

Diffusion Model and Path Space Probabilistic Inference

Jiajun He
University of Cambridge

Outlines

- **Diffusion Model:**

Forward and backward SDEs, time-reversal, and Path RND

- **Path-space Probability Inference:**

Example: Importance Sampling with Path RND;

Variational Inference with Path RND;

Replica Exchange with Path RND.

Diffusion Models

Diffusion Models

Posterior (data \rightarrow noise): $p(x_0)$



$p(x_0)$

Diffusion Models

Posterior (data \rightarrow noise): $p(x_0)q(x_1|x_0)$



$p(x_0)$



$q(x_1|x_0)$

Diffusion Models

Posterior (data \rightarrow noise): $p(x_0)q(x_1|x_0)q(x_2|x_1)$



$p(x_0)$



$q(x_1|x_0)$



$q(x_2|x_1)$

Diffusion Models

Posterior (data \rightarrow noise): $p(x_0)q(x_1|x_0)q(x_2|x_1) \dots$



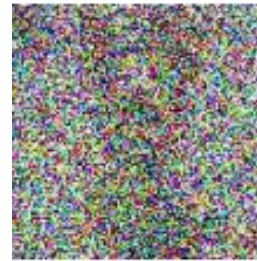
$p(x_0)$



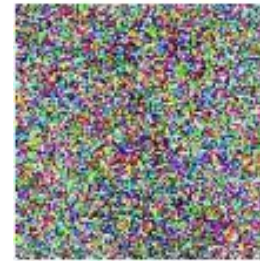
$q(x_1|x_0)$



$q(x_2|x_1)$



...



Diffusion Models

Posterior (data \rightarrow noise): $p(x_0)q(x_1|x_0)q(x_2|x_1) \dots q(x_T|x_{T-1})$



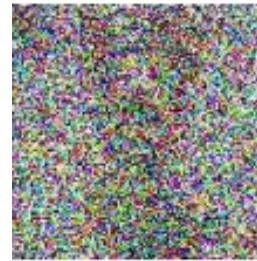
$p(x_0)$



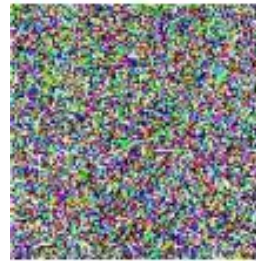
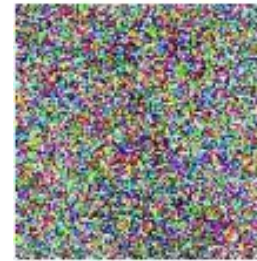
$q(x_1|x_0)$



$q(x_2|x_1)$



...



$q(x_T|x_{T-1})$

Diffusion Models

Posterior (data \rightarrow noise): $p(x_0)q(x_1|x_0)q(x_2|x_1) \dots q(x_T|x_{T-1})$



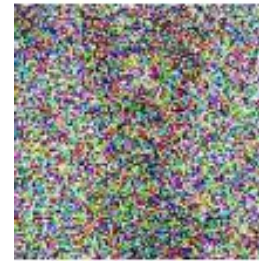
$p(x_0)$



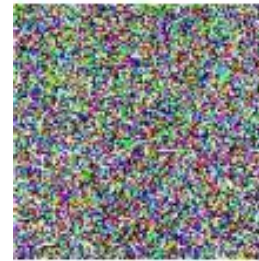
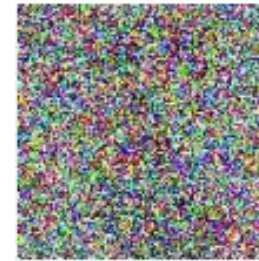
$q(x_1|x_0)$



$q(x_2|x_1)$



...



$q(x_T|x_{T-1})$

Generation (noise \rightarrow data): $p(x_T)$



$p(x_T)$

Diffusion Models

Posterior (data \rightarrow noise): $p(x_0)q(x_1|x_0)q(x_2|x_1) \dots q(x_T|x_{T-1})$



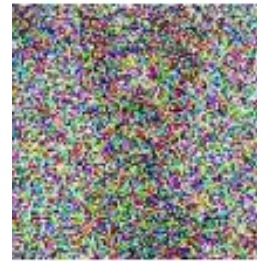
$p(x_0)$



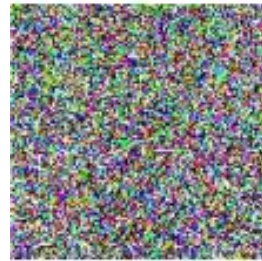
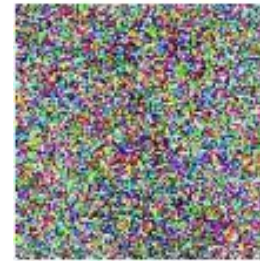
$q(x_1|x_0)$



$q(x_2|x_1)$



...



$q(x_T|x_{T-1})$

Generation (noise \rightarrow data): $p(x_T)p(x_{T-1}|x_T)$



$p(x_T)$



$p(x_{T-1}|x_T)$

Diffusion Models

Posterior (data \rightarrow noise): $p(x_0)q(x_1|x_0)q(x_2|x_1) \dots q(x_T|x_{T-1})$



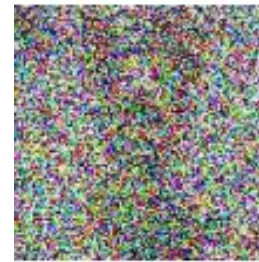
$p(x_0)$



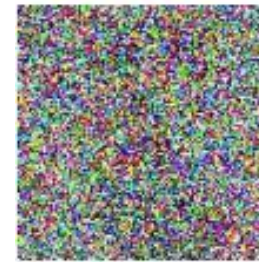
$q(x_1|x_0)$



$q(x_2|x_1)$

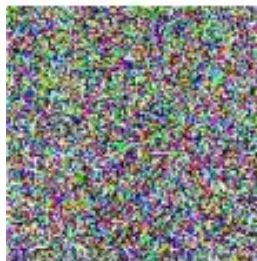


...



$q(x_T|x_{T-1})$

Generation (noise \rightarrow data): $p(x_T)p(x_{T-1}|x_T) \dots$



$p(x_T)$



$p(x_{T-1}|x_T)$



$p(x_{T-2}|x_{T-1})$



...



Diffusion Models

Posterior (data \rightarrow noise): $p(x_0)q(x_1|x_0)q(x_2|x_1) \dots q(x_T|x_{T-1})$



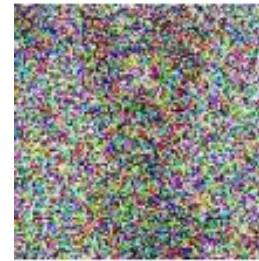
$p(x_0)$



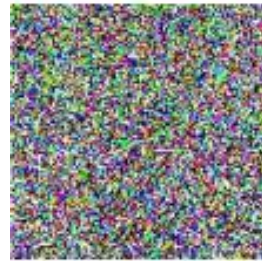
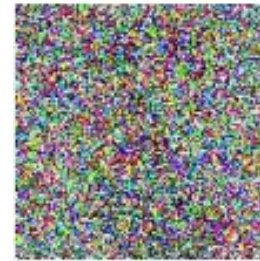
$q(x_1|x_0)$



$q(x_2|x_1)$



...



$q(x_T|x_{T-1})$

Generation (noise \rightarrow data): $p(x_T)p(x_{T-1}|x_T) \dots p(x_0|x_1)$



$p(x_T)$



$p(x_{T-1}|x_T)$



$p(x_{T-2}|x_{T-1})$



...



