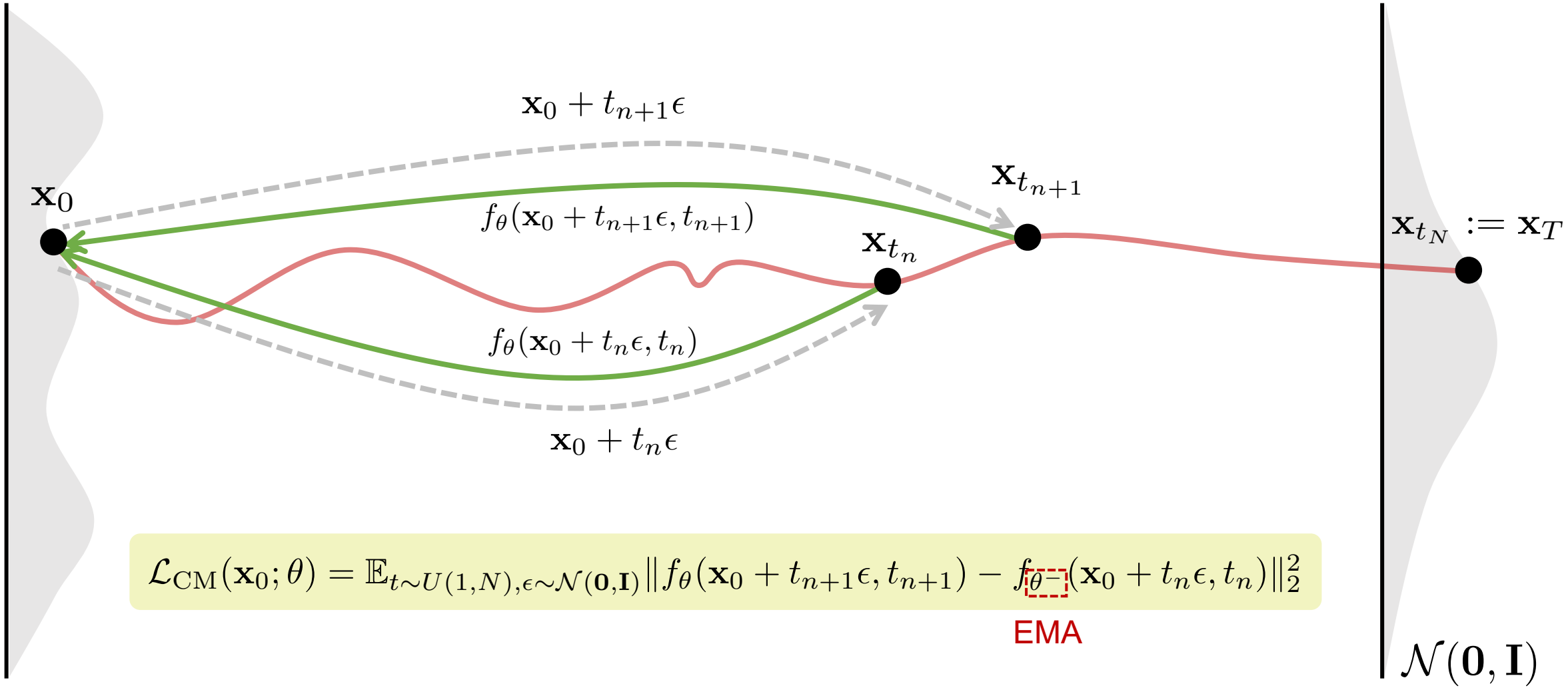
Consistency Models (CM) [Song+ ICML'23]

$$\mathrm{d}\mathbf{x}_t = -t\nabla_{\mathbf{x}_t} \log p_t(\mathbf{x}_t)\mathrm{d}t$$



