



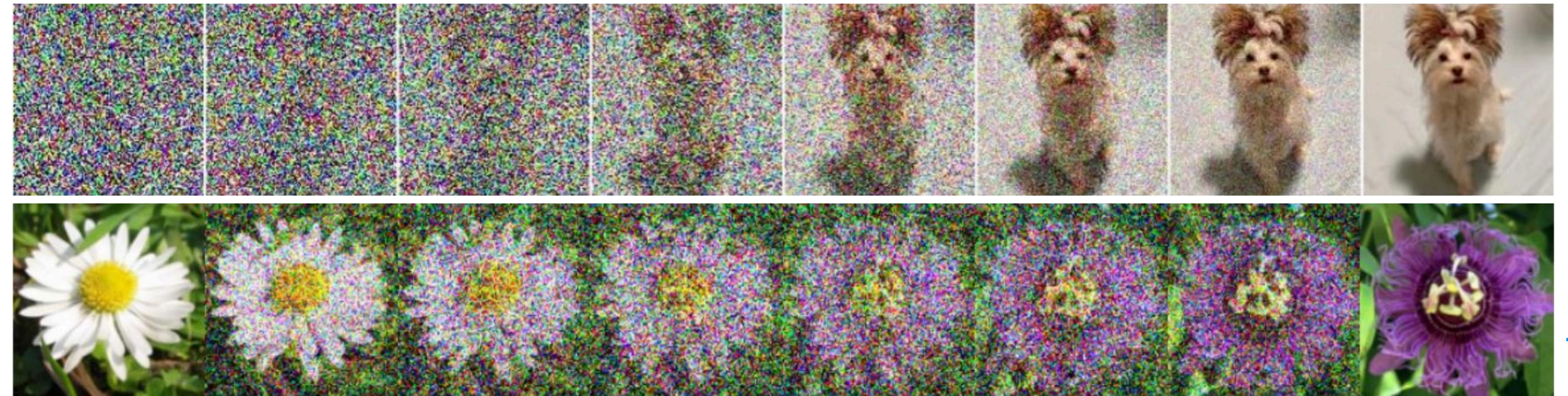
Schrödinger Bridges and Stochastic Control

Denis Rakitin

Translation between distributions

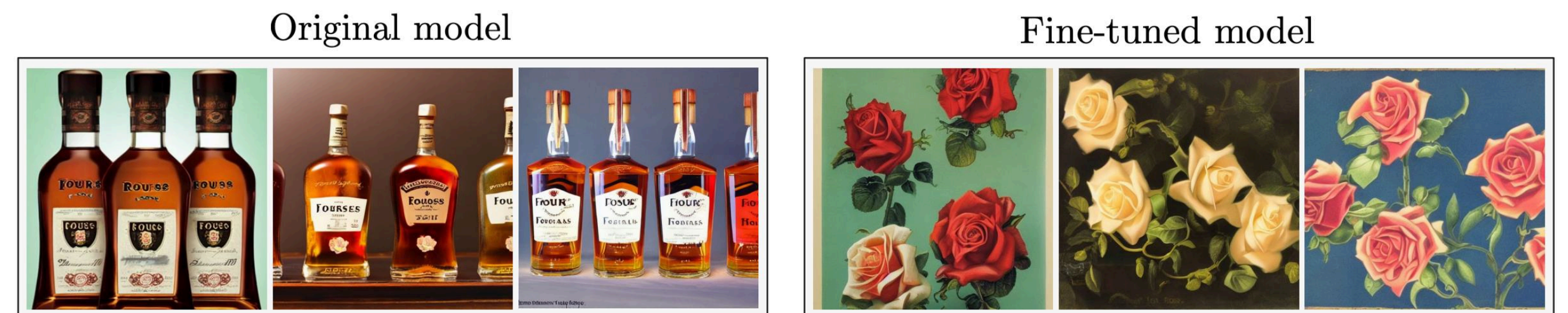
Between what?

- Generative modeling (noise \rightarrow data)
- Image2Image / editing (data \rightarrow data)



Additional settings

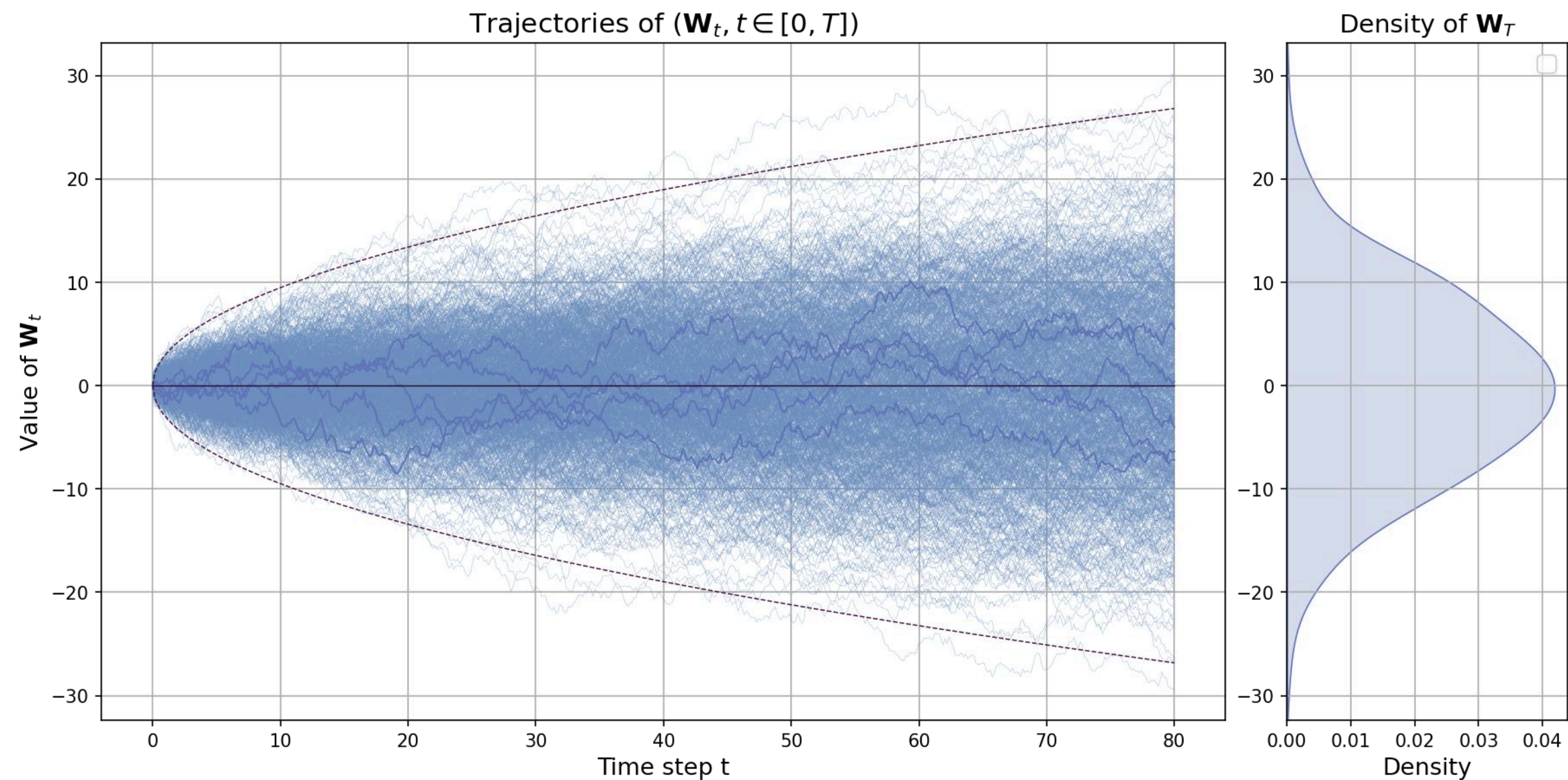
- RL fine-tuning
- Data-free sampling



Continuous time: Wiener process

Process \mathbf{W}_t with the properties of “random walk”:

- $\mathbf{W}_t - \mathbf{W}_s \perp (\mathbf{W}_\tau, \tau \in [0, s]); \mathbf{W}_t - \mathbf{W}_s \sim \mathcal{N}(0, (t - s)I)$