$p(x_0|x_1)$

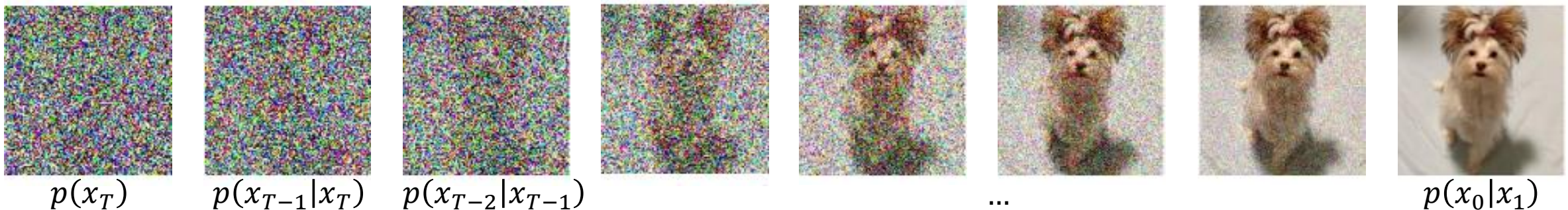
Diffusion Models

Forward SDE (data \rightarrow noise): $x_{t'} = x_t - \beta_t x_t dt + \sqrt{2\beta_t} dt \epsilon$

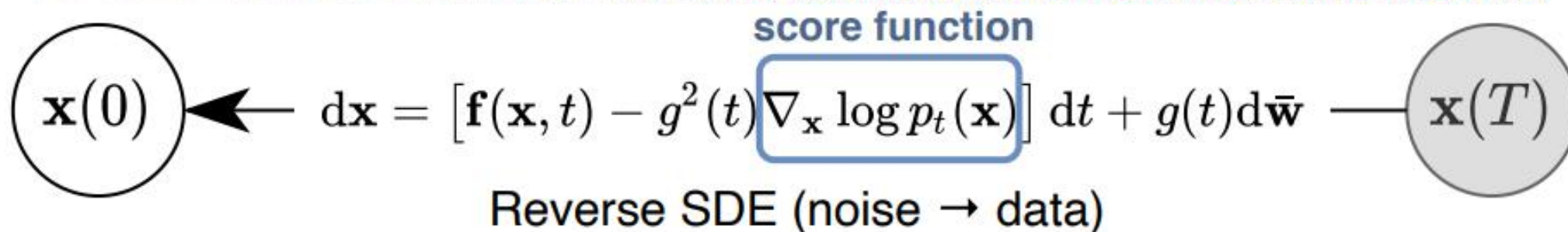
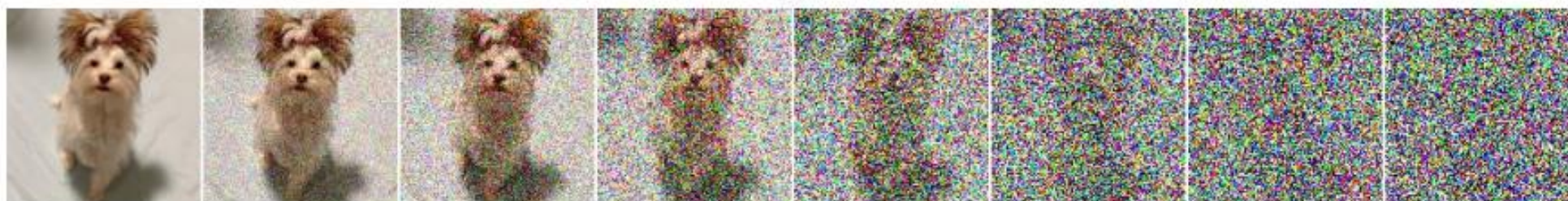
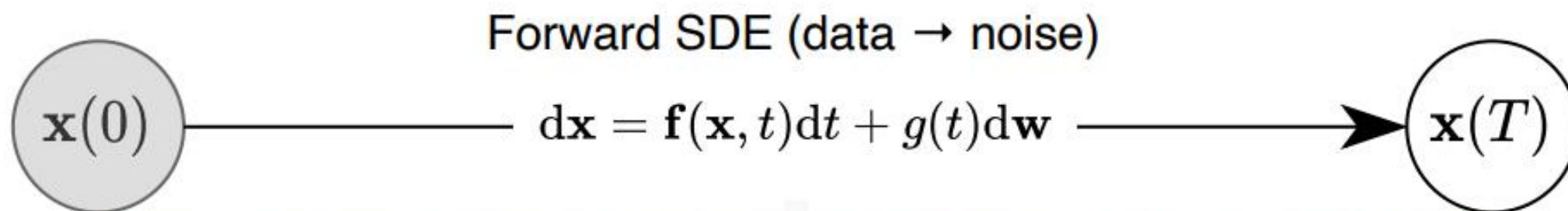


Backward SDE (noise \rightarrow data):

$$x_{t'} = x_t + [\beta_t x_t + 2\beta_t \nabla \log p_t(x_t)] dt + \sqrt{2\beta_t} dt \epsilon'$$



Diffusion Models



Time-reversal and Nelson's relation

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

“time-reversal” iff

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

Time-reversal and Nelson's relation

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

Eular-Maruyama Discretisation:

$$\begin{aligned}X_{n+1} - X_n &= f(X_n, t_n)\Delta t + \sigma_n \sqrt{\Delta t} \epsilon \\X_{n+1} - X_n &= g(X_{n+1}, t_{n+1})\Delta t + \sigma_{n+1} \sqrt{\Delta t} \epsilon'\end{aligned}$$

From Gaussian Density Ratio to Path RND

Now take a closer look at

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

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

From Gaussian Density Ratio to Path RND

Now take a closer look at

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

? 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

Let's look at

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

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

From Gaussian Density Ratio to Path RND

Let's look at

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

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

From Gaussian Density Ratio to Path RND

Let's look at

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

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

💀 density diverge when $\Delta t \rightarrow 0$

From Gaussian Density Ratio to Path RND

But what if we have another kernel:

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

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

From Gaussian Density Ratio to Path RND

But what if we have another kernel:

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

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

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

From Gaussian Density Ratio to Path RND

But what if we have another kernel:

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

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

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

From Gaussian Density Ratio to Path RND

But what if we have another kernel:

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

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

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

 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:

$$\frac{d\mathbf{P}}{d\mathbf{Q}}(X)$$

Path RND and where to find them

- **Path RND:** FF-RND, FB-RND
- **Where to find them?**
 - Importance Sampling
 - Path Space MCMC
 - Parallel Tempering
 - Variational Inference
 - Etc...

A young man with brown hair, wearing a blue coat, holds a glowing wand. The wand's tip emits a bright blue light. In the background, a penguin is visible. The scene is set in a dark, cluttered room with various items hanging on the walls.

FANTASTIC PATH RIND

AND WHERE
TO FIND THEM

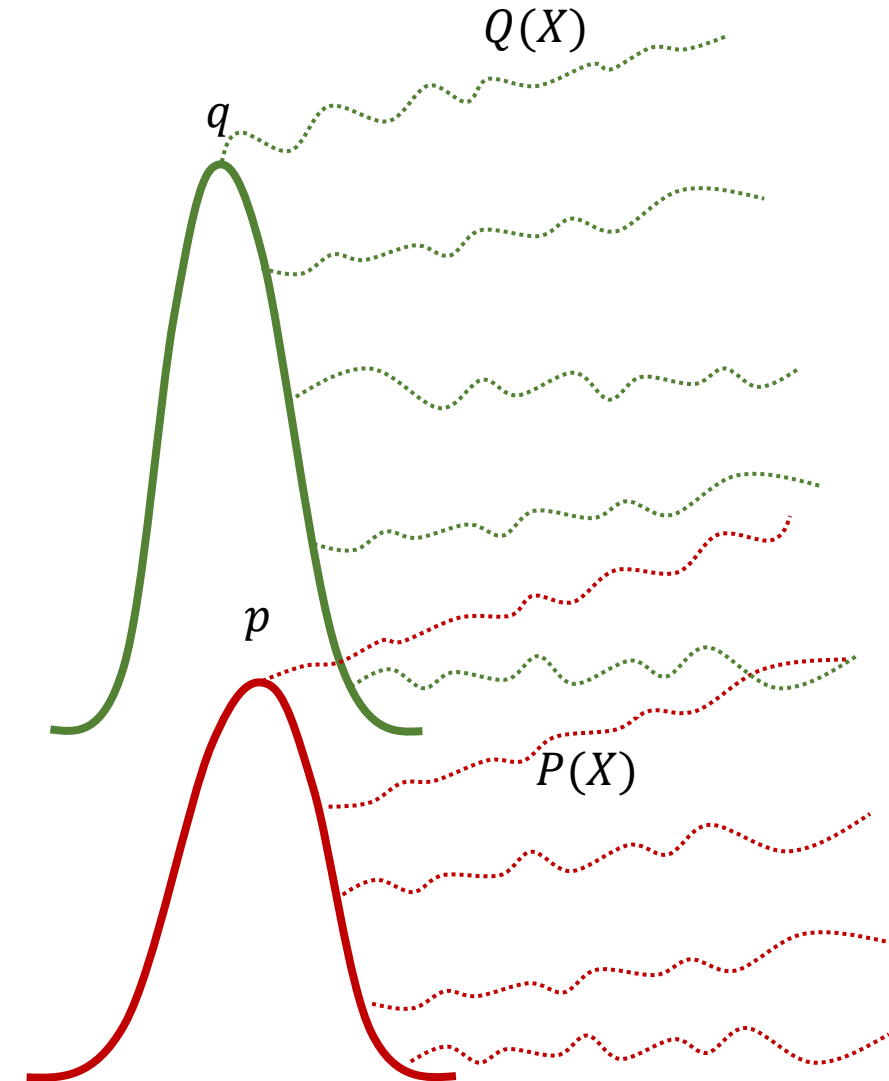
Fantastic Path RND and where to find them