$$f_\theta(\mathbf{x}_t, t) = \mathbf{x}_0, \forall t \in [0, T]$$

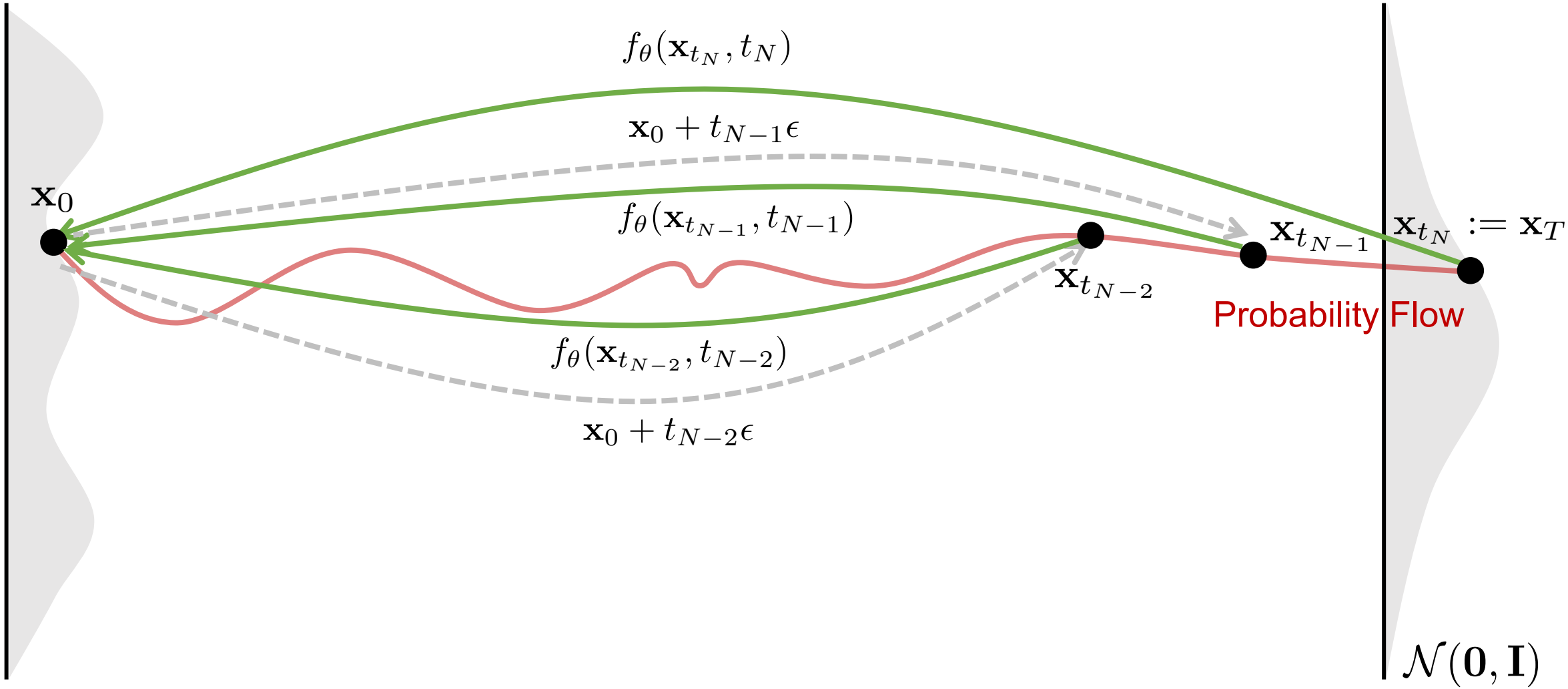
Training CM



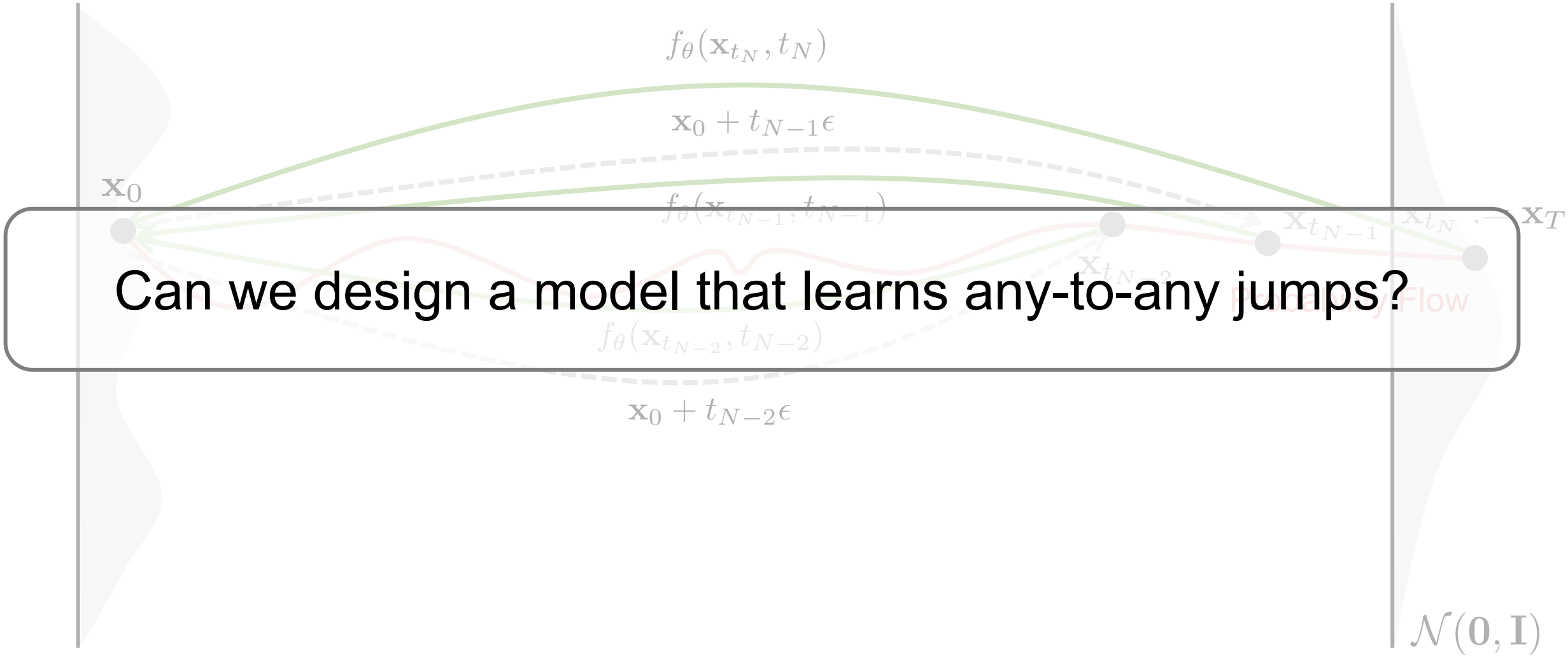
$$\mathcal{L}_{\text{CM}}(\mathbf{x}_0; \theta) = \mathbb{E}_{t\sim U(1,N),\epsilon\sim\mathcal{N}(\mathbf{0},\mathbf{I})} \| f_\theta(\mathbf{x}_0 + t_{n+1}\epsilon, t_{n+1}) - f_{\theta^-}(\mathbf{x}_0 + t_n\epsilon, t_n) \|_2^2$$

