

# Fantastic Path RND and Where to Find Them

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# “Density Ratio” and Radon-Nikodym Derivative

👉 Don't freak out about the name Radon-Nikodym Derivative  
--- it's just the “*density ratio*”

👉 Very informally, let  $\mathbf{P}$  and  $\mathbf{Q}$  be two measures with density  $p$  and  $q$ , their density ratio is the **Radon-Nikodym Derivative (RND)**, denoted as

$$\frac{p(x)}{q(x)} = \frac{d\mathbf{P}}{d\mathbf{Q}}(x)$$

👉 The density is essentially the RND w.r.t to Lebesgue measure

$$p(x) = \frac{d\mathbf{P}}{d\mu}(x), q(x) = \frac{d\mathbf{Q}}{d\mu}(x)$$

👉 RND is helpful for spaces without Lebesgue measure

# Stochastic Differential Equations

▶ Forward SDE

$$dX_t = f(X_t, t)dt + \sigma_t dW_t$$

◀ Backward SDE

$$dX_t = g(X_t, t)dt + \sigma_t \overleftarrow{dW_t}$$



Intuitive understanding by **Eular-Maruyama Discretisation:**

$$X_{n+1} - X_n = f(X_n, t_n)\Delta t + \sigma_n \sqrt{\Delta t} \epsilon$$

$$X_{n+1} - X_n = g(X_{n+1}, t_{n+1})\Delta t + \sigma_{n+1} \sqrt{\Delta t} \epsilon'$$

# From Gaussian Density Ratio to Path RND

$$X_{n+1} - X_n = f(X_n, t_n) \Delta t + \sigma_n \sqrt{\Delta t} \epsilon$$

❓ for a **discretised** path sample  $\{X_1, X_2, \dots, X_N\}$ , what is its density?

✓ **Transition density:**  $p(X_{n+1}|X_n) = N(X_{n+1}|X_n + f(X_n, t_n) \Delta t, \sigma_n^2 \Delta t)$

✓ **Full path density:**  $p(X_1, X_2, \dots, X_N) = p(X_1) \prod p(X_{n+1}|X_n)$

# From Gaussian Density Ratio to Path RND

Now take a closer look at

$$N(X_{n+1}|X_n + f(X_n, t_n)\Delta t, \sigma_n^2\Delta t)$$

$$\log p = \frac{-(\sigma_n \sqrt{\Delta t} \epsilon)^2}{2\sigma_n^2 \Delta t} - \log \sigma_n - \boxed{\frac{1}{2} \log \Delta t} + C$$



density diverge when  $\Delta t \rightarrow 0$

# From Gaussian Density Ratio to Path RND

But what if we have another SDE:

$$p_1 = N(X_{n+1}|X_n + f(X_n, t_n)\Delta t, \sigma_n^2 \Delta t)$$

$$p_2 = N(X_{n+1}|X_n + h(X_n, t_n)\Delta t, \sigma_n^2 \Delta t)$$

$$\log p_1 - \log p_2 = \frac{(2X_{n+1} - 2X_n - h\Delta t - f\Delta t)(h\Delta t - f\Delta t)}{2\sigma_n^2 \Delta t}$$

😎 density ratio did NOT diverge when  $\Delta t \rightarrow 0$

# From Gaussian Density Ratio to Path RND

For solution  $X$  to one SDE:  $dX_t = f(X_t, t)dt + \sigma_t dW_t,$

**we cannot define its density**  $p(X_0) \prod p(X_{t+dt} | X_t)$

But with another SDE:  $dX_t = h(X_t, t)dt + \sigma_t dW_t,$

**we can define density ratio (Radon-Nikodym Derivative) as a whole:**

$$\frac{dP}{dQ}(X)$$

# Forward-forward RND and Girsanov

$$\begin{aligned}\mathbf{P} : \mathrm{d}X_t &= f(X_t, t)\mathrm{d}t + \sigma_t \mathrm{d}W_t, X_0 \sim p_0 \\ \mathbf{Q} : \mathrm{d}X_t &= h(X_t, t)\mathrm{d}t + \sigma_t \mathrm{d}W_t, X_0 \sim q_0\end{aligned}$$

$$\frac{\mathrm{d}\mathbf{P}}{\mathrm{d}\mathbf{Q}}(X) \approx \frac{p(X_0) \prod N_1(X_{n+1}|X_n)}{q(X_0) \prod N_2(X_{n+1}|X_n)}$$

# Forward-forward RND and Girsanov

$$\begin{aligned}\mathbf{P} : \mathrm{d}X_t &= f(X_t, t)dt + \sigma_t \mathrm{d}W_t, X_0 \sim p_0 \\ \mathbf{Q} : \mathrm{d}X_t &= h(X_t, t)dt + \sigma_t \mathrm{d}W_t, X_0 \sim q_0\end{aligned}$$

$$\frac{\mathrm{d}\mathbf{P}}{\mathrm{d}\mathbf{Q}}(X) = \frac{p(X_0)}{q(X_0)} \exp \left( \underbrace{\int \frac{f_t(X_t)}{\sigma_t^2} \cdot \mathrm{d}X_t - \frac{f_t^2(X_t)}{2\sigma_t^2} dt - \int \frac{g_t(X_t)}{\sigma_t^2} \cdot \mathrm{d}X_t + \frac{g_t^2(X_t)}{2\sigma_t^2} dt}_{\text{Forward Ito Integral } \int a_t(X_t) \cdot \mathrm{d}X_t = \lim \sum a_n(X_n) \cdot (X_{n+1} - X_n)} \right)$$

Initial density ratio

# Forward-backward RND

$$\begin{aligned}\mathbf{P} : \mathrm{d}X_t &= f(X_t, t)dt + \sigma_t \overleftarrow{\mathrm{d}W}_t, X_0 \sim p_0 \\ \overleftarrow{\mathbf{Q}} : \mathrm{d}X_t &= g(X_t, t)dt + \sigma_t \overleftarrow{\mathrm{d}W}_t, X_1 \sim q_1\end{aligned}$$

$$\frac{\mathrm{d}\mathbf{P}}{\mathrm{d}\overleftarrow{\mathbf{Q}}}(X) \approx \frac{p_0(X_0) \prod N_1(X_{n+1}|X_n)}{q_1(X_1) \prod N_2(X_n|X_{n+1})}$$

# Forward-backward RND

$$\begin{aligned}\mathbf{P} : dX_t &= f(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_0 \sim p_0 \\ \overleftarrow{\mathbf{Q}} : dX_t &= g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_1 \sim q_1\end{aligned}$$

$$\frac{d\mathbf{P}}{d\overleftarrow{\mathbf{Q}}}(X) = \frac{p_0(X_0)}{q_1(X_1)} \exp \left( \int \underbrace{\frac{f_t(X_t)}{\sigma_t^2} \cdot dX_t - \frac{f_t^2(X_t)}{2\sigma_t^2} dt}_{\text{Initial densities}} - \int \underbrace{\frac{g_t(X_t)}{\sigma_t^2} \cdot \overleftarrow{dX}_t + \frac{g_t^2(X_t)}{2\sigma_t^2} dt}_{\text{Backward Ito Integral}} \right)$$

$$\int a_t(X_t) \cdot \overleftarrow{dX}_t = \lim \sum a_{n+1}(X_{n+1}) \cdot (X_{n+1} - X_n)$$

# Forward-backward RND

$$\begin{aligned} \mathbf{P} : dX_t &= f(X_t, t)dt + \sigma_t dW_t, X_0 \sim p_0 \\ \mathbf{\bar{Q}} : dX_t &= g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_1 \sim q_1 \end{aligned}$$

$$\frac{dP}{d\tilde{Q}}(X) = \frac{p_0(X_0)}{q_1(X_1)} \exp \left( \int \frac{f_t(X_t)}{\sigma_t^2} \cdot dX_t - \frac{f_t^2(X_t)}{2\sigma_t^2} dt - \int \frac{g_t(X_t)}{\sigma_t^2} \cdot \overleftarrow{dX}_t + \frac{g_t^2(X_t)}{2\sigma_t^2} dt \right)$$

Initial densities
lim  $\frac{\prod N_1(X_{n+1}|X_n)}{\prod N_2(X_n|X_{n+1})}$

# A Side Note on Stochastic Integrals

Ito forward integral

$$\int a_t(X_t) \cdot dX_t = \lim \sum a_n(X_n) \cdot (X_{n+1} - X_n)$$

Ito backward integral

$$\int a_t(X_t) \cdot \overleftarrow{dX_t} = \lim \sum a_{n+1}(X_{n+1}) \cdot (X_{n+1} - X_n)$$

Stratonovich integral

$$\int a_t(X_t) \circ dX_t = \lim \sum \frac{a_n(X_n) + a_{n+1}(X_{n+1})}{2} \cdot (X_{n+1} - X_n)$$

# A Side Note on Stochastic Integrals

Ito forward integral

$$\int a_t(X_t) \cdot dX_t = \lim \sum a_n(X_n) \cdot (X_{n+1} - X_n)$$

Ito backward integral

$$\int a_t(X_t) \cdot \overleftarrow{dX_t} = \lim \sum a_{n+1}(X_{n+1}) \cdot (X_{n+1} - X_n)$$

Conversion rule:

$$\int a_t(X_t) \cdot dX_t - \int a_t(X_t) \cdot \overleftarrow{dX_t} = - \int \sigma_t^2 \nabla \cdot a_t dt$$

# Time-reversal and Nelson's relation

$$\begin{aligned}\mathbf{P} : \mathrm{d}X_t &= f(X_t, t)dt + \sigma_t \overleftarrow{\mathrm{d}W}_t, X_0 \sim p_0 \\ \overleftarrow{\mathbf{Q}} : \mathrm{d}X_t &= g(X_t, t)dt + \sigma_t \overleftarrow{\mathrm{d}W}_t, X_1 \sim p_1\end{aligned}$$

$$\overleftarrow{\mathbf{Q}} = \mathbf{P}, \text{ i. e., } \frac{\overleftarrow{\mathrm{d}\mathbf{Q}}}{\mathrm{d}\mathbf{P}} = 1$$

iff

$$g(\cdot, t) = f(\cdot, t) - \sigma_t^2 \nabla \log p_t(\cdot)$$

# Time-reversal and Nelson's relation

$$\begin{aligned}\mathbf{P} : dX_t &= f(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_0 \sim p_0 \\ \overleftarrow{\mathbf{Q}} : dX_t &= g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_1 \sim p_1\end{aligned}$$

$$\overleftarrow{\mathbf{Q}} = \mathbf{P}, \text{ i. e., } \frac{\overleftarrow{d\mathbf{Q}}}{d\mathbf{P}} = 1$$

iff

$$g(\cdot, t) = f(\cdot, t) - \sigma_t^2 \nabla \log p_t(\cdot)$$

e.g., 0 in VE process      score

# Where to Find Path RND?

Path RND is no different than other Density Ratios

- 👉 You can do **Importance Sampling**
- 👉 You can do **Variational Inference**

lead to a variety of methods!

# Importance Sampling with Path RND

**Importance Sampling:**

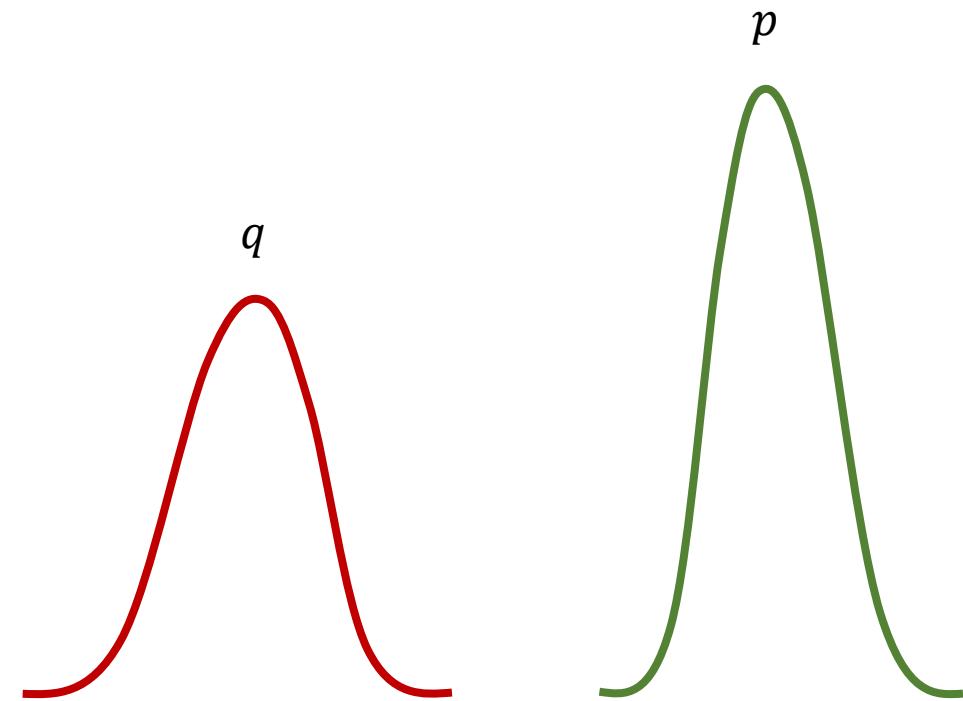
$$\mathbf{E}_{x \sim p}[f(x)] = \mathbf{E}_{x \sim q} \left[ \frac{p(x)}{q(x)} f(x) \right]$$

**Importance Sampling in Path space:**

$$\mathbf{E}_{X \sim \mathbf{P}}[f(X)] = \mathbf{E}_{X \sim \mathbf{Q}} \left[ \frac{d\mathbf{P}}{d\mathbf{Q}}(X) f(X) \right]$$

# Importance Sampling with Path RND: AIS

Estimate:  $\mathbf{E}_{x \sim p}[f(x)]$  with proposal  $q$



# Importance Sampling with Path RND: AIS

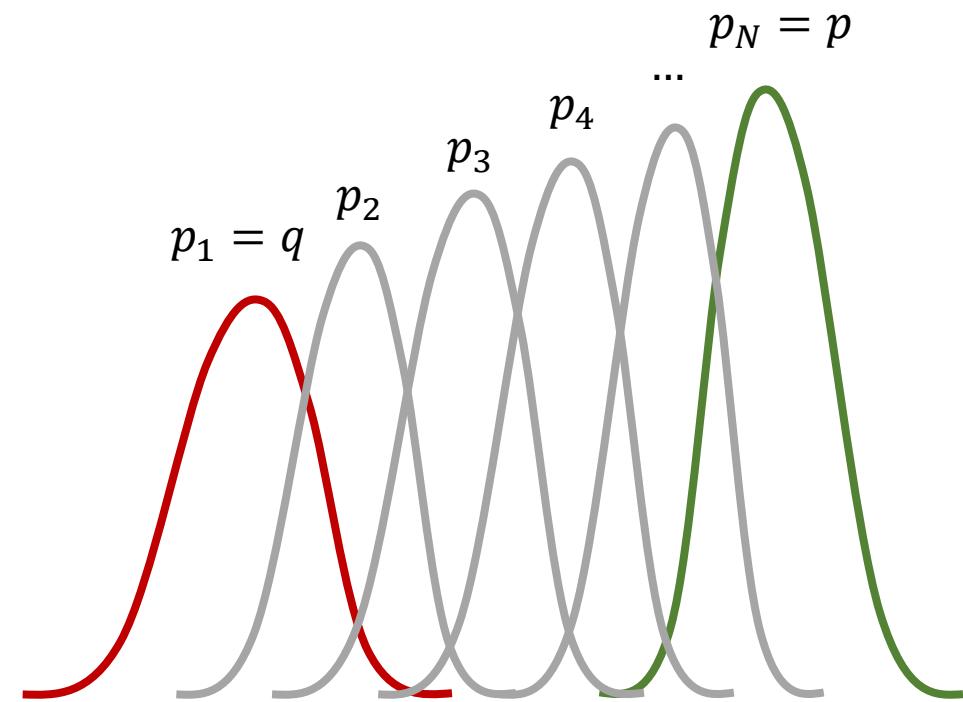
Estimate:  $\mathbf{E}_{x \sim p}[f(x)]$  with proposal  $q$