- **Fantastic Path RND:** FF-RND, FB-RND
- **Where to find them?**
 - Importance Sampling:
 - **Free-energy estimation**, density estimation, SMC
 - **Parallel Tempering**
 - Variational Inference

Forward-forward RND (FF-RND) and Girsanov

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

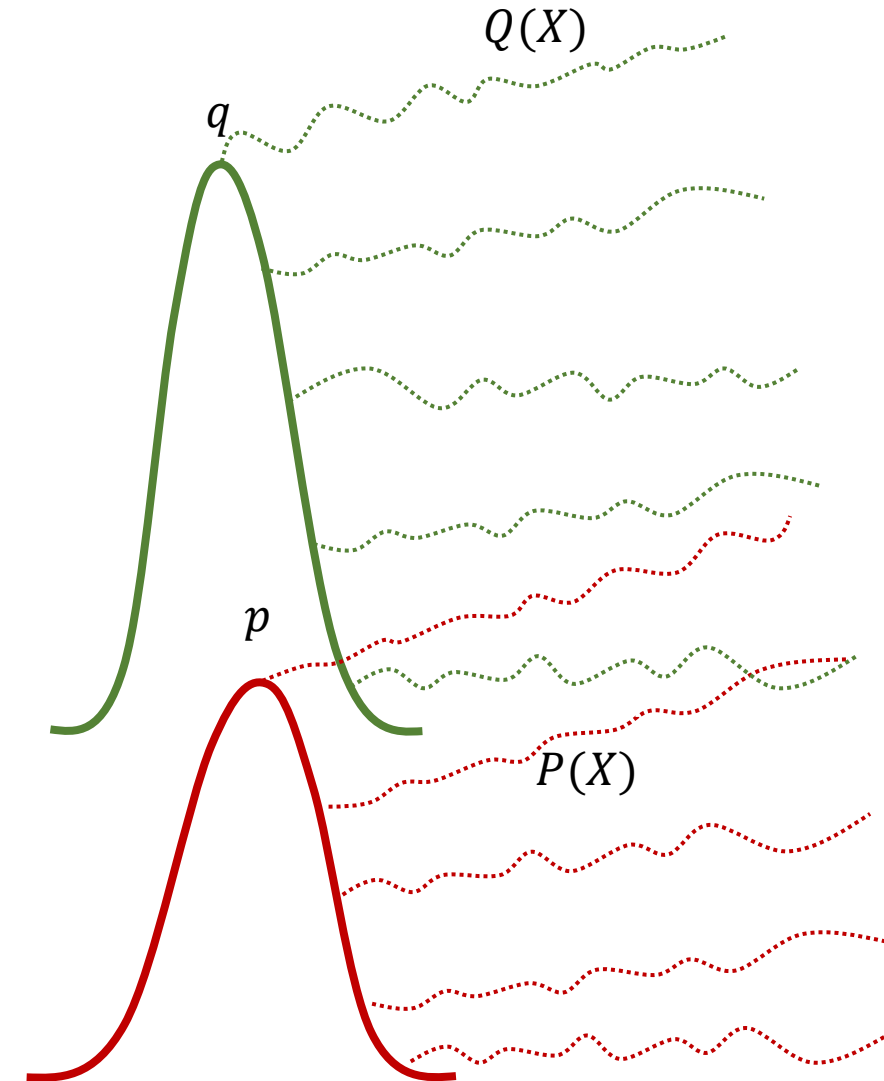
$$Q : dX_t = g(X_t, t)dt + \sigma_t dW_t, X_0 \sim q_0 = q$$



Forward-forward RND (FF-RND) and Girsanov

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

$$\frac{dP}{dQ}(X) = \lim \frac{\underbrace{p(X_0)}_{\text{Initial density ratio}} \underbrace{\prod N_1(X_{n+1}|X_n)}_{\text{Transition kernel ratio}}}{q(X_0) \prod N_2(X_{n+1}|X_n)}$$

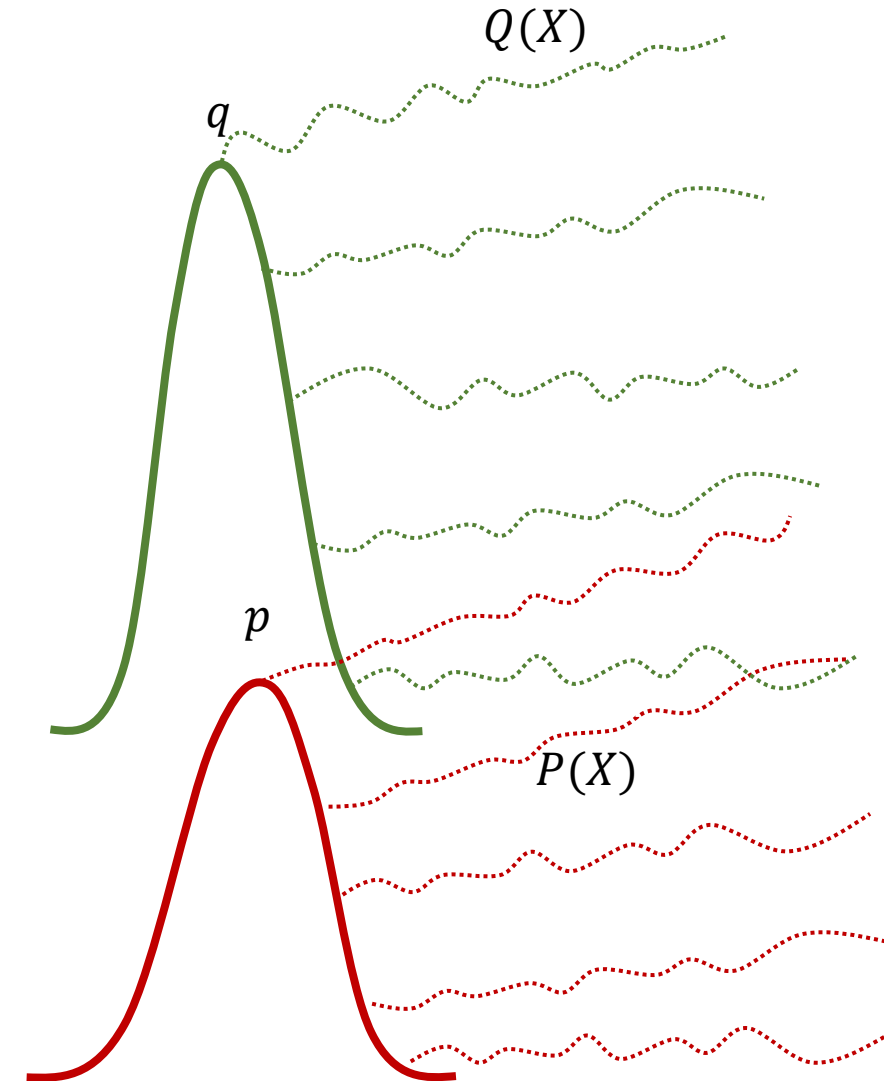


Forward-forward RND (FF-RND) and Girsanov

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

$$Q : dX_t = g(X_t, t)dt + \sigma_t dW_t, X_0 \sim q_0 = q$$

$$\frac{dP}{dQ}(X) = \lim \frac{\underbrace{p(X_0)}_{\text{Initial density ratio}} \prod N_1(X_{n+1}|X_n)}{\underbrace{q(X_0) \prod N_2(X_{n+1}|X_n)}_{\text{Transition kernel ratio}}}$$