EMA

Sampling with CM



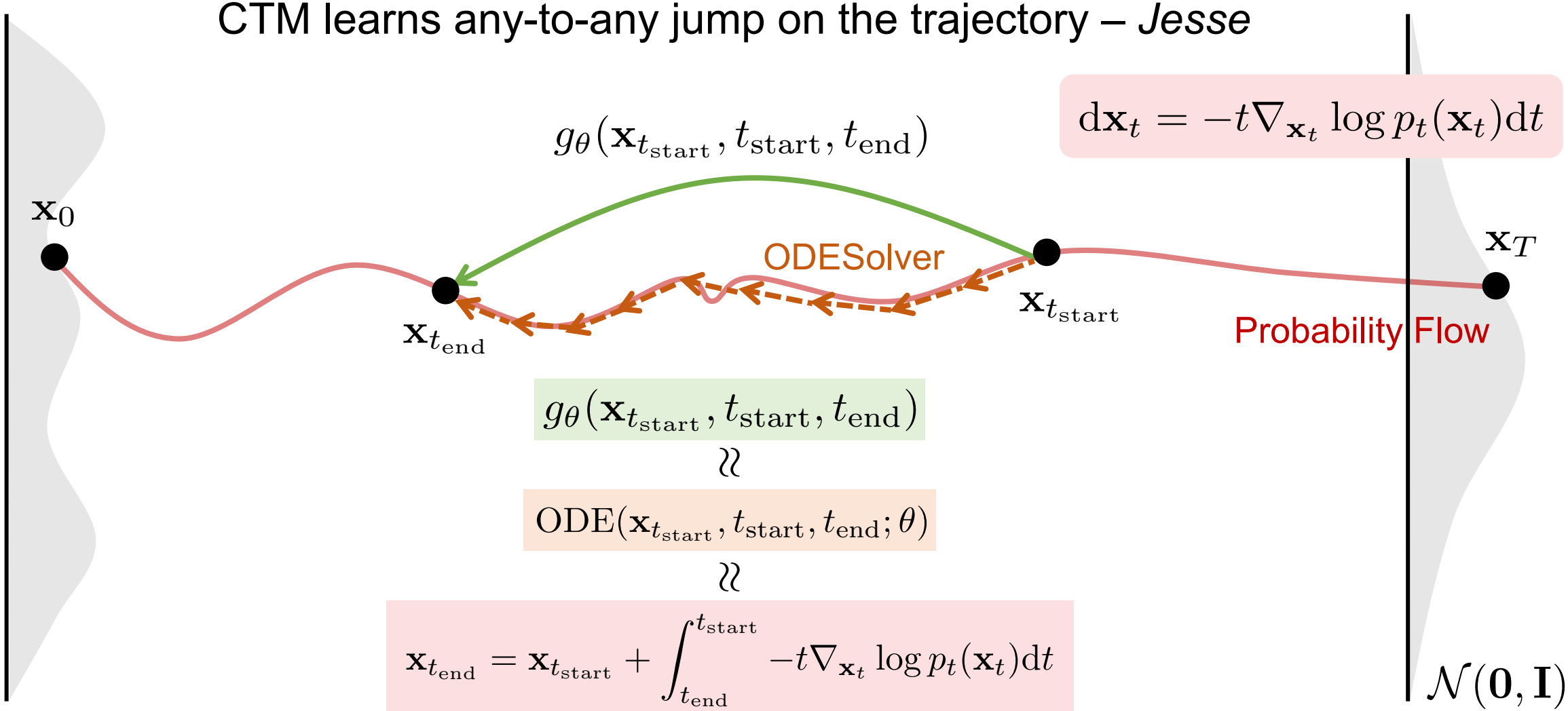
Sampling with CM



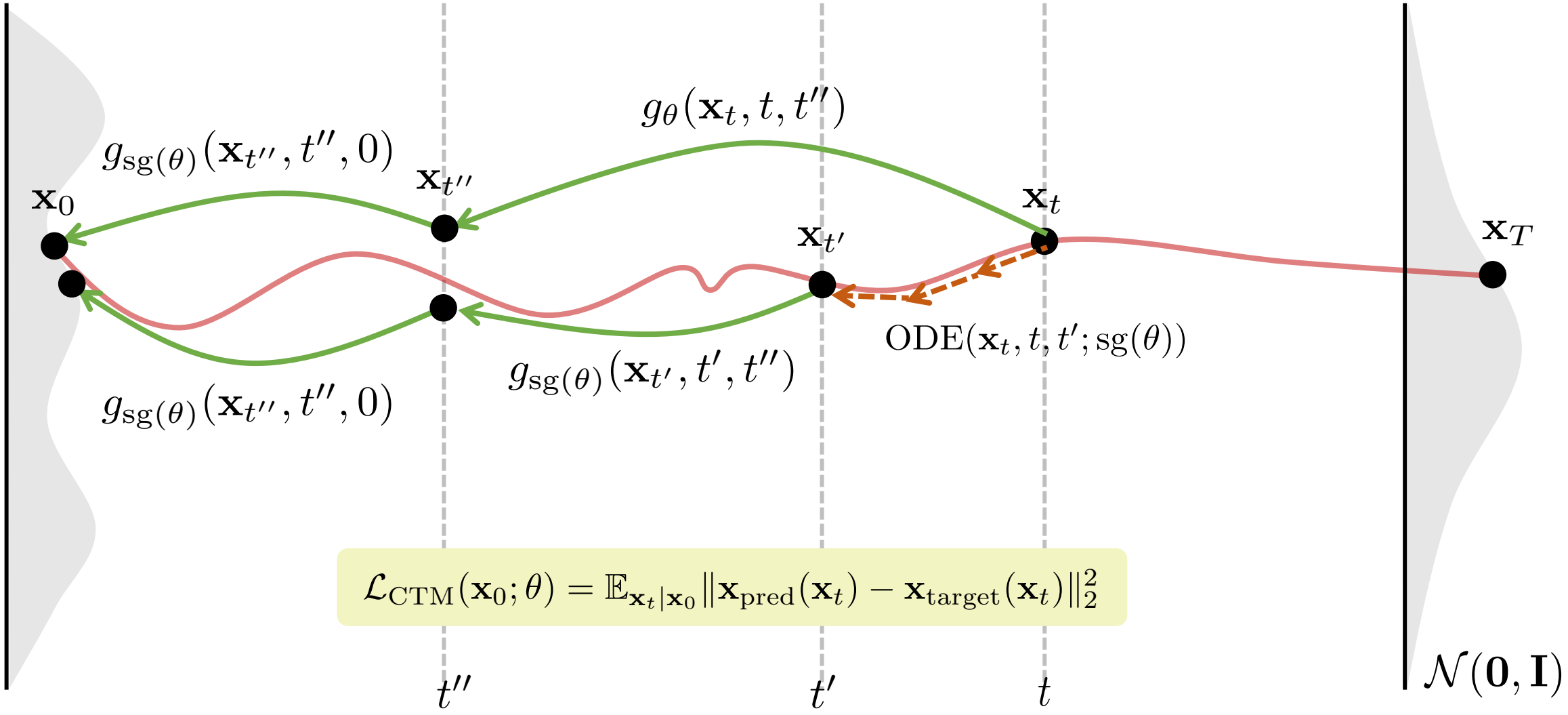
Can we design a model that learns any-to-any jumps?

Consistency Trajectory Models (CTM) [Kim+ ICLR'24]