Stochastic Differential Equations

SDEs: stochastic dynamics that are

- Markovian
- Deterministic velocity + random walk

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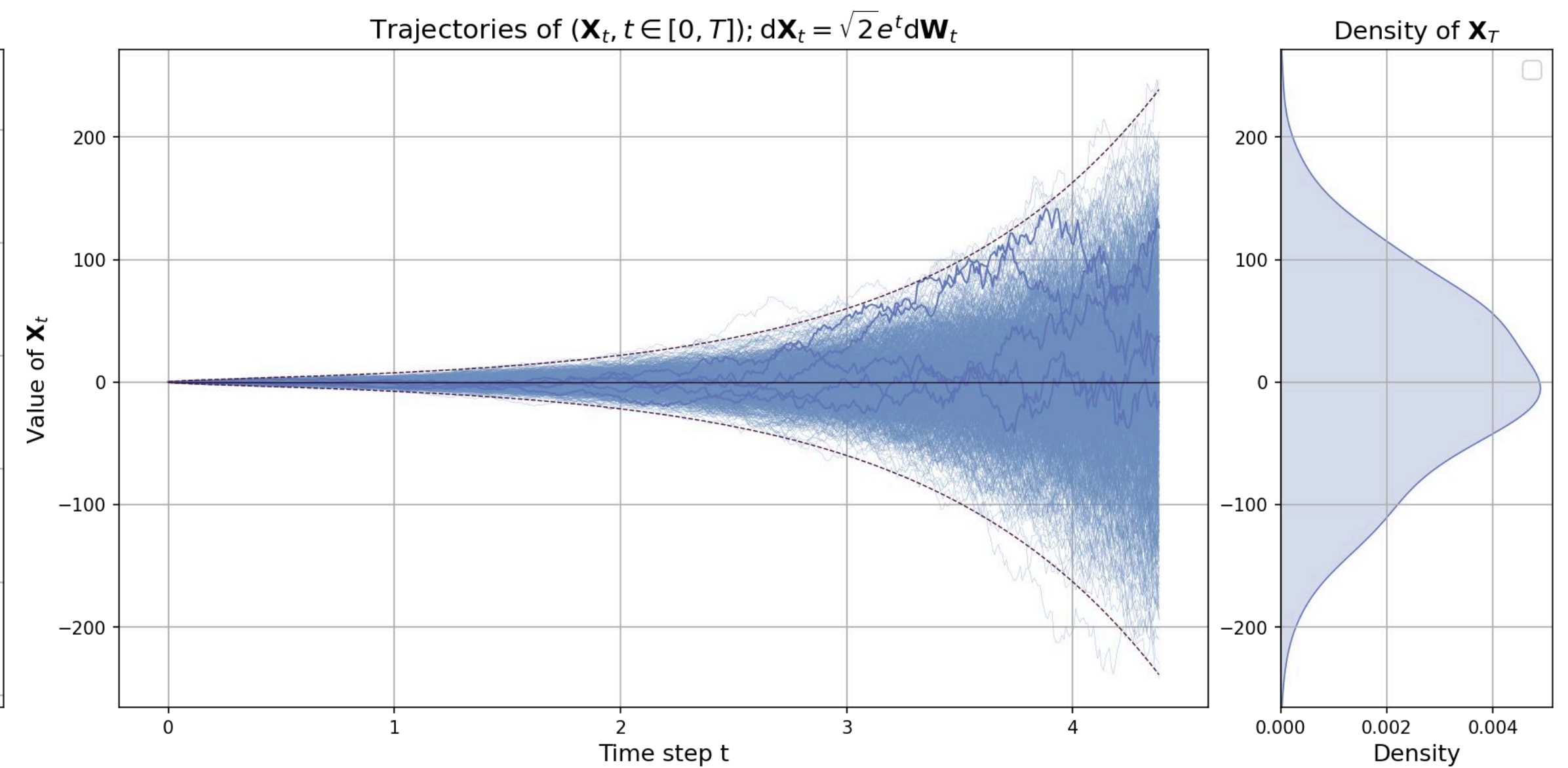
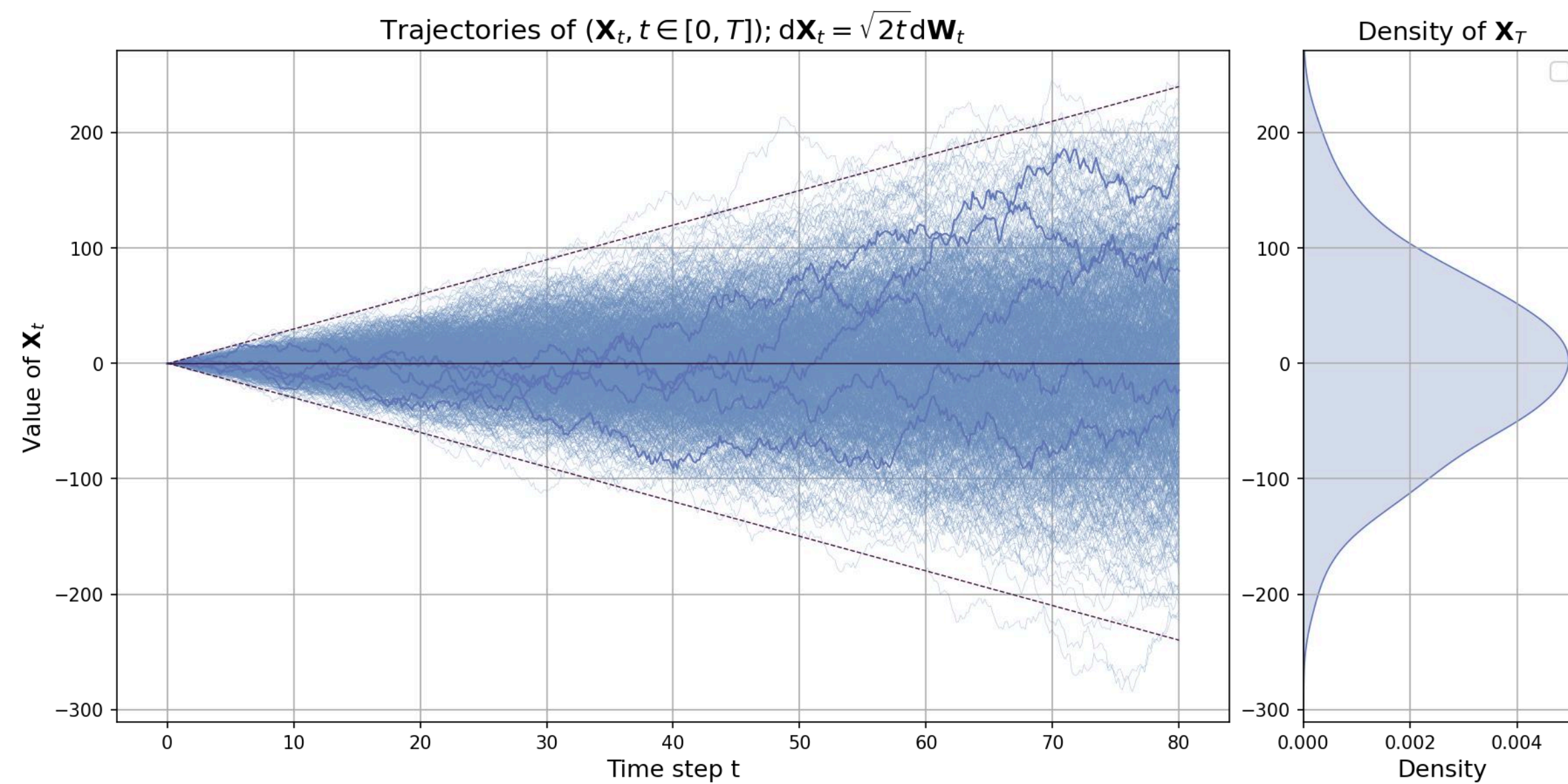
(Pseudo)-definition + Euler scheme

- $d\mathbf{X}_t = f_t(\mathbf{X}_t)dt + g(t)d\mathbf{W}_t$
- $\mathbf{X}_{t+h} \approx \mathbf{X}_t + hf_t(\mathbf{X}_t) + g(t)(\mathbf{W}_{t+h} - \mathbf{W}_t)$
 $\approx \mathbf{X}_t + hf_t(\mathbf{X}_t) + \sqrt{h}g(t)\boldsymbol{\epsilon}_t; \quad \boldsymbol{\epsilon}_t \sim \mathcal{N}(0, I)$

Variance Exploding SDE

$$d\mathbf{X}_t = g(t)d\mathbf{W}_t \quad \mathbf{X}_{t+h} \approx \mathbf{X}_t + \sqrt{h}g(t)\boldsymbol{\epsilon}_t$$

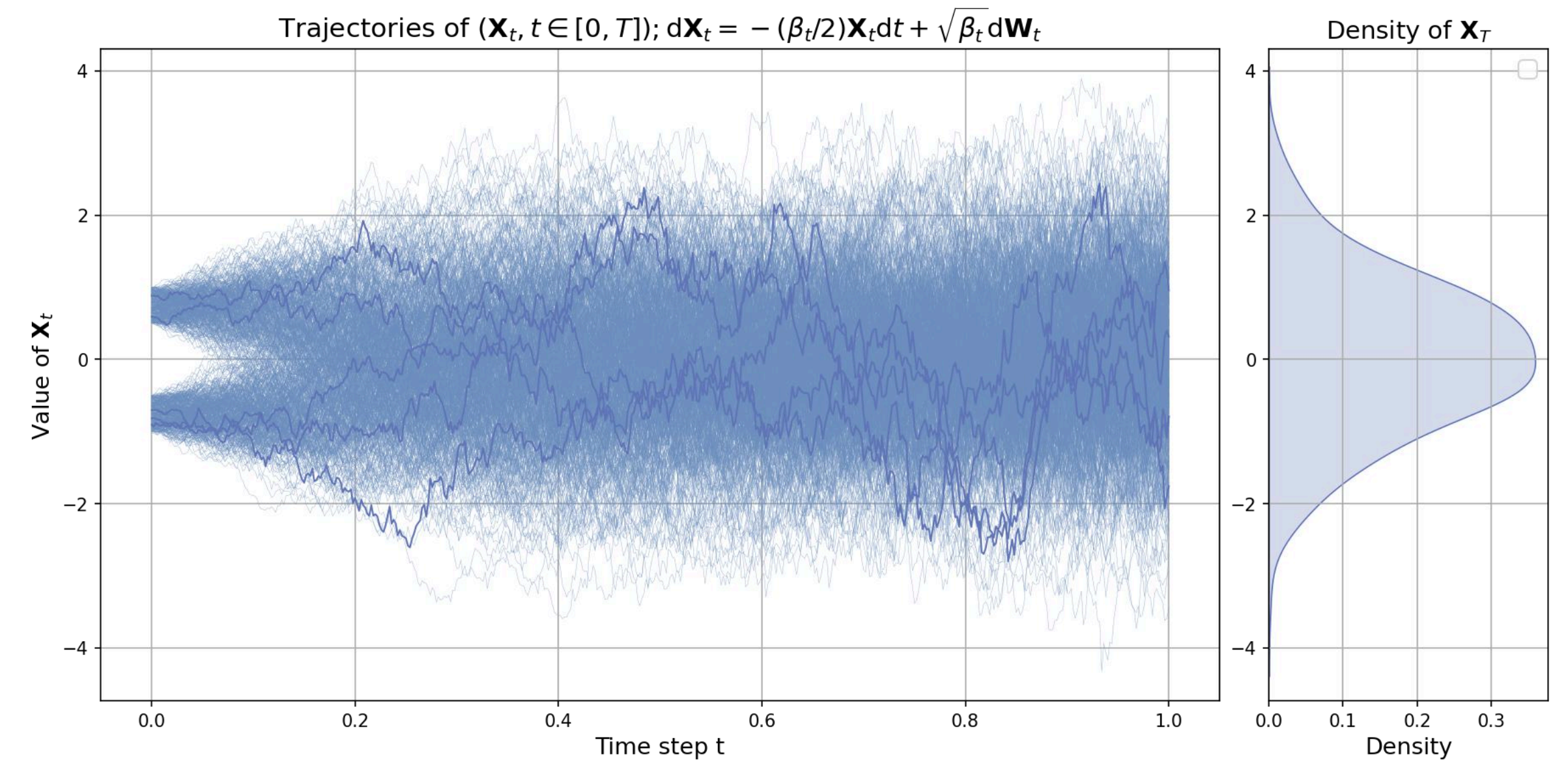
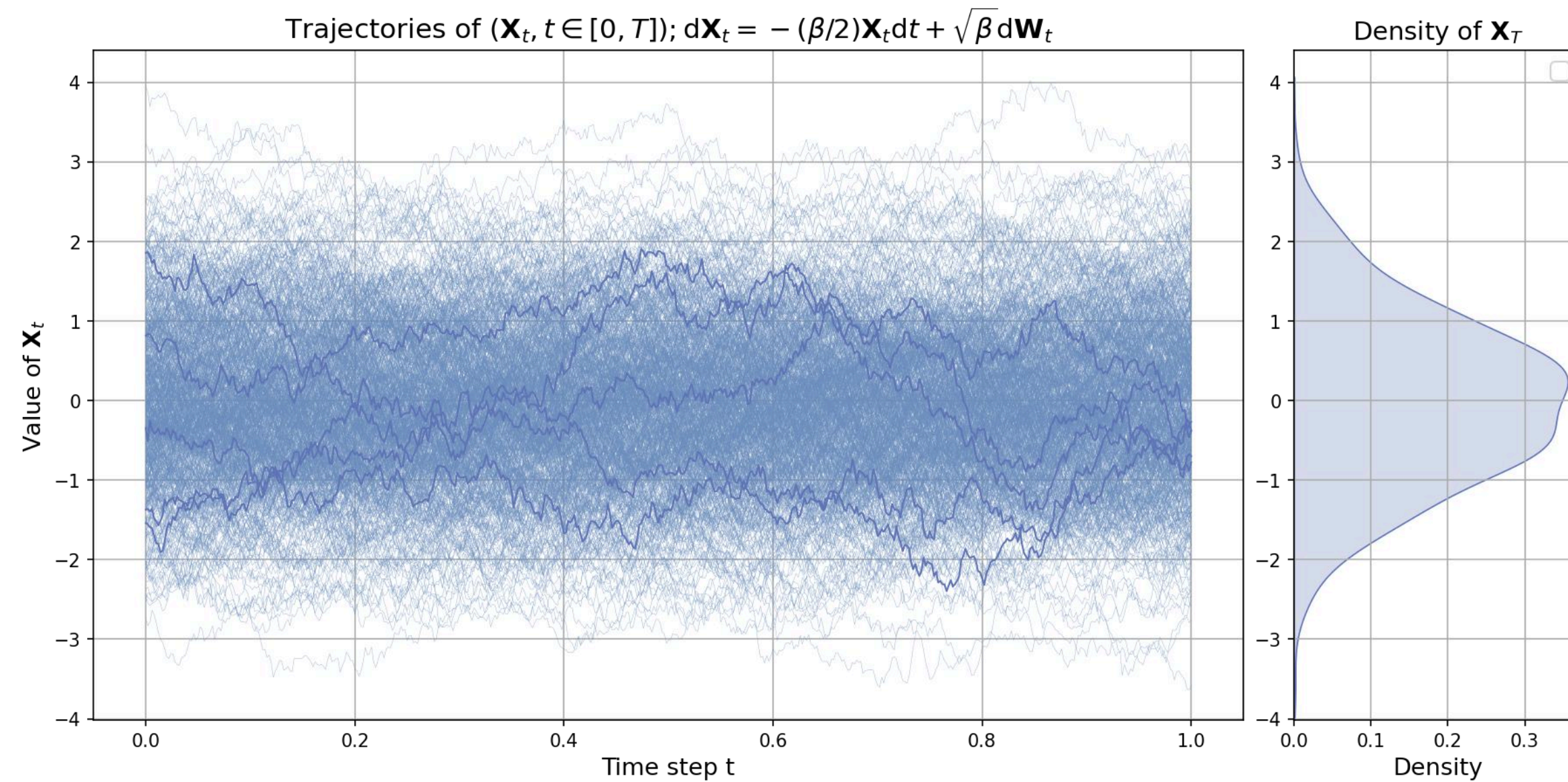
$$p_{\mathbf{X}_t|\mathbf{X}_0}(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}\left(\mathbf{x}_t|\mathbf{x}_0, \int_0^t g^2(s)ds\right)$$