Forward-forward RND (FF-RND) and Girsanov

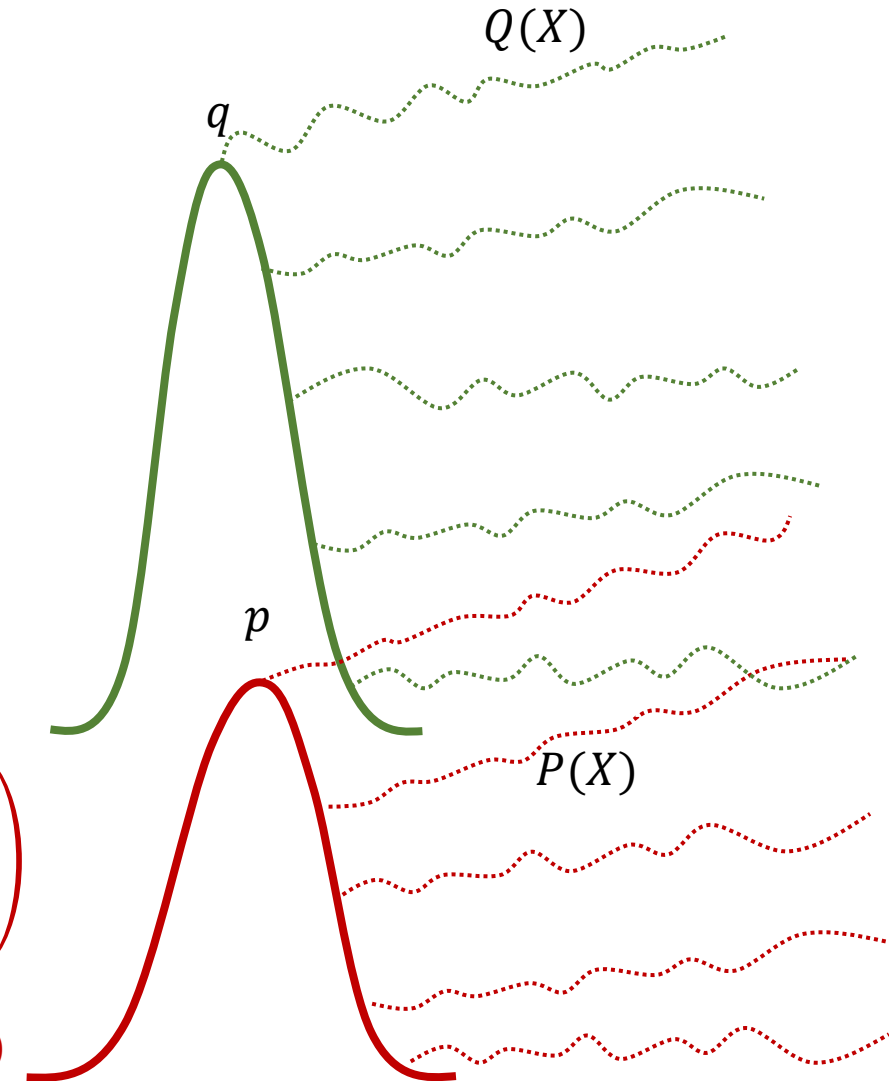
$$P : dX_t = f(X_t, t)dt + \sigma_t dW_t, X_0 \sim p_0 = p$$

$$Q : dX_t = g(X_t, t)dt + \sigma_t dW_t, X_0 \sim q_0 = q$$

$$\frac{dP}{dQ}(X) = \lim \frac{\underbrace{p(X_0)}_{\text{Initial density ratio}} \underbrace{\prod N_1(X_{n+1}|X_n)}_{\text{Transition kernel ratio}}}{q(X_0) \prod N_2(X_{n+1}|X_n)}$$

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

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



Forward-forward RND (FF-RND) and Girsanov

Unnormalised density?

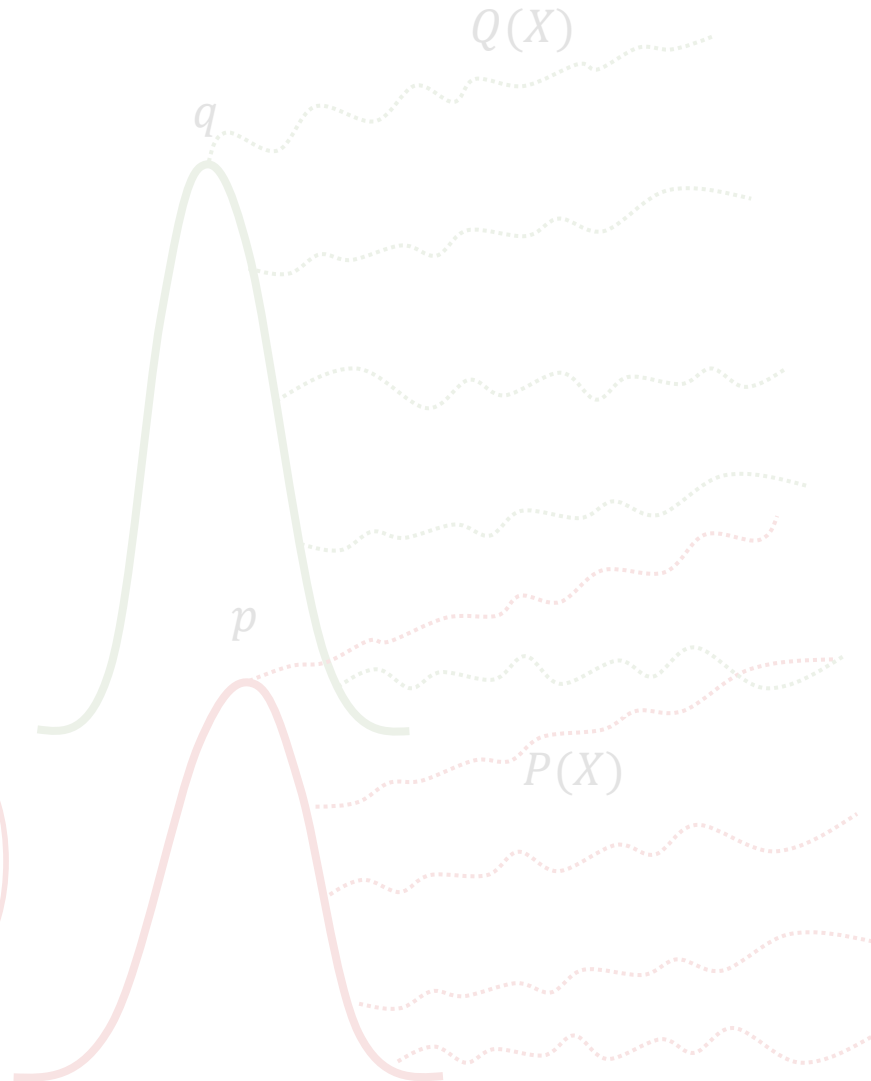
$$P : dX_t = f(X_t, t)dt + \sigma_t dW_t, X_0 \sim p_0 = p$$

$$Q : dX_t = g(X_t, t)dt + \sigma_t dW_t, X_0 \sim q_0 = q$$

$$\frac{dP}{dQ}(X) = \lim \frac{\underbrace{p(X_0)}_{\text{Initial density ratio}} \prod \underbrace{N_1(X_{n+1}|X_n)}_{\text{Transition kernel ratio}}}{q(X_0) \prod N_2(X_{n+1}|X_n)}$$

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

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



Forward-forward RND (FF-RND) and Girsanov

Unnormalised density?