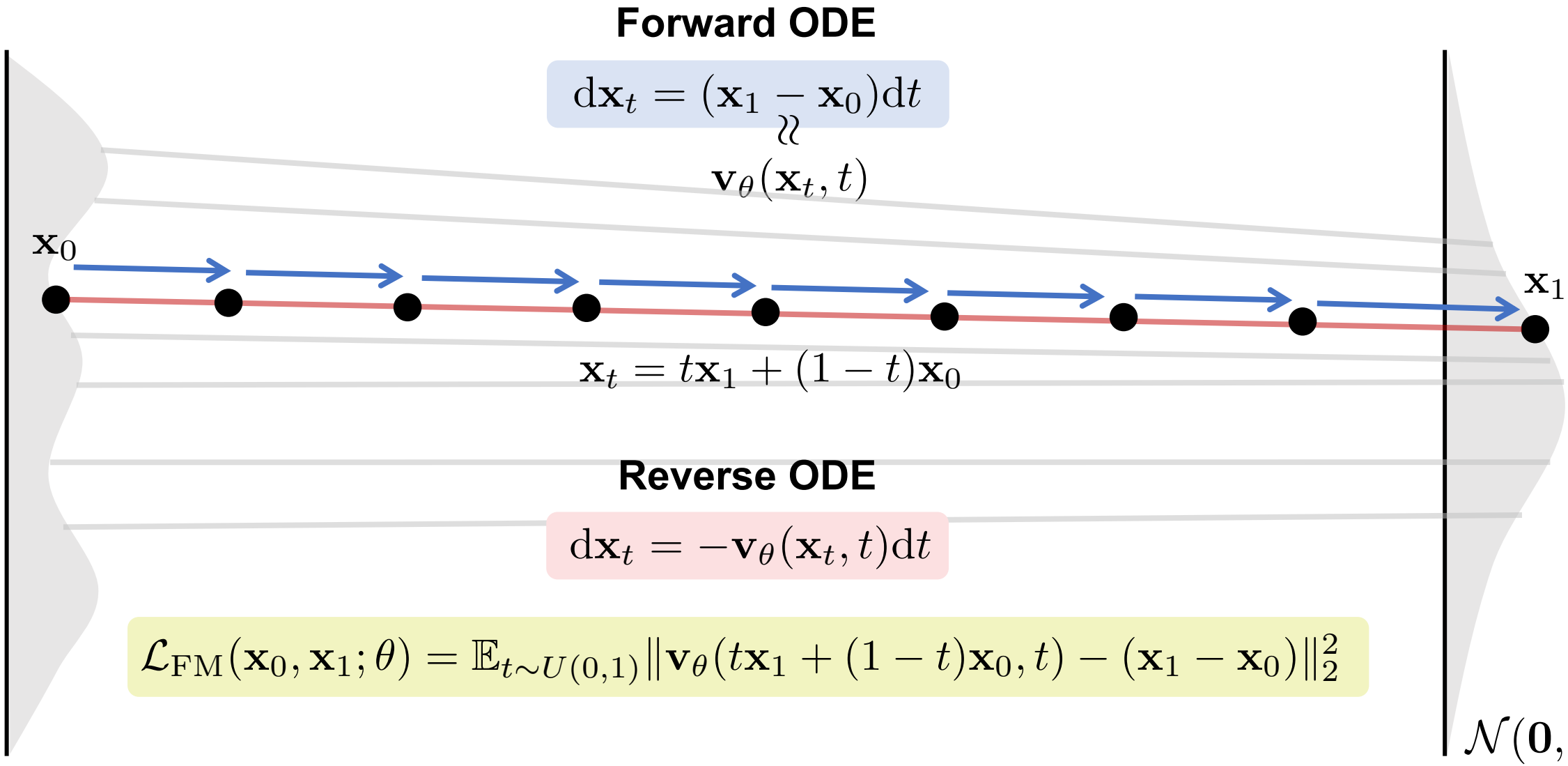
CTM learns any-to-any jump on the trajectory – *Jesse*



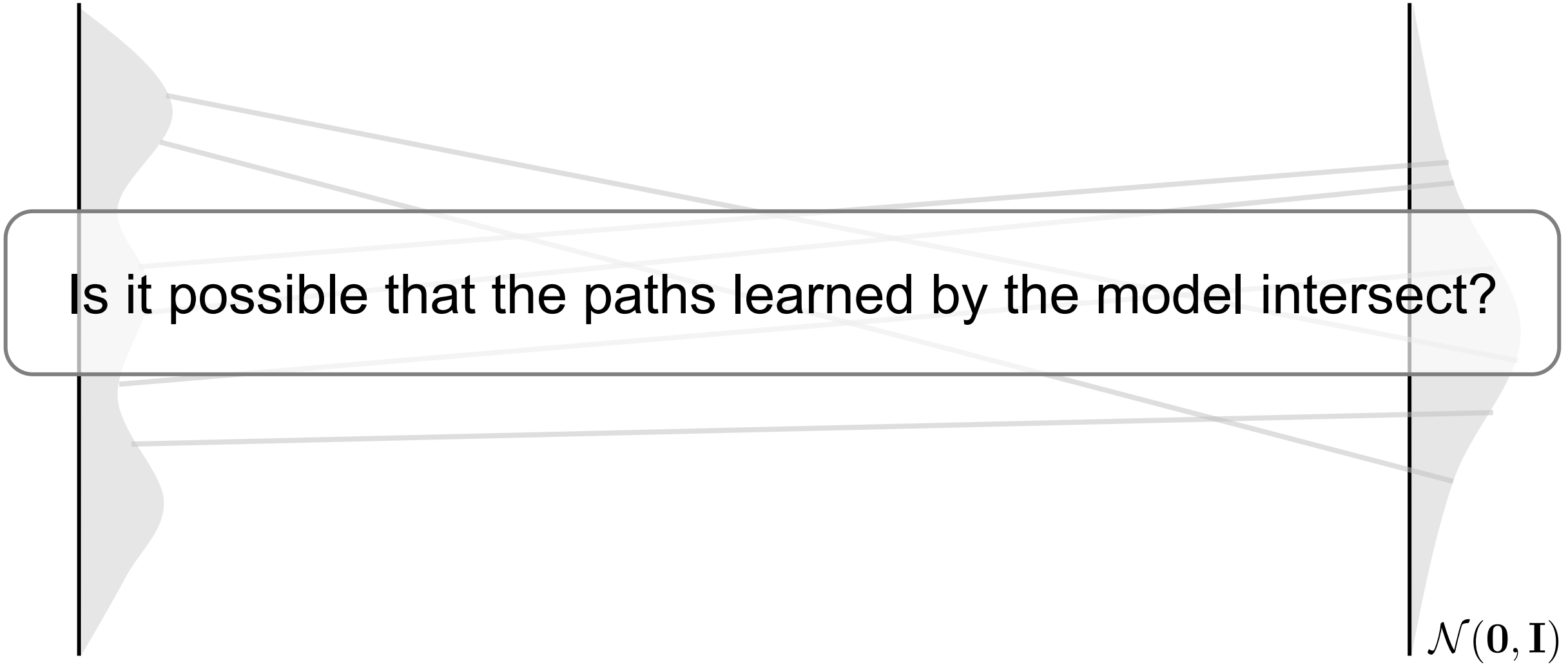
Training CTM



Flow Matching [Lipman+ ICLR'23][Liu+ ICLR'23]

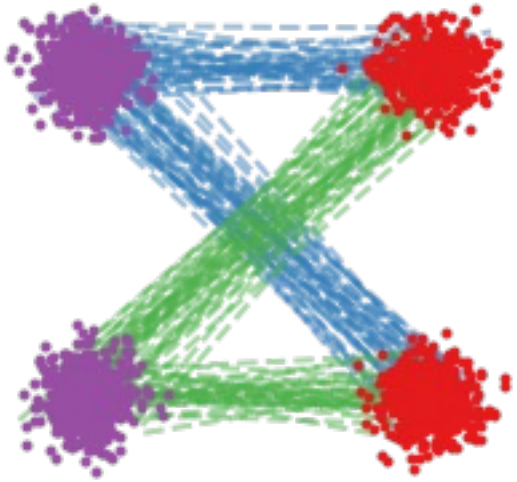


Flow Matching [Lipman+ ICLR'23][Liu+ ICLR'23]



