NEURAL INFORMATION PROCESSING SYSTEMS

IMPERIAL

Canon

Neural Stochastic Flows: Solver-Free Modelling and Inference for SDE Solutions

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Project page

Stochastic Differential Equations (SDEs) are Everywhere

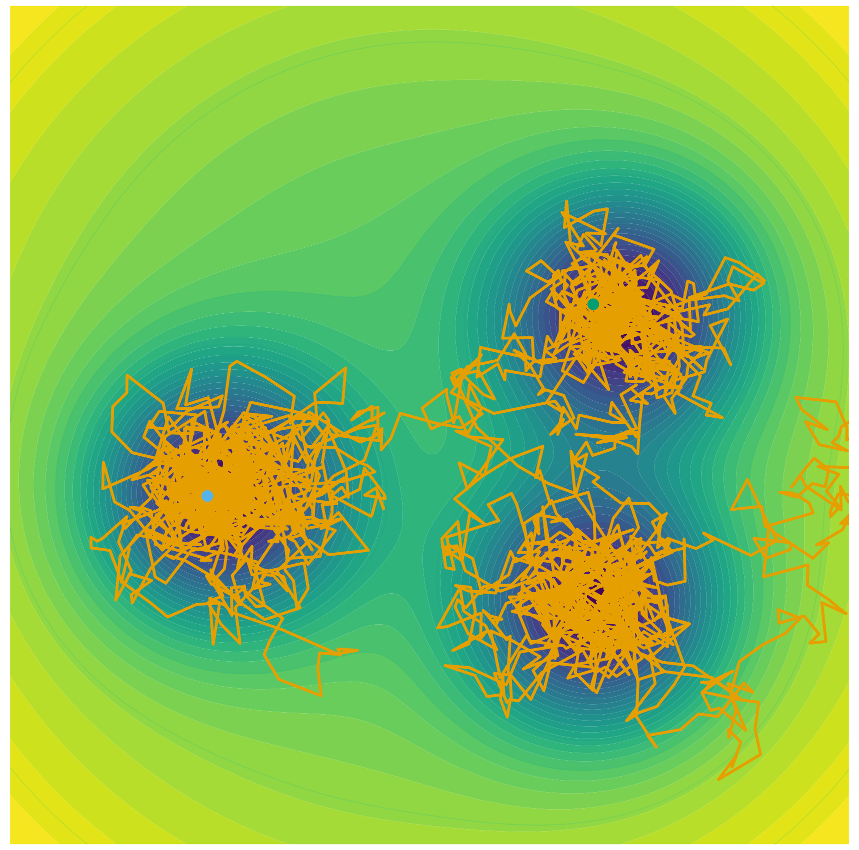
$$\text{Itô SDE:} \qquad dx_t = \boxed{\mu\left(x_t, t\right) dt} + \boxed{\sigma\left(x_t, t\right) dW_t,} \qquad x_0 \sim p_0$$

Drift term (deterministic)

Diffusion term (stochastic)

Finance

Physics



Generative Modelling

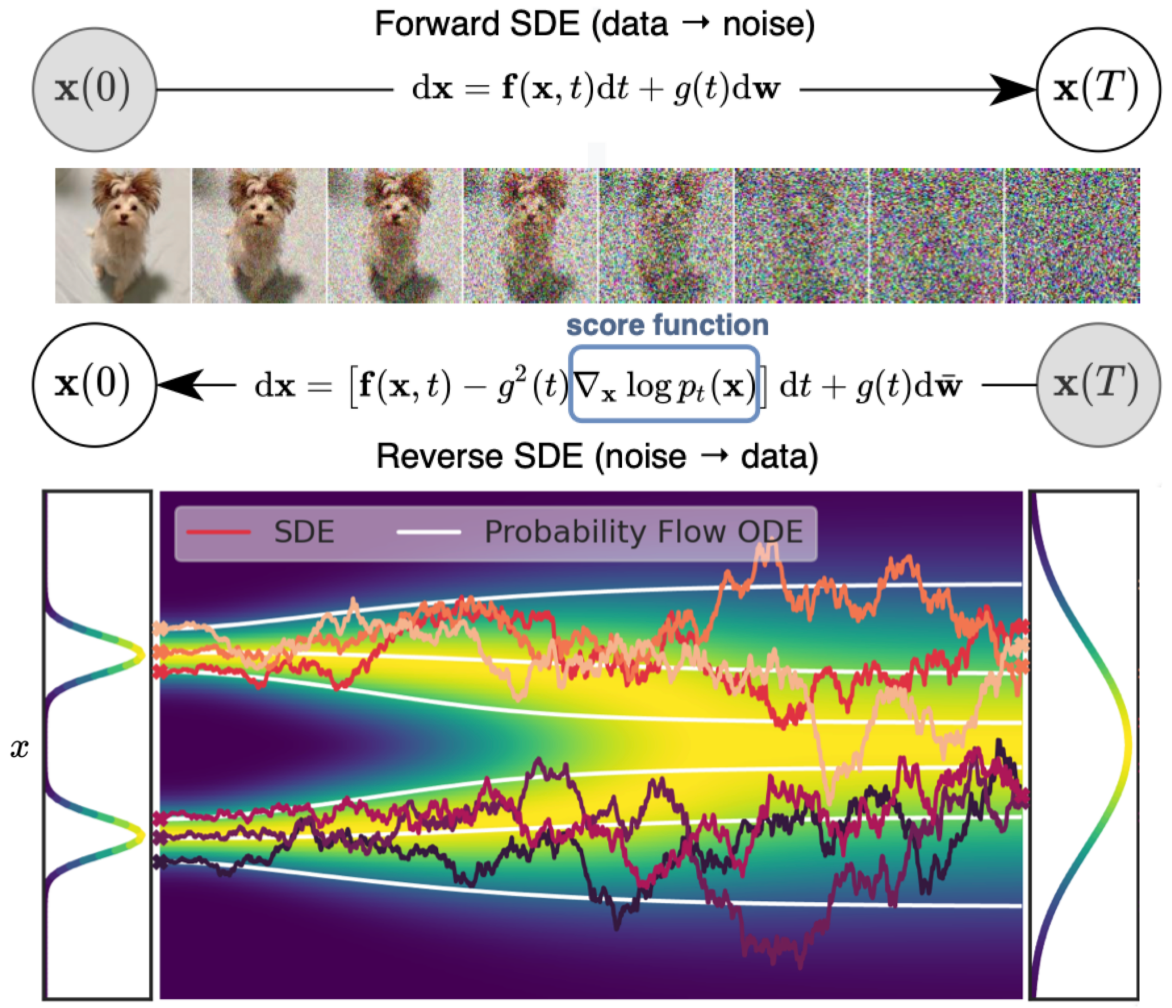


Figure adapted from [47]

Neural SDEs

Modelling SDE Terms using Neural Networks

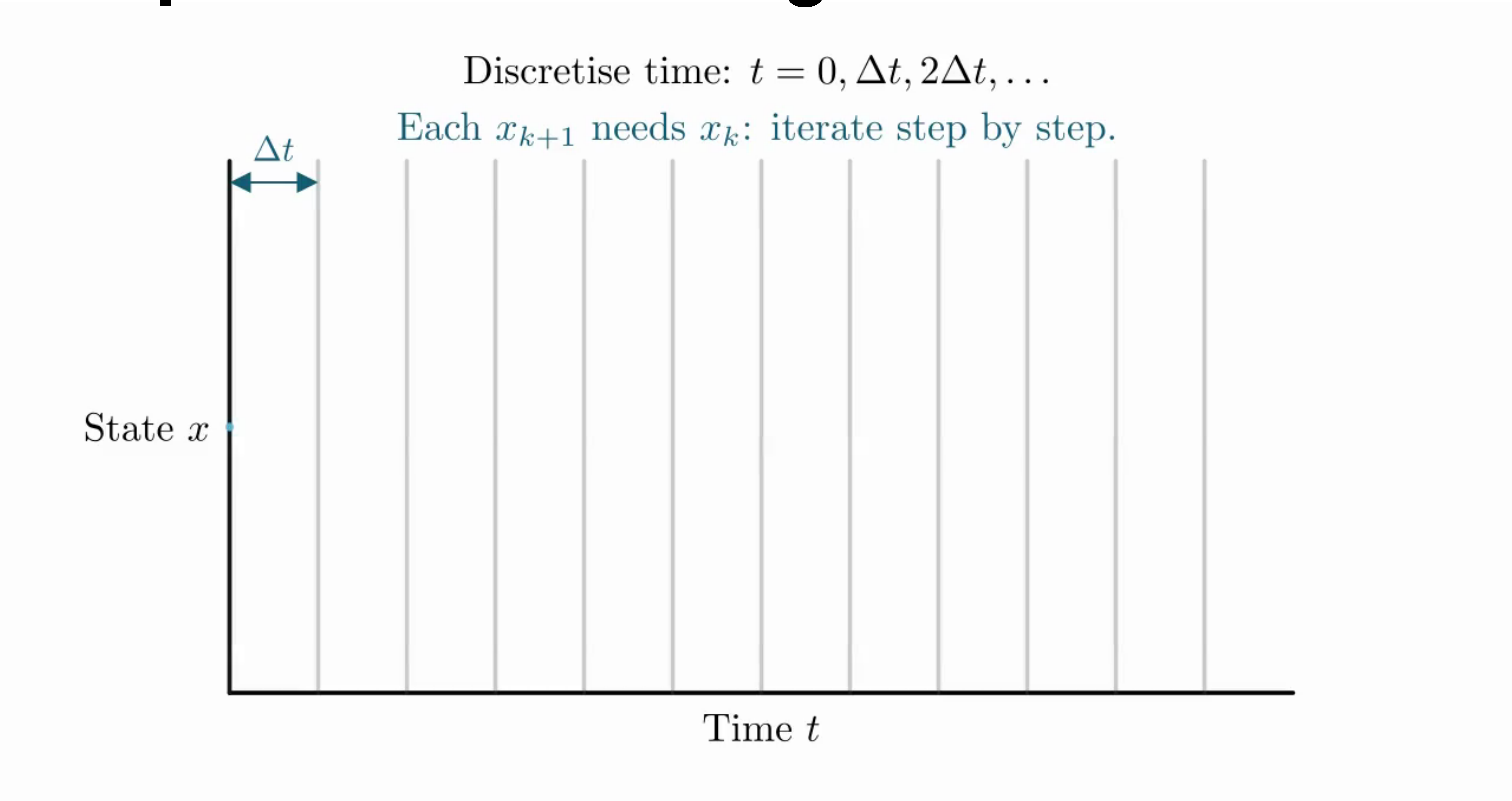
$$\text{Itô SDE:} \qquad dx_t = \boxed{\mu\left(x_t, t\right)} dt + \boxed{\sigma\left(x_t, t\right)} dW_t, \qquad x_0 \sim p_0$$

Modelled by neural networks

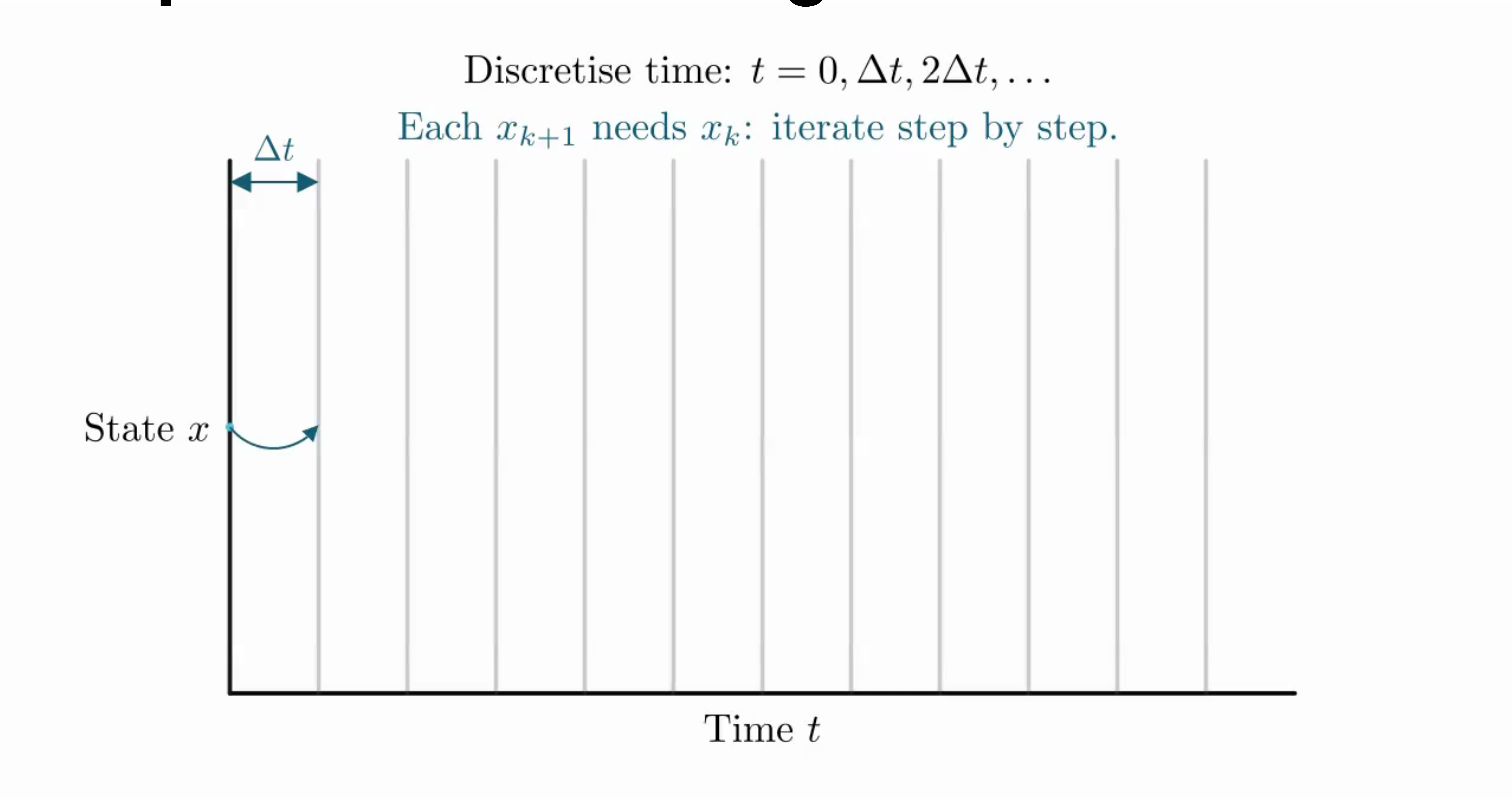
$$x_{t_{k+1}} = x_{t_k} + \mu\left(x_{t_k}, t_k\right) \Delta t + \sigma\left(x_{t_k}, t_k\right) \Delta W_k$$

$$t_k = k\Delta t, \qquad \Delta W_k = W_{t_{k+1}} - W_{t_k} \sim \mathcal{N}(0, \Delta t)$$

Computational Challenges of Neural SDEs



Computational Challenges of Neural SDEs



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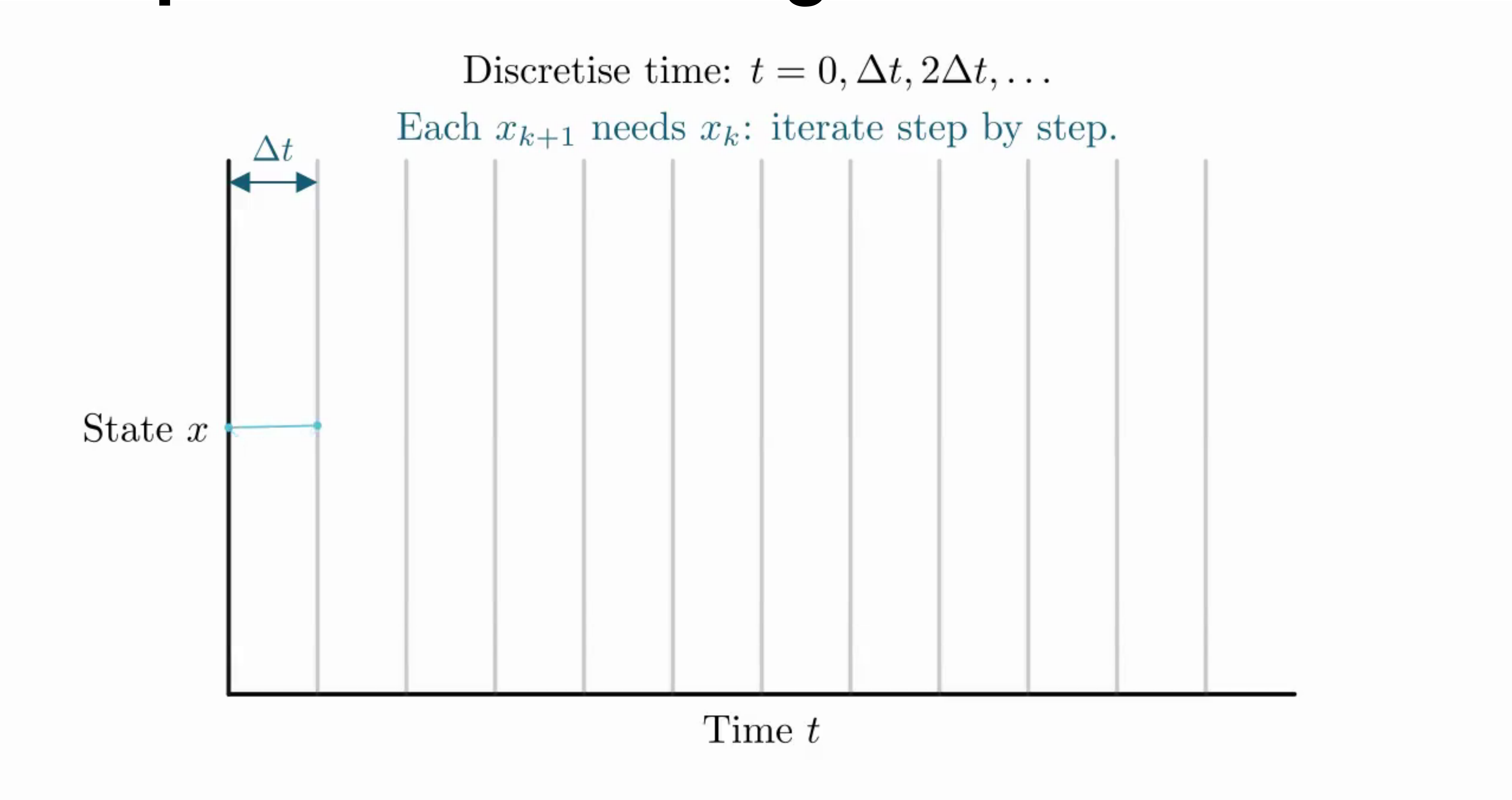