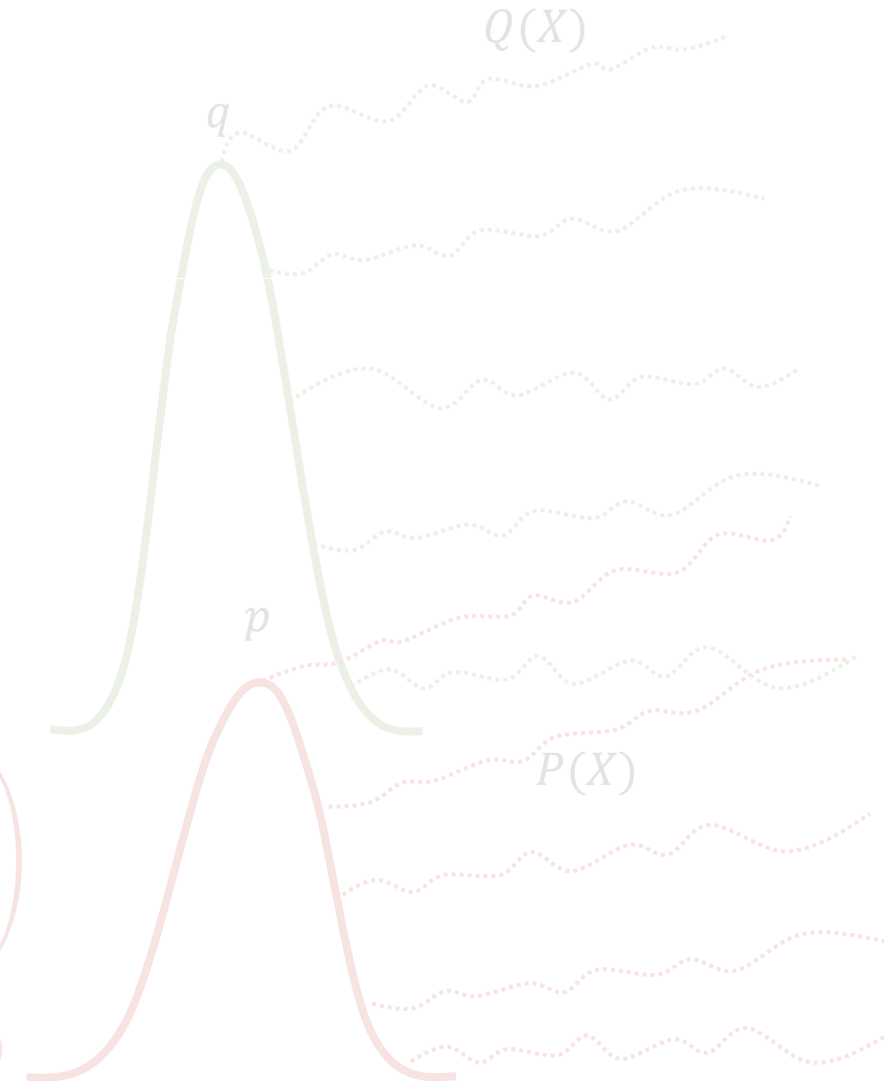
$$P : dX_t = f(X_t, t)dt + \sigma_t dW_t, X_0 \sim \tilde{p}_0 = \tilde{p}$$

$$Q : dX_t = g(X_t, t)dt + \sigma_t dW_t, X_0 \sim \tilde{q}_0 = \tilde{q}$$

$$\frac{dP}{dQ}(X) = \lim \underbrace{\frac{p(X_0)}{q(X_0)}}_{\text{Initial density ratio}} \underbrace{\prod N_1(X_{n+1}|X_n)}_{\text{Transition kernel ratio}} \prod N_2(X_{n+1}|X_n)$$

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

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



Forward-forward RND (FF-RND) and Girsanov

Unnormalised density?

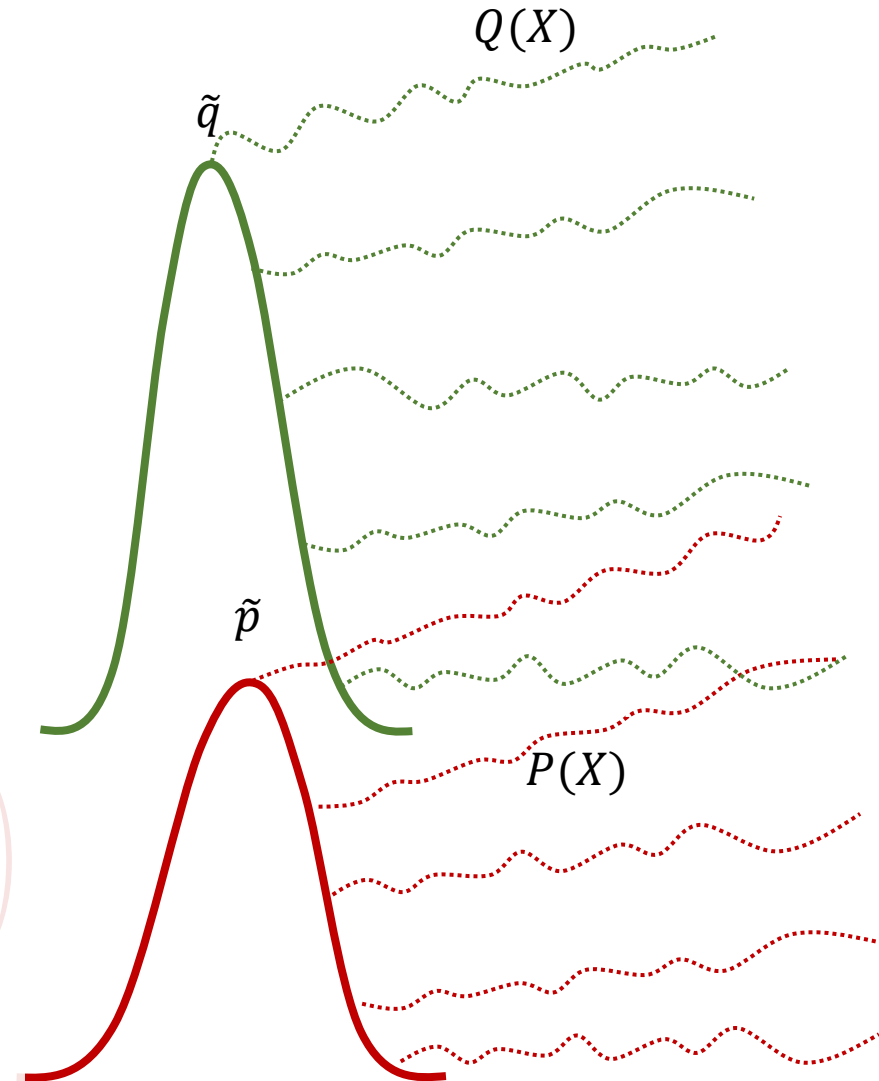
$$P : dX_t = f(X_t, t)dt + \sigma_t dW_t, X_0 \sim \tilde{p}_0 = \tilde{p}$$

$$Q : dX_t = g(X_t, t)dt + \sigma_t dW_t, X_0 \sim \tilde{q}_0 = \tilde{q}$$

$$\frac{dP}{dQ}(X) = \lim \underbrace{\frac{p(X_0)}{q(X_0)}}_{\text{Initial density ratio}} \underbrace{\prod N_1(X_{n+1}|X_n)}_{\text{Transition kernel ratio}} \prod N_2(X_{n+1}|X_n)$$

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

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



Forward-forward RND (FF-RND) and Girsanov

Unnormalised density?

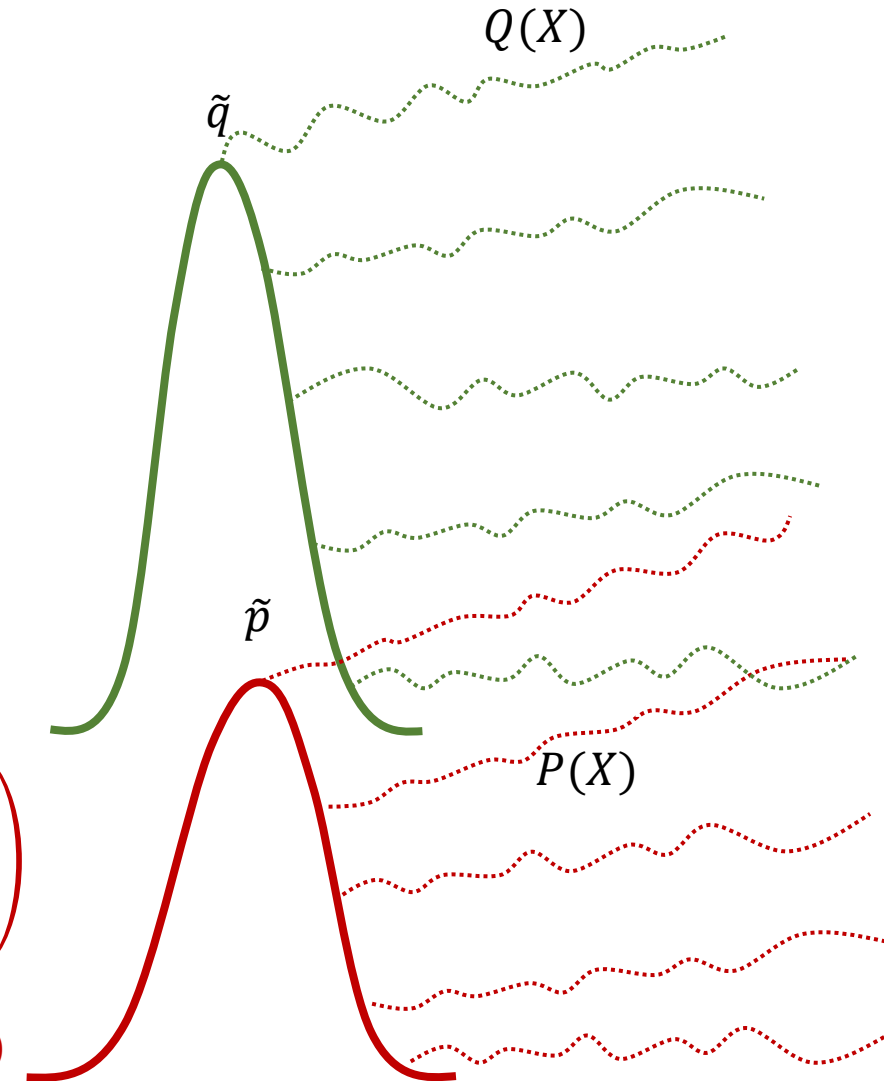
$$P : dX_t = f(X_t, t)dt + \sigma_t dW_t, X_0 \sim \tilde{p}_0 = \tilde{p}$$