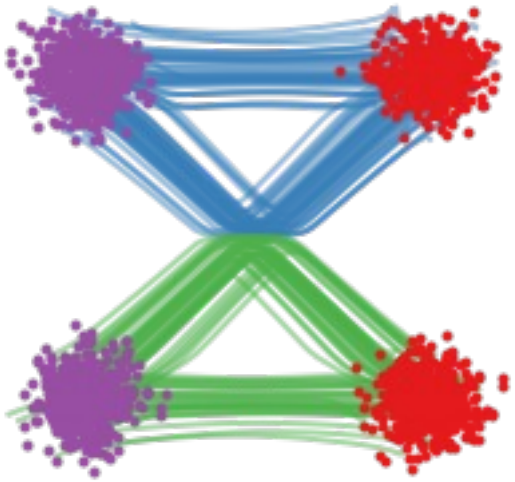
k-Rectified Flow [Liu+ ICLR'23]

Data Noise



$$\mathbf{x}_t = t\mathbf{x}_1 + (1-t)\mathbf{x}_0$$

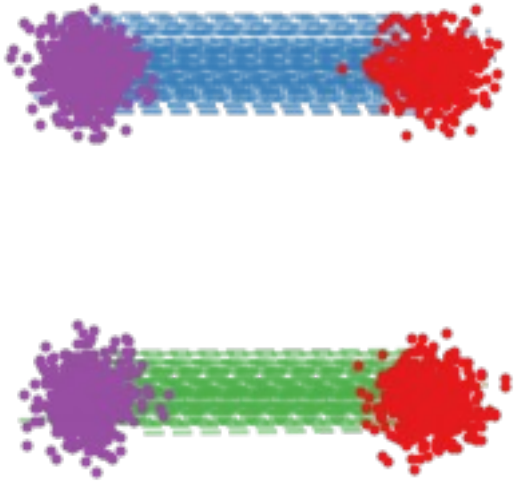
Data Noise



Flow Matching
(1-Rectified Flow)

(not straight but non-crossing)

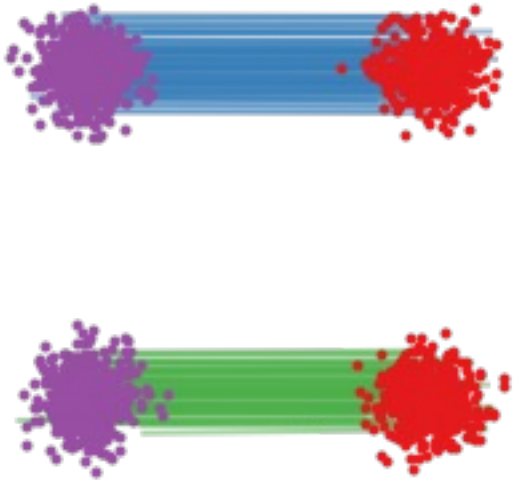
Data Noise



$$\mathbf{x}_t^{(1)} = t\mathbf{x}_1^{(1)} + (1-t)\mathbf{x}_0^{(1)}$$

(Sample the data-noise pair
from 1-Rectified Flow)

Data Noise

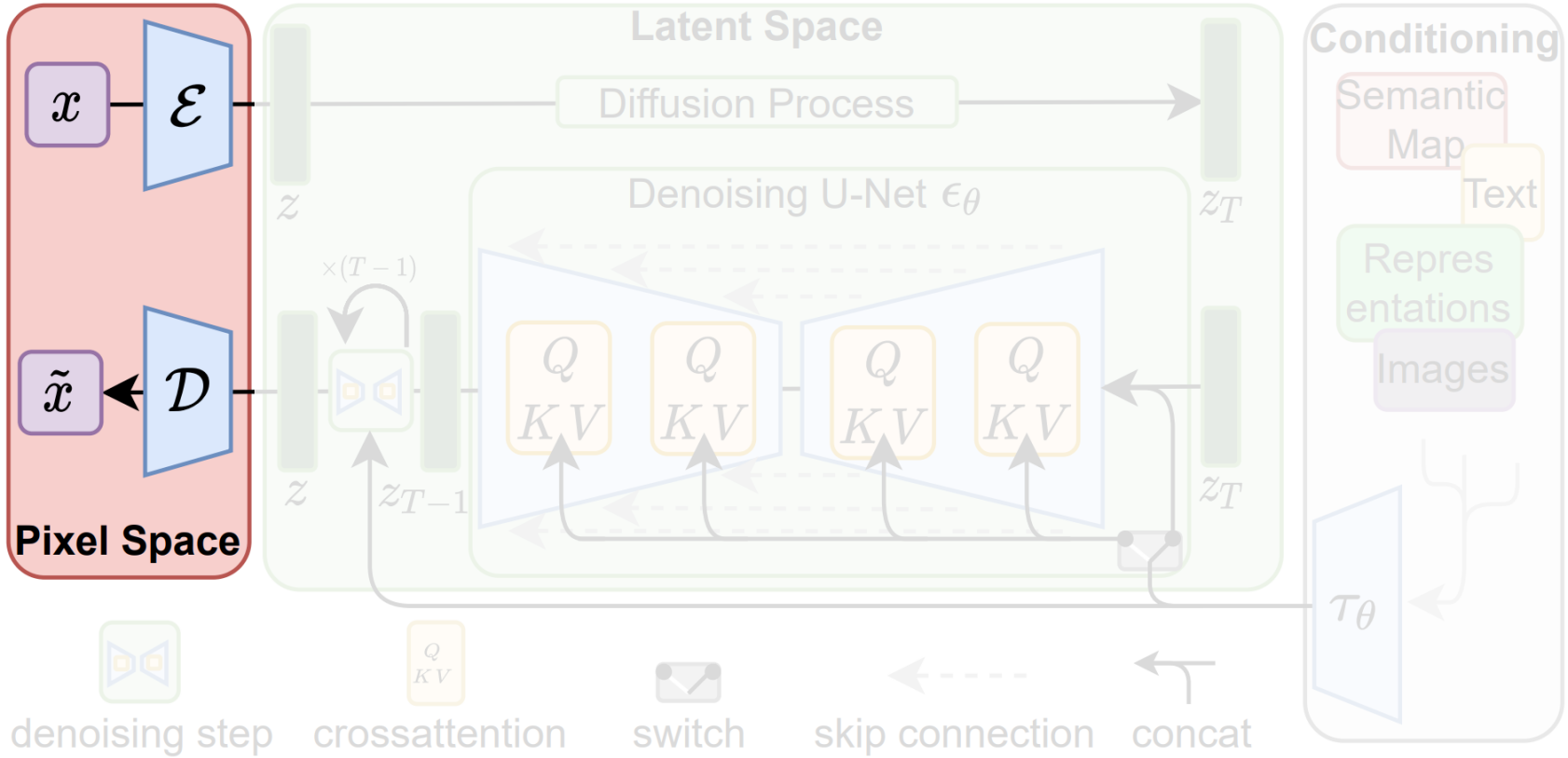


2-Rectified Flow
(straight)

How to reduce the computational cost of diffusion models?