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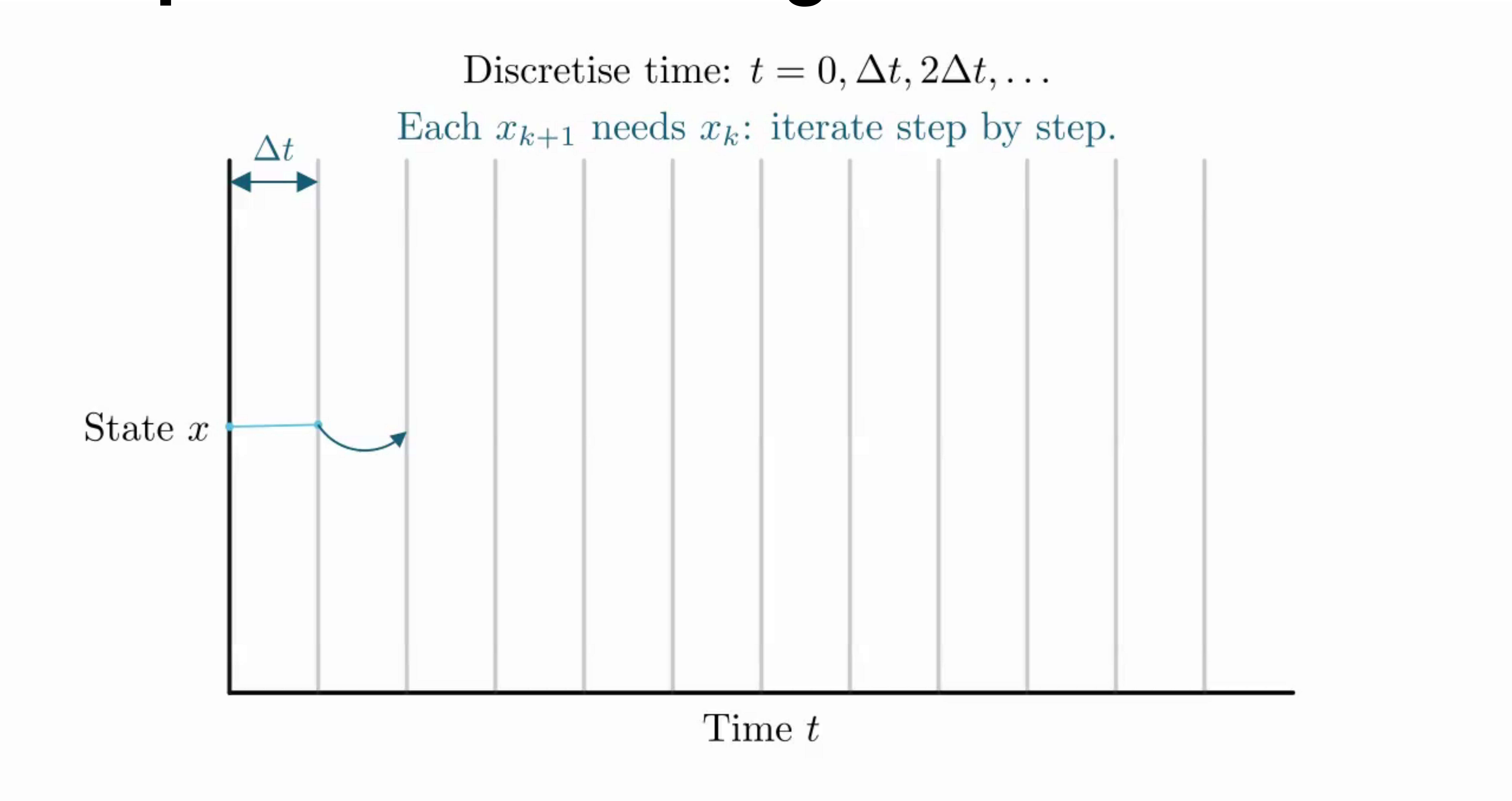
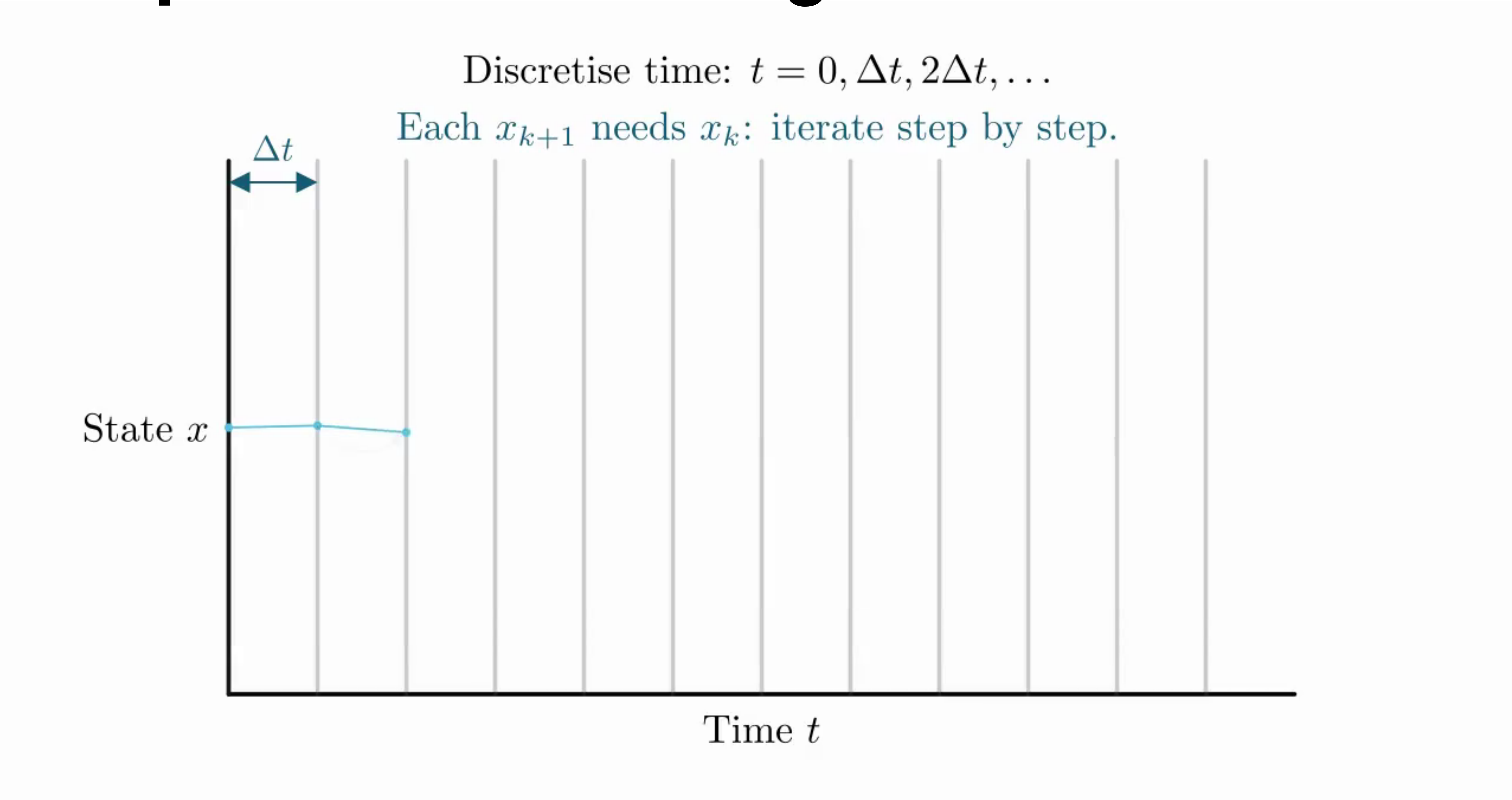
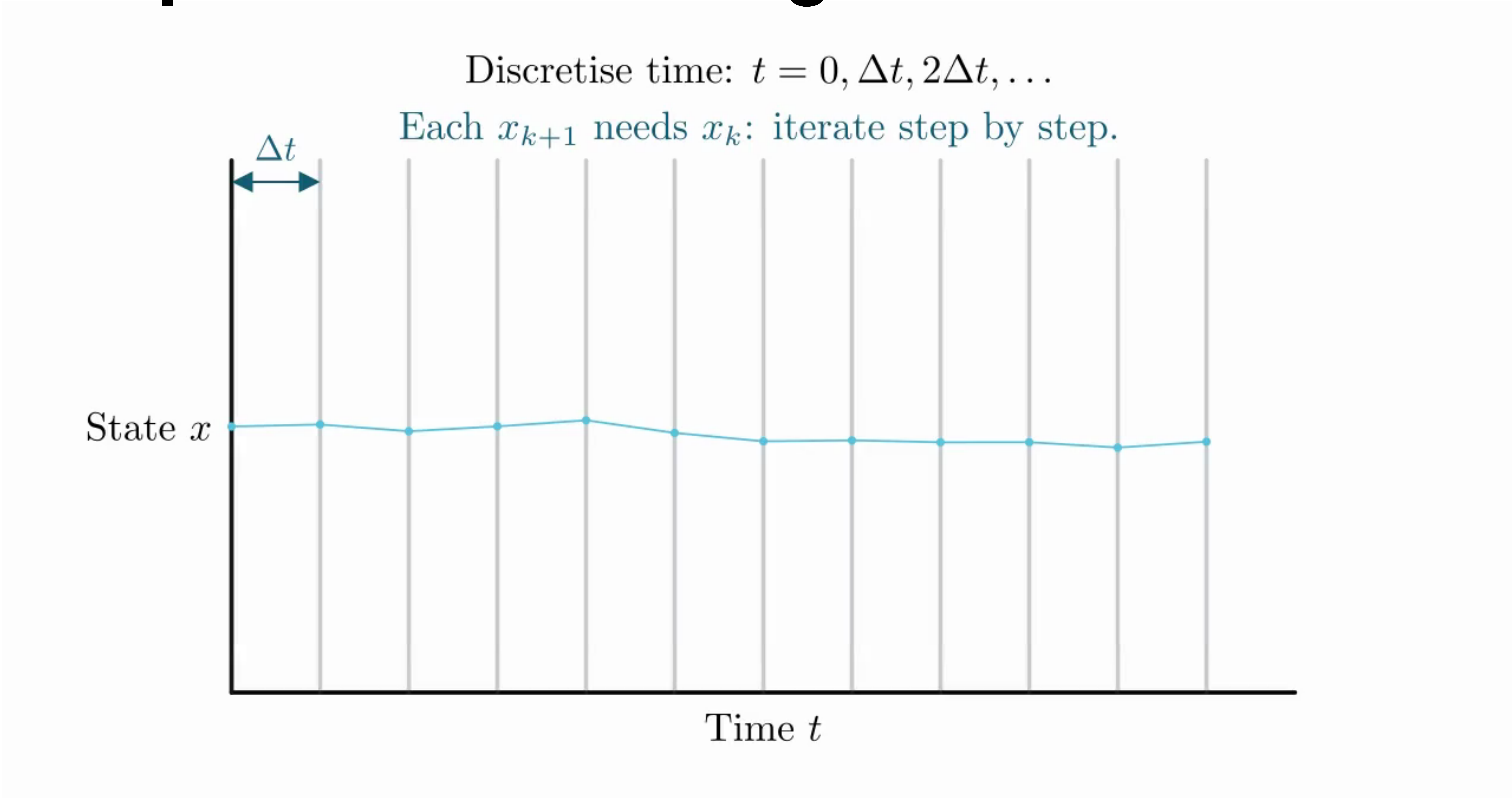