$$Q : dX_t = g(X_t, t)dt + \sigma_t dW_t, X_0 \sim \tilde{q}_0 = \tilde{q}$$

$$w(X) = \frac{Z_p dP}{Z_q dQ}(X) = \lim \frac{\underbrace{\tilde{p}(X_0)}_{\text{Initial density ratio}} \underbrace{\prod N_1(X_{n+1}|X_n)}_{\text{Transition kernel ratio}}}{\tilde{q}(X_0) \prod N_2(X_{n+1}|X_n)}$$

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

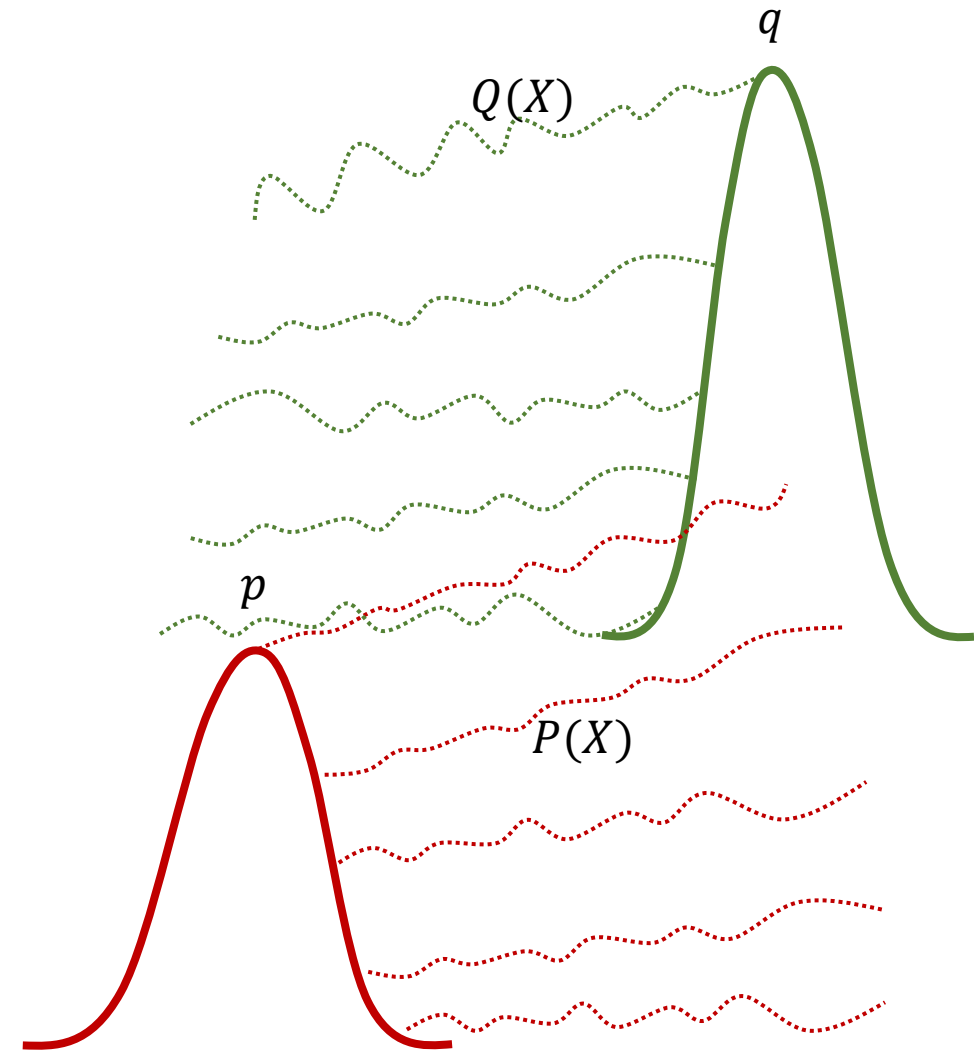
$$\int a_t(X_t) \cdot dX_t = \lim \sum a_n(X_n) \cdot (X_{n+1} - X_n)$$



Forward-backward RND (FB-RND)

$$P : dX_t = f(X_t, t)dt + \sigma_t dW_t, X_0 \sim \tilde{p}_0 = \tilde{p}$$

$$Q : dX_t = g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_1 \sim \tilde{q}_1 = \tilde{q}$$

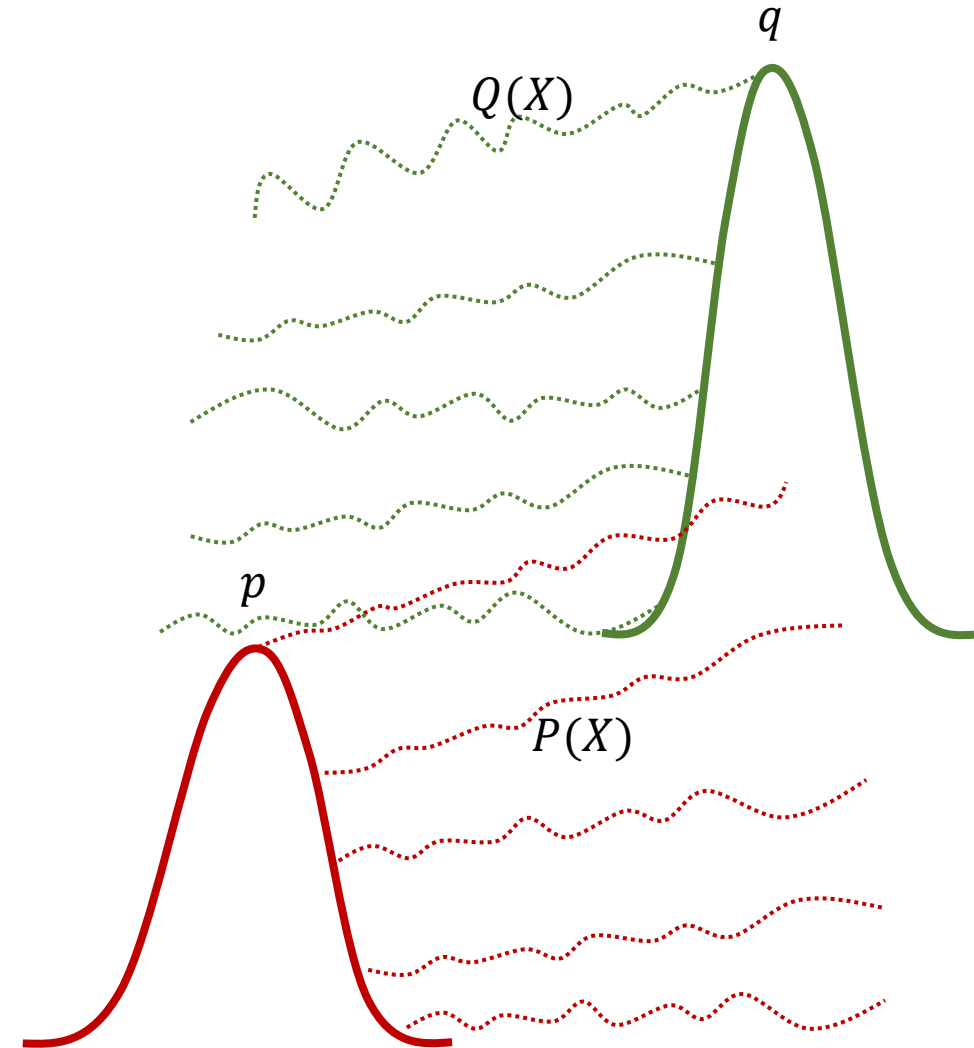


Forward-backward RND (FB-RND)

$$P : dX_t = f(X_t, t)dt + \sigma_t dW_t, X_0 \sim \tilde{p}_0 = \tilde{p}$$

$$Q : dX_t = g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_1 \sim \tilde{q}_1 = \tilde{q}$$

$$w(X) = \frac{Z_p dP}{Z_q d\tilde{Q}}(X) = \lim \frac{\underbrace{\tilde{p}_0(X_0)}_{\text{Initial density ratio}} \prod N_1(X_{n+1}|X_n)}{\underbrace{\tilde{q}_1(X_1) \prod N_2(X_n|X_{n+1})}_{\text{Transition kernel ratio}}}$$