$X_1 \sim p_1$      $X_t \sim \text{MCMC}_{p_t}(X_{t-1})$     “Forward Process”

$X_N \sim p_N$      $X_{t-1} \sim \text{MCMC}_{p_t}(X_t)$     “Backward Process”

$$\begin{aligned}\mathbf{E}_{x \sim p}[f(x)] &= \int f(x_N) p(x_N) \prod p(x_{n-1} | x_n) dx \\ &= \int \frac{f(x_N) p(x_N) \prod p(x_{n-1} | x_n)}{q(x_1) \prod p(x_n | x_{n-1})} q(x_1) \prod p(x_n | x_{n-1}) dx\end{aligned}$$

Proposal



# Importance Sampling with Path RND: AIS

Estimate:  $\mathbf{E}_{x \sim p}[f(x)]$  with proposal  $q$

$$X_1 \sim p_1$$

$$X_N \sim p_N$$

$$X_t \sim \text{ULA}(X_{t-1})$$

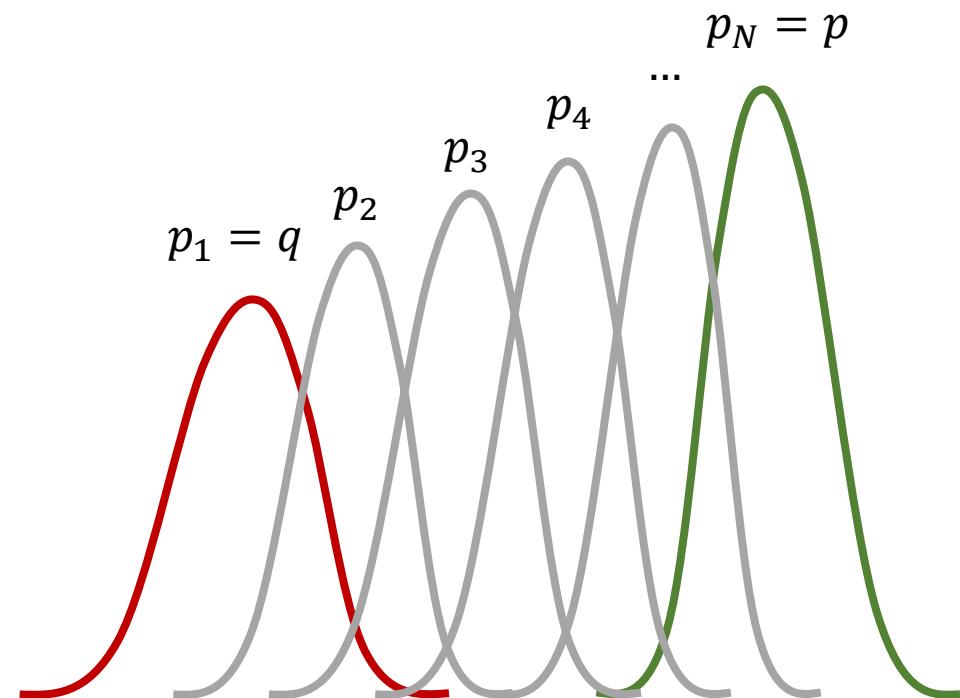
$$X_{t-1} \sim \text{ULA}(X_t)$$

“Forward Process”

“Backward Process”

$$\begin{aligned} \mathbf{E}_{x \sim p}[f(x)] &= \int f(x_N) p(x_N) \prod N(x_{n-1} | x_n) dx \\ &= \int \frac{f(x_N) p(x_N) \prod N(x_{n-1} | x_n)}{q(x_1) \prod N(x_n | x_{n-1})} q(x_1) \prod N(x_n | x_{n-1}) dx \end{aligned}$$

Proposal



# Importance Sampling with Path RND: AIS

Estimate:  $\mathbf{E}_{x \sim p}[f(x)]$  with proposal  $q$

$$X_1 \sim p_1$$

$$X_t \sim \text{ULA}(X_{t-1})$$

“Forward Process”

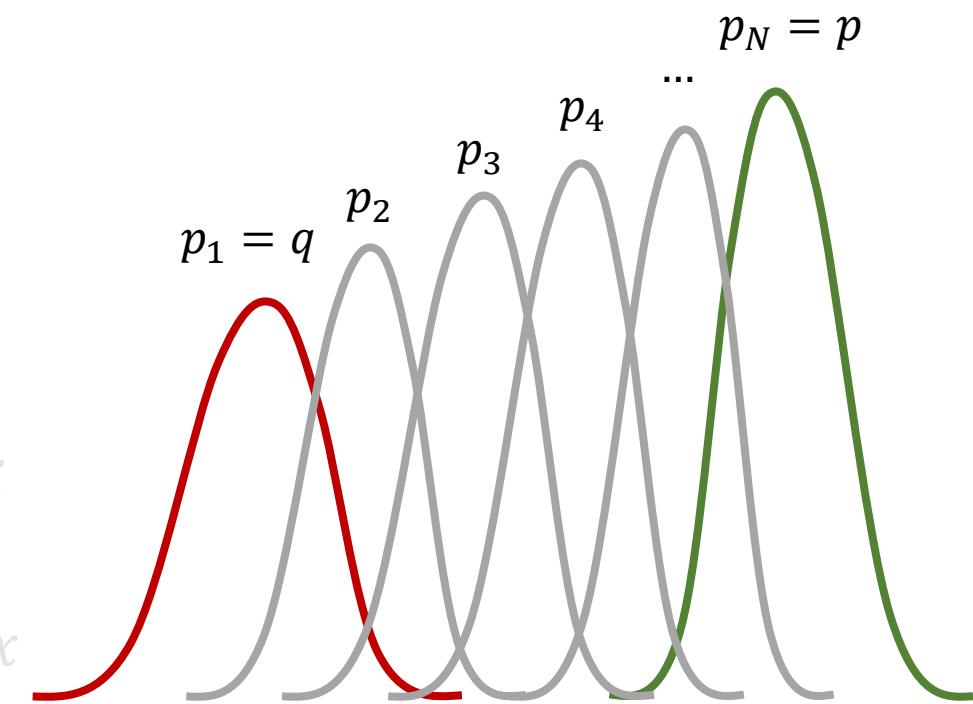
$$X_N \sim p_N$$

$$X_{t-1} \sim \text{ULA}(X_t)$$

“Backward Process”

Taking the limit... ( $\infty$  intermediate distributions)

$$\begin{aligned}\mathbf{E}_{x \sim p}[f(x)] &= \int f(x_N) p(x_N) \prod N(x_{n-1} | x_n) dx \\ &= \int f(x_N) \frac{p(x_N) \prod N(x_{n-1} | x_n)}{q(x_1) \prod N(x_n | x_{n-1})} q(x_1) \prod N(x_n | x_{n-1}) dx\end{aligned}$$



# Importance Sampling with Path RND: AIS

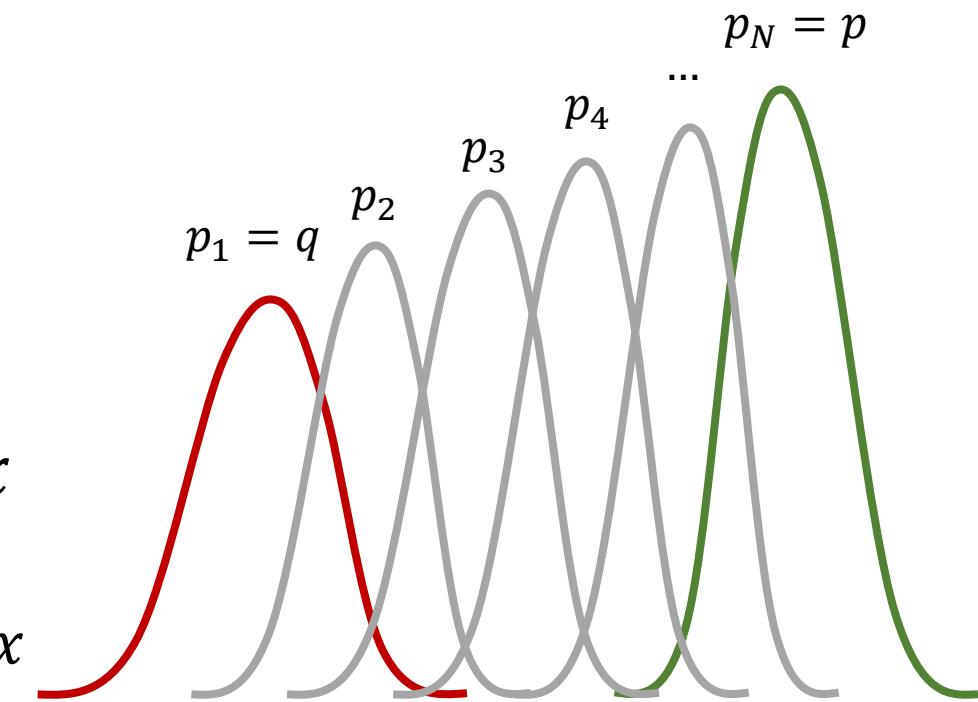
Estimate:  $\mathbf{E}_{x \sim p}[f(x)]$  with proposal  $q$

$$X_1 \sim q = p_1 \quad X_t \sim \text{ULA}(X_{t-1}) \quad \text{"Forward Process"}$$

$$X_N \sim p = p_N \quad X_{t-1} \sim \text{ULA}(X_t) \quad \text{"Backward Process"}$$

$$\mathbf{E}_{x \sim p}[f(x)] = \int f(x_N) p(x_N) \prod N(x_{n-1} | x_n) dx$$

$$= \int f(x_N) \frac{p(x_N) \prod N(x_{n-1} | x_n)}{q(x_1) \prod N(x_n | x_{n-1})} q(x_1) \prod N(x_n | x_{n-1}) dx$$



# Importance Sampling with Path RND: AIS

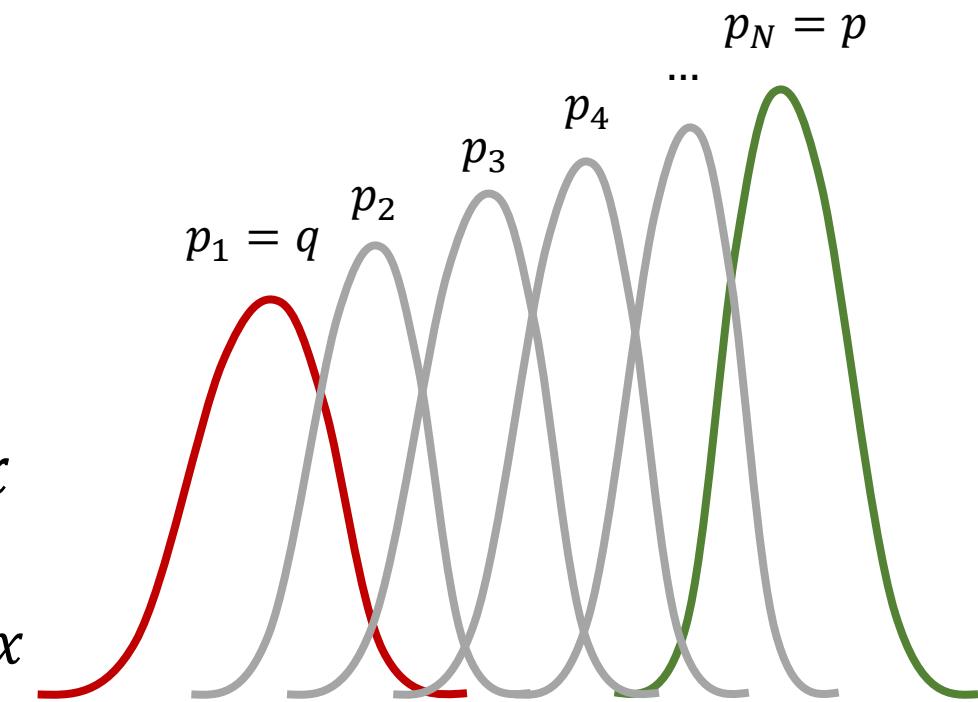
Estimate:  $\mathbf{E}_{x \sim p}[f(x)]$  with proposal  $q$

$$X_1 \sim q = p_1 \quad X_t \text{ d}X_t = -\sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overrightarrow{dW_t} \text{ "forward process"}$$

$$X_N \sim p = p_N \quad X_{t-1} \text{ d}X_t = \sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overleftarrow{dW_t} \text{ "backward process"}$$

$$\mathbf{E}_{x \sim p}[f(x)] = \int f(x_N) p(x_N) \prod N(x_{n-1} | x_n) dx$$

$$= \int f(x_N) \frac{p(x_N) \prod N(x_{n-1} | x_n)}{q(x_1) \prod N(x_n | x_{n-1})} q(x_1) \prod N(x_n | x_{n-1}) dx$$



# Importance Sampling with Path RND: AIS

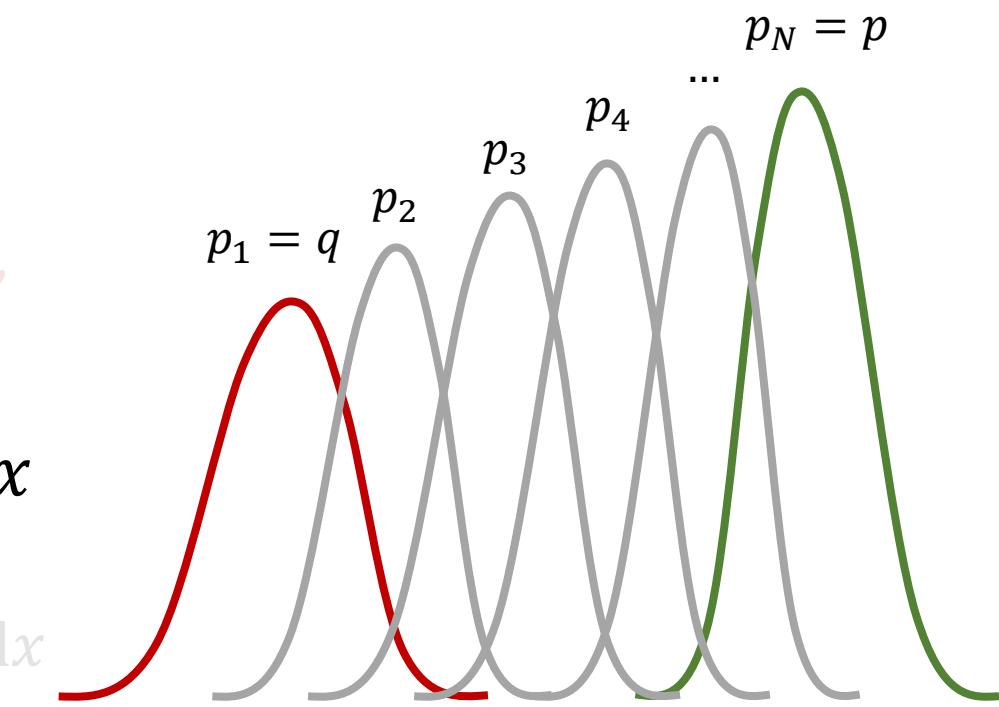
Estimate:  $\mathbf{E}_{x \sim p}[f(x)]$  with proposal  $q$

$$X_1 \sim q = p_1 \quad X_t \quad dX_t = -\sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overrightarrow{dW_t} \text{ "forward process"}$$

$$X_N \sim p = p_N \quad X_{t-1} \quad dX_t = \sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overleftarrow{dW_t} \text{ "backward process"}$$

$$\mathbf{E}_{x \sim p}[f(x)] = \int f(x_N) p(x_N) \prod N(x_{n-1} | x_n) dx$$

$$= \int f(x_N) \frac{p(x_N) \prod \overleftarrow{dP} x_{n-1} | x_n}{q(x_1) \prod \overline{dQ} x_n | x_{n-1}} q(x_1) \prod N(dQ | x_{n-1}) dx$$



$$\mathbf{E}_{X \sim P}[f(X)] = \mathbf{E}_{X \sim Q} \left[ \frac{dP}{dQ}(X) f(X) \right]$$