Variance Preserving SDE

$$d\mathbf{X}_t = -\frac{\beta_t}{2}\mathbf{X}_t dt + \sqrt{\beta_t}d\mathbf{W}_t \quad \mathbf{X}_{t+h} \approx \mathbf{X}_t \left(1 - \frac{h\beta_t}{2}\right) + \sqrt{h\beta_t}\boldsymbol{\epsilon}_t$$

$$p_{\mathbf{X}_t|\mathbf{X}_0}(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t|\sqrt{\alpha_t}\mathbf{x}_0, (1 - \alpha_t)I); \quad \alpha_t = \exp\left(-\int_0^t \beta_s ds\right)$$



Schrödinger Bridges (SB)

Let $d\mathbf{Z}_t = f_t^{\text{base}}(\mathbf{Z}_t)dt + \sqrt{\gamma}d\mathbf{W}_t$ be some “base” SDE (e.g. Wiener process)

Goal: manipulate \mathbf{Z}_t to perform transition between the desired distributions

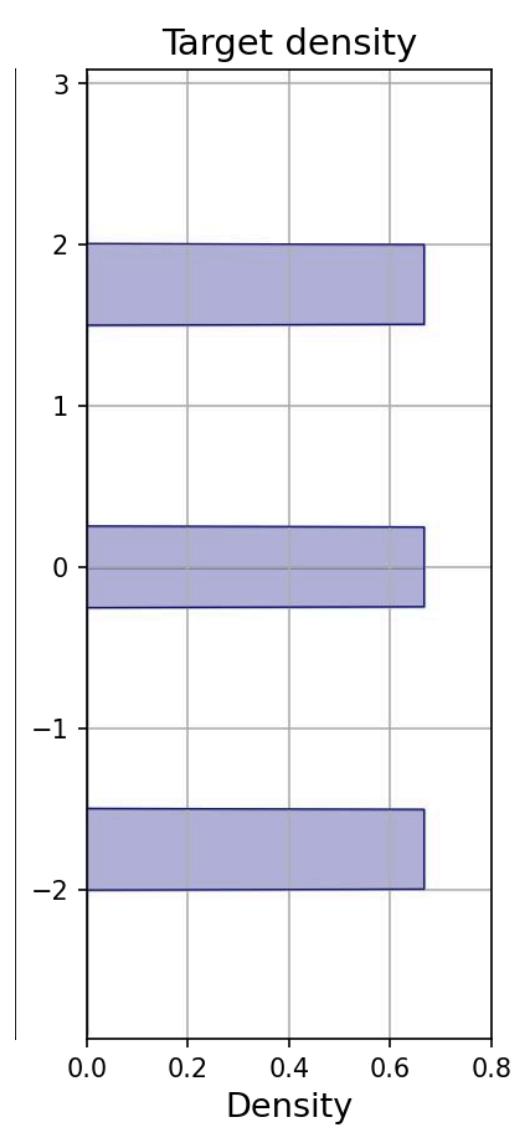
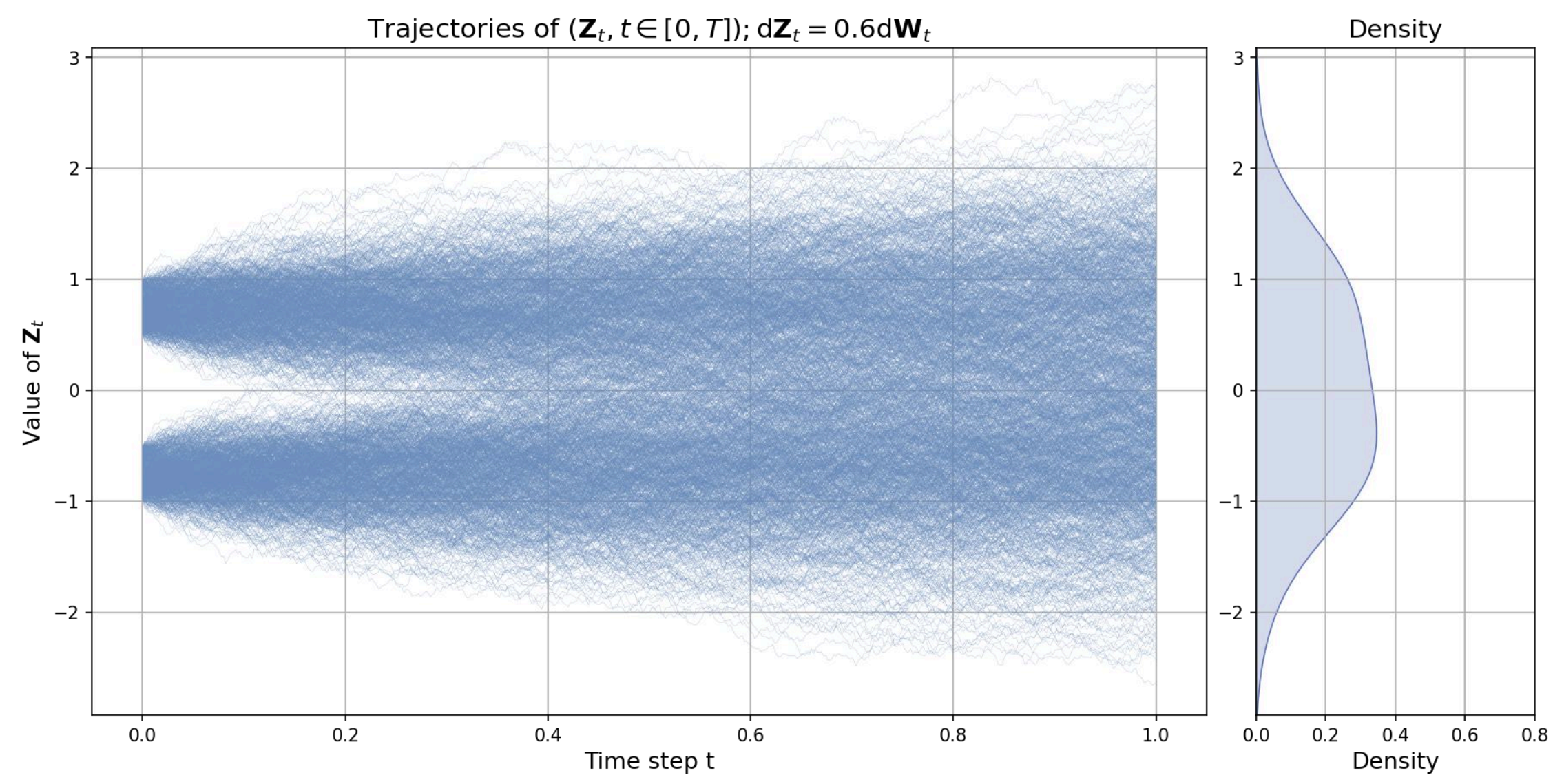
Formalization:

$$\begin{cases} \text{KL}(\mathbf{P}_{\mathbf{X}} \parallel \mathbf{P}_{\mathbf{Z}}) \rightarrow \min_{\mathbf{P}_{\mathbf{X}}}; \\ p_{\mathbf{X}_0} = p^{\mathcal{S}}; p_{\mathbf{X}_1} = p^{\mathcal{T}} \end{cases}$$