Forward-backward RND (FB-RND)

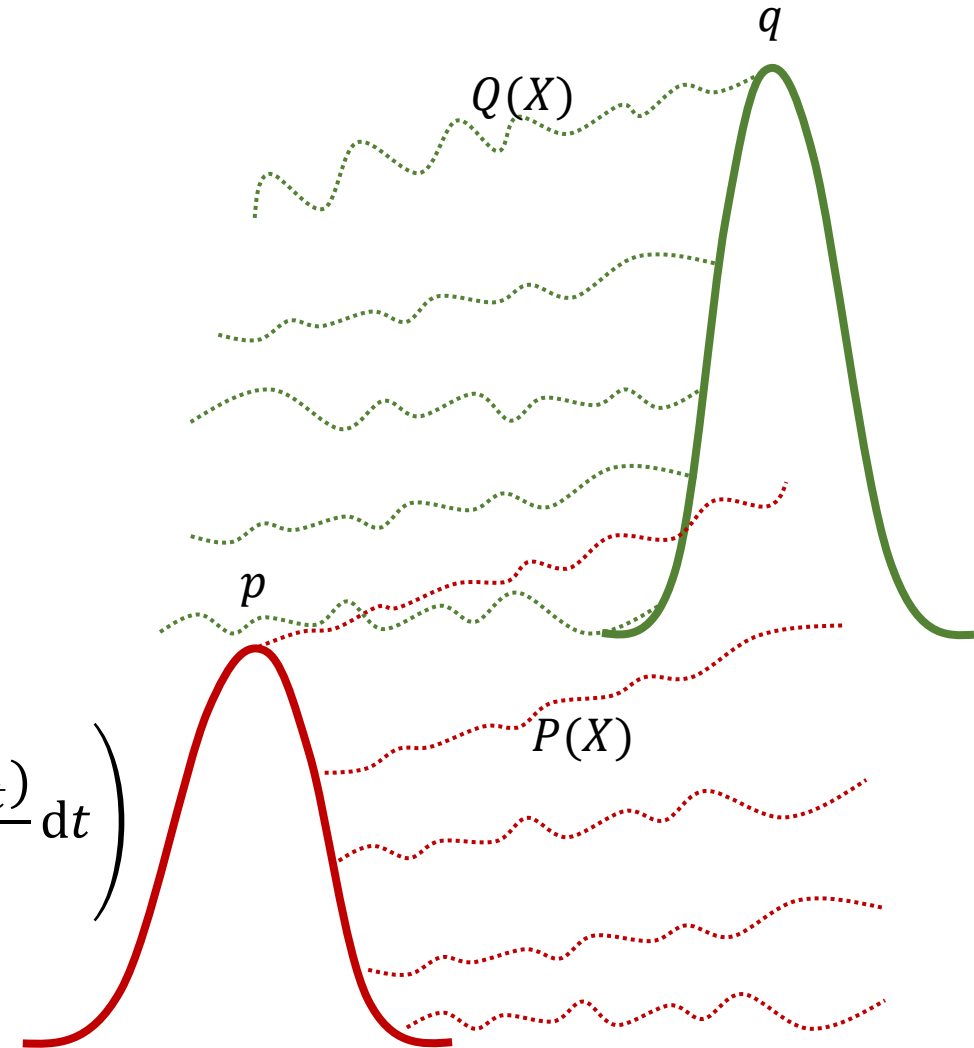
$$P : dX_t = f(X_t, t)dt + \sigma_t dW_t, X_0 \sim \tilde{p}_0 = \tilde{p}$$

$$Q : dX_t = g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_1 \sim \tilde{q}_1 = \tilde{q}$$

$$w(X) = \frac{Z_p dP}{Z_q d\tilde{Q}}(X) = \lim \frac{\underbrace{\tilde{p}_0(X_0)}_{\text{Initial density ratio}} \prod \underbrace{N_1(X_{n+1}|X_n)}_{\text{Transition kernel ratio}}}{\underbrace{\tilde{q}_1(X_1)}_{\text{Initial density ratio}} \prod \underbrace{N_2(X_n|X_{n+1})}_{\text{Transition kernel ratio}}}$$

$$= \frac{\tilde{p}_0(X_0)}{\tilde{q}_1(X_1)} \exp \left(\int \frac{f_t(X_t)}{\sigma_t^2} \cdot dX_t - \frac{f_t^2(X_t)}{2\sigma_t^2} dt - \underbrace{\int \frac{g_t(X_t)}{\sigma_t^2} \cdot \overleftarrow{dX}_t + \frac{g_t^2(X_t)}{2\sigma_t^2} dt}_{\text{Backward Ito Integral}} \right)$$

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



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:

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

Summary

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

Density ratio: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$

- Importance sampling: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$
- FEP: $\Delta F = -\log(\int q(x)w(x) dx)$
- PT Swap: $\alpha = \min\{1, \frac{w(y)}{w(x)}\}$

Background on Free Energy

Background on Free Energy

- Unnormalized density: $\tilde{p}(X) = \exp(-U(X))$

Background on Free Energy

- Unnormalized density: $\tilde{p}(X) = \exp(-U(X))$
- The normalization factor: $Z = \int \tilde{p}(X) dX$

Background on Free Energy

- Unnormalized density: $\tilde{p}(X) = \exp(-U(X))$
- The normalization factor: $Z = \int \tilde{p}(X) dX$
- The free energy: $f = -\log Z$

Background on Free Energy

- Unnormalized density: $\tilde{p}(X) = \exp(-U(X))$
- The normalization factor: $Z = \int \tilde{p}(X) dX$
- The free energy: $f = -\log Z$
- Free energy difference: $\Delta f = f_2 - f_1 = -\log \frac{Z_2}{Z_1}$

Background on Free Energy

- Unnormalized density: $\tilde{p}(X) = \exp(-U(X))$
- The normalization factor: $Z = \int \tilde{p}(X)dX$
- The free energy: $f = -\log Z$
- Free energy difference: $\Delta f = f_2 - f_1 = -\log \frac{Z_2}{Z_1}$

👉 model evidence

👉 binding affinity

👉 potential of mean force

...

Density Ratio and where to find them

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

Density ratio: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$

Density Ratio and where to find them

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

$$\text{Density ratio: } w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$$

- Importance sampling / resampling:
e.g., free-energy estimation:

Density Ratio and where to find them

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

Density ratio: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$

- Importance sampling / resampling:
e.g., free-energy estimation:

$$\begin{aligned}\Delta F &= -\log \frac{Z_p}{Z_q} = -\log \frac{\int \tilde{p}(x) dx}{Z_q} \\ &= -\log \left(\frac{1}{Z_q} \int \tilde{q}(x) \frac{\tilde{p}(x)}{\tilde{q}(x)} dx \right) \\ &= -\log \left(\int \frac{\tilde{q}(x) \tilde{p}(x)}{Z_q \tilde{q}(x)} dx \right) \\ &= -\log \left(\int q(x) \frac{\tilde{p}(x)}{\tilde{q}(x)} dx \right)\end{aligned}$$