# From AIS to Jarzynski Equation & Crooks Theorem

$$X_0 \sim q \quad dX_t = -\sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overrightarrow{dW_t},$$

$$X_1 \sim p \quad dX_t = \sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overleftarrow{dW_t},$$

$$\frac{\overleftarrow{dP}}{\overrightarrow{dQ}} =$$

# From AIS to Jarzynski Equation & Crooks Theorem

$$X_0 \sim q \quad dX_t = -\sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overrightarrow{dW_t},$$

$$X_1 \sim p \quad dX_t = \sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overleftarrow{dW_t},$$

$$\frac{\overleftarrow{dP}}{dQ} = \frac{p(X_1)}{q(X_0)} \exp \left( \int \frac{\nabla U_t}{2} \cdot dX_t + \frac{\sigma_t^2}{4} |\nabla U_t|^2 dt + \int \frac{\nabla U_t}{2} \cdot \overleftarrow{dX_t} - \frac{\sigma_t^2}{4} |\nabla U_t|^2 dt \right)$$

# From AIS to Jarzynski Equation & Crooks Theorem

$$X_0 \sim q \quad dX_t = -\sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overrightarrow{dW_t},$$

$$X_1 \sim p \quad dX_t = \sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overleftarrow{dW_t},$$

$$\begin{aligned}\frac{\overleftarrow{dP}}{dQ} &= \frac{p(X_1)}{q(X_0)} \exp \left( \int \frac{\nabla U_t}{2} \cdot dX_t + \frac{\sigma_t^2}{4} |\nabla U_t|^2 dt + \int \frac{\nabla U_t}{2} \cdot \overleftarrow{dX_t} - \frac{\sigma_t^2}{4} |\nabla U_t|^2 dt \right) \\ &= \frac{p(X_1)}{q(X_0)} \exp \left( \int \frac{\nabla U_t}{2} \cdot dX_t + \int \frac{\nabla U_t}{2} \cdot \overleftarrow{dX_t} \right)\end{aligned}$$

# From AIS to Jarzynski Equation & Crooks Theorem

$$X_0 \sim q \quad dX_t = -\sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overrightarrow{dW_t},$$

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$$\begin{aligned}\frac{\overleftarrow{dP}}{dQ} &= \frac{p(X_1)}{q(X_0)} \exp \left( \int \frac{\nabla U_t}{2} \cdot dX_t + \frac{\sigma_t^2}{4} |\nabla U_t|^2 dt + \int \frac{\nabla U_t}{2} \cdot \overleftarrow{dX_t} - \frac{\sigma_t^2}{4} |\nabla U_t|^2 dt \right) \\ &= \frac{p(X_1)}{q(X_0)} \exp \left( \int \frac{\nabla U_t}{2} \cdot dX_t + \int \frac{\nabla U_t}{2} \cdot \overleftarrow{dX_t} \right)\end{aligned}$$

👉 conversion rule

# From AIS to Jarzynski Equation & Crooks Theorem

$$X_0 \sim q \quad dX_t = -\sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overrightarrow{dW_t},$$

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$$\begin{aligned}\frac{\overleftarrow{dP}}{dQ} &= \frac{p(X_1)}{q(X_0)} \exp \left( \int \frac{\nabla U_t}{2} \cdot dX_t + \frac{\sigma_t^2}{4} |\nabla U_t|^2 dt + \int \frac{\nabla U_t}{2} \cdot \overleftarrow{dX_t} - \frac{\sigma_t^2}{4} |\nabla U_t|^2 dt \right) \\ &= \frac{p(X_1)}{q(X_0)} \exp \left( \int \frac{\nabla U_t}{2} \cdot dX_t + \int \frac{\nabla U_t}{2} \cdot \overleftarrow{dX_t} \right) \quad \text{👉 conversion rule} \\ &= \frac{p(X_1)}{q(X_0)} \exp \left( \int \nabla U_t \cdot dX_t + \int \sigma_t^2 \Delta U_t dt \right)\end{aligned}$$

# From AIS to Jarzynski Equation & Crooks Theorem

$$X_0 \sim q \quad dX_t = -\sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overrightarrow{dW_t},$$

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$$\frac{\overleftarrow{dP}}{dQ} = \frac{p(X_1)}{q(X_0)} \exp \left( \int \nabla U_t \cdot dX_t + \int \sigma_t^2 \Delta U_t dt \right)$$

# From AIS to Jarzynski Equation & Crooks Theorem

$$X_0 \sim q \quad dX_t = -\sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overrightarrow{dW_t},$$

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$$\frac{\overleftarrow{dP}}{dQ} = \frac{p(X_1)}{q(X_0)} \exp \left( \int \nabla U_t \cdot dX_t + \int \sigma_t^2 \Delta U_t dt \right)$$

👉 Ito's lemma

$$df_t(X_t) = (\partial_t f(X_t) + \sigma_t^2 \Delta f) dt + \nabla U_t \cdot dX_t$$

# From AIS to Jarzynski Equation & Crooks Theorem

$$X_0 \sim q \quad dX_t = -\sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overrightarrow{dW_t},$$

$$X_1 \sim p \quad dX_t = \sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overleftarrow{dW_t},$$

$$\begin{aligned}\frac{\overleftarrow{dP}}{dQ} &= \frac{p(X_1)}{q(X_0)} \exp \left( \int \nabla U_t \cdot dX_t + \int \sigma_t^2 \Delta U_t dt \right) \\ &= \frac{p(X_1)}{q(X_0)} \exp \left( \int dU_t(X_t) - \partial_t U_t(X_t) dt \right)\end{aligned}$$

# From AIS to Jarzynski Equation & Crooks Theorem

$$X_0 \sim q \quad dX_t = -\sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overrightarrow{dW_t},$$

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$$\begin{aligned}\frac{\overleftarrow{dP}}{dQ} &= \frac{p(X_1)}{q(X_0)} \exp \left( \int \nabla U_t \cdot dX_t + \int \sigma_t^2 \Delta U_t dt \right) \\ &= \frac{p(X_1)}{q(X_0)} \exp \left( \int dU_t(X_t) - \partial_t U_t(X_t) dt \right) \\ &= \frac{p(X_1)}{q(X_0)} \exp \left( U_1(X_1) - U_0(X_0) + \int -\partial_t U_t(X_t) dt \right)\end{aligned}$$

# From AIS to Jarzynski Equation & Crooks Theorem

$$X_0 \sim q \quad dX_t = -\sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overrightarrow{dW_t},$$

$$X_1 \sim p \quad dX_t = \sigma^2 \nabla U_t(X_t) dt + \sigma \sqrt{2} \overleftarrow{dW_t},$$

$$\begin{aligned}\frac{\overleftarrow{dP}}{dQ} &= \frac{p(X_1)}{q(X_0)} \exp \left( \int \nabla U_t \cdot dX_t + \int \sigma_t^2 \Delta U_t dt \right) \\ &= \frac{p(X_1)}{q(X_0)} \exp \left( \int dU_t(X_t) - \partial_t U_t(X_t) dt \right) \\ &= \frac{Z_0 \exp(-U_1(X_1))}{Z_1 \exp(-U_0(X_0))} \exp \left( U_1(X_1) - U_0(X_0) + \int -\partial_t U_t(X_t) dt \right)\end{aligned}$$

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Crooks Fluctuation Theorem

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Crooks Fluctuation Theorem

$$E_Q \left[ \frac{\overleftarrow{dP}}{dQ} \right] = E_Q \left[ \frac{Z_0}{Z_1} \exp \left( \int -\partial_t U_t(X_t) dt \right) \right] = 1$$

# From AIS to Jarzynski Equation & Crooks Theorem

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Crooks Fluctuation Theorem

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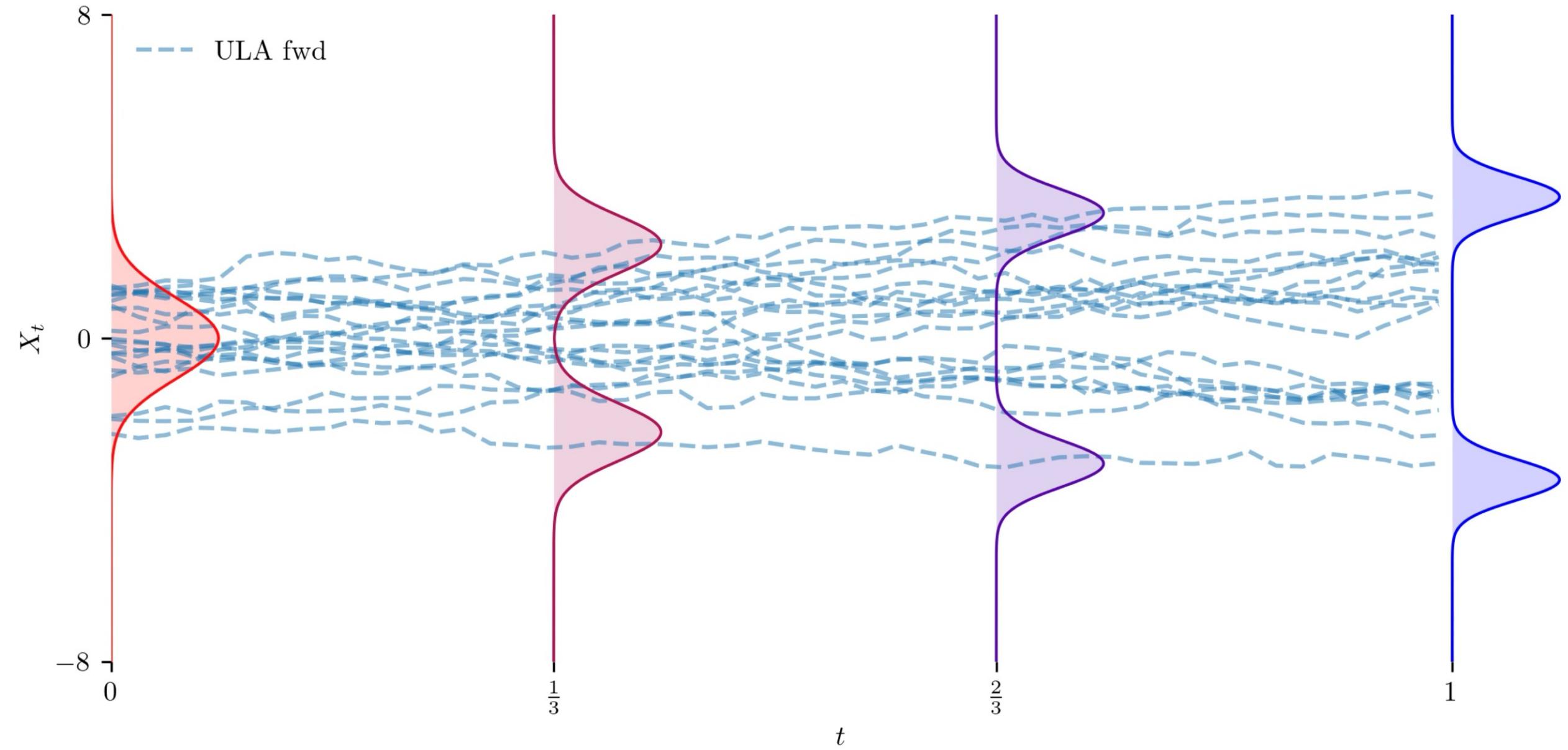
Jarzynski Equation

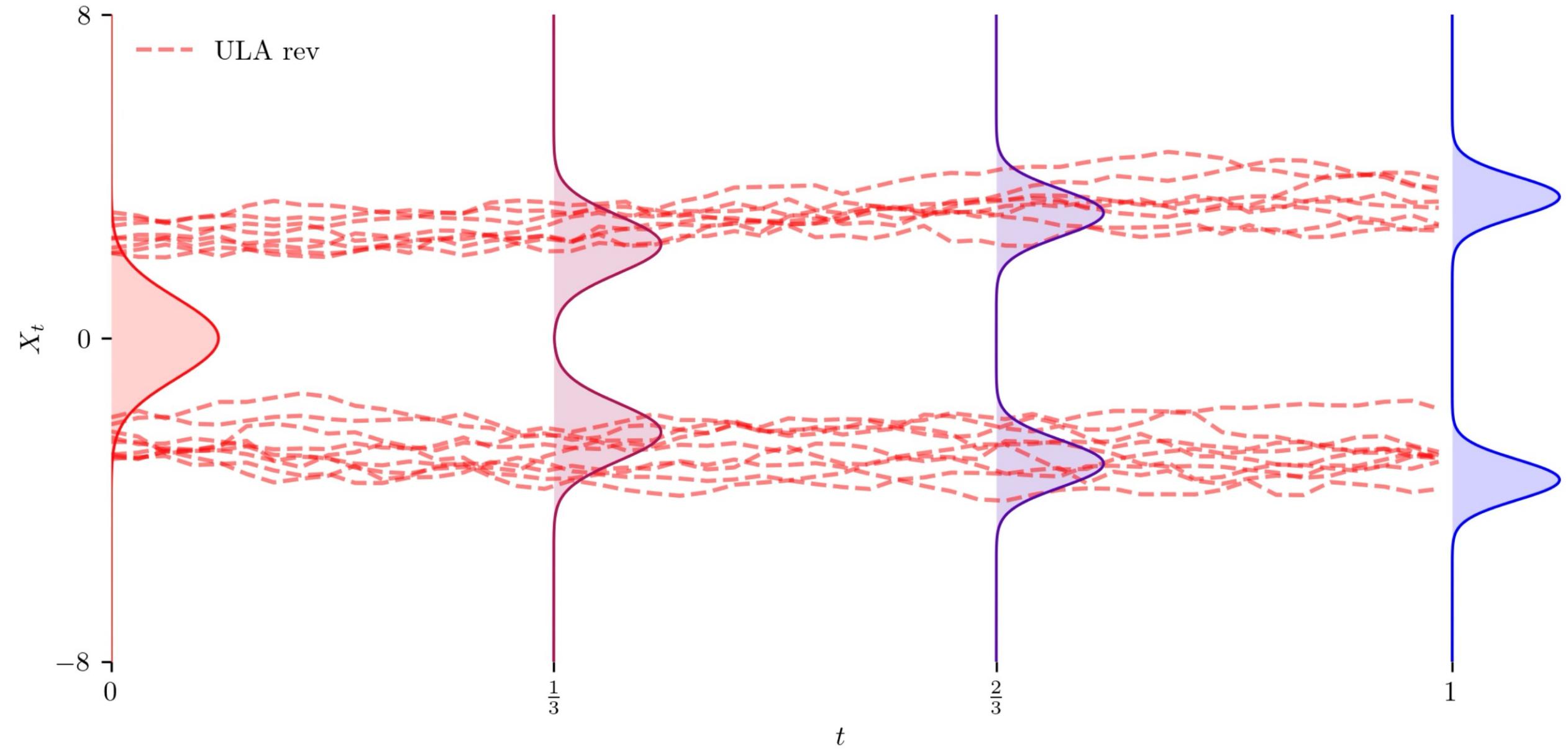
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The evolving of samples is slower than that of energy