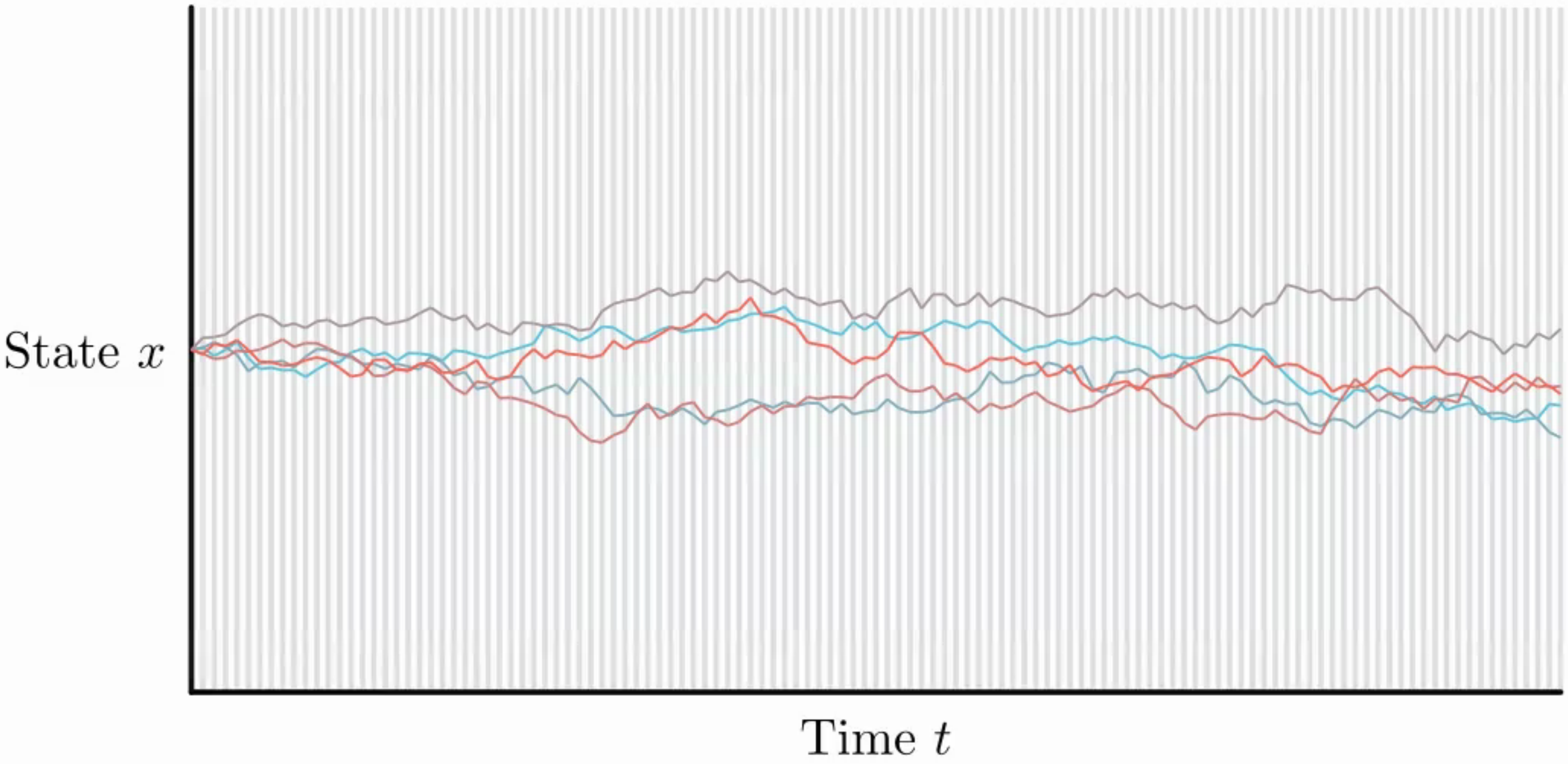
Computational Challenges of Neural SDEs



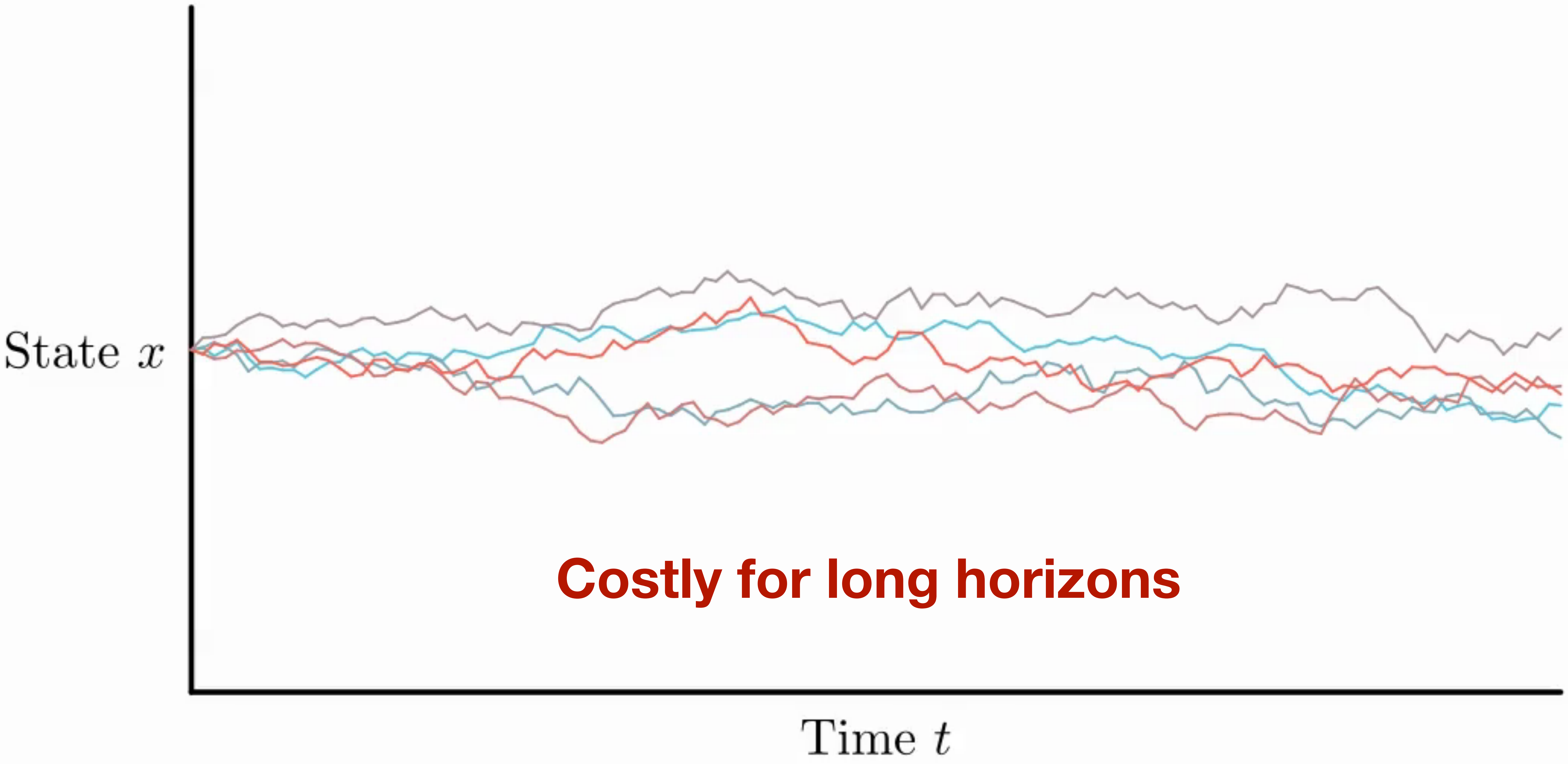
Computational Challenges of Neural SDEs



Computational Challenges of Neural SDEs



Computational Challenges of Neural SDEs



Strong Solution and Weak Solution of the SDEs

$$\text{Itô SDE:} \quad dx_t = \mu(x_t, t)\, dt + \sigma(x_t, t)\, dW_t, \quad x_0 \sim p_0$$

Strong solution

A solution x_t defined on a given probability space with a given Brownian motion. You do not change the noise; x_t must adapt to the fixed W_t.

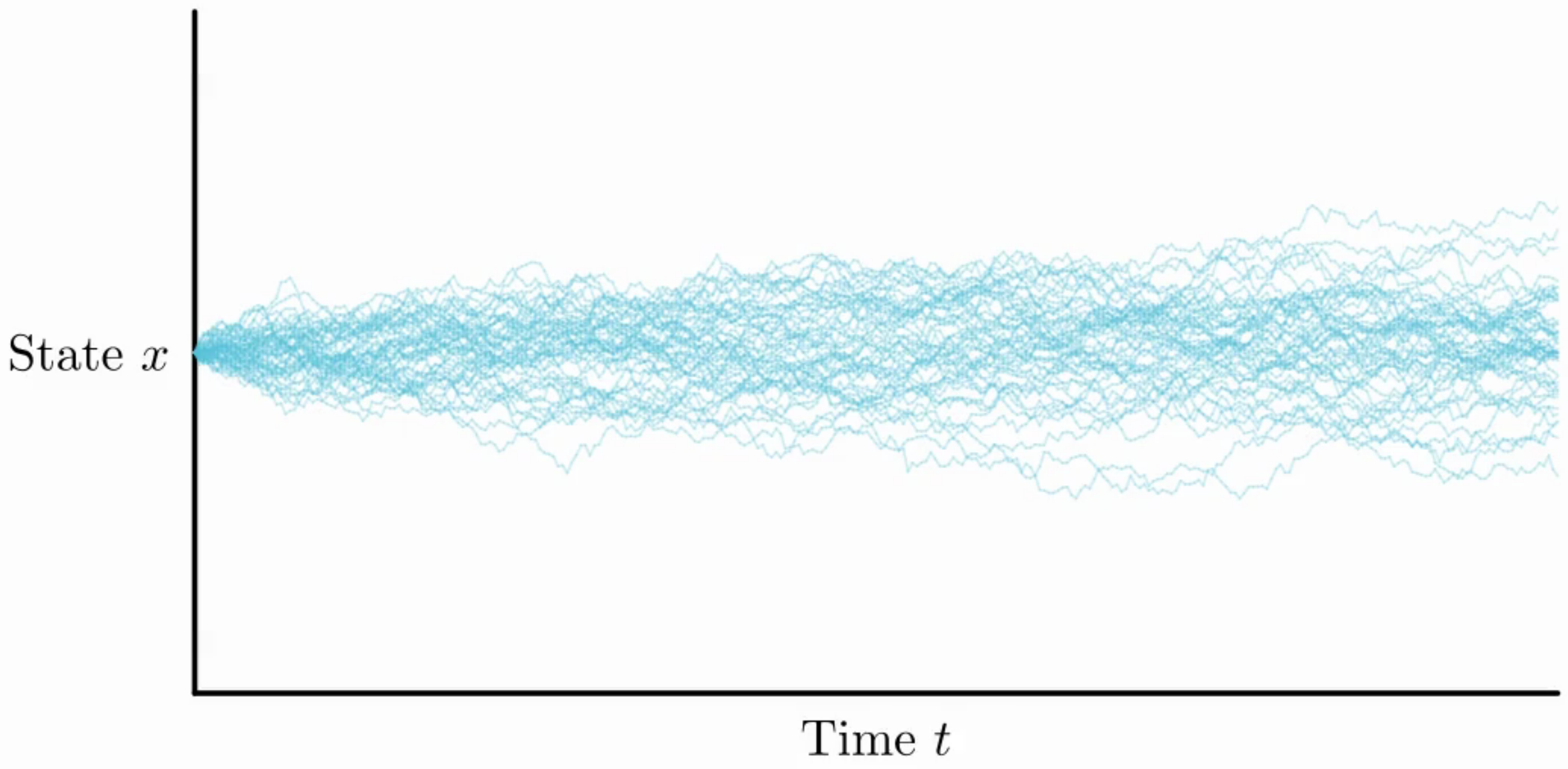
- Neural SDE: model sample paths w.r.t. a fixed Brownian motion.

Weak solution

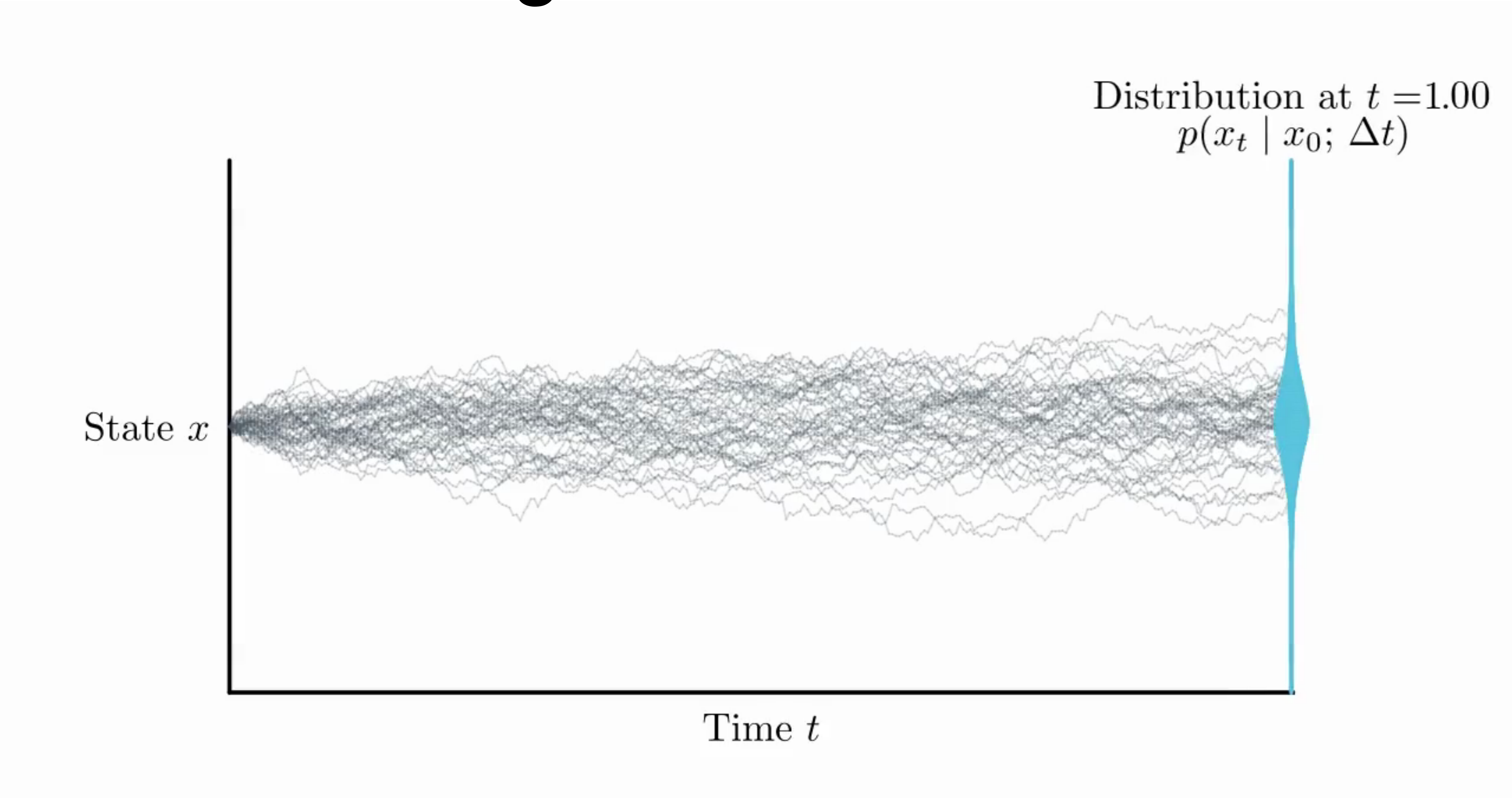
A solution x_t where the probability space and the Brownian motion are part of what you can choose. You only require that x_t and some Brownian motion satisfy the SDE and have the correct distribution.

- **Our idea: SDE as a Markov model—characterised by the transition law $p(x_t \mid x_s)$.**

Direct Modelling of Transition Distributions



Direct Modelling of Transition Distributions



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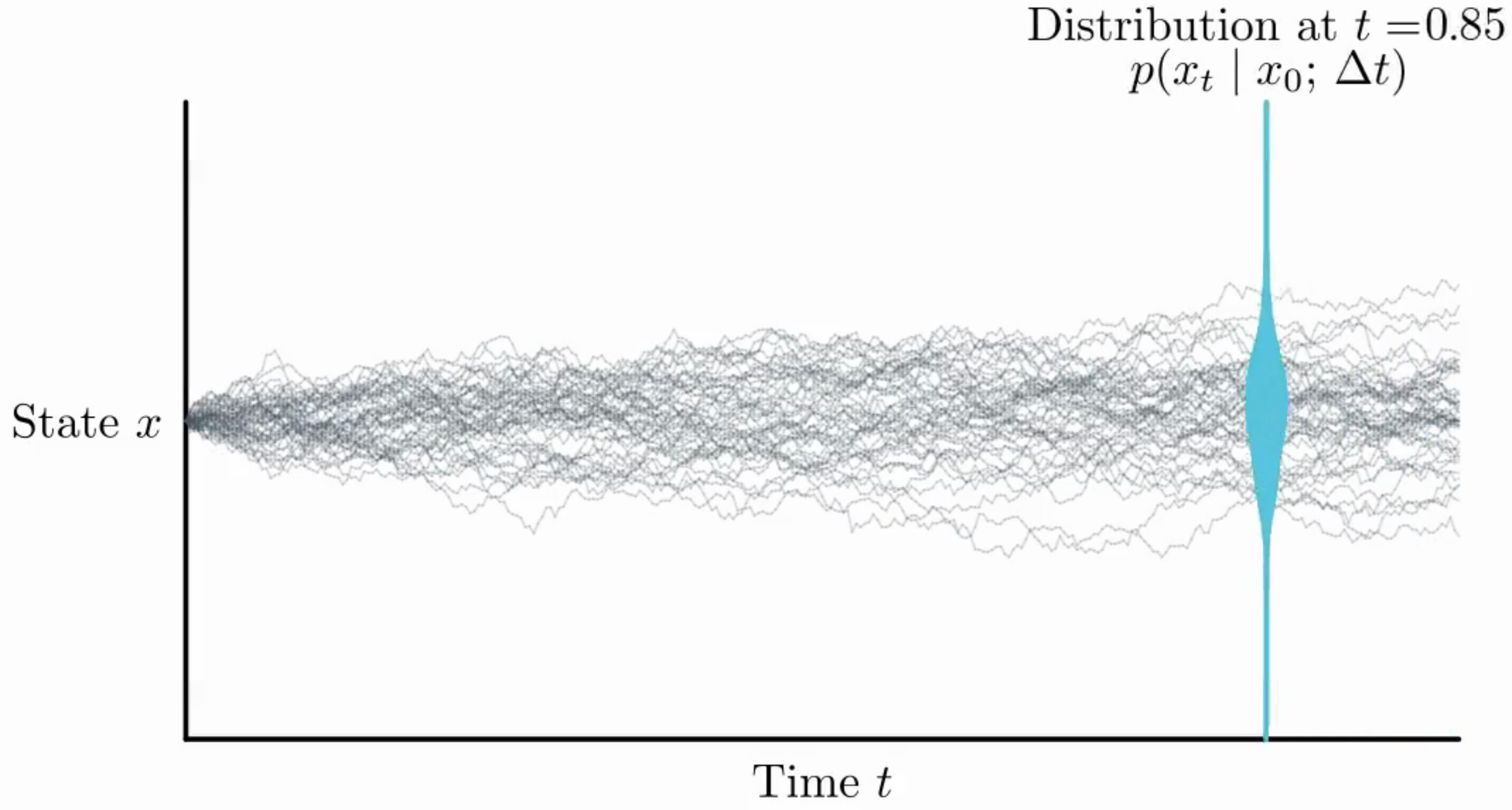
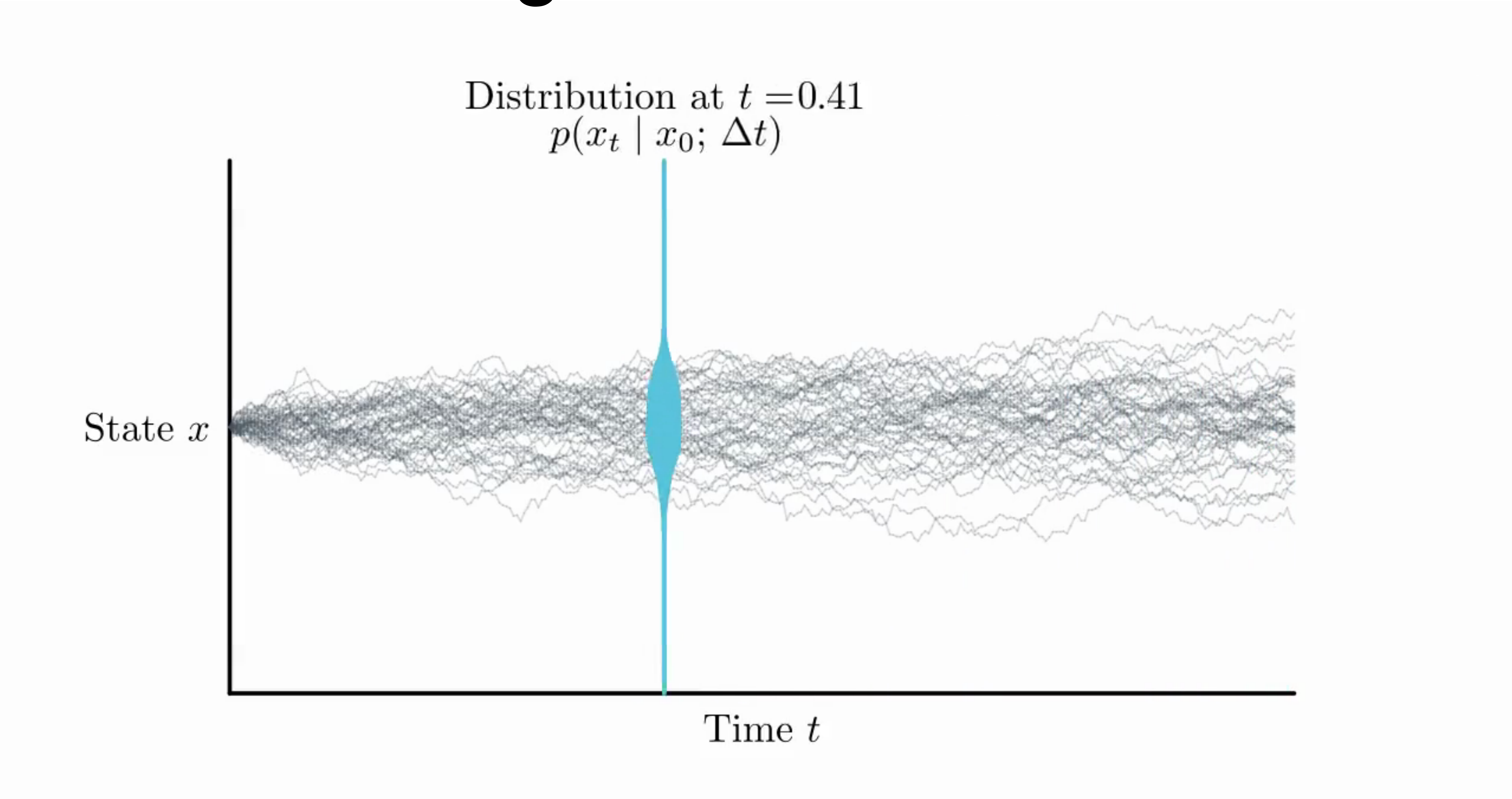