Schrödinger Bridges (SB)

$$d\mathbf{Z}_t = f_t^{\text{base}}(\mathbf{Z}_t)dt + \sqrt{\gamma}d\mathbf{W}_t$$

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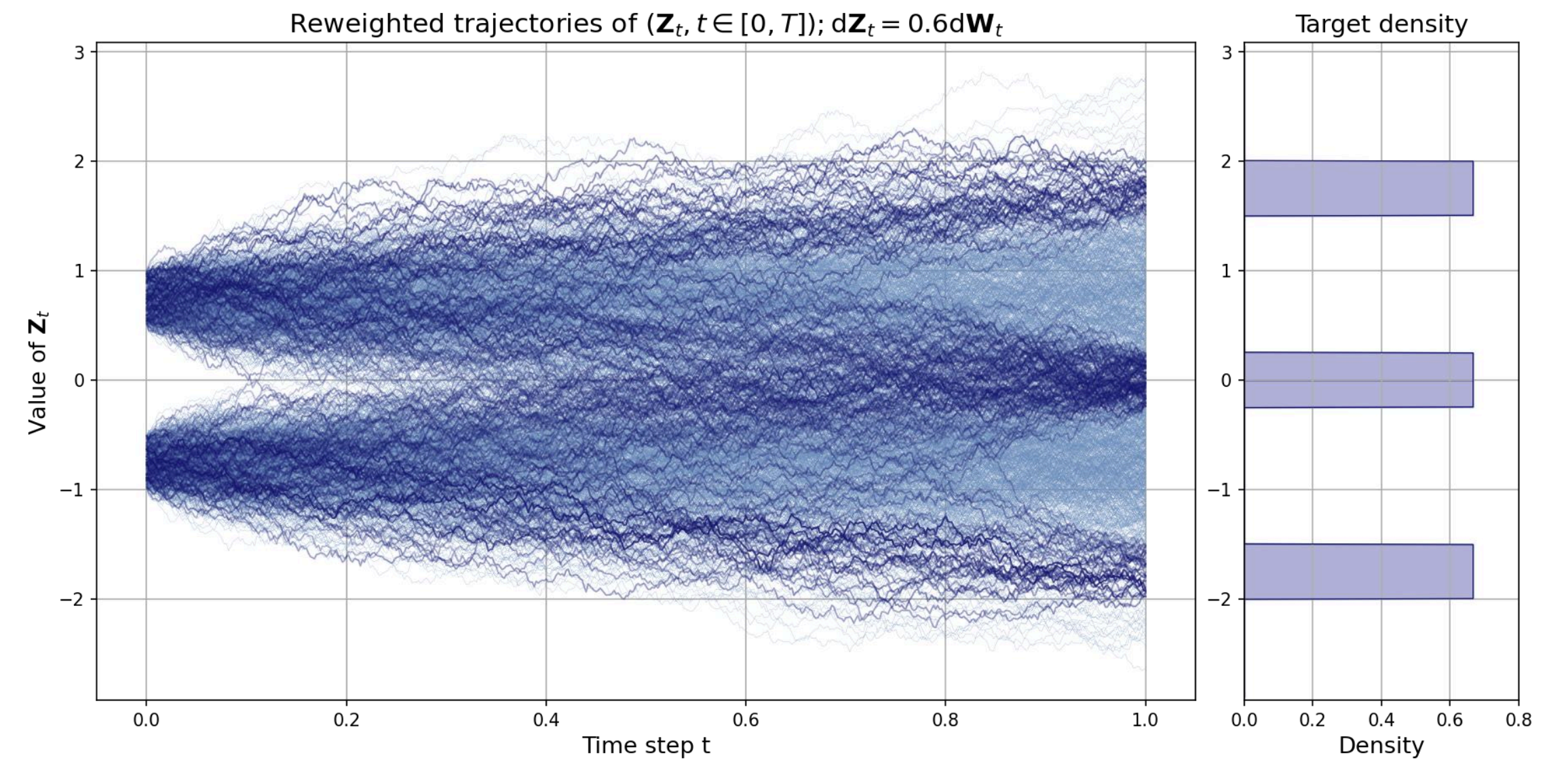
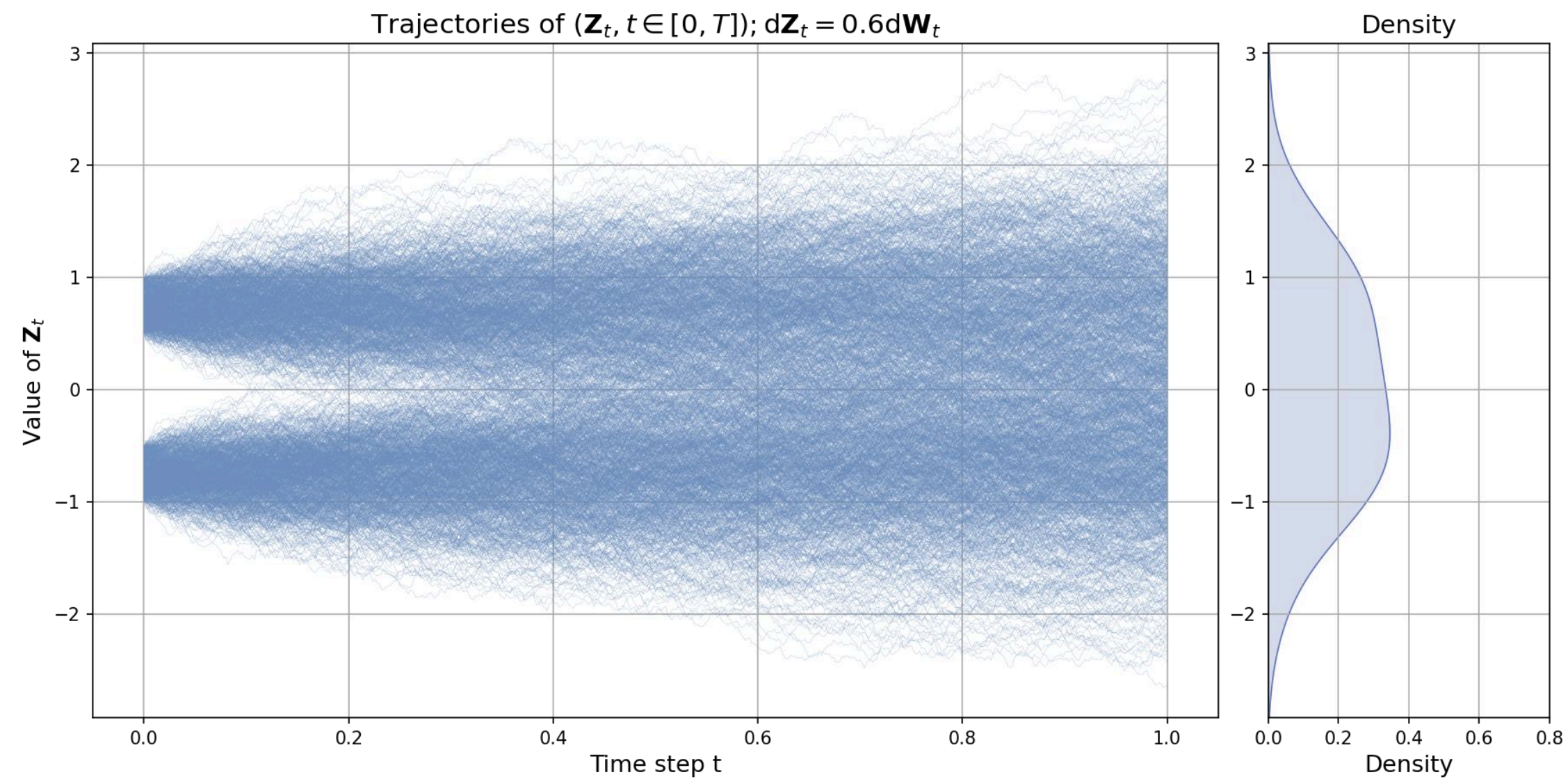


Schrödinger Bridges (SB)

$$d\mathbf{Z}_t = f_t^{\text{base}}(\mathbf{Z}_t)dt + \sqrt{\gamma}d\mathbf{W}_t$$

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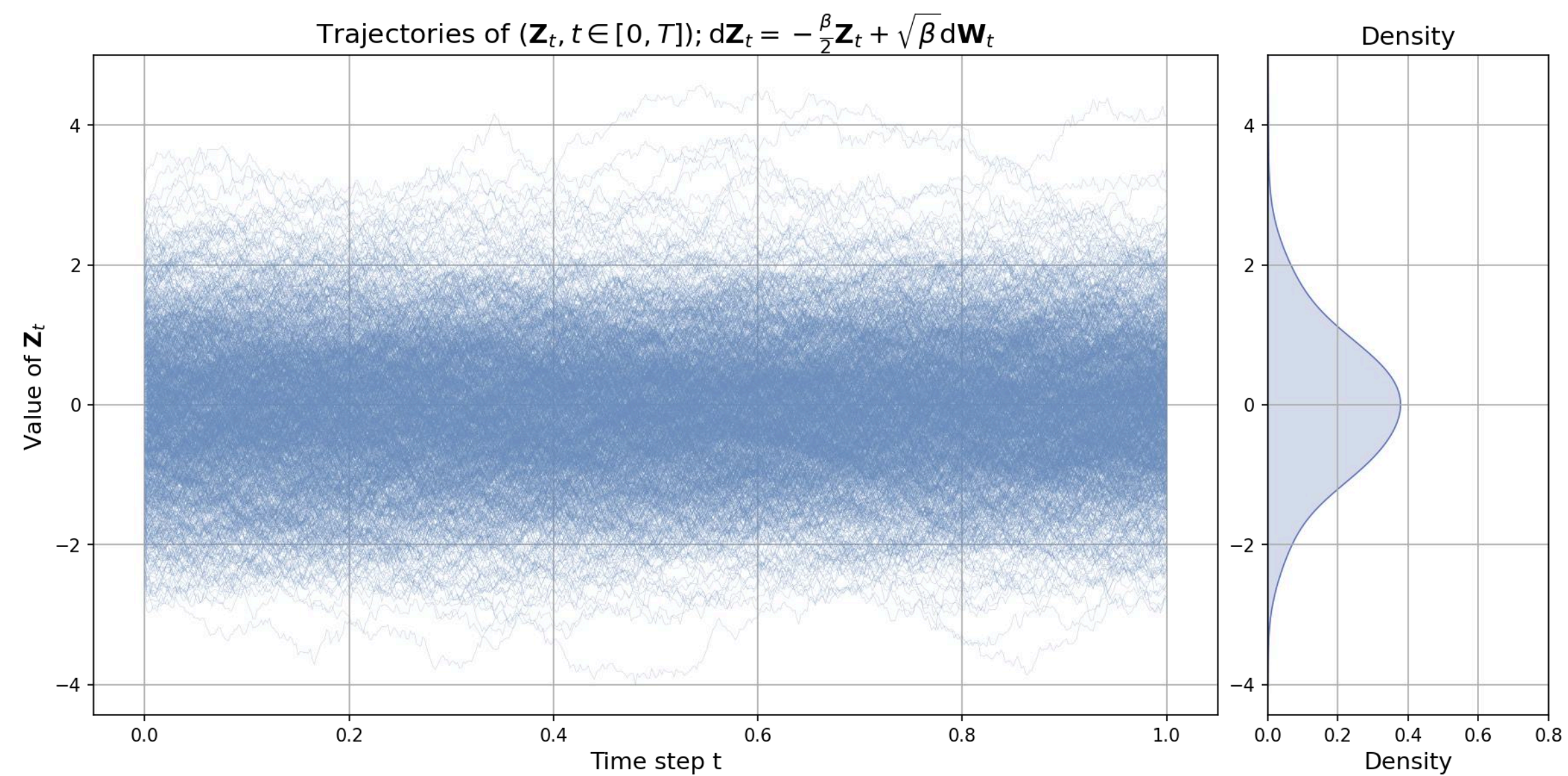
Reweighting as generalization of conditioning