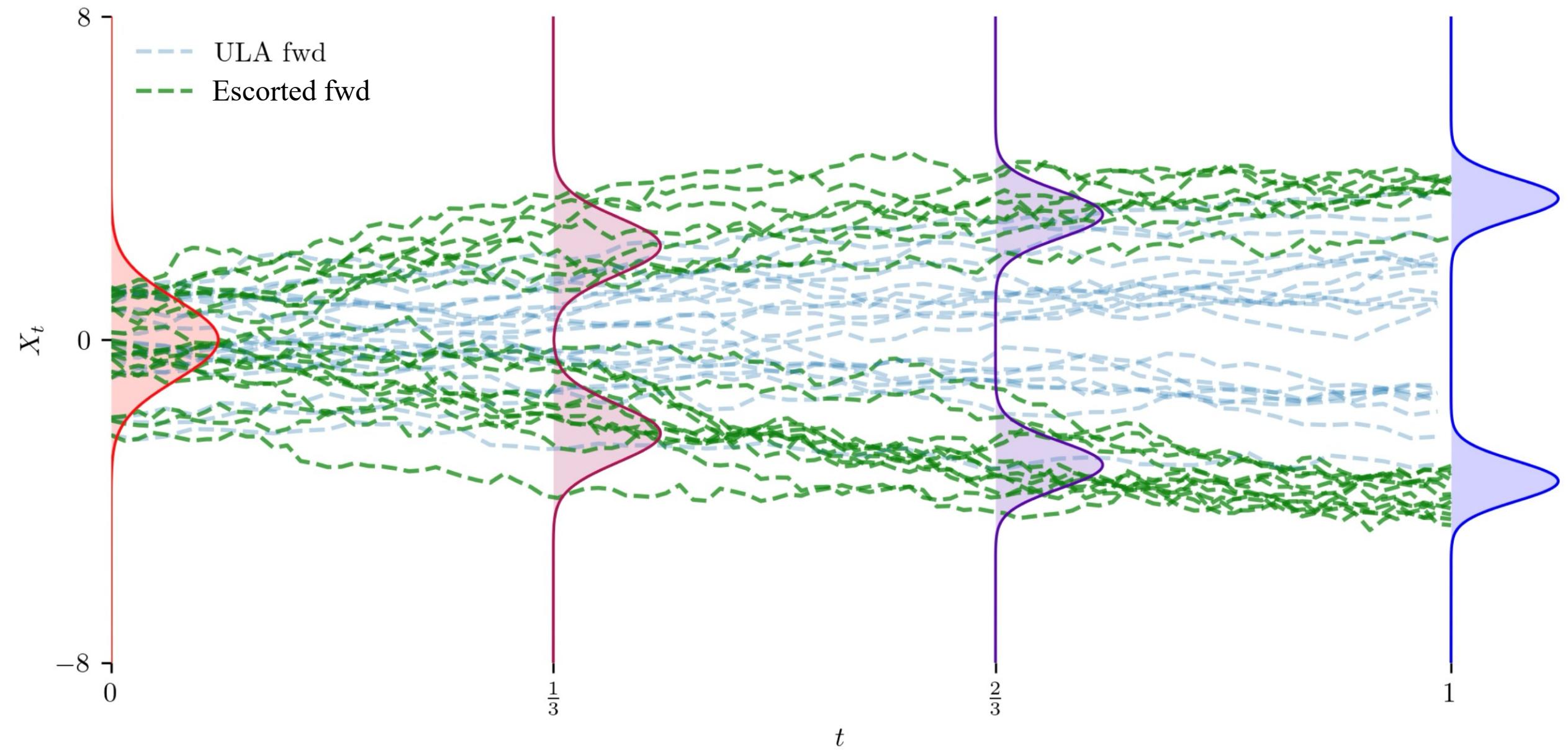


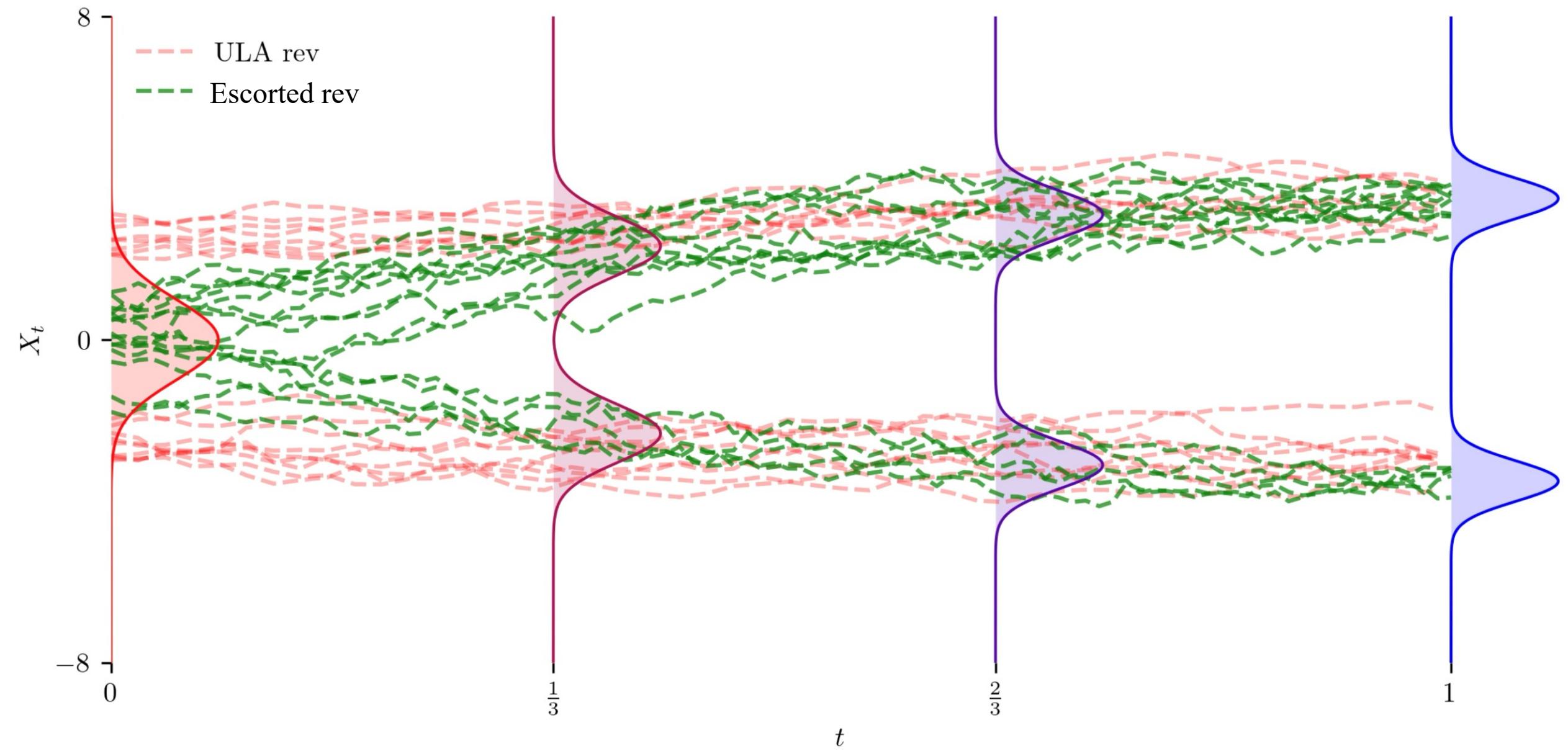
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The evolving of samples is closer to than that of energy





# From Jarzynski to Escorted Jarzynski

$$X_0 \sim q \quad dX_t = [-\sigma^2 \nabla U_t(X_t) + \color{red} u_t(X_t)] dt + \sigma \sqrt{2} \overrightarrow{dW_t},$$

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$$\frac{\overleftarrow{dP}}{dQ} =$$

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$$\frac{\overleftarrow{dP}}{dQ} = \frac{p(X_1)}{q(X_0)} \exp \left( \int \frac{\sigma^2 \nabla U_t - u_t}{2\sigma^2} \cdot dX_t + \frac{1}{4\sigma_t^2} |\sigma_t^2 \nabla U_t - u_t|^2 dt + \int \frac{\sigma^2 \nabla U_t + u_t}{2\sigma^2} \cdot \overleftarrow{dX_t} - \frac{1}{4\sigma_t^2} |\sigma_t^2 \nabla U_t + u_t|^2 dt \right)$$

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...conversion rule...

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...cancel  $U_1$  and  $U_0$ ...

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$$\frac{\overleftarrow{dP}}{dQ} = \frac{Z_0}{Z_1} \exp \left( \int -\partial_t U_t(X_t) dt - \nabla U_t \cdot u_t dt + \nabla \cdot u_t dt \right)$$

# From Jarzynski to Escorted Jarzynski

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Controlled Crooks Fluctuation Theorem

# From Jarzynski to Escorted Jarzynski

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💡 Controlled Crooks Fluctuation Theorem

$$E_Q \left[ \exp \left( \int -\partial_t U_t(X_t) dt - \nabla U_t \cdot u_t dt + \nabla \cdot u_t dt \right) \right] = \frac{Z_1}{Z_0}$$

💡 Escorted Jarzynski Equation

# From Jarzynski to Escorted Jarzynski

$$X_0 \sim q \quad dX_t = [-\sigma^2 \nabla U_t(X_t) + u_t(X_t)]dt + \sigma\sqrt{2} \overrightarrow{dW_t},$$

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Controlled Crooks Fluctuation Theorem

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Escorted Jarzynski Equation

Can also be derived via PDEs [1] / Feynman-Kac formula [2]:

[1] Albergo, M. S., & Vanden-Eijnden, E (2025). NETS: A Non-equilibrium Transport Sampler. *ICML 2025*.

[2] Skreta, M., Akhound-Sadegh, T., Ohanesian, V., Bondesan, R., Aspuru-Guzik, A., Doucet, A., ... & Neklyudov, K. (2025). Feynman-kac correctors in diffusion: Annealing, guidance, and product of experts. *ICML 2025*.

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**Question: How to find  $u_t$ ?**

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**Question: How to find  $u_t$ ?**

👉 Setting 1: access sample for  $q$  + density of  $q$  + energy of  $p$  (neural samplers)

# From Jarzynski to Escorted Jarzynski

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💡 match the forward & backward process

# From Jarzynski to Escorted Jarzynski

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- 💡 match the forward & backward process
- 💡 match the marginal  $p_t$  of sampling process to  $U_t$

# From Jarzynski to Escorted Jarzynski

$$X_0 \sim q \quad dX_t = [-\sigma^2 \nabla U_t(X_t) + u_t(X_t)]dt + \sigma\sqrt{2} \overrightarrow{dW_t},$$

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💡 match the forward & backward process

👉 CMCD [1]

💡 match the marginal  $p_t$  of sampling process to  $U_t$

👉 NETS [2]

[1] Vargas, F., Padhy, S., Blessing, D., & Nüsken, N. (2024). Transport meets variational inference: Controlled monte carlo diffusions. *ICLR 2024*.

[2] Albergo, M. S., & Vanden-Eijnden, E. (2025). Nets: A non-equilibrium transport sampler. *ICML 2025*.

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👉 Setting 2: access sample and energy for  $q$  and  $p$  (e.g., aim to estimate  $Z_0/Z_1$ )

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[2] Albergo, M. S., & Vanden-Eijnden, E. (2025). Nets: A non-equilibrium transport sampler. *ICML 2025*.

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[1] Vargas, F., Padhy, S., Blessing, D., & Nüsken, N. (2024). Transport meets variational inference: Controlled monte carlo diffusions. *ICLR 2024*.

[2] Albergo, M. S., & Vanden-Eijnden, E. (2025). Nets: A non-equilibrium transport sampler. *ICML 2025*.

[3] He, J., Du, Y., Vargas, F., Wang, Y., Gomes, C. P., Hernández-Lobato, J. M., & Vanden-Eijnden, E. (2025). FEAT: Free energy Estimators with Adaptive Transport. *arXiv*.

# Importance Sampling with Path RND

AIS

$$\mathbf{E}_{X \sim \mathbf{P}}[f(X)] = \mathbf{E}_{X \sim \mathbf{Q}} \left[ \frac{d\mathbf{P}}{d\mathbf{Q}}(X) f(X) \right]$$

Jarzynski

$$\mathbf{E}_{\mathbf{Q}} \left[ \exp \left( \int -\partial_t U_t(X_t) dt \right) \right] = \frac{Z_1}{Z_0}$$

Escorted Jarzynski  $\mathbf{E}_{\mathbf{Q}} \left[ \exp \left( \int -\partial_t U_t(X_t) dt - \nabla U_t \cdot u_t dt + \nabla \cdot u_t dt \right) \right] = \frac{Z_1}{Z_0}$

# Importance Sampling with Path RND

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$$Z = \int \exp(-U(X)) dX$$

# Importance Sampling with Path RND

AIS

$$\mathbf{E}_{X \sim \mathbf{P}}[f(X)] = \mathbf{E}_{X \sim \mathbf{Q}} \left[ \frac{d\mathbf{P}}{d\mathbf{Q}}(X) f(X) \right]$$

Jarzynski

$$\mathbf{E}_{\mathbf{Q}} \left[ \exp \left( \int -\partial_t U_t(X_t) dt \right) \right] = \frac{Z_1}{Z_0}$$

Escorted Jarzynski  $\mathbf{E}_{\mathbf{Q}} \left[ \exp \left( \int -\partial_t U_t(X_t) dt - \nabla U_t \cdot u_t dt + \nabla \cdot u_t dt \right) \right] = \frac{Z_1}{Z_0}$

$$Z = \int \exp(-U(X)) dX$$

$$p(X) = \int p(Z, X) dZ$$



$p(X)$  is the normalization factor for  $p(Z|X) \propto p(Z, X)$

# Importance Sampling with Path RND

$$dX_t = g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_1 \sim N(0, \nu)$$

? What is  $p_0(x)$  at  $t = 0$ ?

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$$dX_t = g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_1 \sim N(0, \nu)$$

❓ What is  $p_0(x)$  at  $t = 0$ ?

$$x \sim N(X|Z), p(Z) \sim N(0, \nu)$$

❓ What is  $p(x)$ ?