Direct Modelling of Transition Distributions



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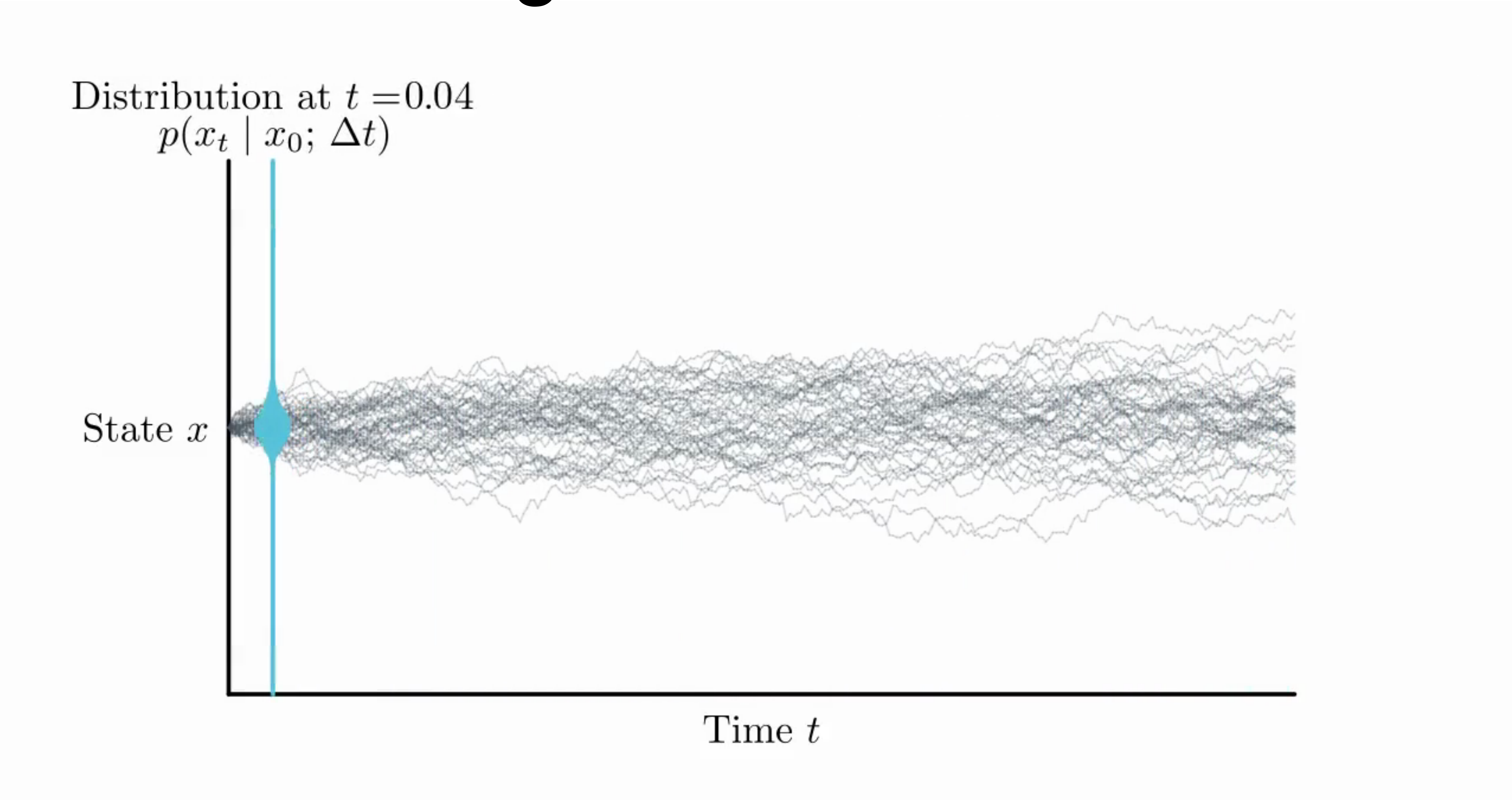

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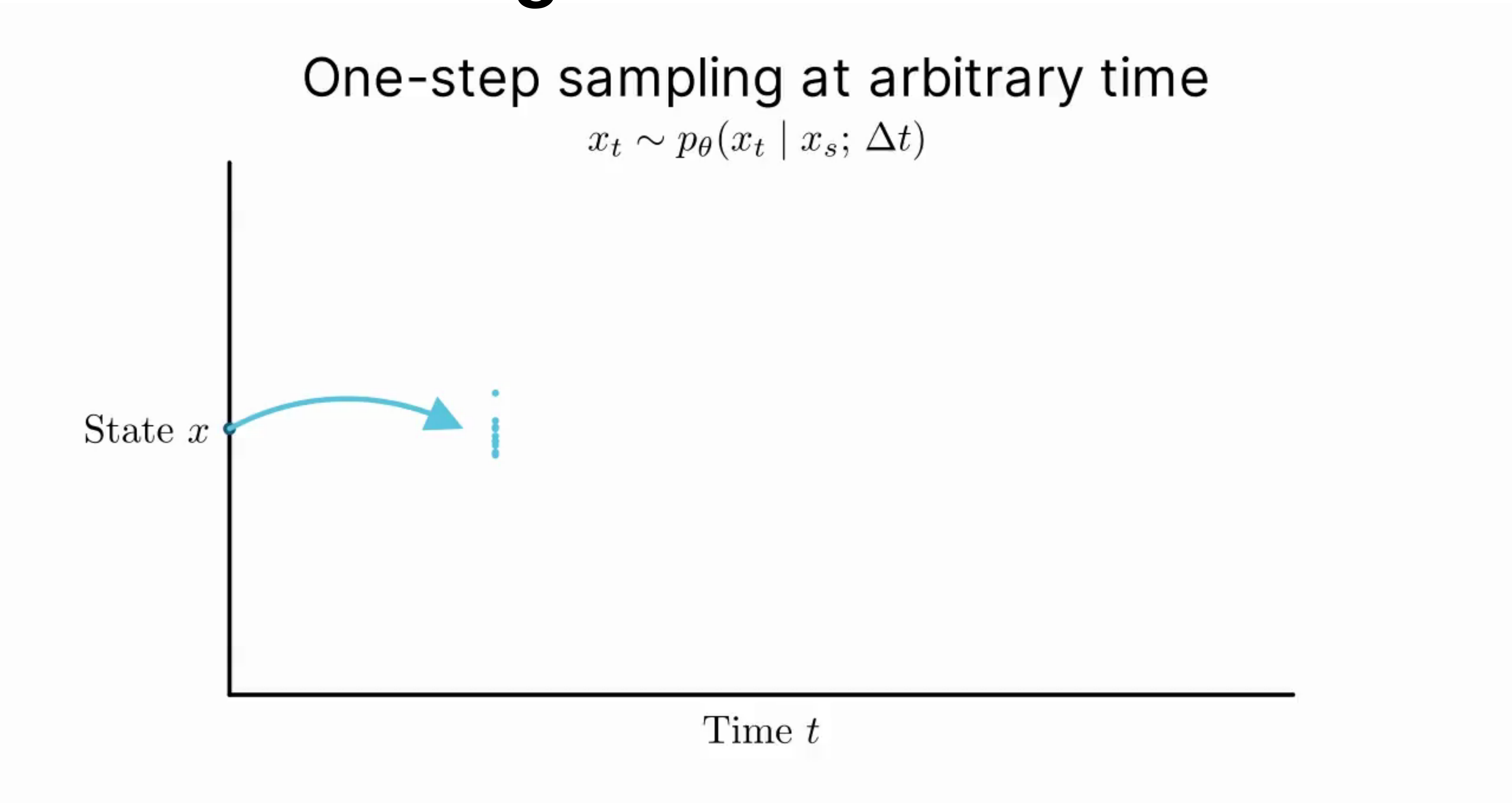

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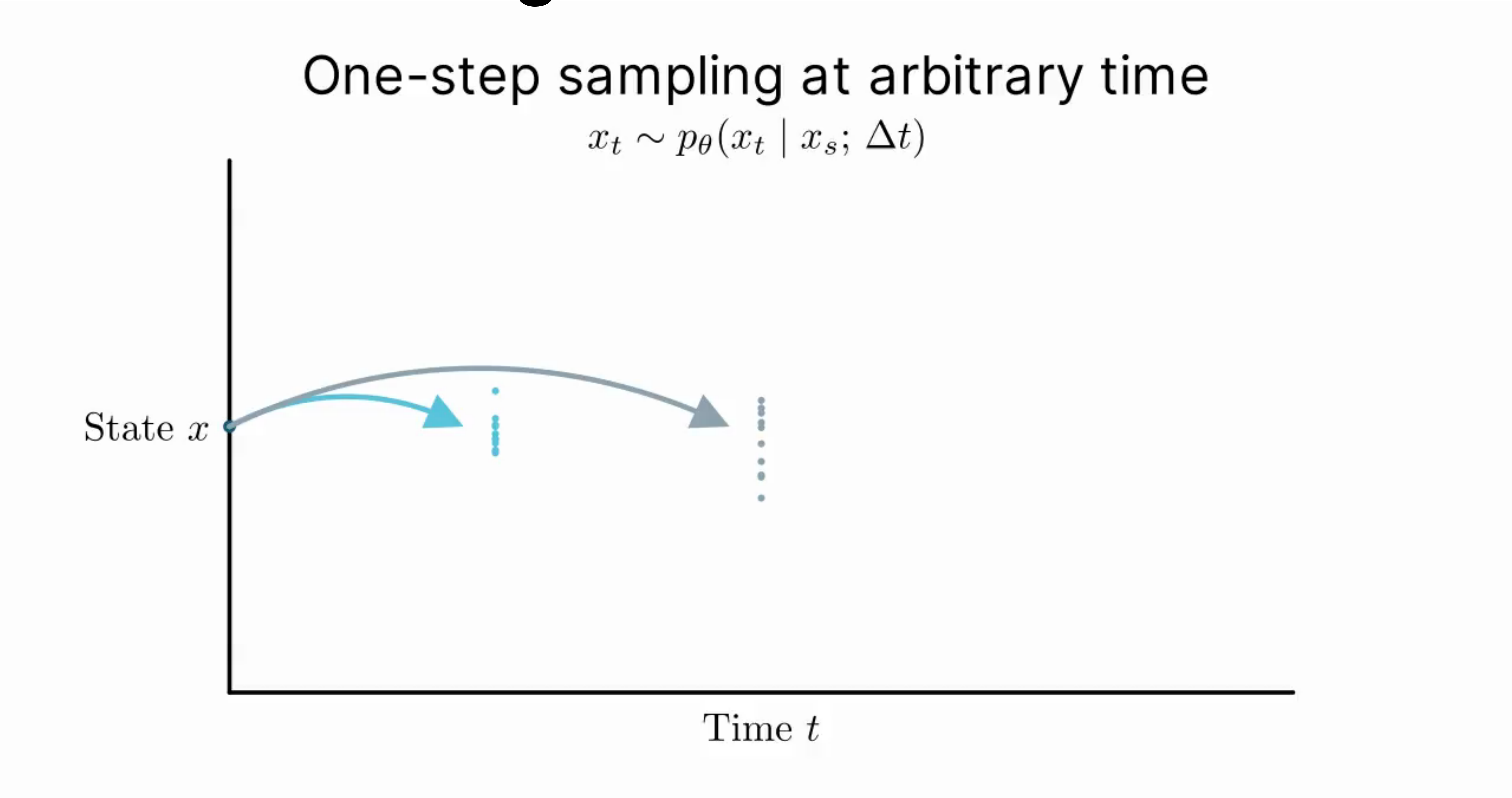

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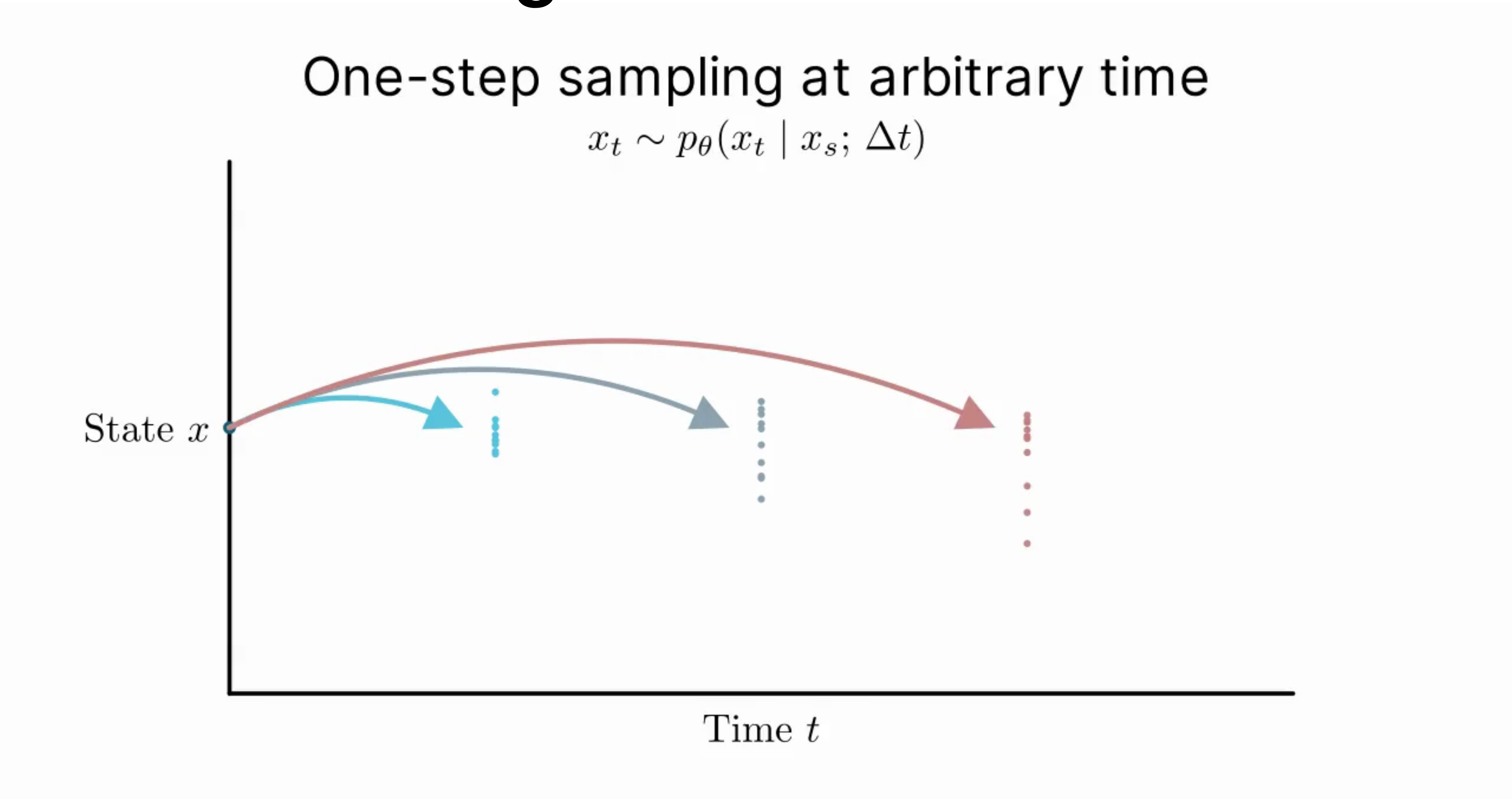