Applications: generative modeling

$$d\mathbf{Z}_t = -\frac{\beta_t}{2}\mathbf{Z}_t dt + \sqrt{\beta_t}d\mathbf{W}_t$$

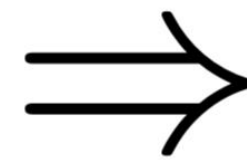
$$\begin{cases} \text{KL}(\mathbf{P}_{\mathbf{X}} \parallel \mathbf{P}_{\mathbf{Z}}) \rightarrow \min; \\ p_{\mathbf{X}_0} = \mathcal{N}(0, I); p_{\mathbf{X}_1} = p^{\text{data}} \end{cases} \Rightarrow$$



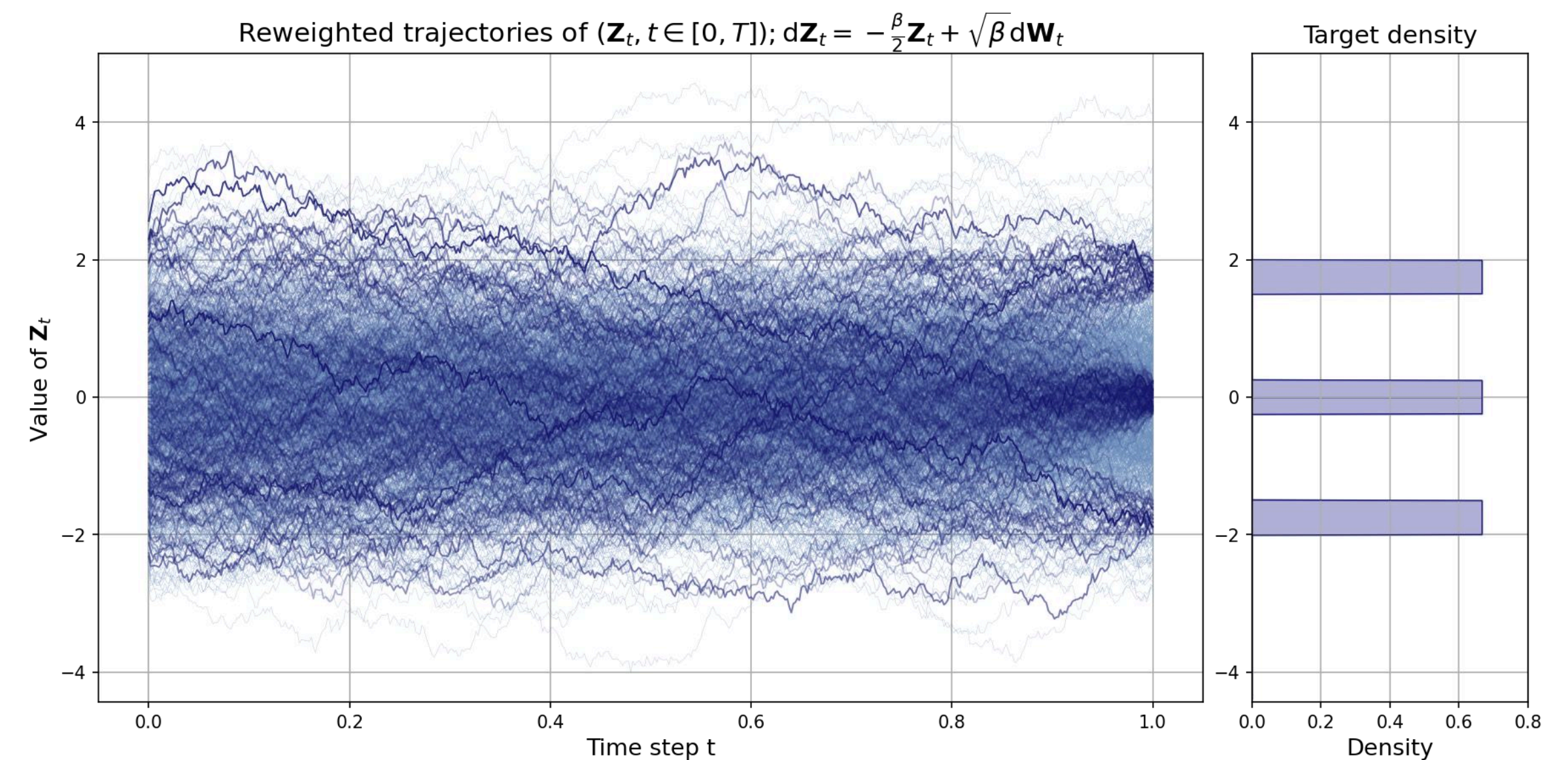
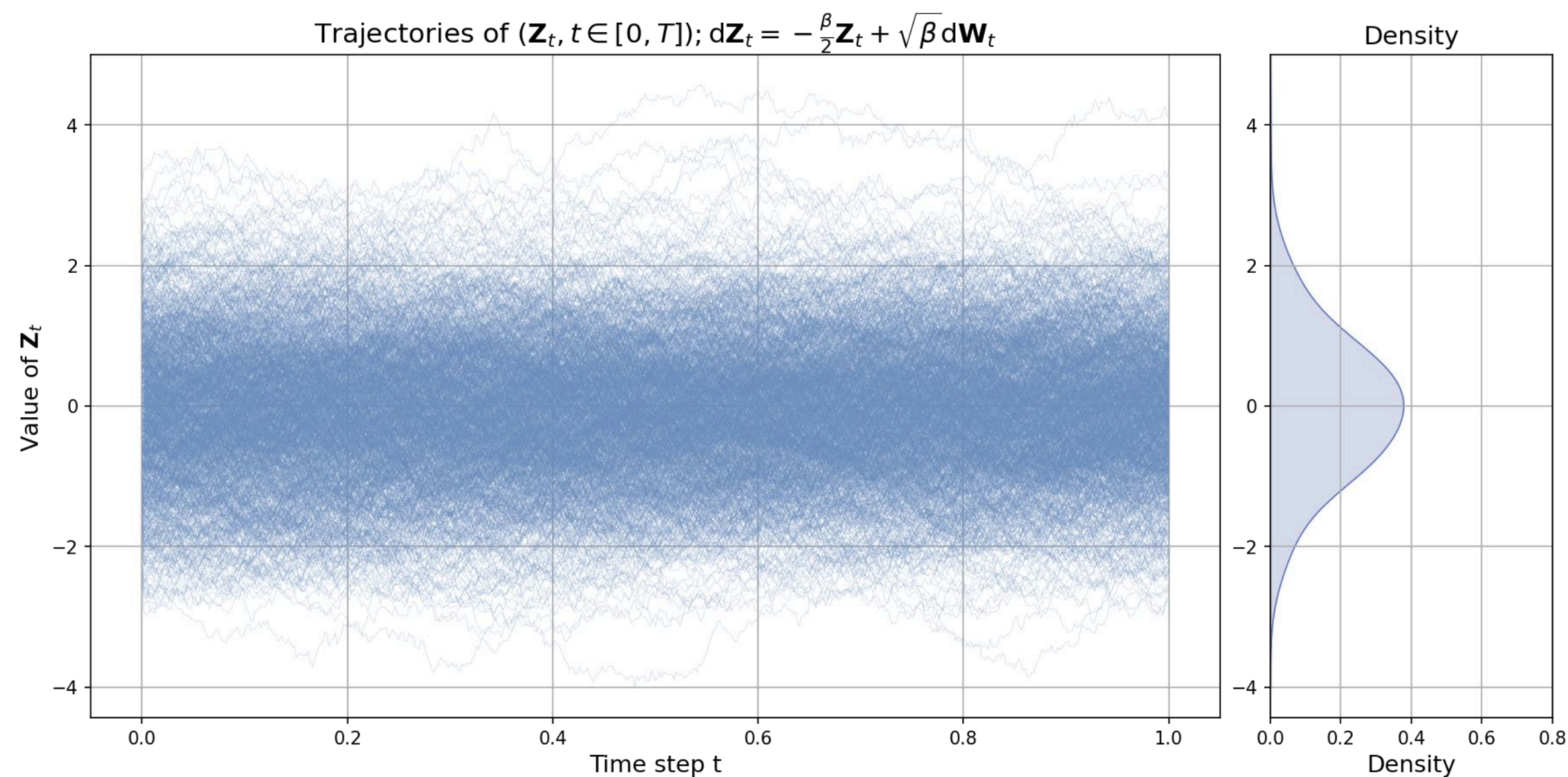
Applications: generative modeling

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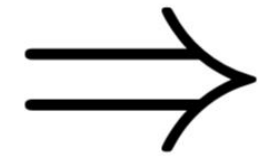


Generative modeling
(Diffusion models)