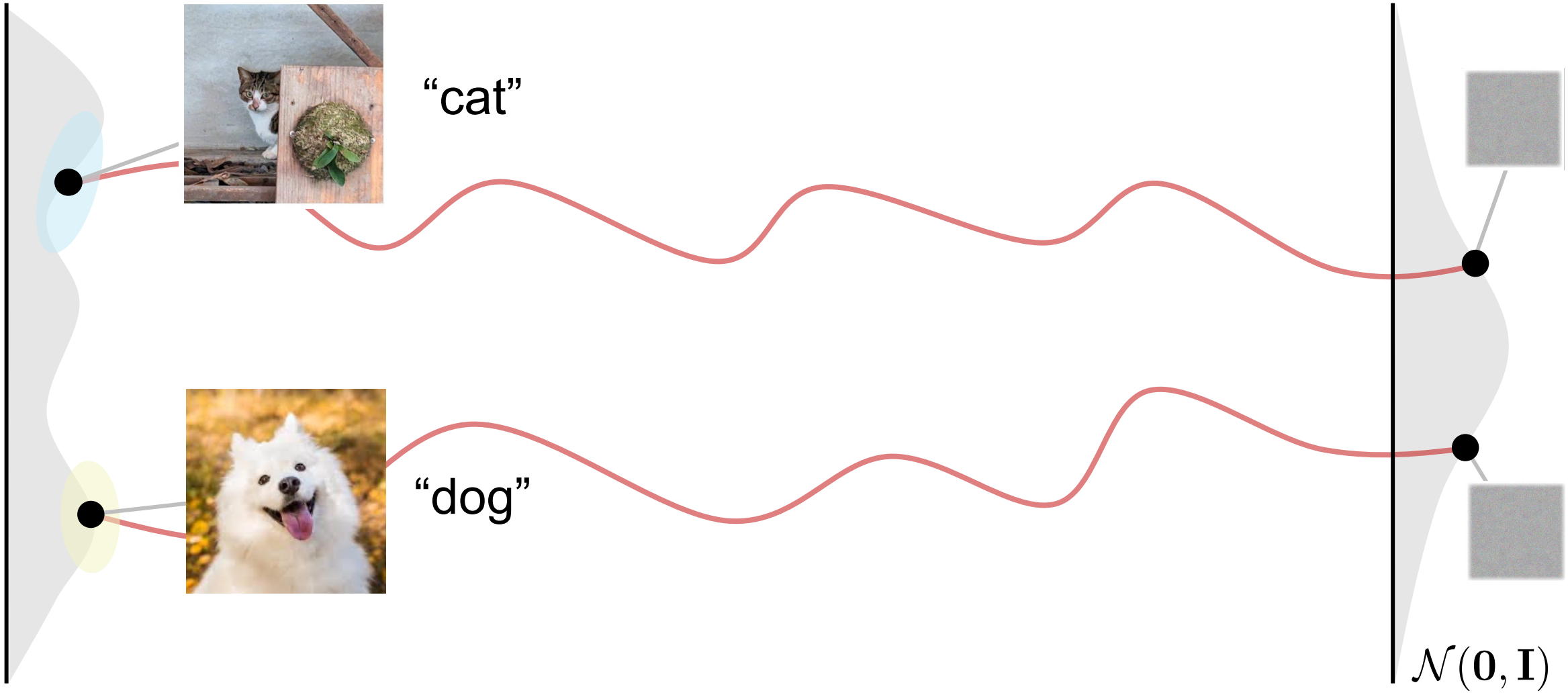
Latent Diffusion Model (LDM) [Rombach+ CVPR'22]

Use the pretrained-VAE to compress the image to latent reducing computation time



Can we control the Diffusion Models?

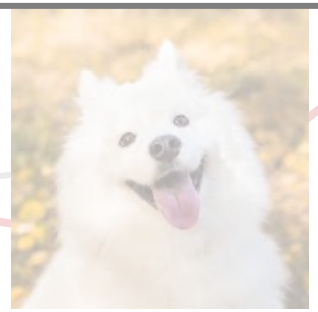
Conditional Diffusion Models



Conditional Diffusion Models

"cat"

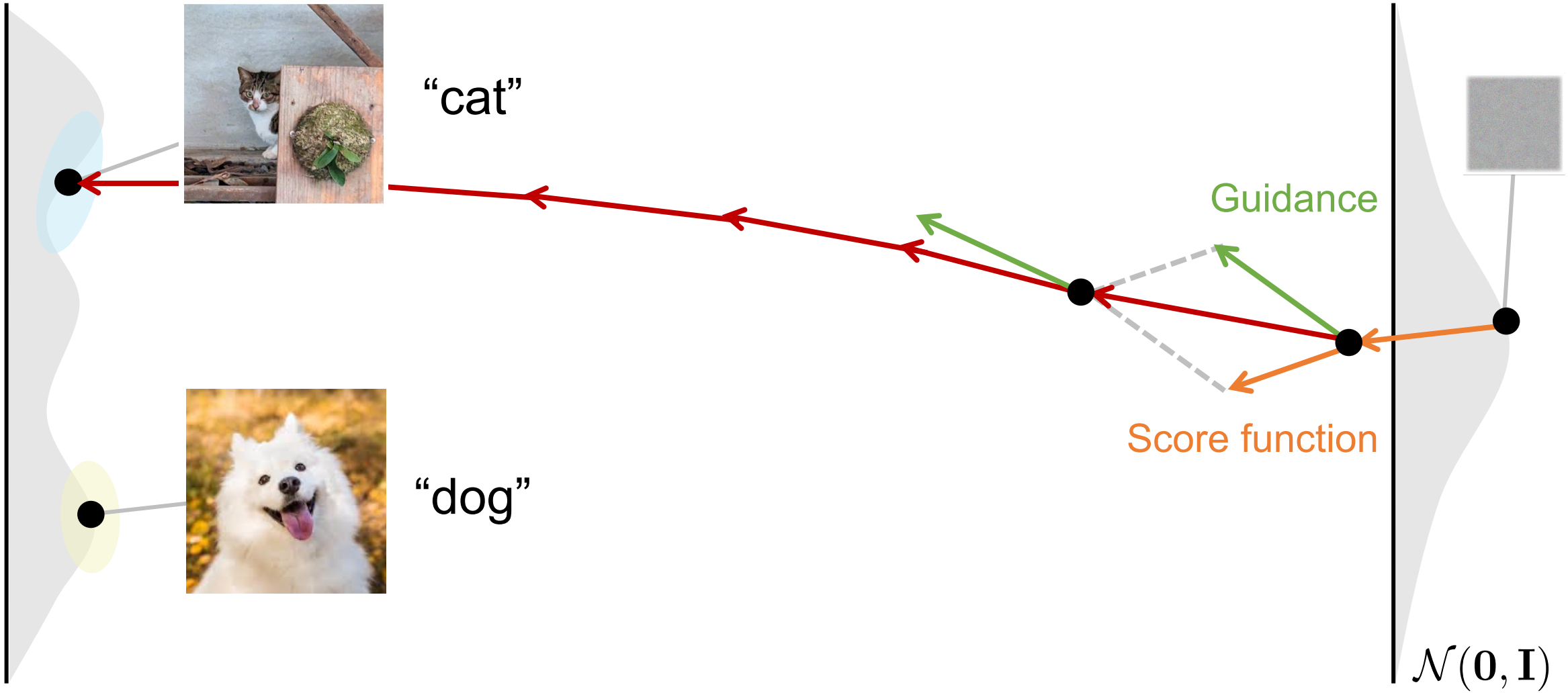
How to control the Diffusion Models?