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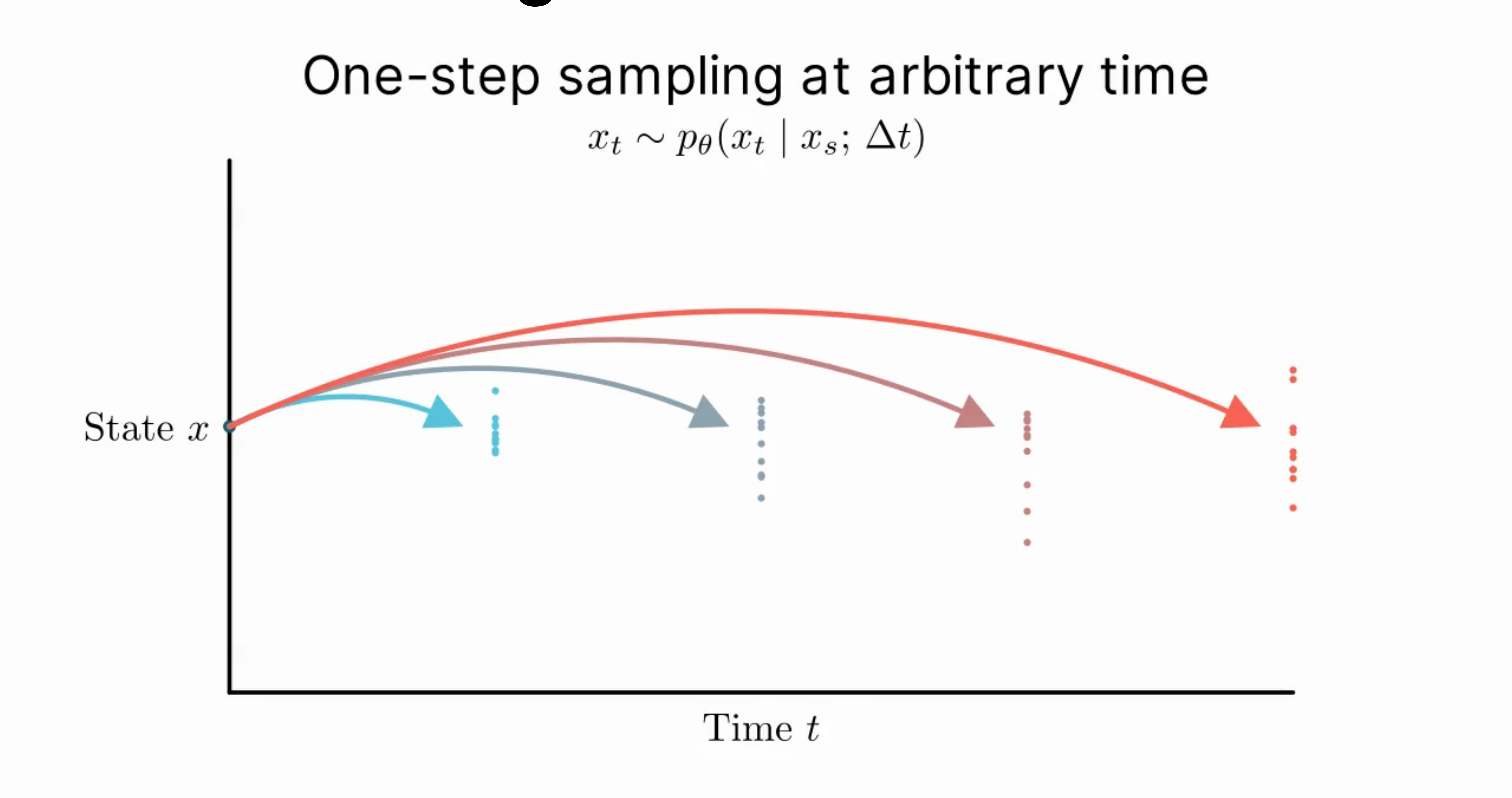

Mathematical Requirements for the Transition Kernel

Properties of $p_{\boldsymbol{\theta}}(\boldsymbol{x}_t \mid \boldsymbol{x}_s; s, \Delta t = t - s)$

1. **Independence.**

   For any $0 \leq t_1 \leq \cdots \leq t_n$, $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_{k+1}} \mid \boldsymbol{x}_{t_k}; t_k, t_{k+1} - t_k)$ are independent.

2. **Identity.**

   When $t = s$, $p_{\boldsymbol{\theta}}(\boldsymbol{x}_t \mid \boldsymbol{x}_s; s, 0) = \delta(\boldsymbol{x}_t - \boldsymbol{x}_s)$

3. **Flow property.**

   For any $0 \leq t_i \leq t_j \leq t_k$, $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_k} \mid \boldsymbol{x}_{t_i}; t_i, t_k - t_i) = \int p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_k} \mid \boldsymbol{x}_{t_j}; t_j, t_k - t_j)\, p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_j} \mid \boldsymbol{x}_{t_i}; t_i, t_j - t_i)\, \mathrm{d}\boldsymbol{x}_{t_j}$

4. **Stationarity (for autonomous SDEs).**

   $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_j} \mid \boldsymbol{x}_s; t_i, t_j - t_i) = p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_j + r} \mid \boldsymbol{x}_s; t_i + r, t_j - t_i)$

Mathematical Requirements for the Transition Kernel

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Architectural Design

Conditional normalising flow for $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_j} \mid \boldsymbol{x}_{t_i}; t_i, \Delta t)$

Base distribution

Using conditioning $\boldsymbol{c} := (\boldsymbol{x}_{t_i}, \Delta t, t_i)$,

$$\boldsymbol{z} = \boldsymbol{x}_{t_i} + \Delta t \cdot \mathrm{MLP}_{\mu}(\boldsymbol{c}; \boldsymbol{\theta}_{\mu}) + \sqrt{\Delta t} \cdot \mathrm{MLP}_{\sigma}(\boldsymbol{c}; \boldsymbol{\theta}_{\sigma}) \odot \boldsymbol{\varepsilon}, \quad \boldsymbol{\varepsilon} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$$

Conditional affine coupling layers [4, 13, 28]

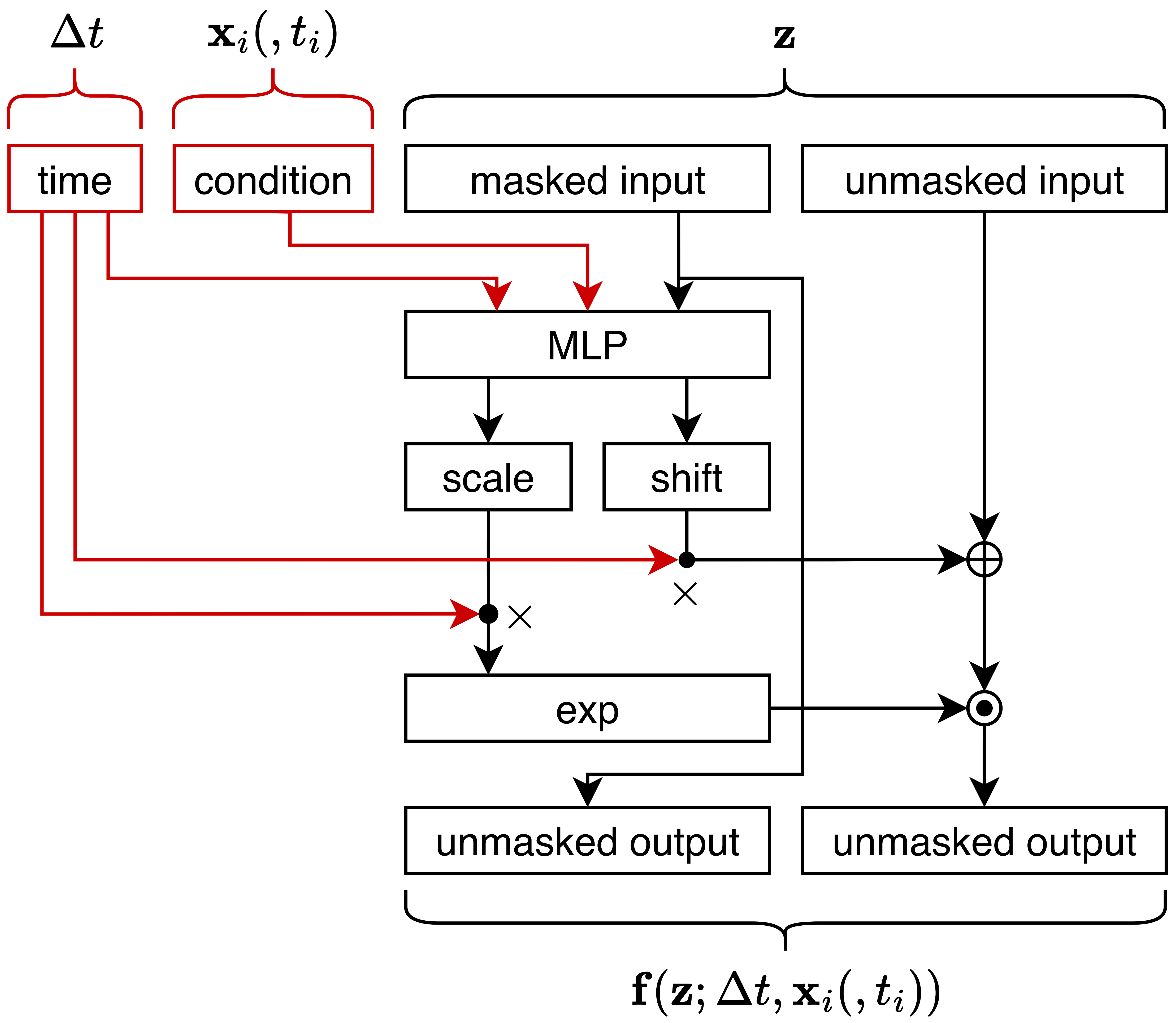
$$\boldsymbol{x}_{t_j} = \boldsymbol{f}_{\boldsymbol{\theta}}(\boldsymbol{z}, \boldsymbol{c}) = \boldsymbol{f}_L(\cdot; \boldsymbol{c}, \boldsymbol{\theta}_L) \circ \boldsymbol{f}_{L-1}(\cdot; \boldsymbol{c}, \boldsymbol{\theta}_{L-1}) \circ \cdots \circ \boldsymbol{f}_1(\boldsymbol{z}; \boldsymbol{c}, \boldsymbol{\theta}_1)$$

With $\boldsymbol{z}_{\mathrm{A}}, \boldsymbol{z}_{\mathrm{B}} = \mathrm{Split}(\boldsymbol{z})$, each layer $\boldsymbol{f}$ is designed as:

$$\mathrm{Concat}\Big(\boldsymbol{z}_{\mathrm{A}}, \boldsymbol{z}_{\mathrm{B}} \odot \exp\big(\Delta t\, \mathrm{MLP}^{(i)}_{\mathrm{scale}}(\boldsymbol{z}_{\mathrm{A}}, \boldsymbol{c}; \boldsymbol{\theta}^{(i)}_{\mathrm{scale}})\big) + \Delta t\, \mathrm{MLP}^{(i)}_{\mathrm{shift}}(\boldsymbol{z}_{\mathrm{A}}, \boldsymbol{c}; \boldsymbol{\theta}^{(i)}_{\mathrm{shift}})\Big)$$

Architectural Design

Conditional affine coupling part for $p_\theta(\boldsymbol{x}_{t_j} \mid \boldsymbol{x}_{t_i}; t_i, \Delta t)$



Architectural Design

Conditional normalising flow for $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_j} \mid \boldsymbol{x}_{t_i}; t_i, \Delta t)$

Base distribution

Using conditioning $\boldsymbol{c} := (\boldsymbol{x}_{t_i}, \Delta t, t_i)$,

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✓ **Identity when $\Delta t = 0$.** ✓ **Stationary when we drop t_i from $\boldsymbol{c}$.**

Mathematical Requirements for the Transition Kernel

Properties of $p_{\boldsymbol{\theta}}(\boldsymbol{x}_t \mid \boldsymbol{x}_s; s, \Delta t = t - s)$

1. **Independence.** **✓ Realised by non-overlapping sampling.**

   For any $0 \leq t_1 \leq \cdots \leq t_n$, $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_{k+1}} \mid \boldsymbol{x}_{t_k}; t_k, t_{k+1} - t_k)$ are independent.

2. **Identity.** **✓ Realised by architecture.**

   When $t = s$, $p_{\boldsymbol{\theta}}(\boldsymbol{x}_t \mid \boldsymbol{x}_s; s, 0) = \delta(\boldsymbol{x}_t - \boldsymbol{x}_s)$

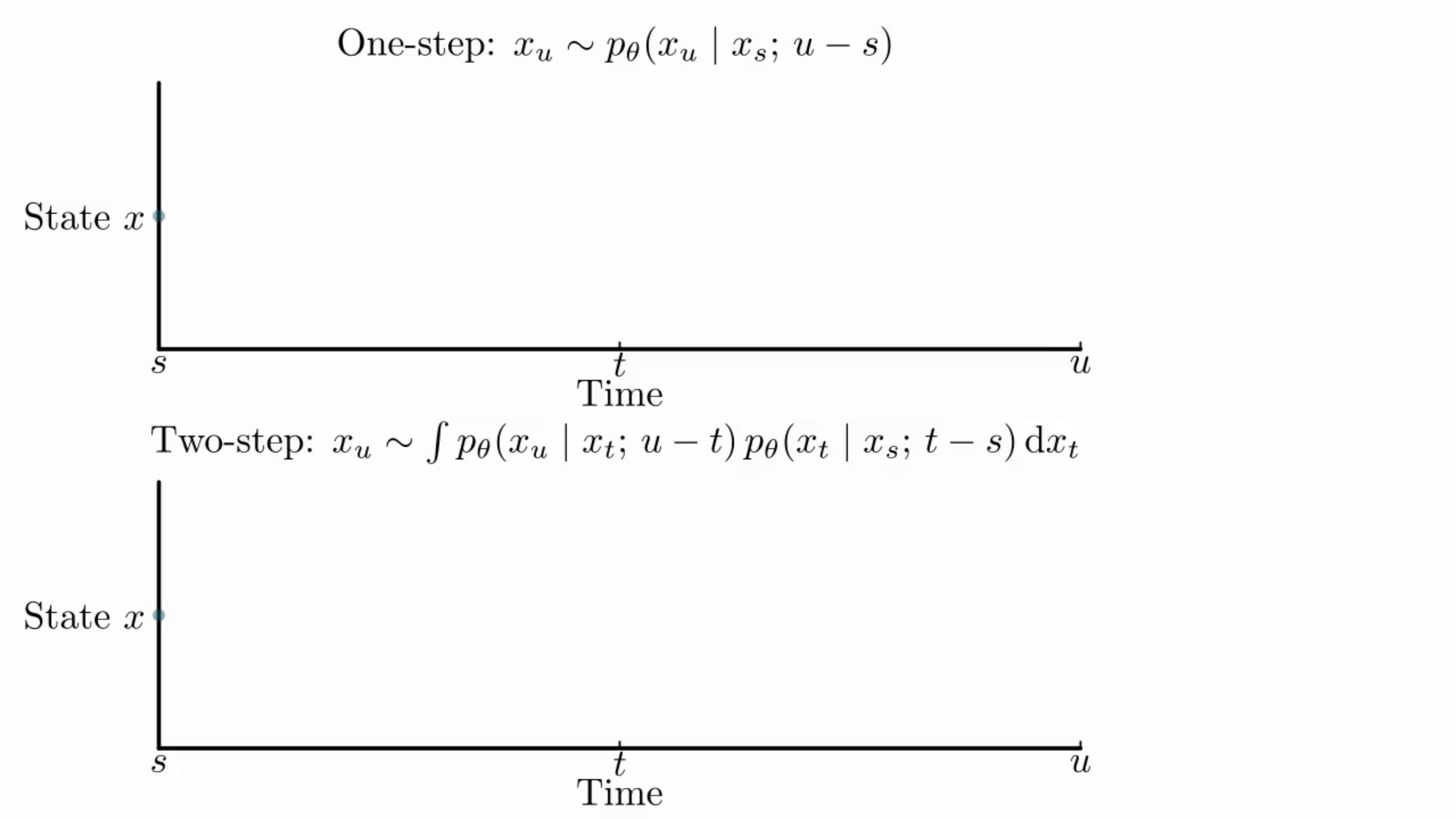
3. **Flow property.**

   For any $0 \leq t_i \leq t_j \leq t_k$, $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_k} \mid \boldsymbol{x}_{t_i}; t_i, t_k - t_i) = \int p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_k} \mid \boldsymbol{x}_{t_j}; t_j, t_k - t_j)\, p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_j} \mid \boldsymbol{x}_{t_i}; t_i, t_j - t_i)\, \mathrm{d}\boldsymbol{x}_{t_j}$

4. **Stationarity (for autonomous SDEs).** **✓ Realised by architecture optionally.**

   $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_j} \mid \boldsymbol{x}_s; t_i, t_j - t_i) = p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_j+r} \mid \boldsymbol{x}_s; t_i + r, t_j - t_i)$