# Importance Sampling with Path RND

Marginal density relation with importance sampling:

$$p(x) = \mathbf{E}_{z \sim p(z|x)}[1]p(x)$$

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# Importance Sampling with Path RND

Marginal density relation with importance sampling:



**Let's rewrite it in a path!**

$$\begin{aligned} p(x) &= \mathbf{E}_{z \sim p(z|x)}[1]p(x) & p_0(x) &= \\ &= \mathbf{E}_{z \sim p(z|x)}[p(x)] & = \\ &= \mathbf{E}_{z \sim q(z|x)} \left[ \frac{p(x)p(z|x)}{q(z|x)} \right] & = \\ &= \mathbf{E}_{z \sim q(z|x)} \left[ \frac{p(z)p(x|z)}{q(z|x)} \right] & = \end{aligned}$$

# Importance Sampling with Path RND

Marginal density relation with importance sampling:



**Let's rewrite it in a path!**

$$\begin{aligned} p(x) &= \mathbf{E}_{z \sim p(z|x)}[1]p(x) & p_0(x) &= \mathbf{E}_{X_{1:N} \sim p(X_{1:N}|X_0=x)}[1]p_0(x) \\ &= \mathbf{E}_{z \sim p(z|x)}[p(x)] & = \\ &= \mathbf{E}_{z \sim q(z|x)} \left[ \frac{p(x)p(z|x)}{q(z|x)} \right] & = \\ &= \mathbf{E}_{z \sim q(z|x)} \left[ \frac{p(z)p(x|z)}{q(z|x)} \right] & = \end{aligned}$$

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Marginal density relation with importance sampling:



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# Importance Sampling with Path RND

$$p(x) = \mathbf{E}_{X_{1:N} \sim q(X_{1:N}|X_0=x)} \left[ \frac{p(X_{1:N}, X_0 = x)}{q(X_{1:N}|X_0 = x)} \right]$$

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$$p: dX_t = g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_N \sim N$$

$$q: dX_t = h(X_t, t)dt + \sigma_t dW_t$$

# Importance Sampling with Path RND

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$$p(x) = \mathbf{E}_{X_{1:N} \sim q(X_{1:N}|X_0=x)} \left[ \frac{\prod N_p(X_n|X_{n+1})}{\prod N_q(X_{n+1}|X_n)} N(X_N) \right]$$

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## Forward-backward RND

$$\begin{aligned} \mathbf{P}: dX_t &= f(X_t, t)dt + \sigma_t dW_t, X_0 \sim p_0 \\ \bar{\mathbf{Q}}: dX_t &= g(X_t, t)dt + \sigma_t dW_t, X_1 \sim q_1 \end{aligned}$$

$$\frac{d\mathbf{P}}{d\bar{\mathbf{Q}}}(X) = \underbrace{\frac{p_0(X_0)}{q_1(X_1)}}_{\text{Initial densities}} \exp \left( \int \underbrace{\frac{f_t(X_t)}{\sigma_t^2} \cdot dX_t - \frac{f_t^2(X_t)}{2\sigma_t^2} dt}_{\text{Backward Ito Integral}} - \int \underbrace{\frac{g_t(X_t)}{\sigma_t^2} \cdot \overline{dX}_t + \frac{g_t^2(X_t)}{2\sigma_t^2} dt} \right)$$

$\int a_t(X_t) \cdot \overline{dX}_t = \lim \sum a_{n+1}(X_{n+1}) \cdot (X_{n+1} - X_n)$

# RECALL: Forward-backward RND

$$\begin{aligned}\mathbf{P} : dX_t &= f(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_0 \sim p_0 \\ \overleftarrow{\mathbf{Q}} : dX_t &= g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_1 \sim q_1\end{aligned}$$

$$\frac{d\mathbf{P}}{d\overleftarrow{\mathbf{Q}}}(X) = \frac{p_0(X_0)}{q_1(X_1)} \exp \left( \underbrace{\int \frac{f_t(X_t)}{\sigma_t^2} \cdot dX_t - \frac{f_t^2(X_t)}{2\sigma_t^2} dt - \int \frac{g_t(X_t)}{\sigma_t^2} \cdot \overleftarrow{dX}_t + \frac{g_t^2(X_t)}{2\sigma_t^2} dt}_{\text{Initial densities}} \right)$$
$$\lim \frac{\prod N_1(X_{n+1}|X_n)}{\prod N_2(X_n|X_{n+1})}$$

# Importance Sampling with Path RND

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$$p(x) = \mathbf{E}_{X_{1:N} \sim q(X_{1:N} | X_0=x)} \left[ \frac{\prod N_g(X_n | X_{n+1})}{\prod N_h(X_{n+1} | X_n)} N(X_N) \right]$$

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$$p(x) = \mathbf{E}_{\mathbf{Q}(\cdot|X_0)} \left[ N(X_1) \exp \left( - \int \frac{f_t(X_t)}{\sigma_t^2} \cdot dX_t + \frac{f_t^2(X_t)}{2\sigma_t^2} dt + \int \frac{g_t(X_t)}{\sigma_t^2} \cdot \overleftarrow{dX_t} - \frac{g_t^2(X_t)}{2\sigma_t^2} dt \right) \right]$$

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$$\int a_t(X_t) \cdot \overleftarrow{dX_t} = \lim \sum a_{n+1}(X_{n+1}) \cdot (X_{n+1} - X_n)$$

For simplicity, we hereafter call

$$R_f^g(X) = \exp \left( - \int \frac{f_t(X_t)}{\sigma_t^2} \cdot dX_t + \frac{f_t^2(X_t)}{2\sigma_t^2} dt + \int \frac{g_t(X_t)}{\sigma_t^2} \cdot \overleftarrow{dX_t} - \frac{g_t^2(X_t)}{2\sigma_t^2} dt \right)$$

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$$\overleftarrow{\mathbf{P}}: dX_t = g(X_t, t)dt + \sigma_t \overleftarrow{dW_t}, X_1 \sim N$$

$$\mathbf{Q}: dX_t = f(X_t, t)dt + \sigma_t dW_t, X_1 \sim q(X_0)$$

$$p(x) = \mathbf{E}_{\mathbf{Q}(\cdot|X_0)} \left[ N(X_1) \exp \left( - \int \frac{f_t(X_t)}{\sigma_t^2} \cdot dX_t + \frac{f_t^2(X_t)}{2\sigma_t^2} dt + \int \frac{g_t(X_t)}{\sigma_t^2} \cdot \overleftarrow{dX_t} - \frac{g_t^2(X_t)}{2\sigma_t^2} dt \right) \right]$$

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$$R_f^g(X) = \lim \frac{\prod N_g(X_n | X_{n+1})}{\prod N_h(X_{n+1} | X_n)}$$

# Importance Sampling with Path RND

$$\overleftarrow{\mathbf{P}}: dX_t = g(X_t, t)dt + \sigma_t \overleftarrow{dW_t}, X_1 \sim N$$

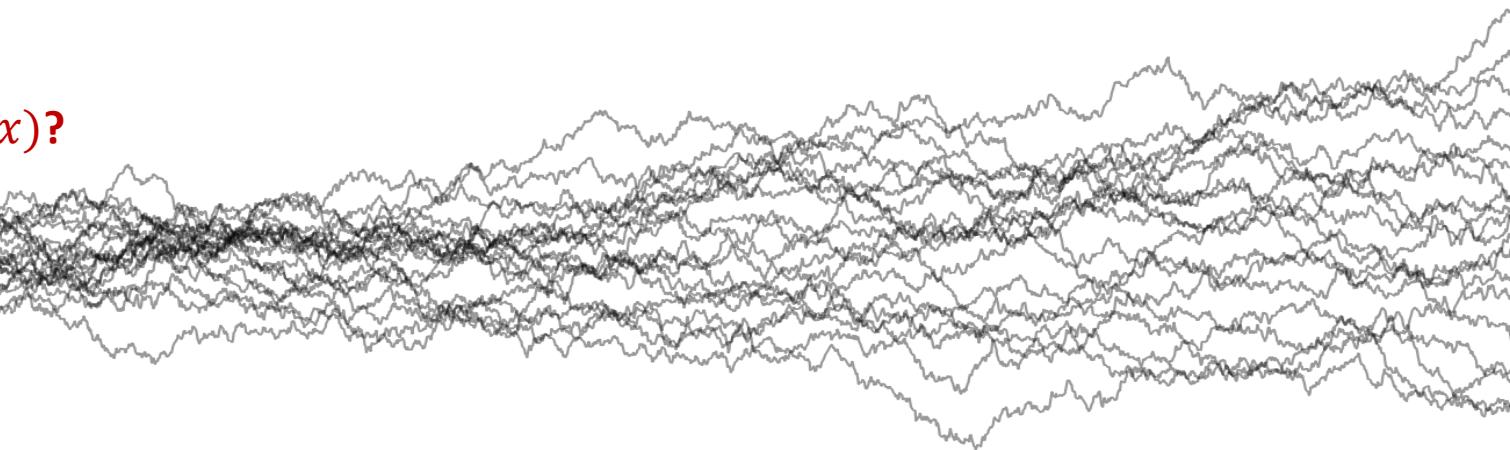
$$\mathbf{Q}: dX_t = f(X_t, t)dt + \sigma_t dW_t, X_1 \sim q(X_0)$$

$$p(x) = \mathbf{E}_{\mathbf{Q}(\cdot|X_0)} \left[ N(X_1) \color{red}{R_f^g(X_{[0,1]})} \right]$$

# Importance Sampling with Path RND

$$\overleftarrow{\mathbf{P}}: dX_t = g(X_t, t)dt + \sigma_t \overleftarrow{dW_t}, X_1 \sim N$$

What's  $p(x)$ ?

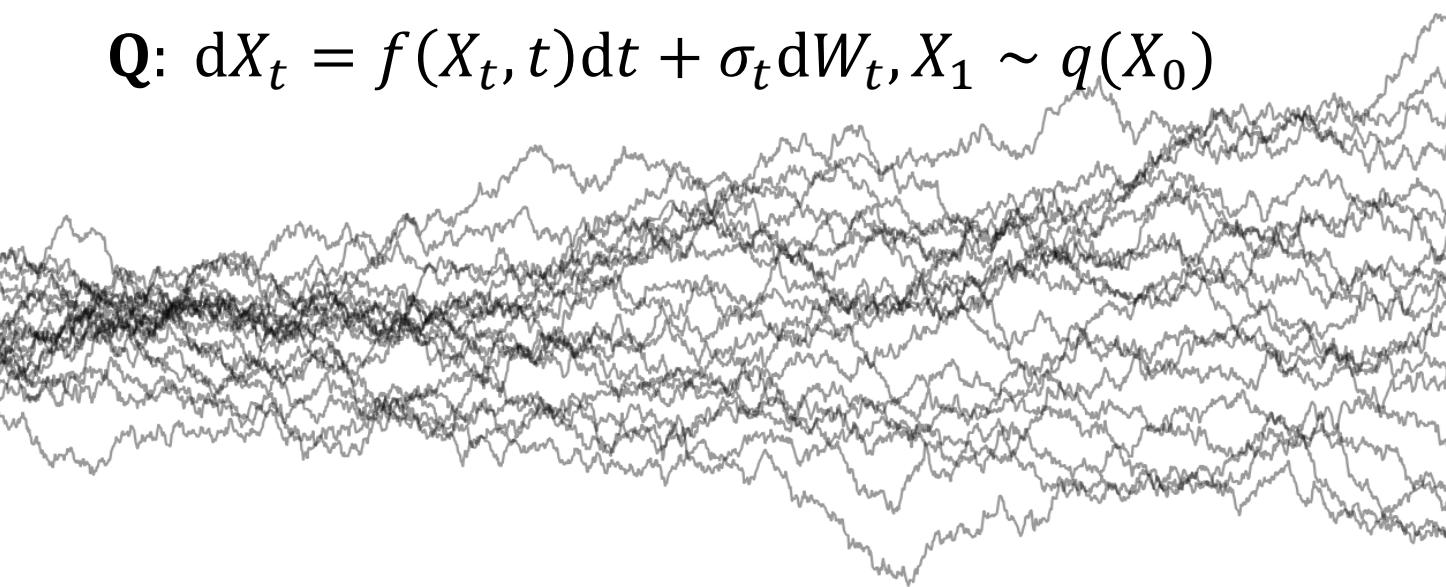


# Importance Sampling with Path RND

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What's  $p(x)$ ?

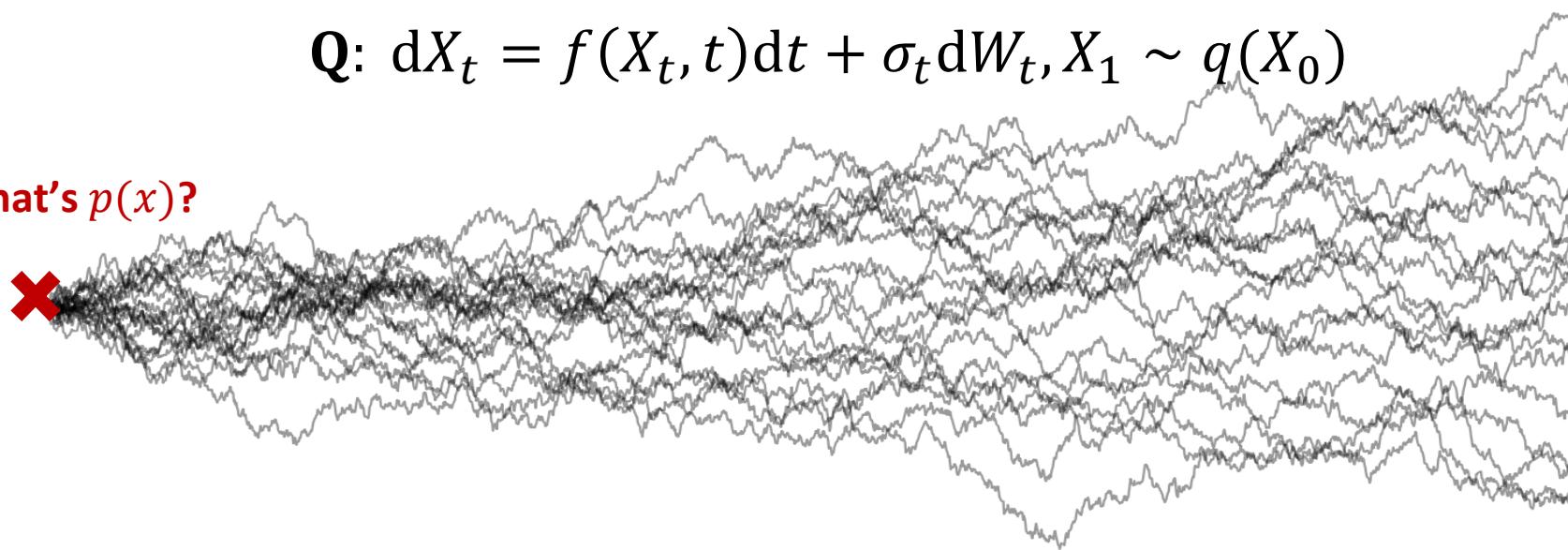


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$$p(x) = \mathbf{E}_{\mathbf{Q}(\cdot|X_0)} \left[ N(X_1) R_f^g(X_{[0,1]}) \right]$$

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$$p(x) = \mathbf{E}_{\mathbf{Q}(\cdot|X_0)} \left[ N(X_1) R_f^g(X_{[0,1]}) \right]$$

Can also be derived from Feynman-Kac formulation as shown in [1] and [2]:

- [1] Huang, C. W., Lim, J. H., & Courville, A. C. (2021). A variational perspective on diffusion-based generative models and score matching. *NeurIPS 2021*.
- [2] Premkumar, A. (2024). Diffusion density estimators. *arXiv*.