"dog"

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

Conditional Diffusion Models



Classifier Guidance (CG) [Dhariwal+ NeurIPS'21]

- **Bayes' Rule:**

$$P\left(\mathbf{x}_t = \text{  } \,\middle|\, \mathbf{y} = \text{“cat”}\right) = \frac{p(\mathbf{x}_t)p(\mathbf{y}|\mathbf{x}_t)}{p(\mathbf{y})}$$

- **Bayes' Rule for Score Function:**

$$\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}) = \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t) + \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t) - \nabla_{\mathbf{x}_t} \log p(\mathbf{y})$$

0

$$= \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t) + \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t)$$

Unconditional score

Classifier (need to additional training)

Classifier-Free Guidance (CFG) [Ho+ NeurIPSW'21]

From CG, we have

$$\nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t) = \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}) - \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t)$$

Reweight the coefficient between unconditional score and classifier score

$$\nabla_{\mathbf{x}_t} \log \tilde{p}(\mathbf{x}_t|\mathbf{y}) := \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t) + \gamma \nabla_{\mathbf{x}_t} \log p(\mathbf{y}|\mathbf{x}_t)$$

$$= \gamma \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}) + (1-\gamma) \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t)$$

Conditional score

Unconditional score

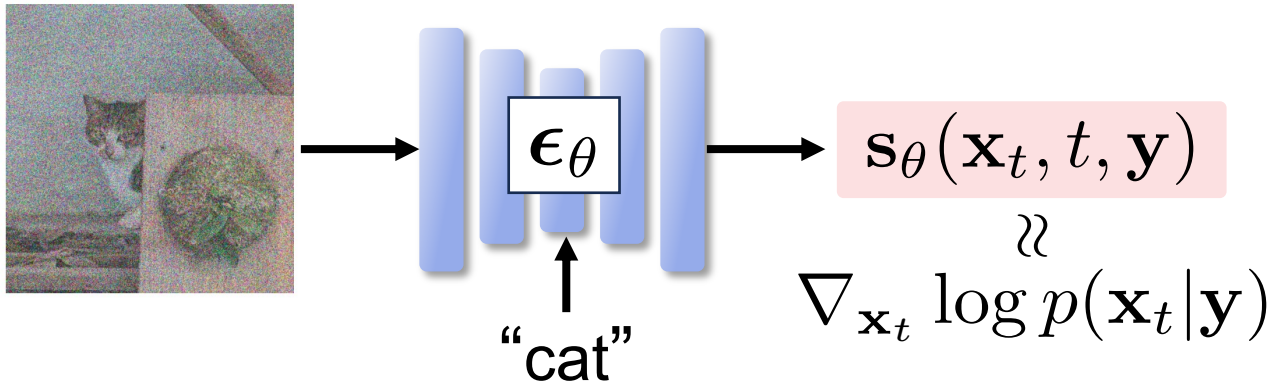
Training CFG

$$\nabla_{\mathbf{x}_t} \log \tilde{p}(\mathbf{x}_t|\mathbf{y}) = \gamma \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}) + (1-\gamma) \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t)$$

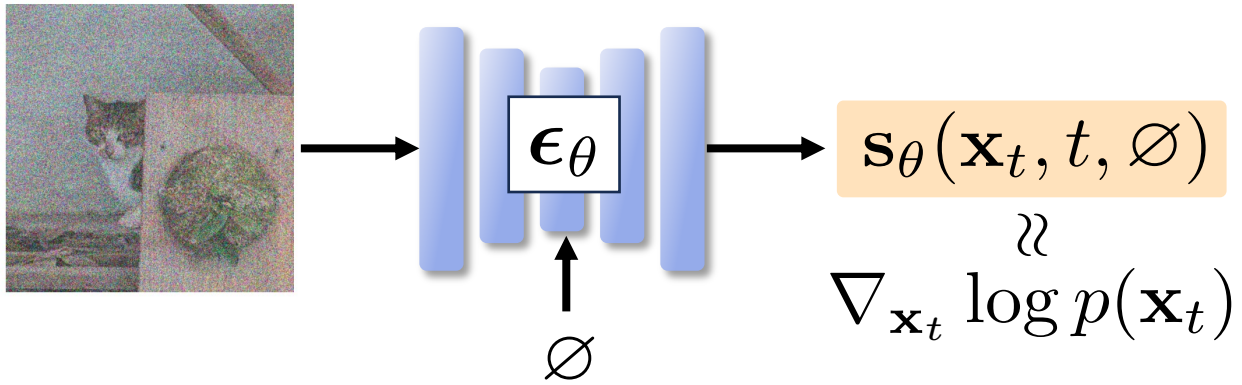
Conditional score

Unconditional score

Predict Conditional Score



Predict Unconditional Score



Training CFG

$$\nabla_{\mathbf{x}_t} \log \tilde{p}(\mathbf{x}_t|\mathbf{y}) = \gamma \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y}) + (1-\gamma) \nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t)$$

Conditional score

Unconditional score

Predict Conditional Score

ϵ_θ

"cat"

$\mathbf{s}_\theta(\mathbf{x}_t, t, \mathbf{y})$

$\approx$

$\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t|\mathbf{y})$

Can we control the semantic details of an image?