Regularisation for Flow Consistency



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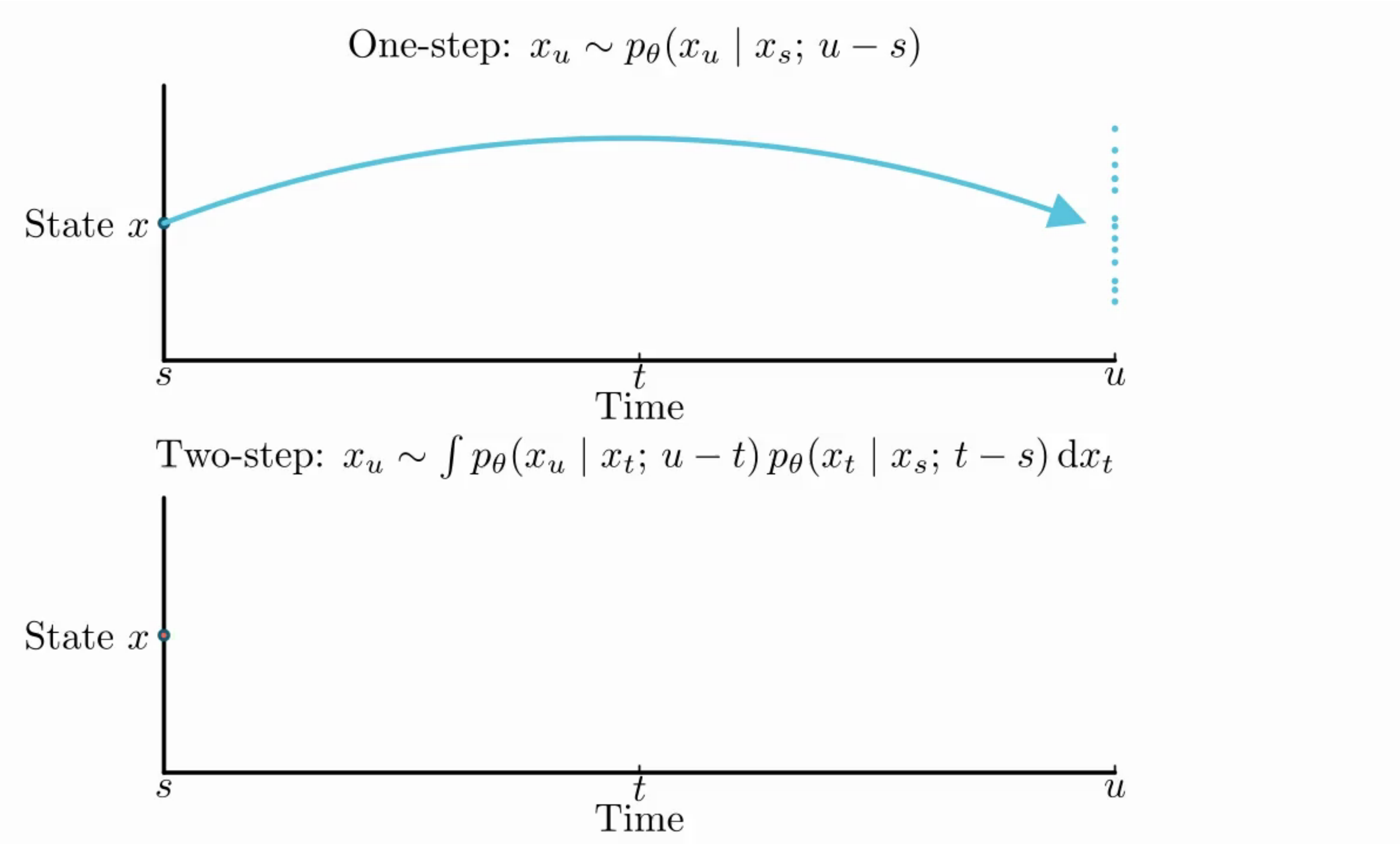

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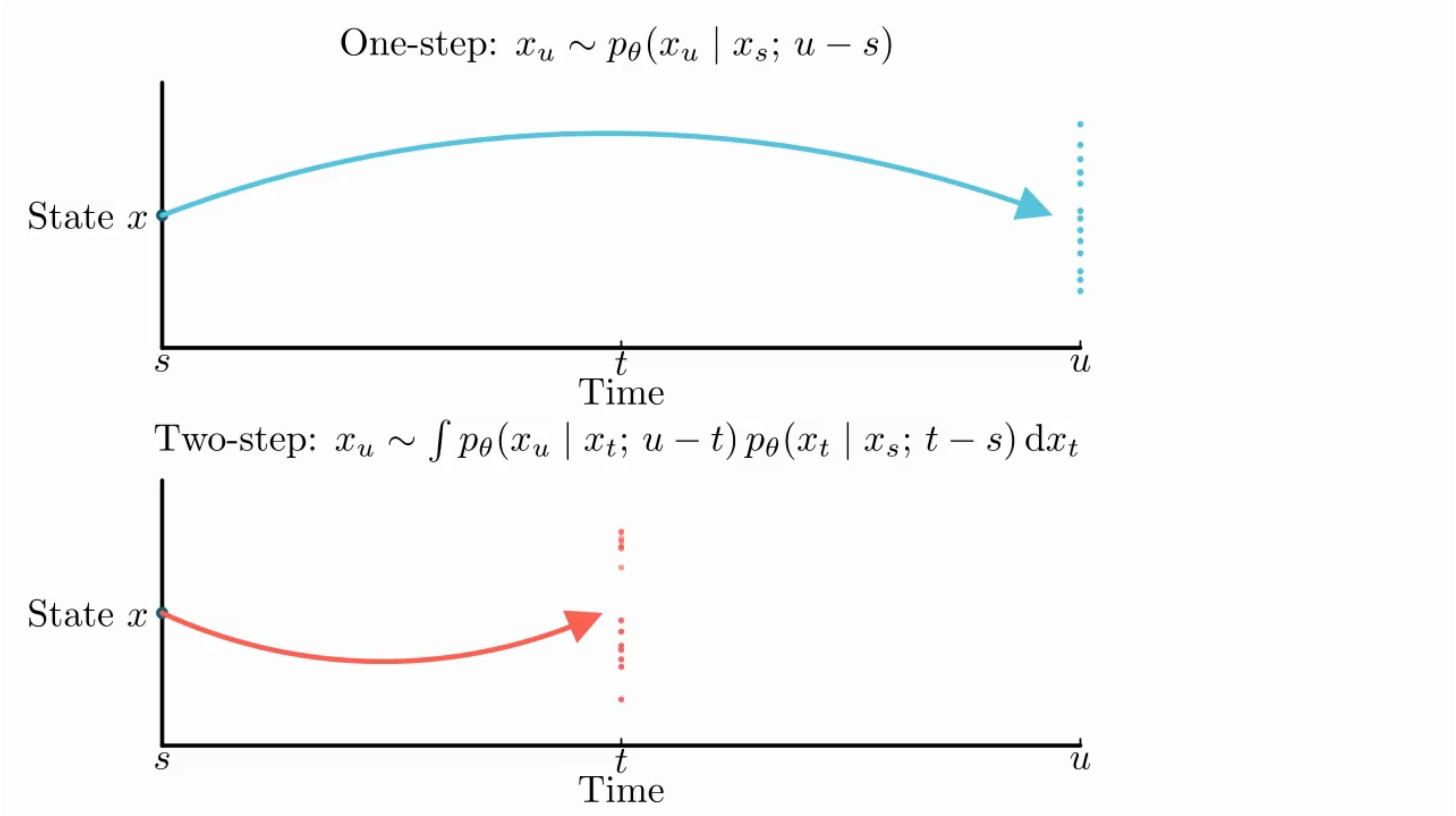

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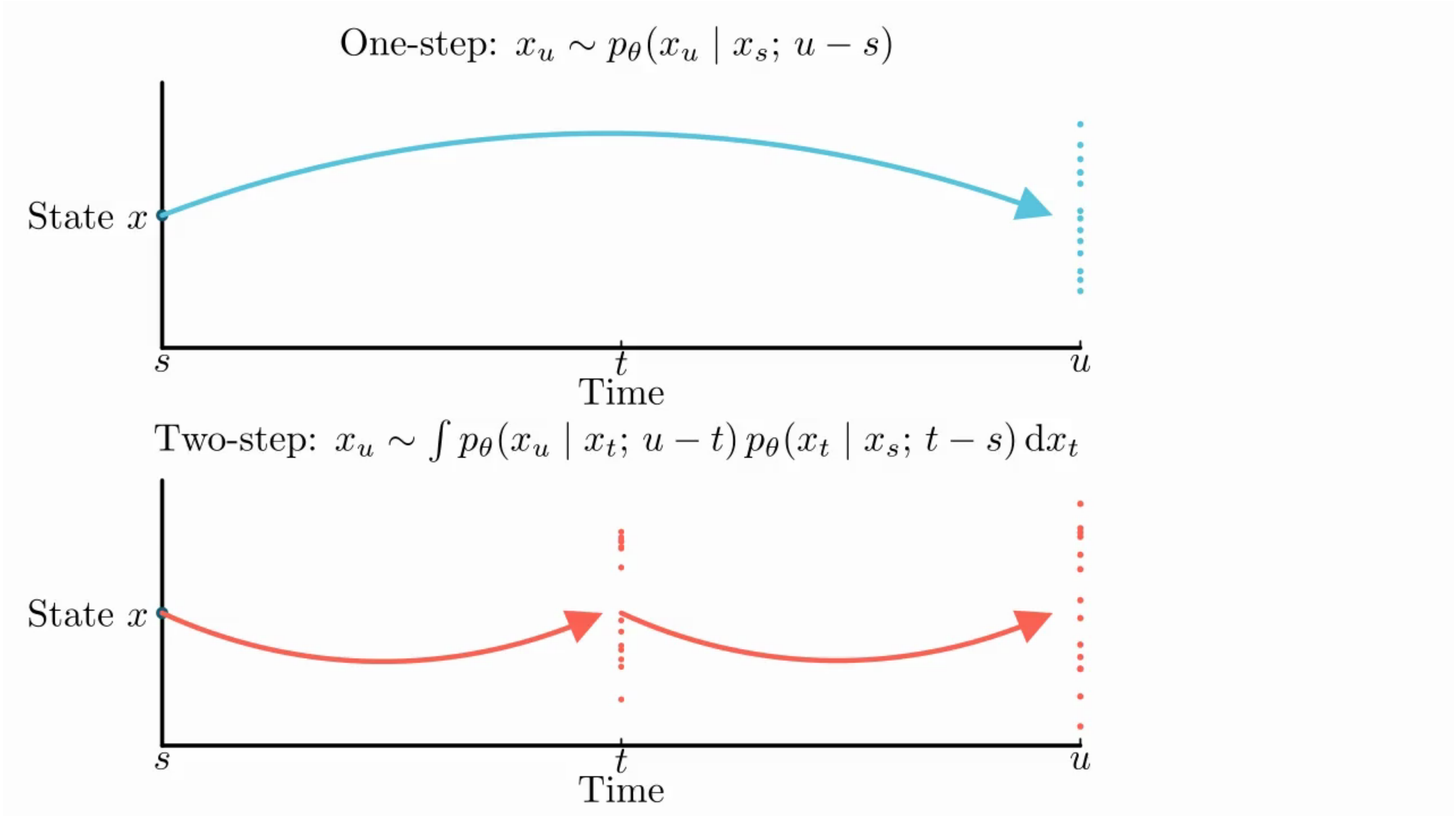

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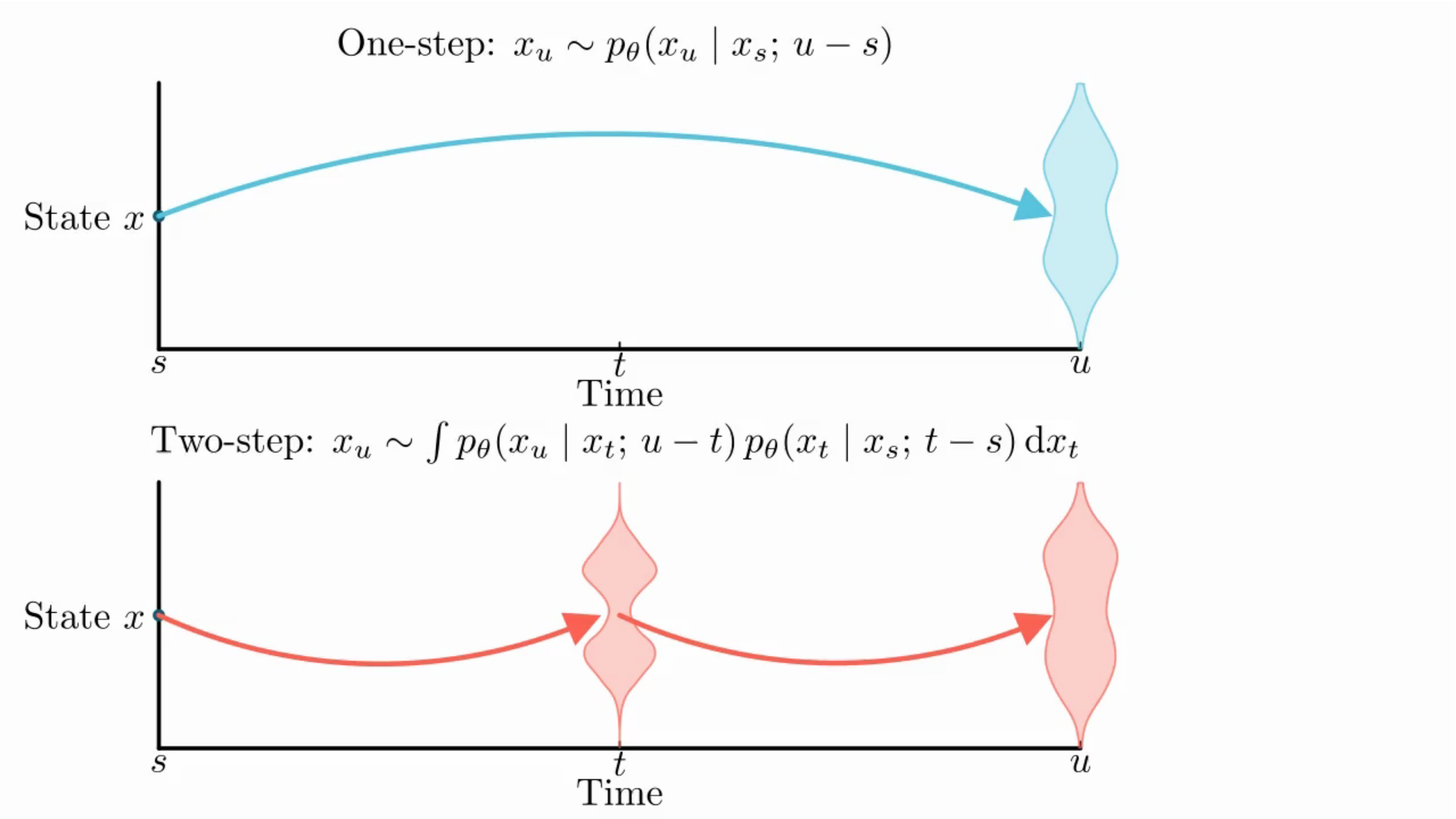
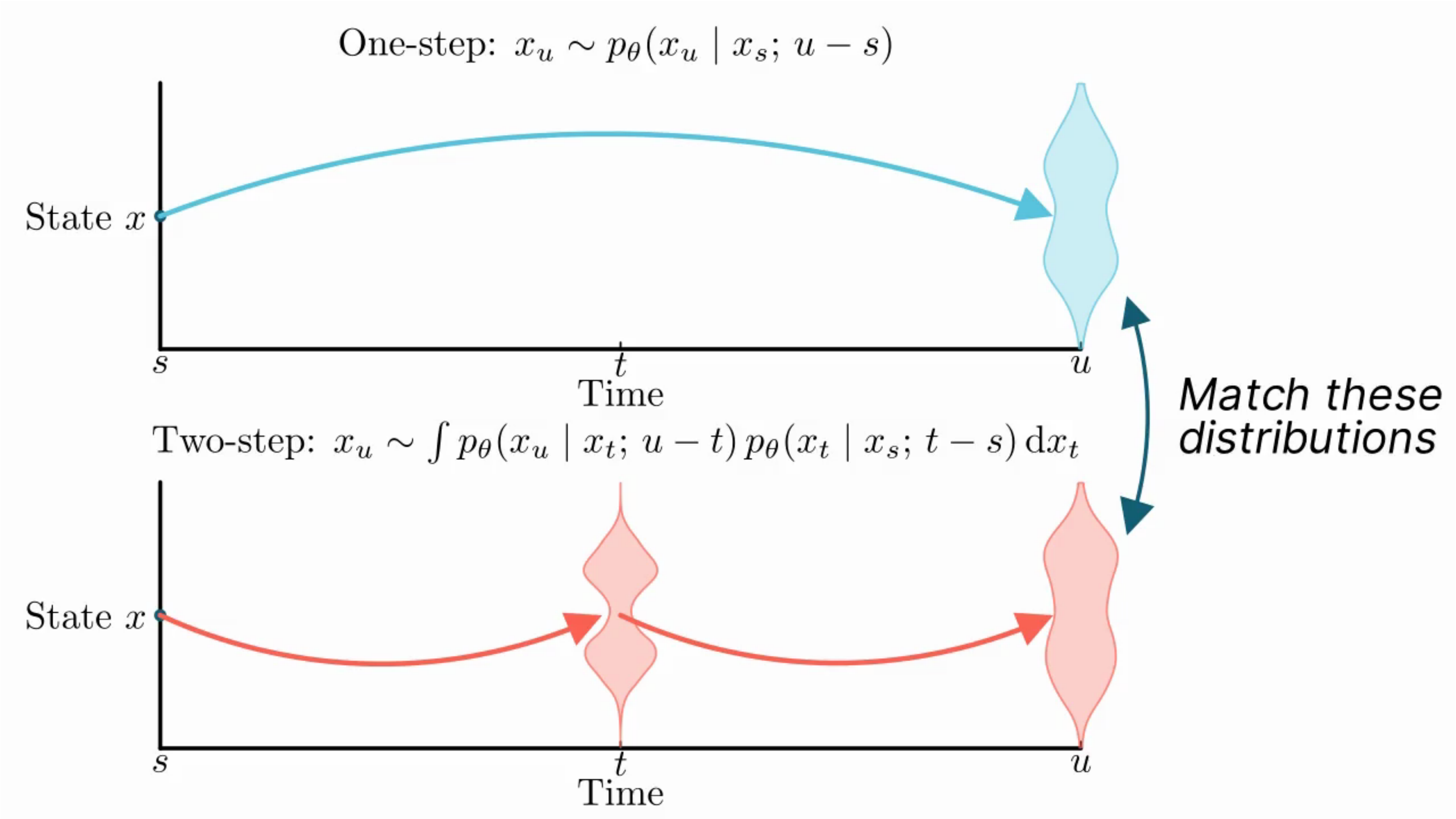