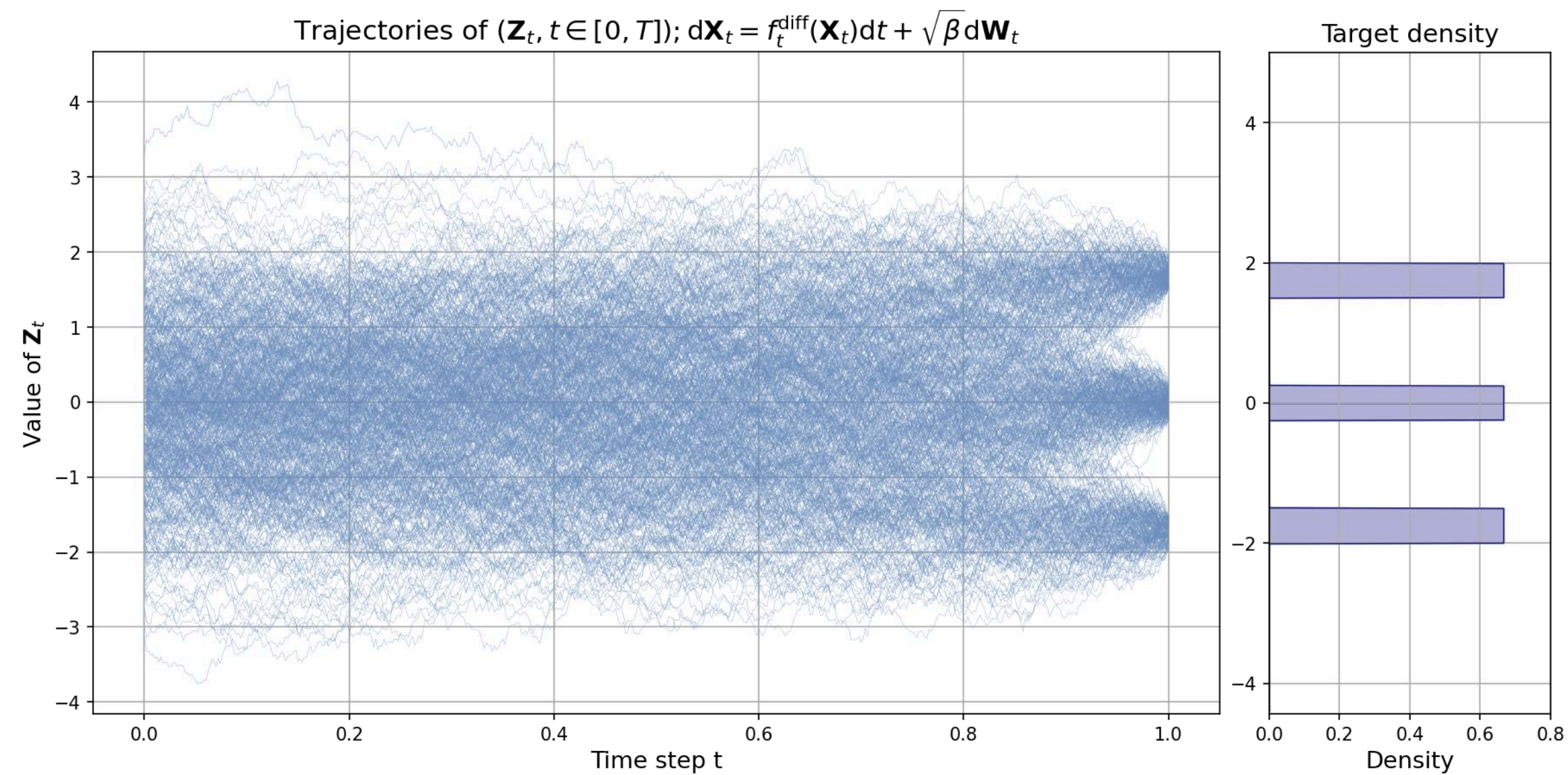
Applications: finetuning

$$d\mathbf{Z}_t = f_t^{\text{diff}}(\mathbf{Z}_t)dt + g(t)d\mathbf{W}_t$$



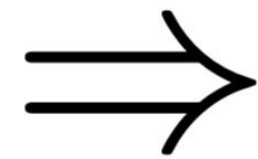
$$\begin{cases} \text{KL}(\mathbf{P}_{\mathbf{X}} \parallel \mathbf{P}_{\mathbf{Z}}) \rightarrow \min_{\mathbf{P}_{\mathbf{X}}}; \\ p_{\mathbf{X}_0} = \mathcal{N}(0, I); p_{\mathbf{X}_1}(\mathbf{x}_1) \propto p^{\text{data}}(\mathbf{x}_1) \cdot \exp(R(\mathbf{x}_1)) \end{cases}$$

$$R(\mathbf{x}_1) = |\mathbf{x}_1|$$



Applications: finetuning

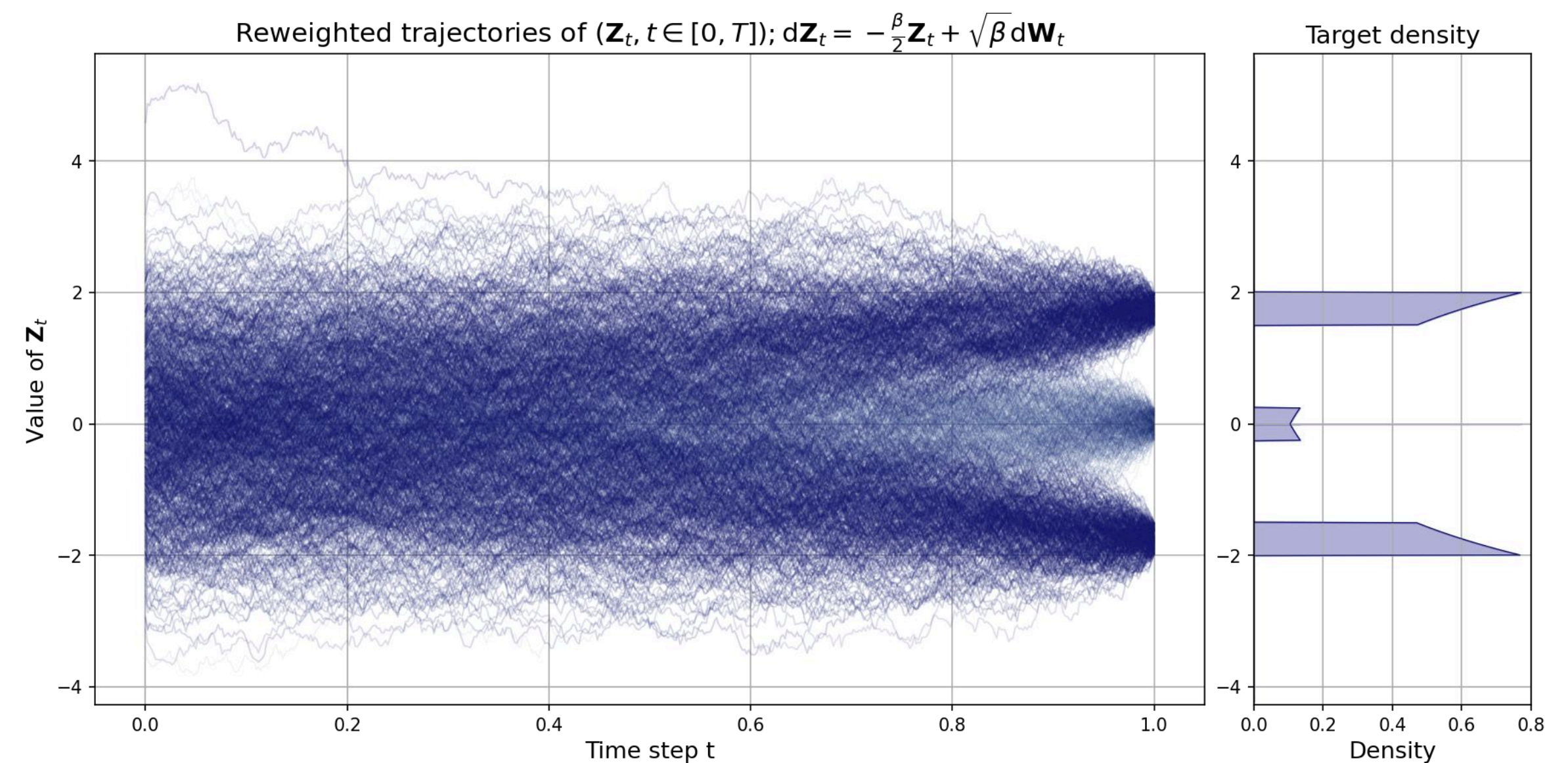
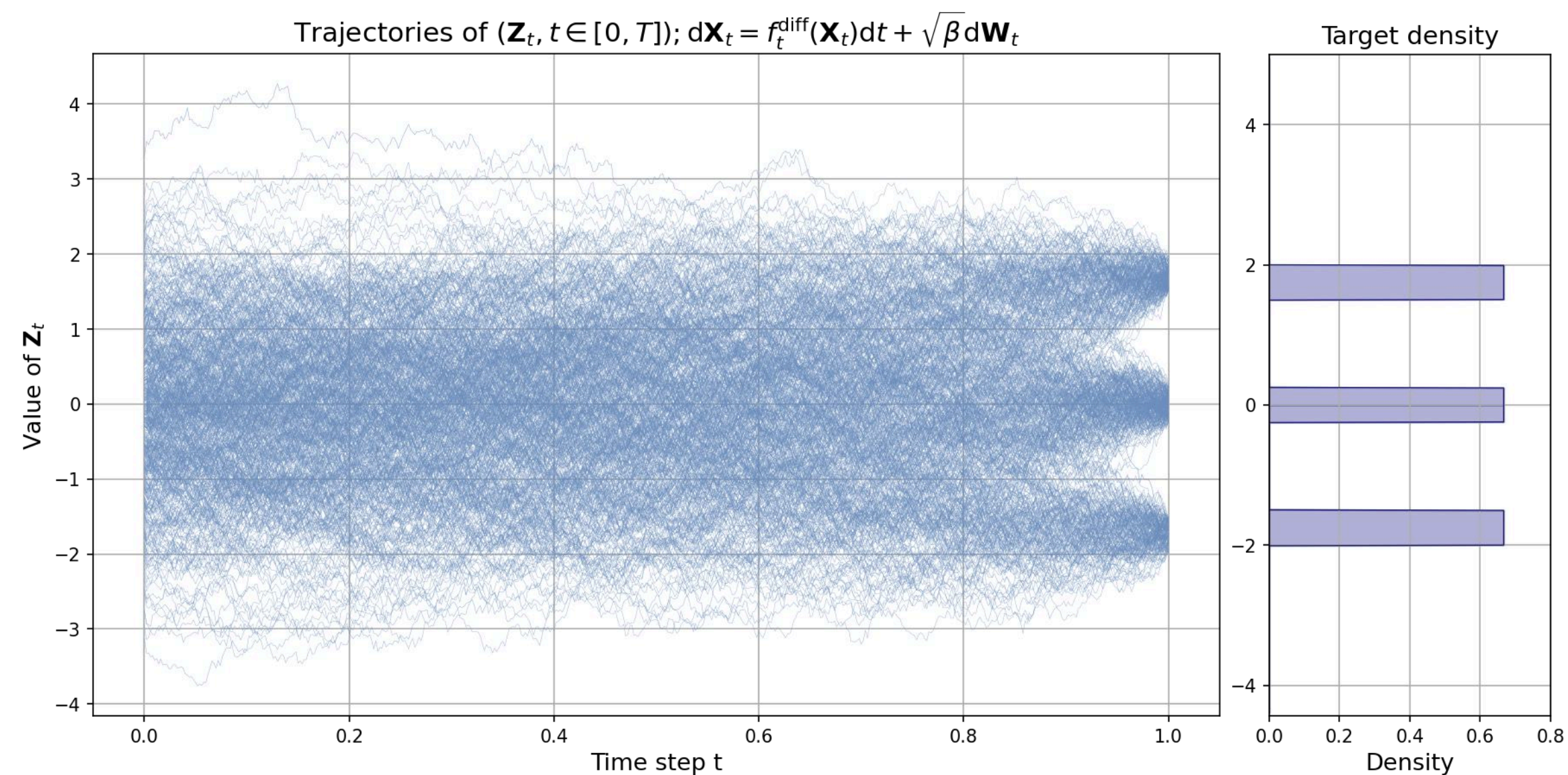
$$d\mathbf{Z}_t = f_t^{\text{diff}}(\mathbf{Z}_t)dt + g(t)d\mathbf{W}_t$$