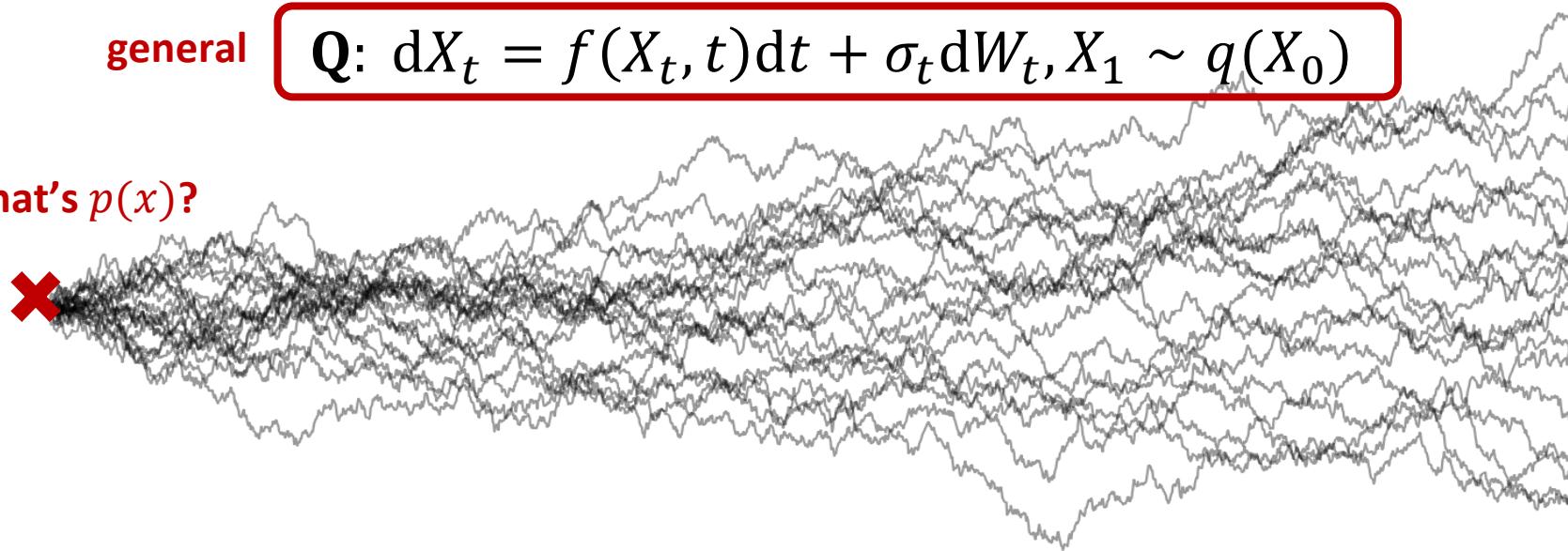
# Importance Sampling with Path RND

$$\stackrel{\leftarrow}{\mathbf{P}}: dX_t = g(X_t, t)dt + \sigma_t \overleftarrow{dW_t}, X_1 \sim N$$

general

$$\mathbf{Q}: dX_t = f(X_t, t)dt + \sigma_t dW_t, X_1 \sim q(X_0)$$

What's  $p(x)$ ?



# Importance Sampling with Path RND

Special Case: **time-reversal proposal**

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$$\mathbf{P}: dX_t = f(X_t, t)dt + \sigma_t dW_t, X_0 \sim p_0$$

# Importance Sampling with Path RND

Special Case: **time-reversal proposal**

$$\begin{aligned}\bar{\mathbf{P}}: dX_t &= g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_1 \sim N \\ \mathbf{P}: dX_t &= f(X_t, t)dt + \sigma_t dW_t, X_0 \sim p_0\end{aligned}$$

$$\frac{\overleftarrow{d\mathbf{P}}}{d\mathbf{P}}(X_0 = x, X_{(0,1]}) = 1$$

## Forward-backward RND

$$\begin{aligned}\mathbf{P}: dX_t &= f(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_0 \sim p_0 \\ \bar{\mathbf{Q}}: dX_t &= g(X_t, t)dt + \sigma_t \overrightarrow{dW}_t, X_1 \sim q_1\end{aligned}$$

$$\frac{d\mathbf{P}}{d\bar{\mathbf{Q}}}(X) = \underbrace{\frac{p_0(X_0)}{q_1(X_1)}}_{\text{Initial densities}} \exp \left( \int \underbrace{\frac{f_t(X_t)}{\sigma_t^2} \cdot dX_t}_{\text{Forward Itô Integral}} - \frac{f_t^2(X_t)}{2\sigma_t^2} dt - \int \underbrace{\frac{g_t(X_t)}{\sigma_t^2} \cdot \overrightarrow{dX}_t}_{\text{Backward Itô Integral}} + \frac{g_t^2(X_t)}{2\sigma_t^2} dt \right)$$

$$\int a_t(X_t) \cdot \overrightarrow{dX}_t = \lim \sum a_{n+1}(X_{n+1}) \cdot (X_{n+1} - X_n)$$

# Importance Sampling with Path RND

Special Case: **time-reversal proposal**

$$\begin{aligned}\overleftarrow{\mathbf{P}}: dX_t &= g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_1 \sim N \\ \mathbf{P}: dX_t &= f(X_t, t)dt + \sigma_t dW_t, X_0 \sim p_0\end{aligned}$$

$$\frac{N(X_1)}{p_0(X_0 = x)} R_f^g(X_{[0,1]}) = 1$$

$$\frac{\overleftarrow{d\mathbf{P}}}{d\mathbf{P}}(X_0 = x, X_{(0,1]}) = 1$$

## Forward-backward RND

$$\begin{aligned}\mathbf{P}: dX_t &= f(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_0 \sim p_0 \\ \overleftarrow{\mathbf{Q}}: dX_t &= g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_1 \sim q_1\end{aligned}$$

$$\frac{d\mathbf{P}}{d\overleftarrow{\mathbf{Q}}}(X) = \underbrace{\frac{p_0(X_0)}{q_1(X_1)}}_{\text{Initial densities}} \exp \left( \int \underbrace{\frac{f_t(X_t)}{\sigma_t^2} \cdot dX_t}_{\text{Forward Itô Integral}} - \frac{f_t^2(X_t)}{2\sigma_t^2} dt - \int \underbrace{\frac{g_t(X_t)}{\sigma_t^2} \cdot \overleftarrow{dX}_t}_{\text{Backward Itô Integral}} + \frac{g_t^2(X_t)}{2\sigma_t^2} dt \right)$$

Initial densities

Backward Itô Integral

$$\int a_t(X_t) \cdot \overleftarrow{dX}_t = \lim \sum a_{n+1}(X_{n+1}) \cdot (X_{n+1} - X_n)$$

# Importance Sampling with Path RND

Special Case: **time-reversal proposal**

$$\begin{aligned}\overleftarrow{\mathbf{P}}: dX_t &= g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_1 \sim N \\ \mathbf{P}: dX_t &= f(X_t, t)dt + \sigma_t dW_t, X_0 \sim p_0\end{aligned}$$



$$\frac{\overleftarrow{d\mathbf{P}}}{d\mathbf{P}}(X_0 = x, X_{[0,1]}) = 1$$

$$N(X_1)R_f^g(X_{[0,1]}) = p_0(X_0 = x)$$

## Forward-backward RND

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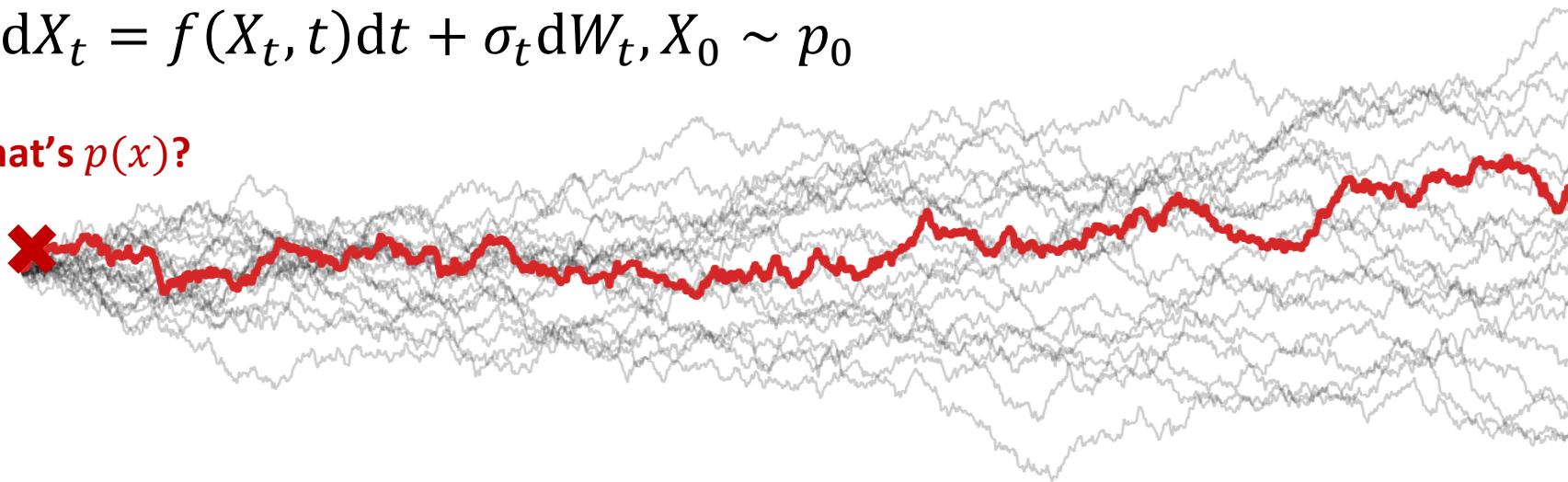
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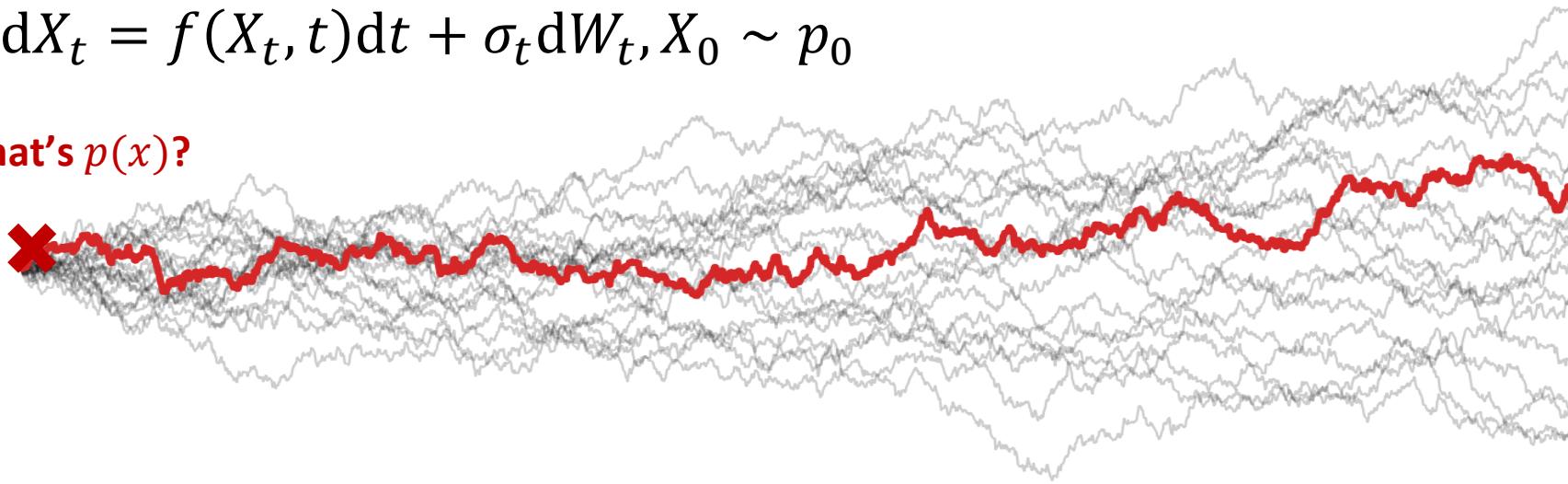
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Can be derived by PDEs as shown in [1] and [2]:

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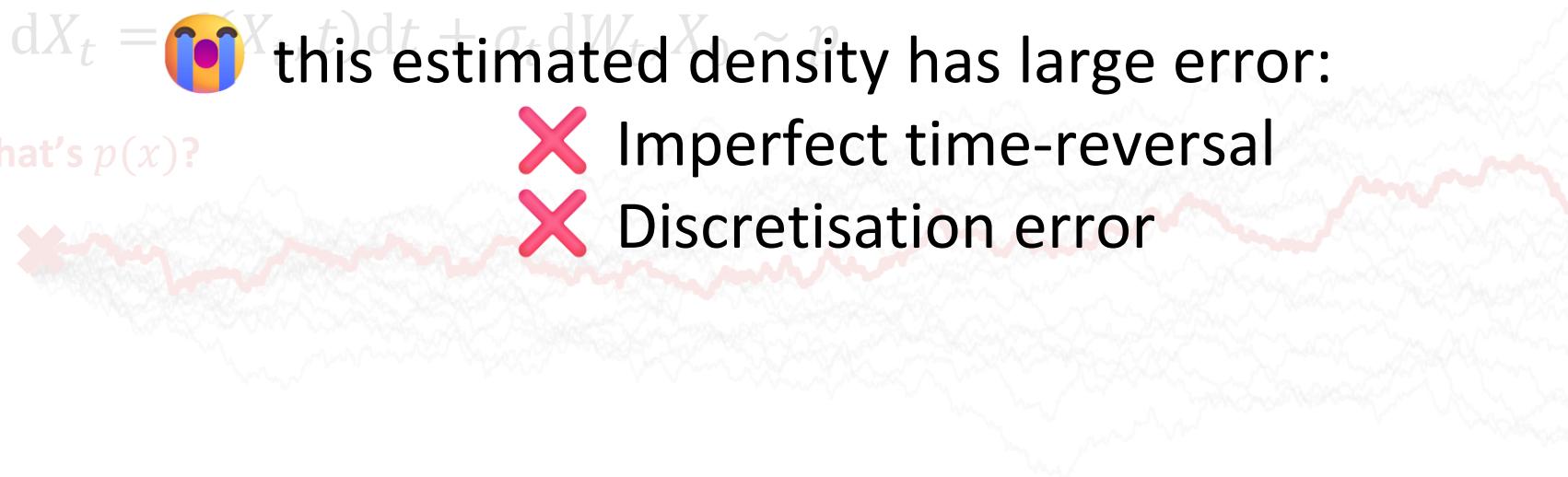
$$P: dX_t = h(X_t, t)dt + \sigma_t dW_t, X_0 \sim n$$



this estimated density has large error:

What's  $p(x)$ ?