Regularisation for Flow Consistency



Regularisation for Flow Consistency

$$\mathcal{L}_{\text{flow}} \; = D\left[p_{\boldsymbol{\theta}}^{1}\left(\mathbf{x}_{t_k} \mid \mathbf{x}_{t_i}\right), \int p_{\boldsymbol{\theta}}^{2}\left(\mathbf{x}_{t_k} \mid \mathbf{x}_{t_j}\right) p_{\boldsymbol{\theta}}^{2}\left(\mathbf{x}_{t_j} \mid \mathbf{x}_{t_i}\right) d\mathbf{x}_{t_j}\right]$$

Challenges in computing the flow loss

- The marginalisation is generally intractable
  → **Direct access to the marginalised density is not available**
- Naive Monte Carlo estimation would require many samples

We derive the upper bounds for KL divergences

Regularisation for Flow Consistency

Upper bounds for KL divergences

1-step → 2-step KL divergence

$$D_{\mathrm{KL}}\left(p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_k} \mid \boldsymbol{x}_{t_i}) \,\middle\|\, \int p_{\boldsymbol{\theta}}\left(\boldsymbol{x}_{t_k} \mid \boldsymbol{x}_{t_j}\right) p_{\boldsymbol{\theta}}\left(\boldsymbol{x}_{t_j} \mid \boldsymbol{x}_{t_i}\right) \mathrm{d}\boldsymbol{x}_{t_j}\right)$$

$$\leq \mathbb{E}_{\boldsymbol{x}_{t_k} \sim p_{\boldsymbol{\theta}}(\cdot \mid \boldsymbol{x}_{t_i})}\left[\mathbb{E}_{\boldsymbol{x}_{t_j} \sim b_{\boldsymbol{\xi}}(\cdot \mid \boldsymbol{x}_{t_i}, \boldsymbol{x}_{t_k})}\left[\log\left(\frac{p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_k} \mid \boldsymbol{x}_{t_i})\, b_{\boldsymbol{\xi}}\left(\boldsymbol{x}_{t_j} \mid \boldsymbol{x}_{t_i}, \boldsymbol{x}_{t_k}\right)}{p_{\boldsymbol{\theta}}\left(\boldsymbol{x}_{t_k} \mid \boldsymbol{x}_{t_j}\right) p_{\boldsymbol{\theta}}\left(\boldsymbol{x}_{t_j} \mid \boldsymbol{x}_{t_i}\right)}\right)\right]\right] =: \mathcal{L}_{\text{flow, 1-to-2}}(\boldsymbol{\theta}, \boldsymbol{\xi}; t_i, t_j, t_k)\,.$$

2-step → 1-step KL divergence

$$D_{\mathrm{KL}}\left(\int p_{\boldsymbol{\theta}}\left(\boldsymbol{x}_{t_k} \mid \boldsymbol{x}_{t_j}\right) p_{\boldsymbol{\theta}}\left(\boldsymbol{x}_{t_j} \mid \boldsymbol{x}_{t_i}\right) \mathrm{d}\boldsymbol{x}_{t_j} \,\middle\|\, p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_k} \mid \boldsymbol{x}_{t_i})\right)$$

$$\leq \mathbb{E}_{\boldsymbol{x}_{t_j} \sim p_{\boldsymbol{\theta}}(\cdot \mid \boldsymbol{x}_{t_i})}\left[\mathbb{E}_{\boldsymbol{x}_{t_k} \sim p_{\boldsymbol{\theta}}(\cdot \mid \boldsymbol{x}_{t_j})}\left[\log\left(\frac{p_{\boldsymbol{\theta}}\left(\boldsymbol{x}_{t_j} \mid \boldsymbol{x}_{t_i}\right) p_{\boldsymbol{\theta}}\left(\boldsymbol{x}_{t_k} \mid \boldsymbol{x}_{t_j}\right)}{b_{\boldsymbol{\xi}}\left(\boldsymbol{x}_{t_j} \mid \boldsymbol{x}_{t_i}, \boldsymbol{x}_{t_k}\right) p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_k} \mid \boldsymbol{x}_{t_i})}\right)\right]\right] =: \mathcal{L}_{\text{flow, 2-to-1}}(\boldsymbol{\theta}, \boldsymbol{\xi}; t_i, t_j, t_k)\,.$$

$$\mathcal{L}_{\text{flow}}(\boldsymbol{\theta}, \boldsymbol{\xi}) := \mathop{\mathbb{E}}_{p(t_i, t_j, t_k)}\left[\mathcal{L}_{\text{flow, 1-to-2}}(\boldsymbol{\theta}, \boldsymbol{\xi}; t_i, t_j, t_k) + \mathcal{L}_{\text{flow, 2-to-1}}(\boldsymbol{\theta}, \boldsymbol{\xi}; t_i, t_j, t_k)\right]$$

Mathematical Requirements for the Transition Kernel

Properties of $p_{\boldsymbol{\theta}}(\boldsymbol{x}_t \mid \boldsymbol{x}_s; s, \Delta t = t - s)$

1. **Independence.** **✓ Realised by non-overlapping sampling.**

   For any $0 \leq t_1 \leq \cdots \leq t_n$, $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_{k+1}} \mid \boldsymbol{x}_{t_k}; t_k, t_{k+1} - t_k)$ are independent.

2. **Identity.** **✓ Realised by architecture.**

   When $t = s$, $p_{\boldsymbol{\theta}}(\boldsymbol{x}_t \mid \boldsymbol{x}_s; s, 0) = \delta(\boldsymbol{x}_t - \boldsymbol{x}_s)$

3. **Flow property.** **✓ Approximately realised by flow loss.**

   For any $0 \leq t_i \leq t_j \leq t_k$, $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_k} \mid \boldsymbol{x}_{t_i}; t_i, t_k - t_i) = \int p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_k} \mid \boldsymbol{x}_{t_j}; t_j, t_k - t_j)\, p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_j} \mid \boldsymbol{x}_{t_i}; t_i, t_j - t_i)\, \mathrm{d}\boldsymbol{x}_{t_j}$

4. **Stationarity (for autonomous SDEs).** **✓ Realised by architecture optionally.**

   $p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_j} \mid \boldsymbol{x}_s; t_i, t_j - t_i) = p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_j + r} \mid \boldsymbol{x}_s; t_i + r, t_j - t_i)$

Training Objective

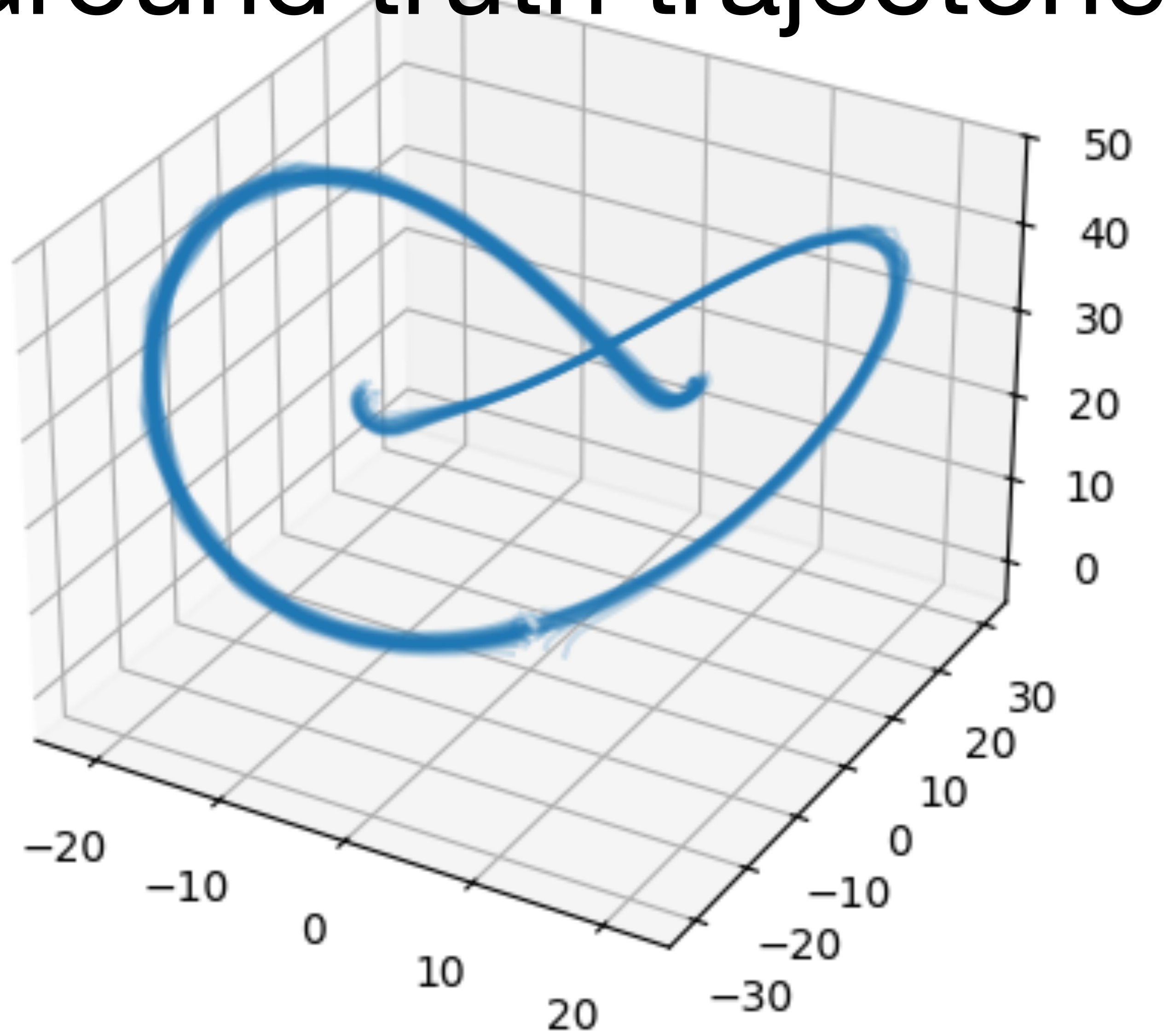
$$\mathcal{L} = \mathop{\mathbb{E}}_{\boldsymbol{x}_{t_j}, \boldsymbol{x}_{t_i} \sim \mathcal{D}} \left[\log p_{\boldsymbol{\theta}}(\boldsymbol{x}_{t_j} \mid \boldsymbol{x}_{t_i}) \right] + \lambda \mathcal{L}_{\text{flow}}(\boldsymbol{\theta}, \boldsymbol{\xi})$$

Negative log likelihood **Flow loss**

Experimental Configurations

Chaotic dynamics—Stochastic Lorenz Attractor

Ground truth trajectories



$$\mathrm{d}x = \sigma(y - x)\mathrm{d}t + \alpha_x \, \mathrm{d}W_1$$

$$\mathrm{d}y = (x(\rho - z) - y)\mathrm{d}t + \alpha_y \, \mathrm{d}W_2$$

$$\mathrm{d}z = (xy - \beta z)\mathrm{d}t + \alpha_z \, \mathrm{d}W_3$$

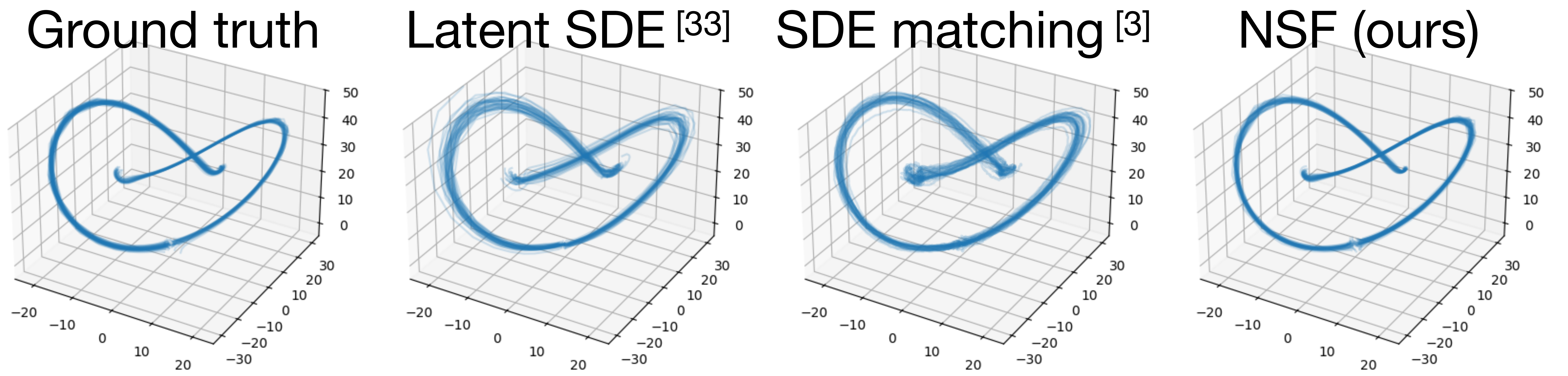
$$\sigma = 10, \rho = 28, \beta = 8/3, \alpha = (0.15, 0.15, 0.15)$$

$$\text{Initial state: } \mathcal{N}(0, I); \text{ Duration: } t \in [0, 1]$$

Trained on 1,024 trajectories, tested on 1,024 trajectories.

Experimental Results

With a comparable network size



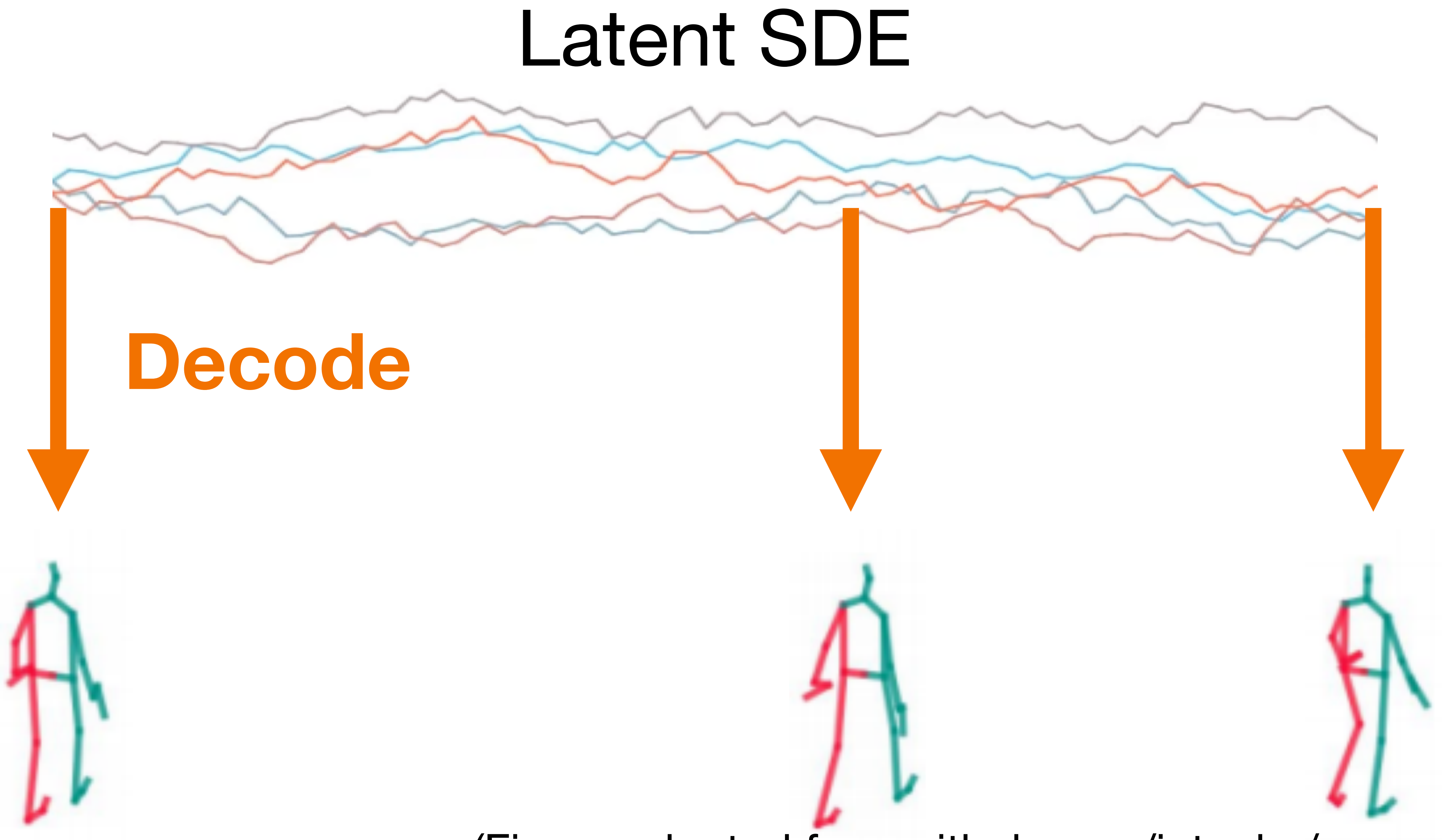
Method	t = 0.25		t = 0.5		t = 0.75		t = 1.0	
	KL ↓	kFLOPs ↓	KL ↓	kFLOPs ↓	KL ↓	kFLOPs ↓	KL ↓	kFLOPs ↓
Latent SDE [33]	2.1 ± 0.9	959	1.8 ± 0.1	1,917	0.9 ± 0.3	2,839	1.5 ± 0.5	3,760
SDE matching [3]	6.3 ± 0.4	1,917	11.7 ± 0.5	3,834	7.9 ± 0.3	5,677	6.0 ± 0.3	7,520
NSF (ours)	**0.8 ± 0.7**	**53**	**1.3 ± 0.1**	**53**	**0.6 ± 0.3**	**53**	**0.2 ± 0.6**	**53**