$$\begin{cases} \text{KL}(\mathbf{P}_{\mathbf{X}} \parallel \mathbf{P}_{\mathbf{Z}}) \rightarrow \min; \\ p_{\mathbf{X}_0} = \mathcal{N}(0, I); p_{\mathbf{X}_1}(\mathbf{x}_1) \propto p^{\text{data}}(\mathbf{x}_1) \cdot \exp(R(\mathbf{x}_1)) \end{cases}$$

Diffusion models +
fine-tuning on reward

$$R(\mathbf{x}_1) = |\mathbf{x}_1|$$



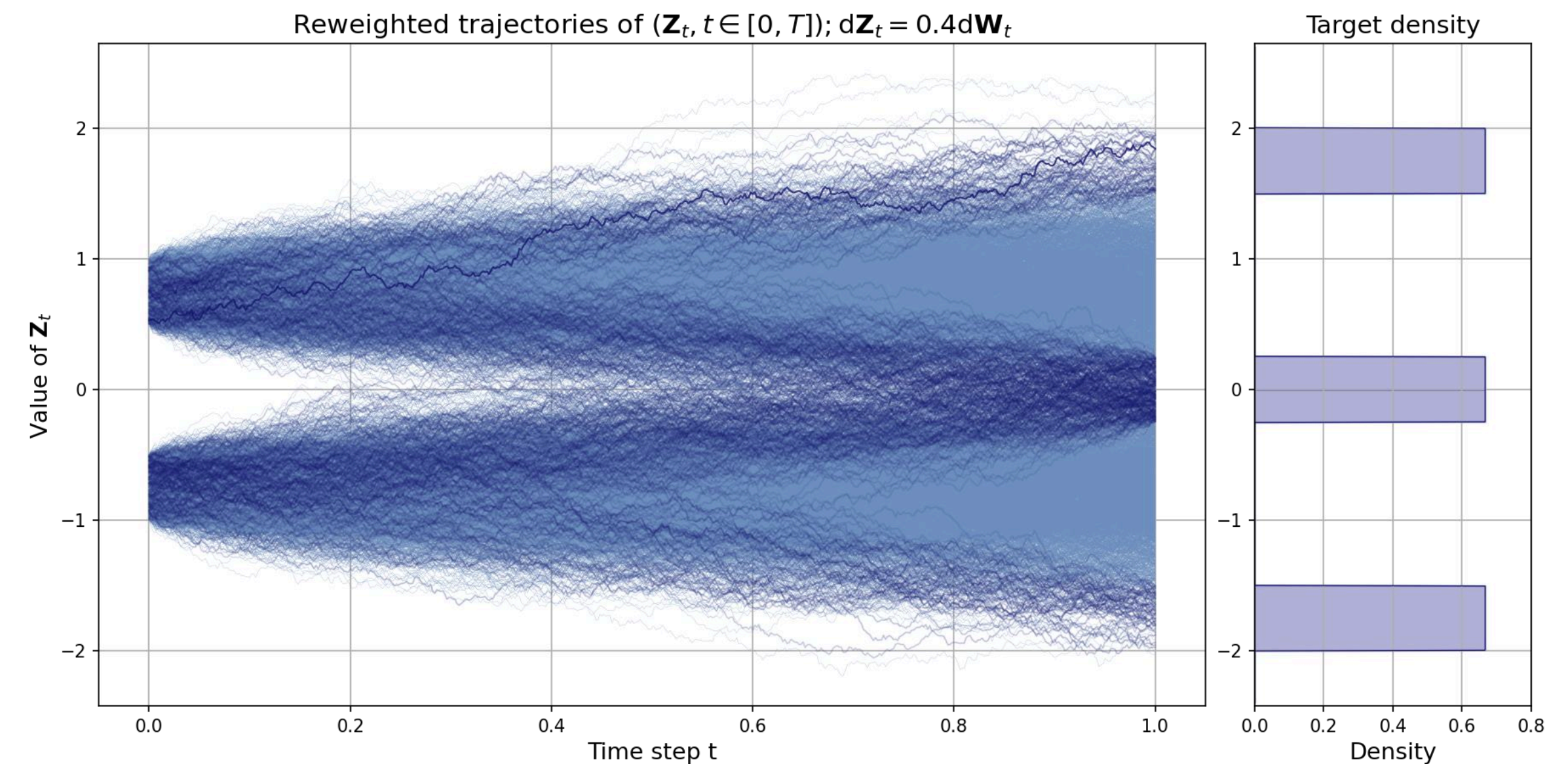
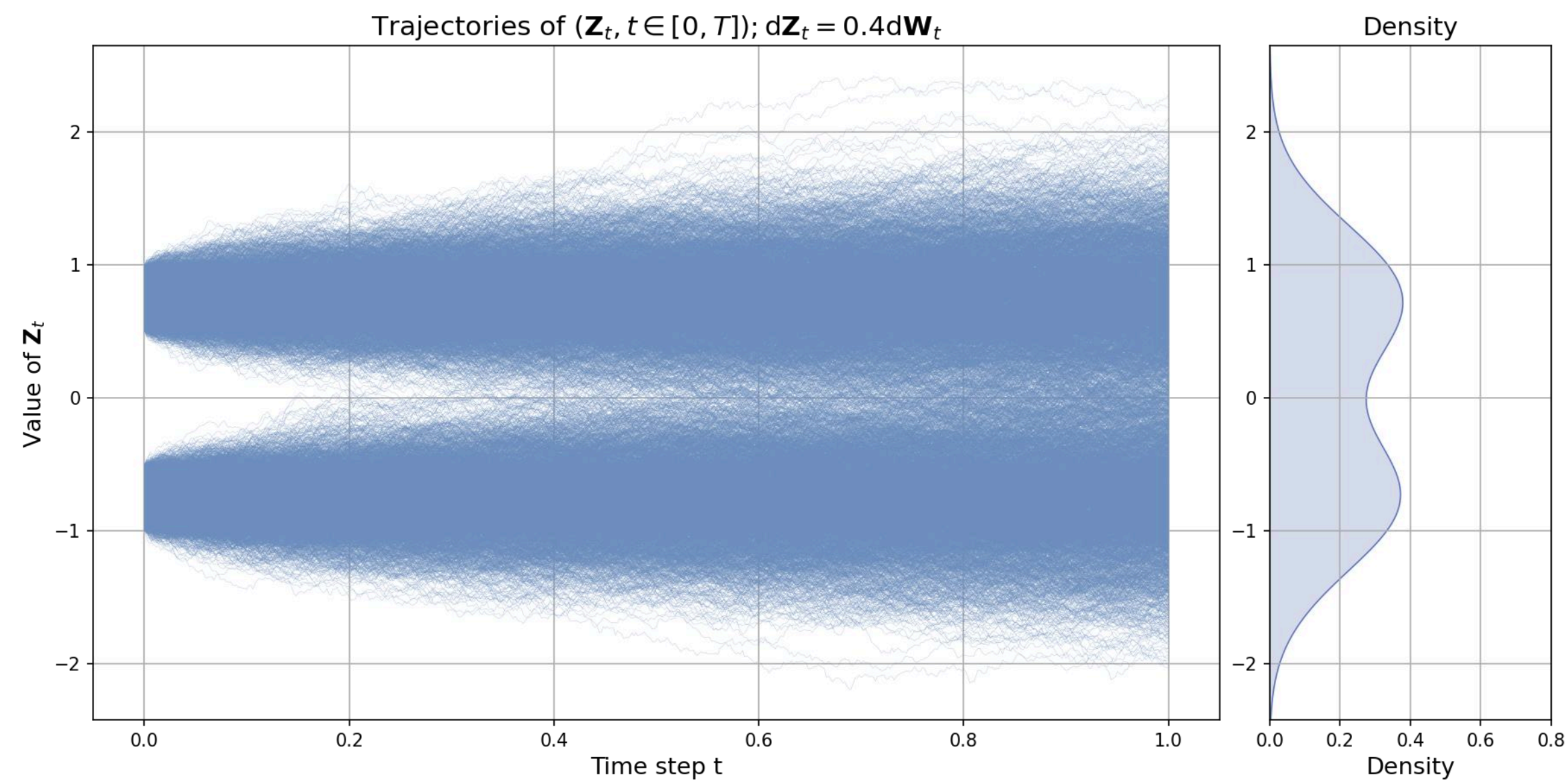
Applications: optimal transport

$$d\mathbf{Z}_t = \sqrt{\gamma} d\mathbf{W}_t$$

$$\begin{cases} \text{KL}(\mathbf{P}_{\mathbf{X}} \parallel \mathbf{P}_{\mathbf{Z}}) \rightarrow \min; \\ p_{\mathbf{X}_0} = p^{\mathcal{S}}; p_{\mathbf{X}_1} = p^{\mathcal{T}} \end{cases}$$