- ✗ Imperfect time-reversal
- ✗ Discretisation error



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✓ Only look at small intervals

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# Importance Sampling with Path RND

- Only look at small intervals

$$\begin{aligned}\bar{\mathbf{P}}: \mathrm{d}X_t &= g(X_t, t)dt + \sigma_t \overleftarrow{\mathrm{d}W}_t & X_{\tau'} &\sim p_{\tau'} & t \in [\tau, \tau'] \\ \mathbf{P}: \mathrm{d}X_t &= f(X_t, t)dt + \sigma_t \mathrm{d}W_t & X_\tau &\sim p_\tau & t \in [\tau, \tau']\end{aligned}$$

$$\rightarrow \frac{\overleftarrow{\mathrm{d}\mathbf{P}}}{\mathrm{d}\mathbf{P}}(X_{[\tau, \tau']}) = 1$$

$$\frac{p_{\tau'}(X_{\tau'})}{p_\tau(X_\tau)} R_f^g(X_{[\tau, \tau']}) = 1$$

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$$\rightarrow \frac{\overleftarrow{d\mathbf{P}}}{d\mathbf{P}}(X_{[\tau, \tau']}) = 1$$

👉 Equal density sampling:  
for two diffusion models, find sample has **same density under both models**

👉 Calculate SMC weights:  
for one (or several) DMs, **steer the distribution** by tilting/annealing/composition

👉 Energy regularisation:  
Train **an energy-based diffusion model** by ensuring this relation for all time intervals

# Example: Diffusion Inference-time Steering with Path RND



Problem Setup:

Given a pretrained model for  $p_0$ , generate samples  $\sim p_0(x)\exp(r(x))$

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- Choose a heuristic guidance process;
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We already learned about this pipeline from Raghav (Feynman-Kac Steering); Marta (Feynman-Kac Corrector); Luhuan (RDSMC) during the talks

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have  $\{x\} \sim q_{\tau'}$ , how to obtain exact sample  $\{x\} \sim q_\tau$

- Choose a heuristic guidance process;

$$dX_t = (\text{score} + \text{guidance}) dt + \sigma_t \overleftarrow{dW}_t, \quad X_{\tau'} \sim q_{\tau'}$$

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**“target”?**  $X_\tau \sim q_\tau$

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$$w \propto \frac{\text{target}}{\text{proposal}}$$

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$$w \propto \frac{\text{target}}{q_{\tau'}(X_{\tau'}) \prod N_a(X_n | X_{n+1})}$$

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$$w \propto \frac{q_{\tau}(X_{\tau}) \prod N_b(X_{n+1}|X_n)}{q_{\tau'}(X_{\tau'}) \prod N_a(X_n|X_{n+1})}$$

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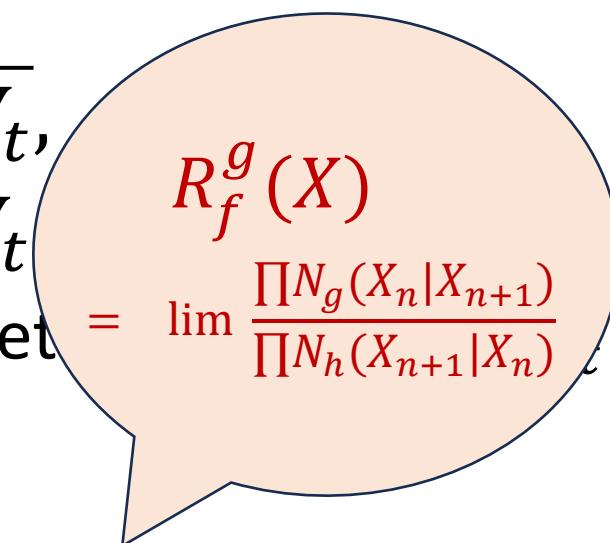
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- Define a sequence of intermediate target

- Do **importance-resampling**


$$R_f^g(X) = \lim \frac{\prod N_g(X_n | X_{n+1})}{\prod N_h(X_{n+1} | X_n)}(x_t) \exp(r_t(x_t));$$

$$w \propto \frac{q_{\tau}(X_{\tau}) \prod N_b(X_{n+1} | X_n)}{q_{\tau'}(X_{\tau'}) \prod N_a(X_n | X_{n+1})}$$

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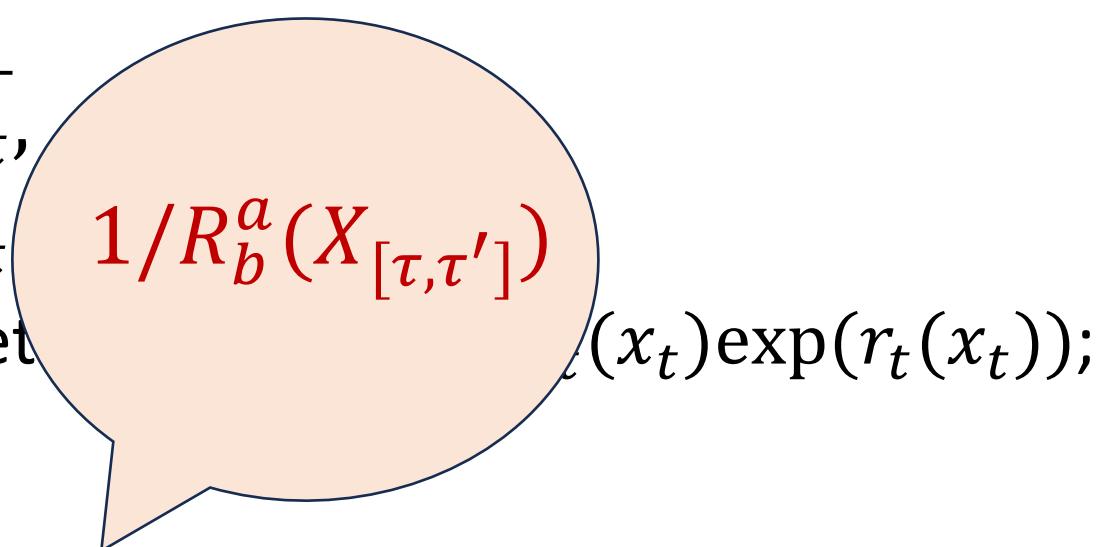
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$(x_t) \exp(r_t(x_t));$

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$$w \propto \frac{q_\tau(X_\tau)}{q_{\tau'}(X_{\tau'})} \textcolor{red}{1/R_b^a(X_{[\tau,\tau']})}$$

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# Example: Diffusion Inference-time Steering with Path RND

- Choose a heuristic guidance process;  
“proposal”  $\tilde{\mathbf{P}}: dX_t = \text{diffusion denoising } dt + \sigma_t \overleftarrow{dW_t} \quad X_{\tau'} \sim p_{\tau'} \quad t \in [\tau, \tau']$
- “target”?  $\mathbf{P}: dX_t = \text{diffusion noising } dt + \sigma_t \overrightarrow{dW_t}, \quad X_{\tau} \sim p_{\tau} \quad t \in [\tau, \tau']$
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“target”  $dX_t = b(X_t, t)dt + \sigma_t dW_t, \quad X_\tau \sim q_\tau$

- Define a sequence of intermediate target densities  $q_t \propto p_t(x_t) \exp(r_t(x_t))$ ;
- Do **importance-resampling**

$$w \propto R_f^g(X_{[\tau, \tau']}) \frac{\exp(r_\tau(x_\tau))}{\exp(r_{\tau'}(x_{\tau'}))} 1/R_b^a(X_{[\tau, \tau']})$$

# Example: Diffusion Inference-time Steering with Path RND

$$w \propto R_f^g(X_{[\tau,\tau']}) \frac{\exp(r_\tau(x_\tau))}{\exp(r_{\tau'}(x_{\tau'}))} 1/R_b^a(X_{[\tau,\tau']})$$

## Summary:

- 👉 Define proposal and target process
- 👉 Define intermediate densities  $q_t$  (by steering diffusion's  $p_t$ )
- 👉 Replace ratio between  $p_t$  by forward-backward kernel ratio  $R$

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🌟 Anneal target  $p_t^\beta$

🌟 Composition/CFG between 2 diffusions  $\left(p_t^{(1)}\right)^\beta \left(p_t^{(2)}\right)^\alpha$

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$$w \propto \left[ R_f^g(X_{[\tau, \tau']}) \right]^\beta 1/R_b^a(X_{[\tau, \tau']})$$

🌟 Composition/CFG between 2 diffusions  $\left(p_t^{(1)}\right)^\beta \left(p_t^{(2)}\right)^\alpha$

$$w \propto \left[ R_{f_1}^{g_1}(X_{[\tau, \tau']}) \right]^\beta \left[ R_{f_2}^{g_2}(X_{[\tau, \tau']}) \right]^\alpha 1/R_b^a(X_{[\tau, \tau']})$$

## Example: Diffusion Inference-time Steering with Path RND

$$R_f^g(X) = \exp \left( - \int \frac{f_t(X_t)}{\sigma_t^2} \cdot dX_t + \frac{f_t^2(X_t)}{2\sigma_t^2} dt + \int \frac{g_t(X_t)}{\sigma_t^2} \cdot d\overline{X}_t - \frac{g_t^2(X_t)}{2\sigma_t^2} dt \right)$$

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If we (1) plug-in this  $R$ ,  
and (2) choose target process  $f$  to be simple noising process:



We recover a path RND perspective for FKC [1]:

[1] Skreta, M., Akhound-Sadegh, T., Ohanesian, V., Bondesan, R., Aspuru-Guzik, A., Doucet, A., ... & Neklyudov, K. (2025). Feynman-kac correctors in diffusion: Annealing, guidance, and product of experts. *ICML 2025*.

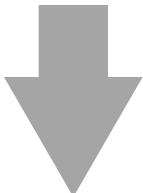
## Example: Diffusion Inference-time Steering with Path RND

$$R_f^g(X) = \lim \frac{\prod N_g(X_n|X_{n+1})}{\prod N_h(X_{n+1}|X_n)}$$

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$$R_f^g(X) = \lim \frac{\prod N_g(X_n|X_{n+1})}{\prod N_h(X_{n+1}|X_n)}$$

If we (1) plug-in this  $R$ ,  
and (2) choose target process  $f$  to be simple noising process,  
and (3) focus on reward-tilting



We recover a path RND perspective for TDS [1] / FKS[2]:

- [1] Wu, L., Trippe, B., Naesseth, C., Blei, D., & Cunningham, J. P. (2023). Practical and asymptotically exact conditional sampling in diffusion models. *NeurIPS 2023*.
- [2] Singhal, R., Horvitz, Z., Teehan, R., Ren, M., Yu, Z., McKeown, K., & Ranganath, R. (2025). A general framework for inference-time scaling and steering of diffusion models. *ICML 2025*.

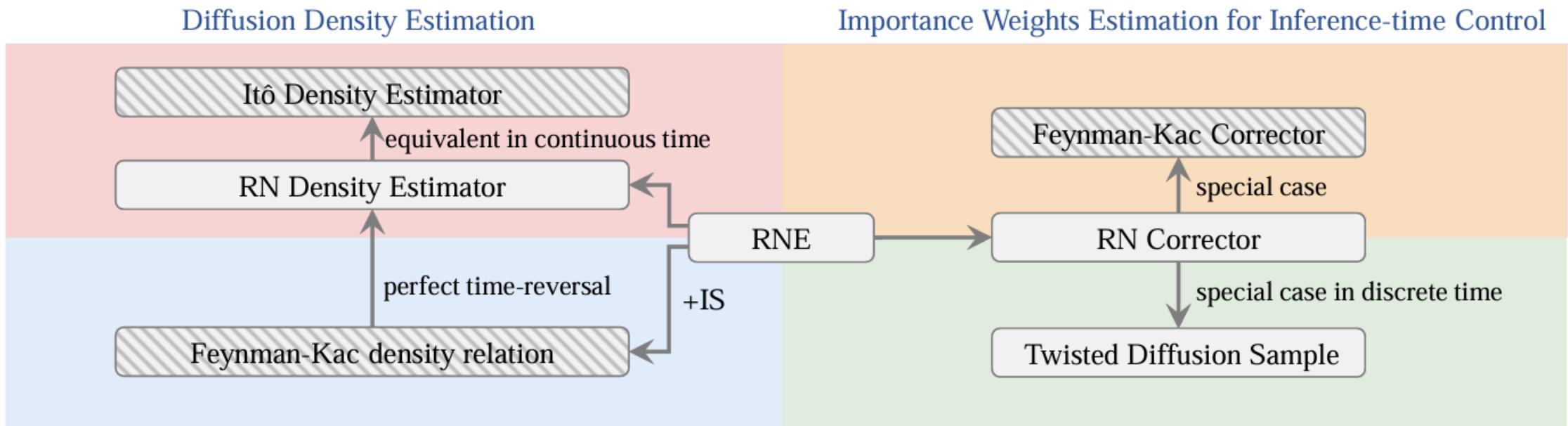
# Example: Diffusion Inference-time Steering with Path RND

## Inference-time control with path RND (RN Estimator) [1]:

- 👉 flexible! (any target process, any proposal process)
- 👉 plug-and-play! (as long as there is some  $p_t/p_{t'}$ )
- 👉 Unifying! (Ito density estimator/FKC/TDS/FKS...)

[1] He, J., Hernández-Lobato, J. M., Du, Y., & Vargas, F. (2025). RNE: a plug-and-play framework for diffusion density estimation and inference-time control. *arXiv*.

# Example: Diffusion Inference-time Steering with Path RND



# Example: Diffusion Inference-time Steering with Path RND

Inference-time Annealing: (Alanine Dipeptide 800K to 300K)

Metric	Energy TV( $\downarrow$ )	Distance TV( $\downarrow$ )	Sample $W_2(\downarrow)$
Anneal score (wo SMC)	0.794	0.023	<b>0.173*</b>
FKC	0.338	0.022	0.289
In theory = FKC ➡️ RNC ( $c_a = 1, c_b = 0$ )	0.386	0.017	0.282
Flexible choices ➡️ RNC ( $c_a = 0.6, c_b = 0.4$ )	<b>0.034</b>	<b>0.011</b>	0.253

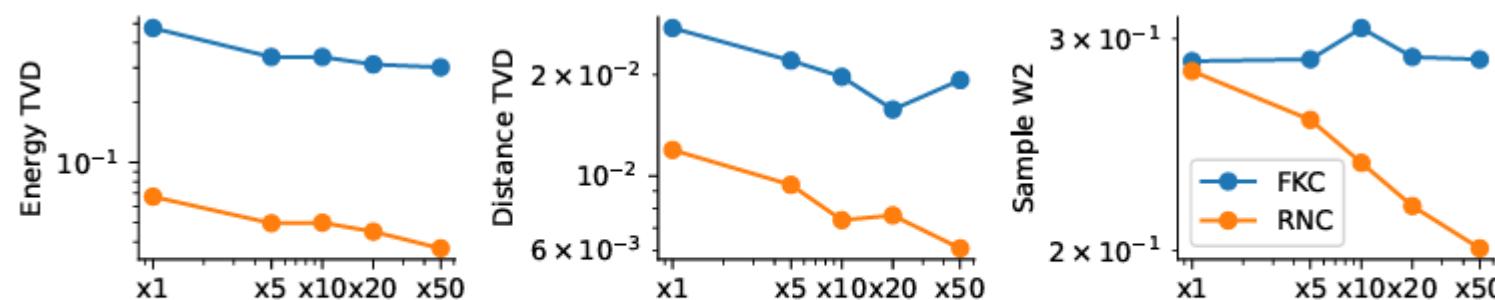


Figure 6: Performance scaling with particle numbers in SMC.

## Takeaways So Far...

# Path RND connects transition kernels with marginal densities

- 👉 Density estimation
  - 👉 SMC corrector

# Takeaways So Far...

# Path RND connects transition kernels with marginal densities

- 👉 Density estimation
  - 👉 SMC corrector
  - ❓ What else? Where do we also need density?