Latent SDEs and Latent Neural Stochastic Flows

Extension for partially-observed/high-dimensional data

Real-world time-series data is often:

- Partially-observed
- Irregularly-sampled
- High-dimensional



(Figure adapted from github.com/jutanke/mocap)

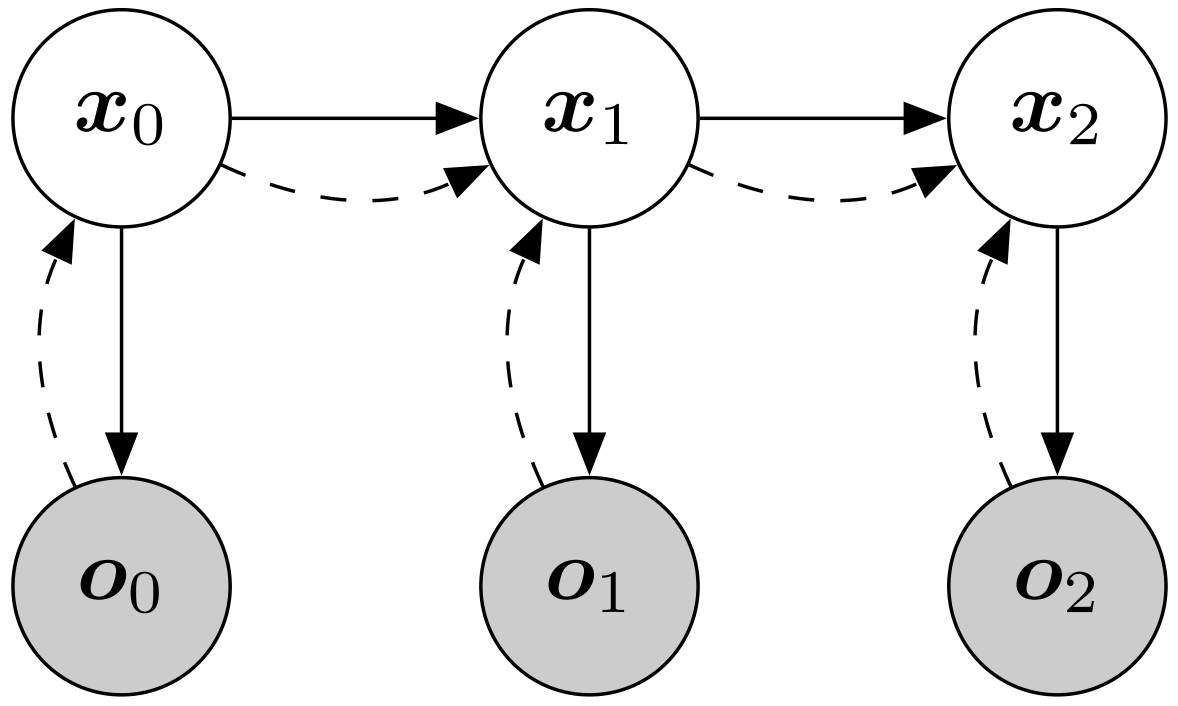
Latent SDEs are powerful tools, but they require high computational costs.

We replace SDEs with Neural Stochastic Flows.

Latent Neural Stochastic Flows

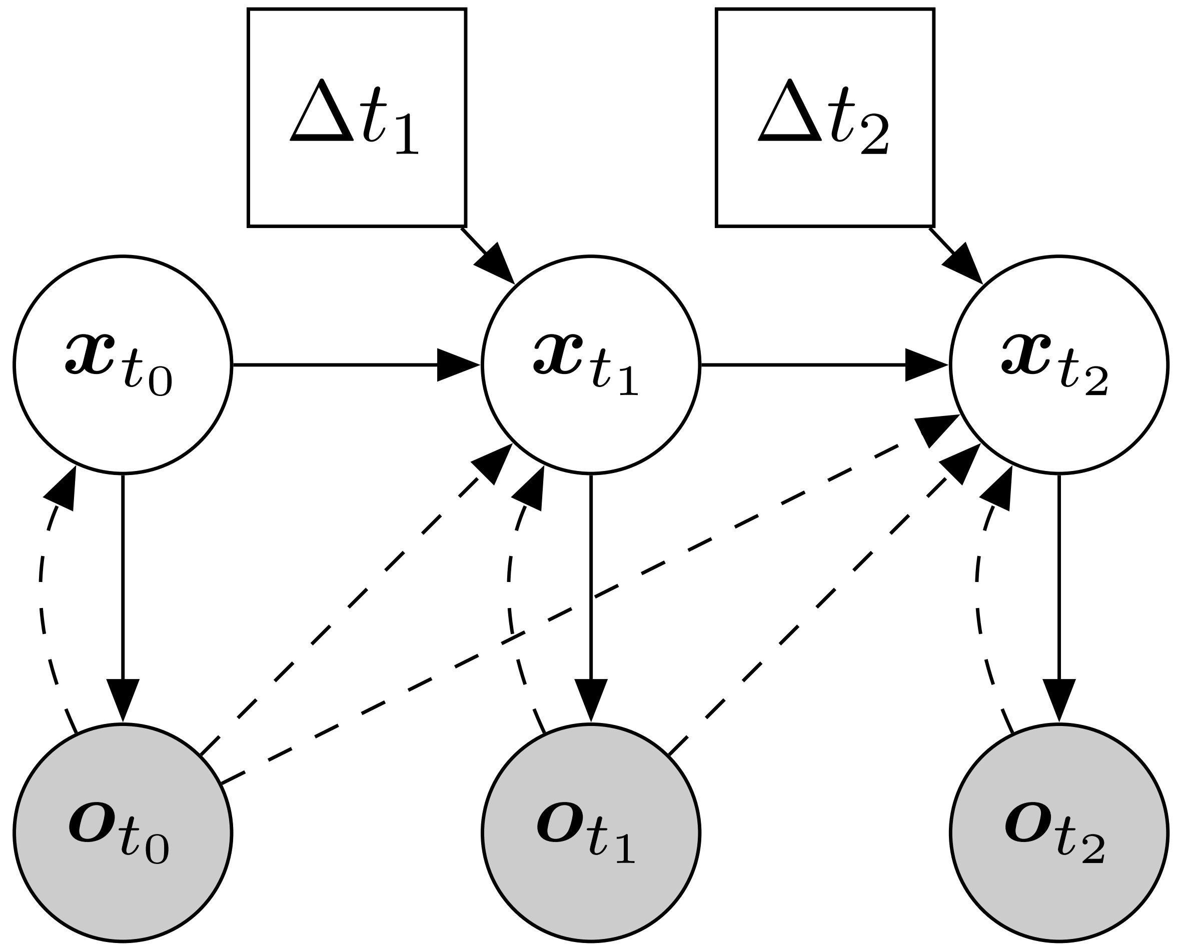
Extension for partially-observed/high-dimensional data

Variational State Space Model [8, 21, 22, 31]



A proven template for sequential modelling, including RL (PlaNet[16], Dreamer, etc.)

Latent NSF (ours)



✓ **VSSM structure remains the same by NSF's closed-form log density**

✓ **One-step transition for arbitrary Δt**

Experimental Results with Latent NSF

Real-world/high-dimensional sequential prediction

CMU Motion Capture (50-dims.)

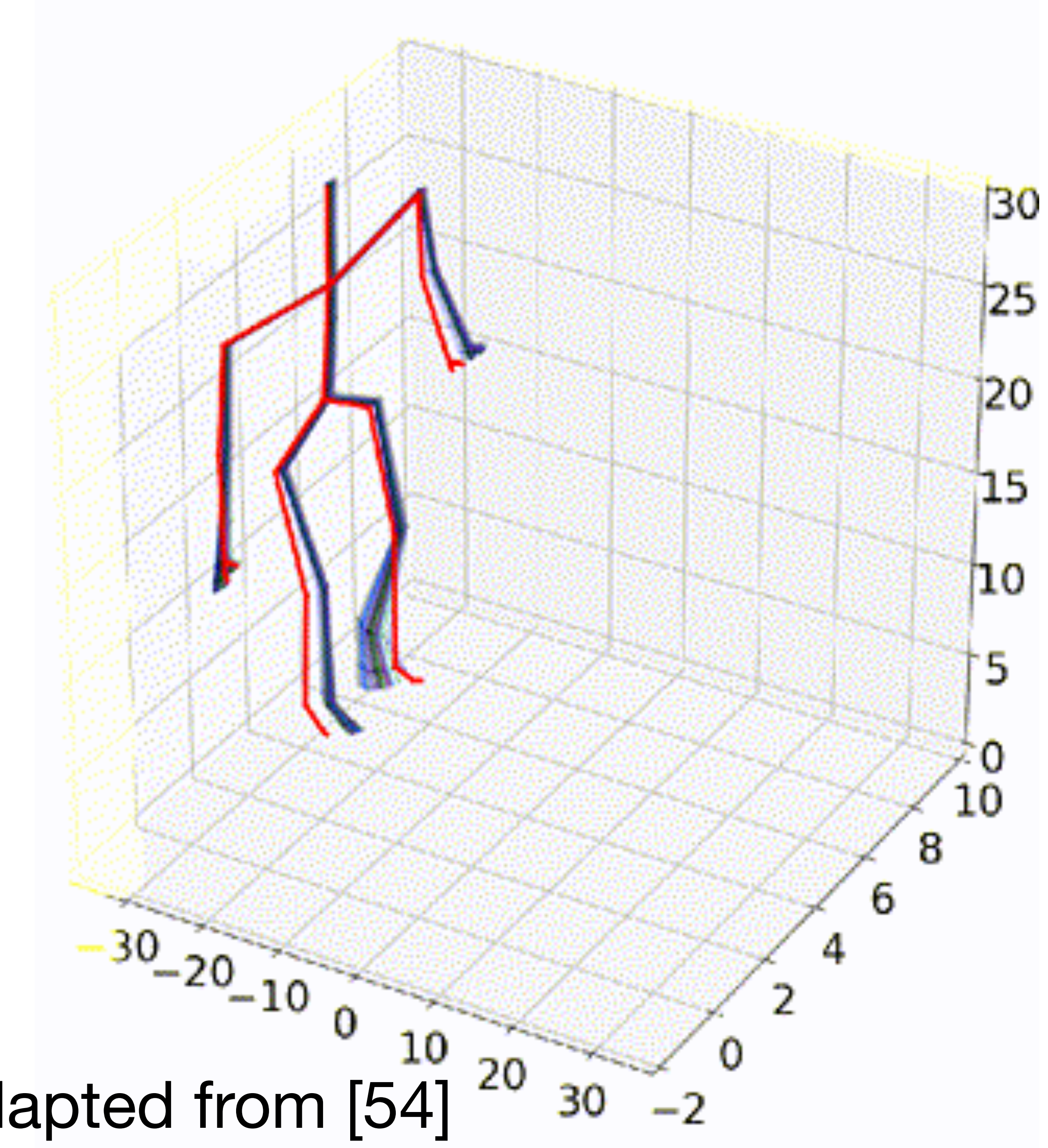


Figure adapted from [54]

Setup 1: The same length for train/test

Setup 2: Training length < Test length

Stochastic Moving MNIST (64x64 px)

Experimental Results with Latent NSF

Real-world/high-dimensional sequential prediction

CMU Motion Capture (50-dims.)

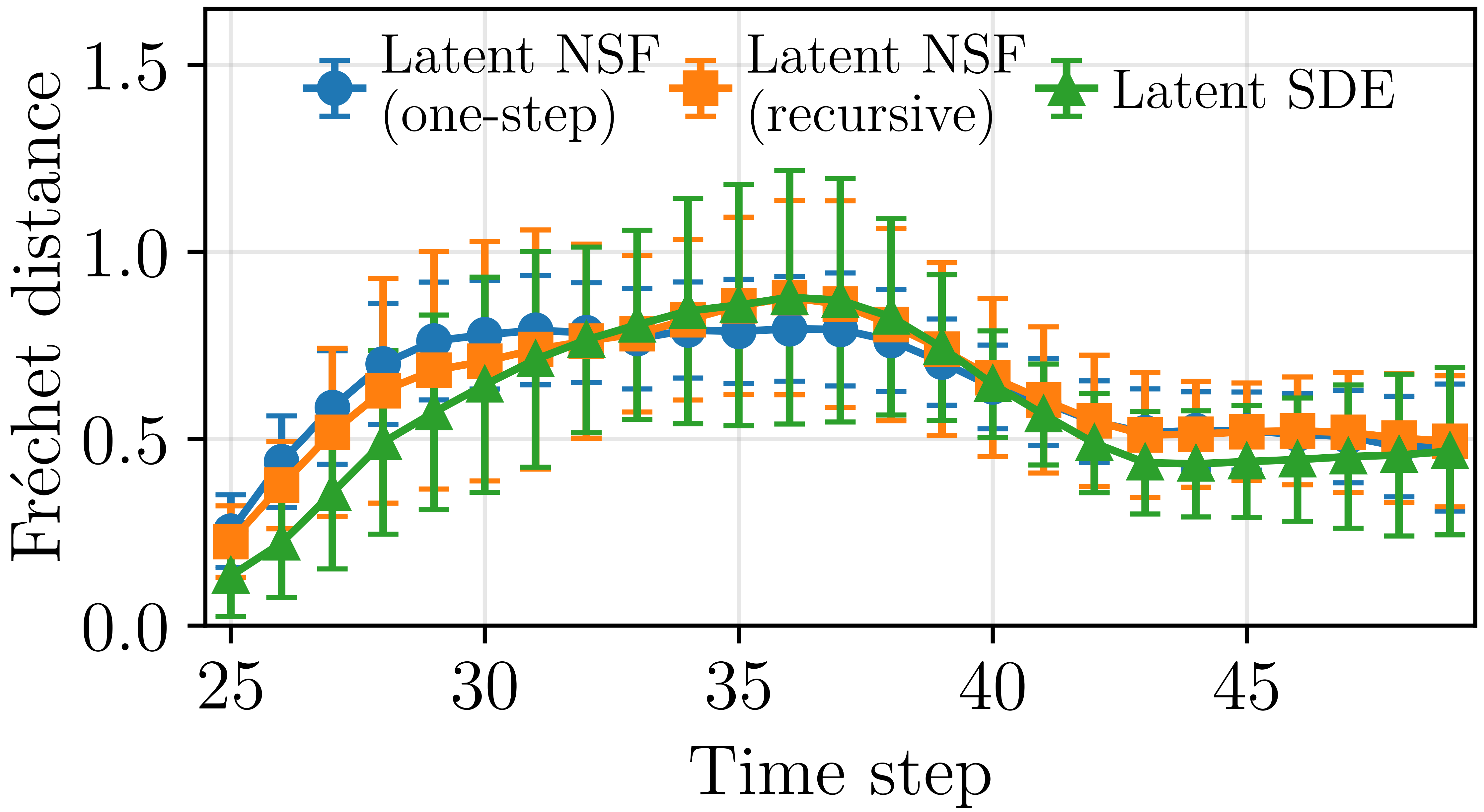
Compared by mean square error

Methods	Setup 1	Setup 2
npODE [17]	$22.96^{\dagger}$	–
Neural ODE [6]	$22.49 \pm 0.88^{\dagger}$	–
ODE2VAE-KL [54]	$8.09 \pm 1.95^{\dagger}$	–
Latent ODE [43]	$5.98 \pm 0.28^{*}$	$31.62 \pm 0.05^{\S}$
Latent SDE [33]	12.91 ± 2.90^{1}	$9.52 \pm 0.21^{\S}$
Latent Approx SDE [46]	$7.55 \pm 0.05^{\S}$	10.50 ± 0.86
ARCTA [9]	$7.62 \pm 0.93^{\ddagger}$	9.92 ± 1.82
NCDSSM [2]	$5.69 \pm 0.01^{\S}$	$4.74 \pm 0.01^{\S}$
SDE matching [3]	$\mathbf{5.20} \pm \mathbf{0.43}^{2}$	4.26 ± 0.35
Latent NSF (ours)	8.62 ± 0.32	$\mathbf{3.41} \pm \mathbf{0.27}$

✔ Best/tied-best performance

✔ Two orders of magnitude faster

Stochastic Moving MNIST (64x64 px)



✔ Comparable performance

✔ 2x faster

Position of Our Work

Method(s)	**Target dynamics**	**Solver-free training**	**Solver-free inference**
Neural ODEs [6]	General ODEs	✗	✗
Neural flows [4]	General ODEs	✓	✓
Score-based diffusion via reverse SDEs/PF-ODEs [47]; flow matching [34]	Pre-defined diffusion SDEs/ODEs	✓	✗
Progressive distillation [44]	Pre-defined diffusion SDEs/ODEs	✗	✓
Consistency models [26, 48]; rectified flows [35]	Pre-defined diffusion SDEs/ODEs	✓	✓
Neural (latent) SDEs [25, 33, 38, 46, 50]	**General Itô SDEs**	✗	✗
ARCTA [9]; SDE matching [3]	**General Itô SDEs**	✓	✗
Neural Stochastic Flows (ours)	**General Itô SDEs**	✓	✓

Summary

- **We proposed Neural Stochastic Flows, which enable solver-free in both training and inference, with closed-form log-densities.**
- **Extended to Latent NSF: a variational state-space model using NSF as the latent transition for partially-observed/high-dimensional data.**

Key Benefits:

- **One-step prediction** for arbitrary time gaps.
- **Speed**: up to two orders of magnitude faster.
- **Stable training** with tractable densities.

Limitations:

- **Chapman–Kolmogorov relation is enforced approximately.**
- Affine-coupling design constrains **expressivity**.

Project page

Paper & Refs.