Optimal transport:
target density + in/out similarity



Stochastic optimal control (SOC)

$$\begin{cases} \mathbb{E}_{\mathbf{p}_f} \left[\int_0^1 V_t(\mathbf{X}_t^f) dt + \beta(\mathbf{X}_1^f) \right] \rightarrow \min_f; \\ d\mathbf{X}_t^f = \left(f_t^{\text{base}}(\mathbf{X}_t^f) + g(t)f_t(\mathbf{X}_t^f) \right) dt + g(t)d\mathbf{W}_t \end{cases}$$

Stochastic optimal control (SOC)

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Environment transition Action

Stochastic optimal control (SOC)

Current reward

Final reward

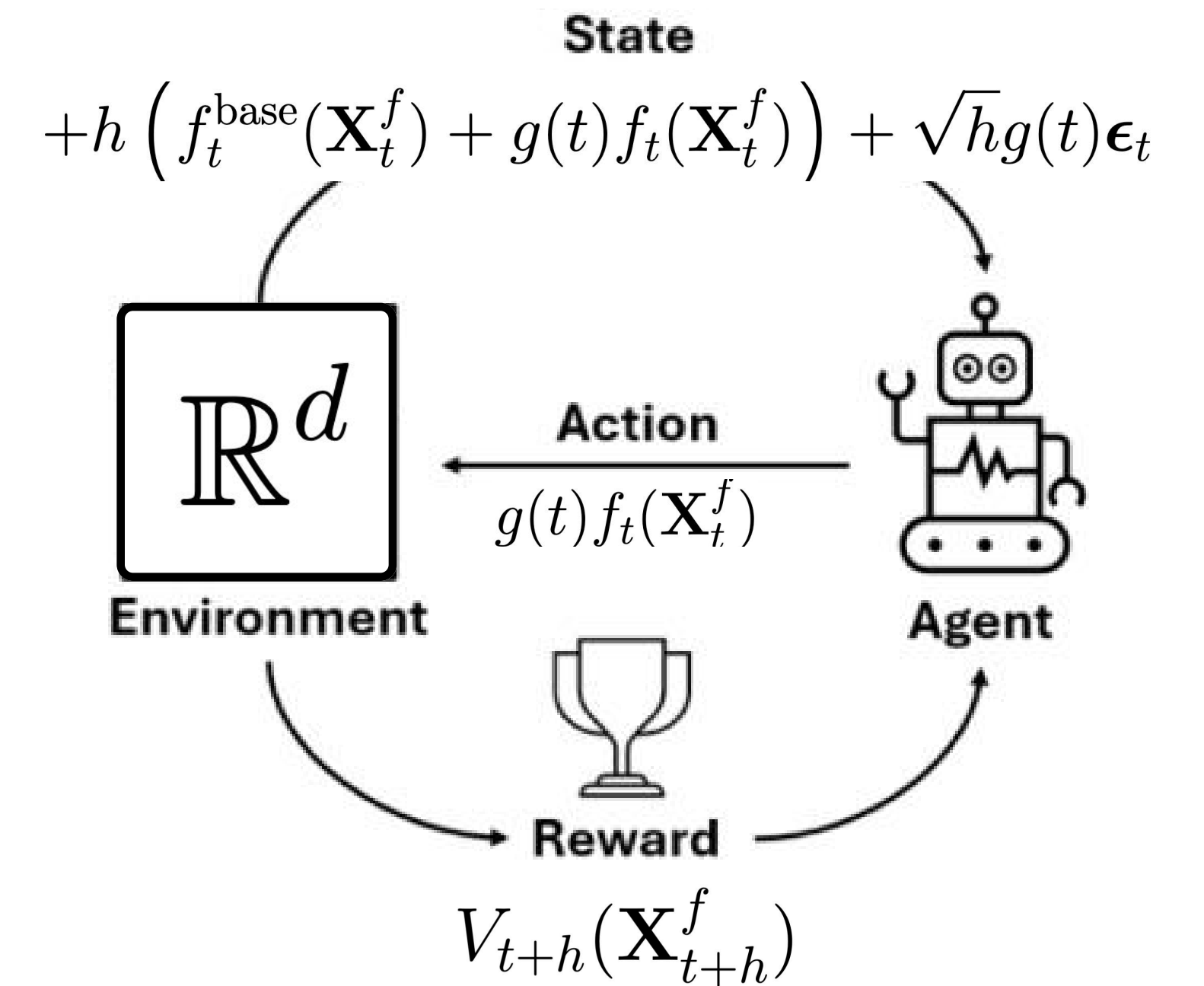
$$\begin{cases} \mathbb{E}_{\mathbf{p}_f} \left[\int_0^1 V_t(\mathbf{X}_t^f) dt + \beta(\mathbf{X}_1^f) \right] \rightarrow \min; \\ d\mathbf{X}_t^f = \left(f_t^{\text{base}}(\mathbf{X}_t^f) + g(t)f_t(\mathbf{X}_t^f) \right) dt + g(t)d\mathbf{W}_t \end{cases}$$

Environment transition

Action

Stochastic optimal control (SOC)

$$\begin{cases} \mathbb{E}_{\mathbf{p}_f} \left[\int_0^1 \text{Current reward } V_t(\mathbf{X}_t^f) dt + \text{Final reward } \beta(\mathbf{X}_1^f) \right] \rightarrow \min; \\ d\mathbf{X}_t^f = \left(\text{Environment transition } f_t^{\text{base}}(\mathbf{X}_t^f) + \text{Action } g(t)f_t(\mathbf{X}_t^f) \right) dt + g(t)d\mathbf{W}_t \end{cases}$$



SB through SOC

$$d\mathbf{Z}_t = f_t^{\text{base}}(\mathbf{Z}_t)dt + \sqrt{\gamma}d\mathbf{W}_t$$

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\Leftrightarrow

$$\begin{cases} \mathbb{E}_{\mathbf{P}^f} \int_0^1 \frac{1}{2} \|f_t(\mathbf{X}_t^f)\|^2 dt \rightarrow \min_f; \\ d\mathbf{X}_t^f = \left(f_t^{\text{base}}(\mathbf{X}_t^f) + g(t)f_t(\mathbf{X}_t^f) \right) dt + g(t)d\mathbf{W}_t; \\ \mathbf{X}_0^f \sim p^{\mathcal{S}}; \mathbf{X}_1^f \sim p^{\mathcal{T}} \end{cases}$$

SB through SOC

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- For some β that defines $p^{\mathcal{T}}$

SB through SOC

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- For some β that defines $p^{\mathcal{T}}$
- β acts as “discriminator”

SB through SOC

$$d\mathbf{Z}_t = f_t^{\text{base}}(\mathbf{Z}_t)dt + \sqrt{\gamma}d\mathbf{W}_t$$

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- For some β that defines $p^{\mathcal{T}}$
- β acts as “discriminator”
- Known for generative modeling and fine-tuning

SOC: typical solutions

$$\begin{cases} \mathbb{E}_{\mathbf{P}^\theta} \left[\int_0^1 \frac{1}{2} \|f_t^\theta(\mathbf{X}_t^\theta)\|^2 dt + \beta(\mathbf{X}_1^\theta) \right] \rightarrow \min_{\theta} \\ d\mathbf{X}_t^\theta = \left(f_t^{\text{base}}(\mathbf{X}_t^\theta) + g(t)f_t^\theta(\mathbf{X}_t^\theta) \right) dt + g(t)d\mathbf{W}_t; \end{cases}$$

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$$\nabla_{\theta} \mathcal{L}(\theta) \approx \nabla_{\theta} \left(\sum_{i=0}^{N-1} \frac{1}{2} \|f_{t_i}^\theta(\mathbf{X}_{t_i}^\theta)\|^2 \Delta t_i + \beta(\mathbf{X}_1^\theta) \right) \quad [4]$$

$$\mathbf{X}_{t_{i+1}}^\theta = \mathbf{X}_{t_i}^\theta + \left(f_{t_i}^{\text{base}}(\mathbf{X}_{t_i}^\theta) + g(t_i)f_{t_i}^\theta(\mathbf{X}_{t_i}^\theta) \right) \Delta t_i + g(t) \sqrt{\Delta t_i} \boldsymbol{\epsilon}_i$$

SOC: typical solutions

$$\begin{cases} \mathbb{E}_{\mathbf{P}^\theta} \left[\int_0^1 \frac{1}{2} \|f_t^\theta(\mathbf{X}_t^\theta)\|^2 dt + \beta(\mathbf{X}_1^\theta) \right] \rightarrow \min_{\theta} \\ d\mathbf{X}_t^\theta = \left(f_t^{\text{base}}(\mathbf{X}_t^\theta) + g(t)f_t^\theta(\mathbf{X}_t^\theta) \right) dt + g(t)d\mathbf{W}_t; \end{cases}$$

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Here: N forward, N backward

SOC: typical solutions

$$\begin{cases} \mathbb{E}_{\mathbf{P}^\theta} \left[\int_0^1 \frac{1}{2} \|f_t^\theta(\mathbf{X}_t^\theta)\|^2 dt + \beta(\mathbf{X}_1^\theta) \right] \rightarrow \min_{\theta} \\ d\mathbf{X}_t^\theta = (f_t^{\text{base}}(\mathbf{X}_t^\theta) + g(t)f_t^\theta(\mathbf{X}_t^\theta)) dt + g(t)d\mathbf{W}_t; \end{cases}$$

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Here: N forward, N backward

Possible: N forward, K backward [5]

SOC: typical solutions

$$\begin{cases} \mathbb{E}_{\mathbf{P}^\theta} \left[\int_0^1 \frac{1}{2} \|f_t^\theta(\mathbf{X}_t^\theta)\|^2 dt + \beta(\mathbf{X}_1^\theta) \right] \rightarrow \min_{\theta} \\ d\mathbf{X}_t^\theta = (f_t^{\text{base}}(\mathbf{X}_t^\theta) + g(t)f_t^\theta(\mathbf{X}_t^\theta)) dt + g(t)d\mathbf{W}_t; \end{cases}$$

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Here: N forward, N backward

Possible: N forward, K backward [5]

Goal: K forward, K backward

References

- [1] Song Y. et al. Score-based generative modeling through stochastic differential equations;
- [2] Stochastic Interpolants: A Unifying Framework for Flows and Diffusions;
- [3] DPOK: Reinforcement Learning for Fine-tuning Text-to-Image Diffusion Models;
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- [5] Adjoint Sampling: Highly Scalable Diffusion Samplers via Adjoint Matching;

[1+] Rakitin D., Oganov A. Diffusion-based Generative Models Course.