Predict Unconditional Score

ϵ_θ

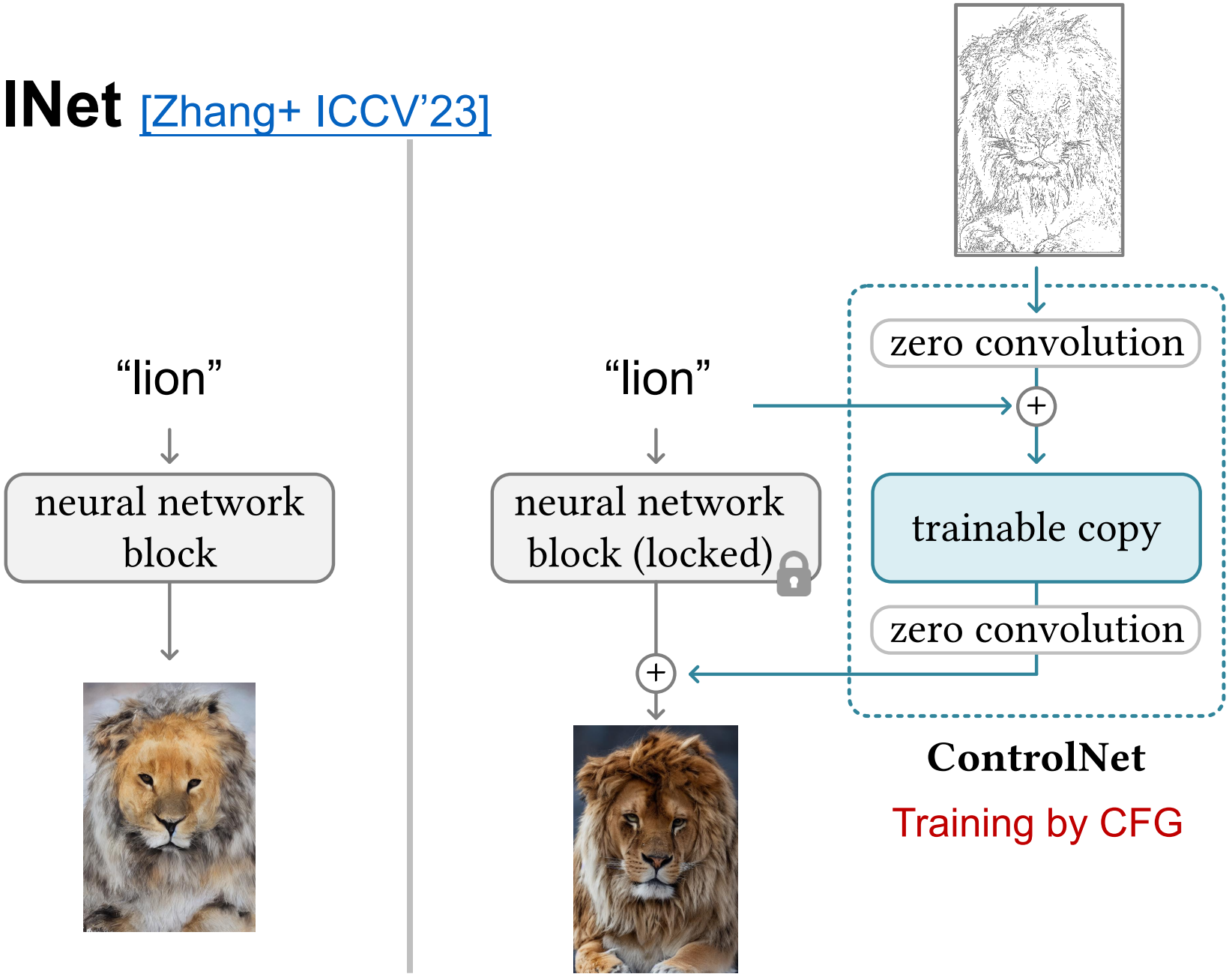
$\varnothing$

$\mathbf{s}_\theta(\mathbf{x}_t, t, \varnothing)$

$\approx$

$\nabla_{\mathbf{x}_t} \log p(\mathbf{x}_t)$

ControlNet [Zhang+ ICCV'23]



Applications of Diffusion Models in 3D Vision

Zero-1-to-3
2023 / 5

Magic123
2023 / 6

One-2-3-45++
2023 / 11

DreamFusion
2022 / 9

One-2-3-45
2023 / 6

Zero123++
2023 / 10

Stable Zero123
2023 / 12

Takeaway

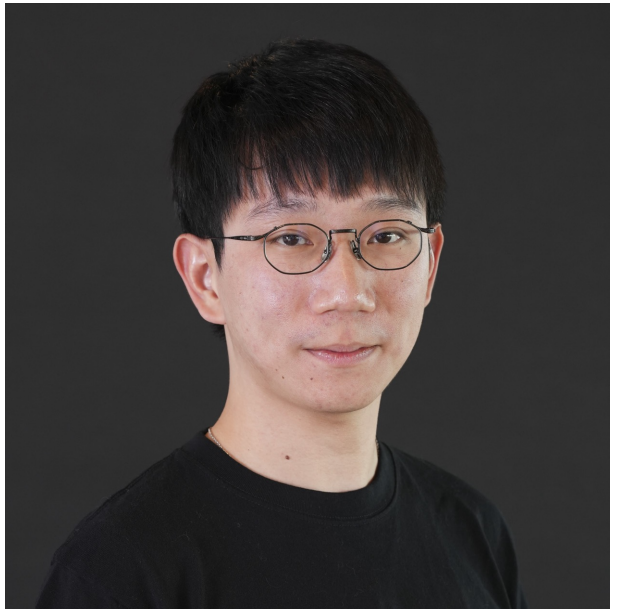
- Diffusion models build a bridge between noise and data, forming a powerful generative modeling framework.
- Score-based models leverage SDE/ODE formulations and score functions to guide the reverse process.
- Variants like DDIM, CM, CTM, and Flow Matching offer trade-offs in speed, quality, and control.
- Conditional methods like CFG and ControlNet significantly improve controllability and application scope.
- Diffusion models are already widely applied in 2D/3D image synthesis, speech, and multi-modal generation.

Acknowledgement

Some concepts and insights in these slides are inspired by Yang Song and Jesse

Yang Song

Research Scientist at OpenAI



Chieh-Hsin (Jesse) Lai

Research Scientist at Sony AI

Thank you