# Example: Energy-parameterised Diffusion Training



Problem Setup:

train a diffusion model, parameterised by energy instead of score

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$$\begin{aligned} \widetilde{\mathbf{P}}: dX_t &= g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t & X_{\tau'} &\sim p_{\tau'} & t \in [\tau, \tau'] \\ \mathbf{P}: dX_t &= f(X_t, t)dt + \sigma_t dW_t & X_\tau &\sim p_\tau & t \in [\tau, \tau'] \end{aligned} \quad \rightarrow \frac{\overleftarrow{d\mathbf{P}}}{d\mathbf{P}}(X_{[\tau, \tau']}) = 1$$

$$\frac{p_{\tau'}(X_{\tau'})}{p_\tau(X_\tau)} R_f^g(X_{[\tau, \tau']}) = 1$$

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Learned network👉

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Learned network  $\bar{\mathbf{P}}$ :  $dX_t = g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t$      $X_{\tau'} \sim p_{\tau'} \quad t \in [\tau, \tau']$      $\frac{\overleftarrow{d\mathbf{P}}}{d\mathbf{P}}(X_{[\tau, \tau']}) = 1$

Noising process  $\mathbf{P}$ :  $dX_t = f(X_t, t)dt + \sigma_t dW_t$      $X_\tau \sim p_\tau \quad t \in [\tau, \tau']$

$$\frac{p_{\tau'}(X_{\tau'})}{p_{\tau}(X_{\tau})} R_f^g(X_{[\tau, \tau']}) = 1$$

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Learned network

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$$\left\| \frac{p_{\tau'}(X_{\tau'})}{p_{\tau}(X_{\tau})} R_f^g(X_{[\tau, \tau']}) - 1 \right\|^2$$

# Example: Energy-parameterised Diffusion Training



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Learned network

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$$\left\| \frac{p_{\tau'}(X_{\tau'})}{p_{\tau}(X_{\tau})} R_f^g(X_{[\tau, \tau']}) - 1 \right\|^2$$

$\tau' = \tau + \Delta t$

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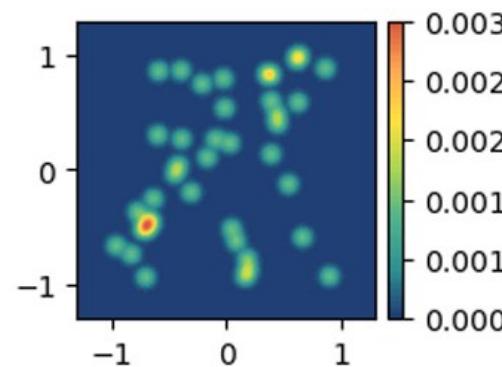
Learned network

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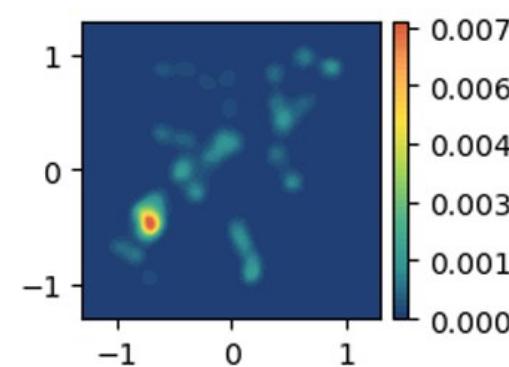
$$\left\| \frac{p_{\tau'}(X_{\tau'})}{p_{\tau}(X_{\tau})} R_f^g(X_{[\tau, \tau']}) - 1 \right\|^2 + \text{DSM}$$

$\tau' = \tau + \Delta t$

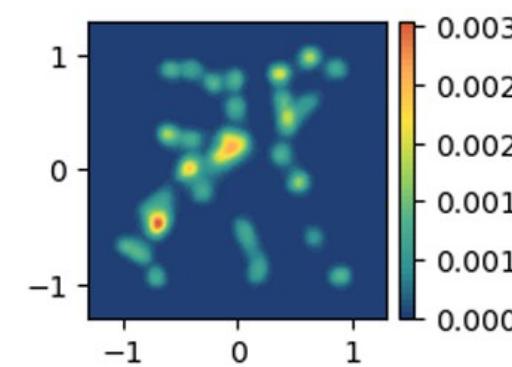
# Example: Energy-parameterised Diffusion Training



(a) Ground truth



(b) DSM

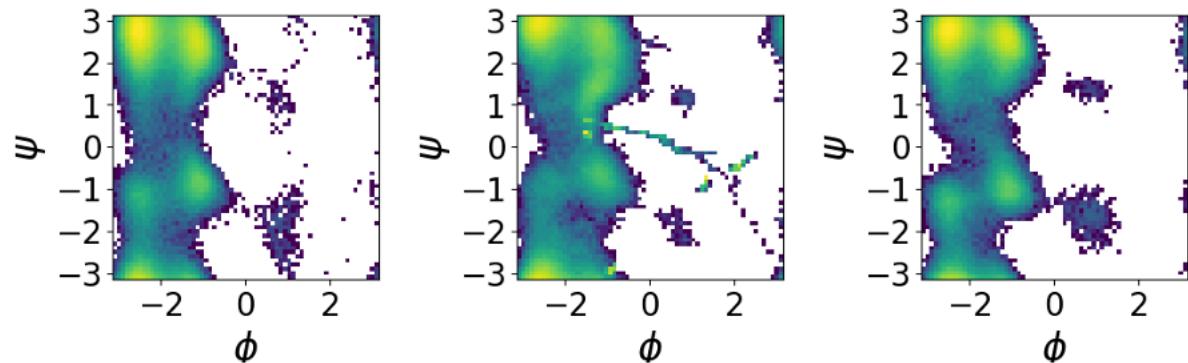


(c) RNE regularise

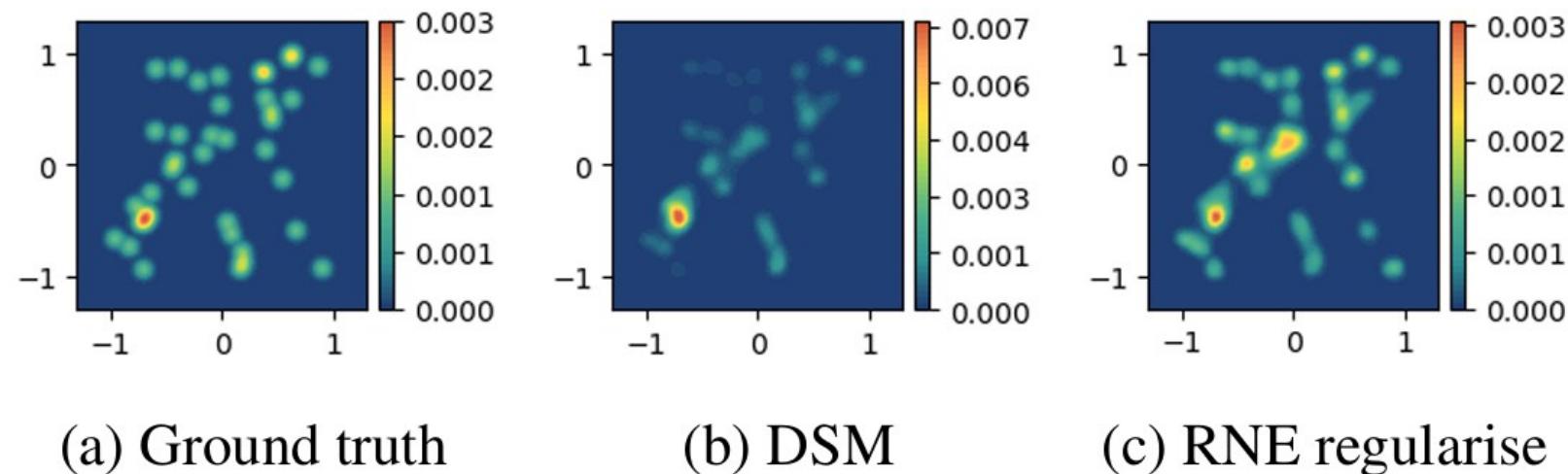
# Example: Energy-parameterised Diffusion Training

Table 4: Quality of samples obtained by running denoising process (denoted as DM) and running MCMC on learned energy at  $t = 0$ .

Training method	Sample Method	Sample $W2$
DSM	DM	0.1811
	MCMC	0.9472
RNE Reg	DM	0.1809
	MCMC	0.1836



(a) Ground truth      (b) DSM      (c) RNE regularise  
 Figure 8: Ramachandran plot of samples by MCMC (with Metropolis–Hastings) on learned energy.



# Importance Sampling with Path RND

**Importance Sampling:**

$$\mathbf{E}_{x \sim p}[f(x)] = \mathbf{E}_{x \sim q} \left[ \frac{p(x)}{q(x)} f(x) \right]$$

**Importance Sampling in Path space:**

$$\mathbf{E}_{X \sim \mathbf{P}}[f(X)] = \mathbf{E}_{X \sim \mathbf{Q}} \left[ \frac{d\mathbf{P}}{d\mathbf{Q}}(X) f(X) \right]$$

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? What is the optimal proposal for  $f > 0$ ?

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$$q \propto pf$$

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$$\frac{d\mathbf{Q}}{d\mathbf{P}} \propto f$$

# Importance Sampling with Path RND

**Importance Sampling:**

$$\mathbf{E}_{x \sim p}[f(x)] = \mathbf{E}_{x \sim q} \left[ \frac{p(x)}{q(x)} f(x) \right]$$

? What is the optimal proposal for  $L > 0$ ?

$$q \propto pL$$

**Importance Sampling in Path space:**

$$\mathbf{E}_{X \sim \mathbf{P}}[f(X)] = \mathbf{E}_{X \sim \mathbf{Q}} \left[ \frac{d\mathbf{P}}{d\mathbf{Q}}(X) f(X) \right]$$

$$\frac{d\mathbf{Q}}{d\mathbf{P}} \propto L$$

Likelihood

# Variational Inference with Path RND

**Importance Sampling:**

$$\mathbf{E}_{x \sim p}[f(x)] = \mathbf{E}_{x \sim q} \left[ \frac{p(x)}{q(x)} f(x) \right]$$

**Importance Sampling in Path space:**

$$\mathbf{E}_{X \sim \mathbf{P}}[f(X)] = \mathbf{E}_{X \sim \mathbf{Q}} \left[ \frac{d\mathbf{P}}{d\mathbf{Q}}(X) f(X) \right]$$

**Variational Inference:**

$$\begin{aligned} q^* &\propto pL \\ q &= \min D[q, q^*] \end{aligned}$$

**Variational Inference in Path space:**

$$\frac{d\mathbf{Q}^*}{d\mathbf{P}} \propto L$$

$$\mathbf{Q} = \min D[\mathbf{Q}, \mathbf{Q}^*]$$

# Variational Inference with Path RND

**Variational Inference in Path space:**

$$\frac{dQ^*}{dP} \propto L$$

$$Q = \min D[Q, Q^*]$$

# Variational Inference with Path RND

**Variational Inference in Path space:**

$$\frac{d\mathbf{Q}^*}{d\mathbf{P}} \propto L$$

$$\mathbf{Q} = \min D[\mathbf{Q}, \mathbf{Q}^*]$$

$$\mathbf{P}: dX_t = b(X_t, t)dt + \sigma_t dW_t \quad X_0 \sim p_0$$

$$\mathbf{Q}: dX_t = (b + \sigma_t u)(X_t, t)dt + \sigma_t dW_t \quad X_0 \sim p_0$$

# Variational Inference with Path RND

**Variational Inference in Path space:**

$$\frac{dQ^*}{dP} \propto L$$

$$Q = \min KL[Q||Q^*]$$

$$P: dX_t = b(X_t, t)dt + \sigma_t dW_t \quad X_0 \sim p_0$$

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# Variational Inference with Path RND

**Variational Inference in Path space:**

$$\frac{dQ^*}{dP} \propto L$$

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# Variational Inference with Path RND

**Variational Inference in Path space:**

$$\frac{dQ^*}{dP} \propto L$$

$$Q = \min E_Q \left[ \log \frac{dQ}{dQ^*} \right] = \min E_Q \left[ \log \frac{dQ}{dP} + \log \frac{dP}{dQ^*} \right]$$

$$P: dX_t = b(X_t, t)dt + \sigma_t dW_t \quad X_0 \sim p_0$$

$$Q: dX_t = (b + \sigma_t u)(X_t, t)dt + \sigma_t dW_t \quad X_0 \sim p_0$$

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$$\frac{dQ^*}{dP} \propto L$$

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$$X_0 \sim p_0$$

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**Forward-forward RND and Girsanov**

$$P: dX_t = f(X_t, t)dt + \sigma_t dW_t, X_0 \sim p_0$$
$$Q: dX_t = h(X_t, t)dt + \sigma_t dW_t, X_0 \sim q_0$$

$$\frac{dP}{dQ}(X) = \underbrace{\frac{p(X_0)}{q(X_0)}}_{\text{Initial density ratio}} \exp \left( \int \underbrace{\frac{f_t(X_t)}{\sigma_t^2} \cdot dX_t}_{\text{Forward Ito Integral}} - \frac{f_t^2(X_t)}{2\sigma_t^2} dt - \int \frac{g_t(X_t)}{\sigma_t^2} \cdot dX_t + \frac{g_t^2(X_t)}{2\sigma_t^2} dt \right)$$

Forward Ito Integral  $\int a_t(X_t) \cdot dX_t = \lim \sum a_n(X_n) \cdot (X_{n+1} - X_n)$

# Variational Inference with Path RND

**Variational Inference in Path space:**

$$\frac{dQ^*}{dP} \propto L$$

$$Q = \min E_Q \left[ \log \frac{dQ}{dQ^*} \right] = \min E_Q \left[ \int \frac{1}{2} ||u_t||^2 dt - \log L \right]$$

$$P: dX_t = b(X_t, t)dt + \sigma_t dW_t \quad X_0 \sim p_0$$

$$Q: dX_t = (b + \sigma_t u)(X_t, t)dt + \sigma_t dW_t \quad X_0 \sim p_0$$

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$$X_0 \sim p_0$$

**stochastic optimal control**

$$Q: dX_t = (b + \sigma_t u)(X_t, t)dt + \sigma_t dW_t \quad X_0 \sim p_0$$

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$$Q: dX_t = (b + \sigma_t u)(X_t, t)dt + \sigma_t dW_t \quad X_0 \sim p_0$$

👉 fine-tune diffusion models [1]  
👉 neural samplers [2,3,4...]

- [1] Domingo-Enrich, C., Drozdzal, M., Karrer, B., & Chen, R. T. (2024). Adjoint matching: Fine-tuning flow and diffusion generative models with memoryless stochastic optimal control. ICLR 2025.
- [2] Havens, A., Miller, B. K., Yan, B., Domingo-Enrich, C., Sriram, A., Wood, B., ... & Chen, R. T. (2025). Adjoint sampling: Highly scalable diffusion samplers via adjoint matching. ICML 2025.
- [3] Liu, G. H., Choi, J., Chen, Y., Miller, B. K., & Chen, R. T. (2025). Adjoint Schrodinger Bridge Sampler. arXiv.
- [4] Zhu, Y., Guo, W., Choi, J., Liu, G. H., Chen, Y., & Tao, M. (2025). MDNS: Masked Diffusion Neural Sampler via Stochastic Optimal Control. arXiv.

# Collaborators on FEAT



# Collaborators on RNE



# Fantastic Path RNDs

- ★ *intuitive understand from sequence of Gaussian kernels*
- ★ *Forward-forward RND with Girsanov theorem*
- ★ *Forward-backward RND*

# Where to Find Them?

## Importance Sampling with Path RND

*AIS, Jarzynski and Crook's Fluctuation Theorem*

*Free-energy estimation*

*Density estimation*

*Generation control*

*Energy regularisation*

## Variational Inference with Path RND

*Neural samplers*

*Diffusion model fine-tuning*

# Thank You!

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