Density Ratio and where to find them

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

Density ratio: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$

- Importance sampling / resampling:
e.g., free-energy estimation:

$$\begin{aligned}\Delta F &= -\log \frac{Z_p}{Z_q} = -\log \frac{\int \tilde{p}(x) dx}{Z_q} \\ &= -\log \left(\frac{1}{Z_q} \int \tilde{q}(x) \frac{\tilde{p}(x)}{\tilde{q}(x)} dx \right) \\ &= -\log \left(\int \frac{\tilde{q}(x) \tilde{p}(x)}{Z_q \tilde{q}(x)} dx \right) \\ &= -\log \left(\int q(x) \frac{\tilde{p}(x)}{\tilde{q}(x)} dx \right)\end{aligned}$$

Density Ratio and where to find them

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

Density ratio: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$

- Importance sampling / resampling:
e.g., free-energy estimation:

$$\begin{aligned}\Delta F &= -\log \frac{Z_p}{Z_q} = -\log \frac{\int \tilde{p}(x) dx}{Z_q} \\ &= -\log \left(\frac{1}{Z_q} \int \tilde{q}(x) \frac{\tilde{p}(x)}{\tilde{q}(x)} dx \right) \\ &= -\log \left(\int \frac{\tilde{q}(x) \tilde{p}(x)}{Z_q \tilde{q}(x)} dx \right) \\ &= -\log \left(\int q(x) \frac{\tilde{p}(x)}{\tilde{q}(x)} dx \right)\end{aligned}$$

Density Ratio and where to find them

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

Density ratio: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$

- Importance sampling / resampling:
e.g., free-energy estimation:

$$\begin{aligned}\Delta F &= -\log \frac{Z_p}{Z_q} = -\log \frac{\int \tilde{p}(x) dx}{Z_q} \\ &= -\log \left(\frac{1}{Z_q} \int \tilde{q}(x) \frac{\tilde{p}(x)}{\tilde{q}(x)} dx \right) \\ &= -\log \left(\int \frac{\tilde{q}(x)}{Z_q} \frac{\tilde{p}(x)}{\tilde{q}(x)} dx \right) \\ &= -\log \left(\int q(x) \frac{\tilde{p}(x)}{\tilde{q}(x)} dx \right)\end{aligned}$$

Density Ratio and where to find them

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

Density ratio: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$

- Importance sampling / resampling:
e.g., free-energy estimation:

$$\begin{aligned}\Delta F &= -\log \frac{Z_p}{Z_q} = -\log \frac{\int \tilde{p}(x) dx}{Z_q} \\ &= -\log \left(\frac{1}{Z_q} \int \tilde{q}(x) \frac{\tilde{p}(x)}{\tilde{q}(x)} dx \right) \\ &= -\log \left(\int \frac{\tilde{q}(x) \tilde{p}(x)}{Z_q \tilde{q}(x)} dx \right) \\ &= -\log \left(\int q(x) w(x) dx \right)\end{aligned}$$

Density Ratio and where to find them

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

Density ratio: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$

Free-energy Perturbation

- Importance sampling / resampling:
e.g., free-energy estimation:

$$\begin{aligned}\Delta F &= -\log \frac{Z_p}{Z_q} = -\log \frac{\int \tilde{p}(x) dx}{Z_q} \\ &= -\log \left(\frac{1}{Z_q} \int \tilde{q}(x) \frac{\tilde{p}(x)}{\tilde{q}(x)} dx \right) \\ &= -\log \left(\int \frac{\tilde{q}(x) \tilde{p}(x)}{Z_q \tilde{q}(x)} dx \right) \\ &= -\log \left(\int q(x) w(x) dx \right)\end{aligned}$$

Density Ratio and where to find them

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

Density ratio: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$

- Parallel Tempering:

Parallel tempering

- **An MCMC algorithm for target density $\tilde{\pi}_N$**
- Workflow:
 - Choose an easy-to-sample reference $\tilde{\pi}_0$
 - Design multiple intermediate targets $\tilde{\pi}_n$
 - Design two MCMC kernels with invariant measure as $\tilde{\pi}_0 \times \tilde{\pi}_1 \times \cdots \times \tilde{\pi}_N$

Parallel tempering

- An MCMC algorithm for target density $\tilde{\pi}_N$
- Workflow:
 - Choose an easy-to-sample reference $\tilde{\pi}_0$
 - Design multiple intermediate targets $\tilde{\pi}_n$
 - Design two MCMC kernels with invariant measure as $\tilde{\pi}_0 \times \tilde{\pi}_1 \times \cdots \times \tilde{\pi}_N$

Parallel tempering

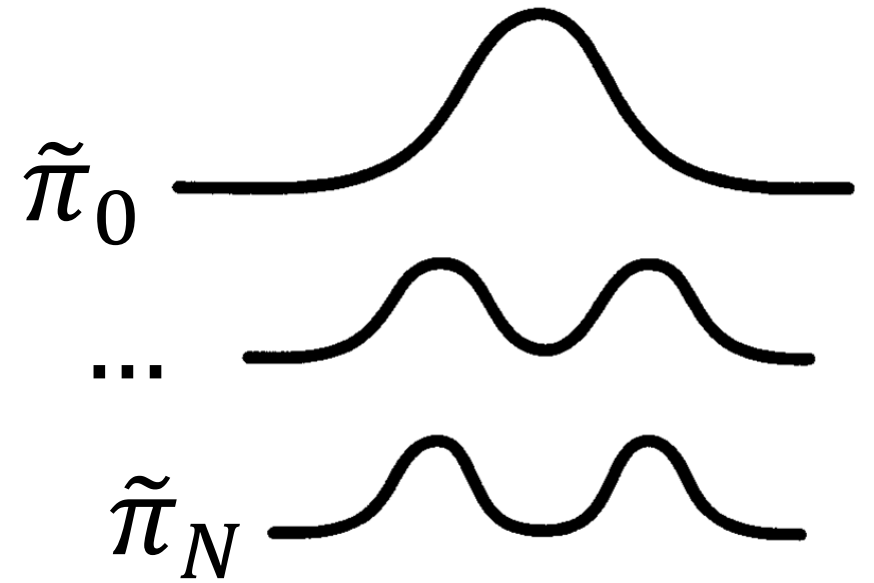
- An MCMC algorithm for target density $\tilde{\pi}_N$
- Workflow:
 - Choose an easy-to-sample reference $\tilde{\pi}_0$
 - Design multiple intermediate targets $\tilde{\pi}_n$
 - Design two MCMC kernels with invariant measure as $\tilde{\pi}_0 \times \tilde{\pi}_1 \times \cdots \times \tilde{\pi}_N$

Parallel tempering

- An MCMC algorithm for target density $\tilde{\pi}_N$
- Workflow:
 - Choose an easy-to-sample reference $\tilde{\pi}_0$
 - Design multiple intermediate targets $\tilde{\pi}_n$
 - Design two MCMC kernels with invariant measure as $\tilde{\pi}_0 \times \tilde{\pi}_1 \times \cdots \times \tilde{\pi}_N$

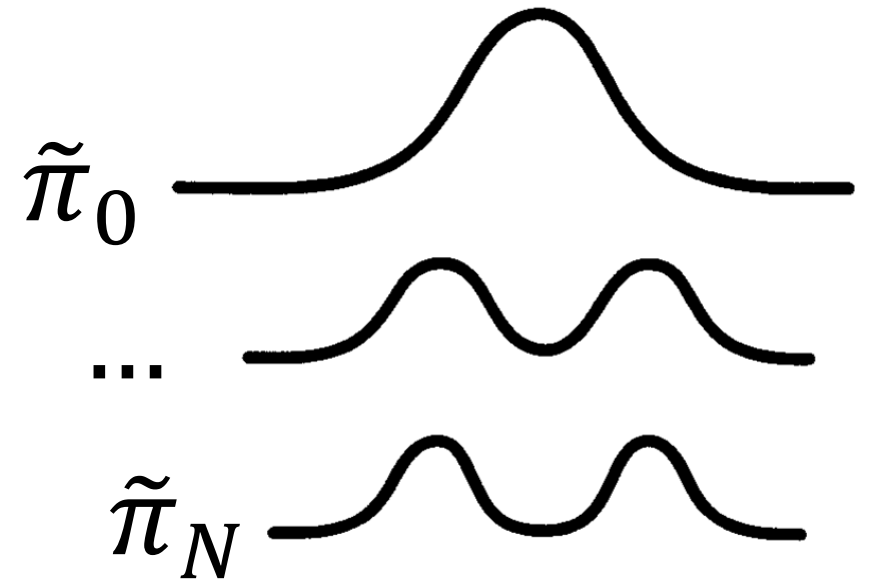
Parallel tempering

- An MCMC algorithm for target density $\tilde{\pi}_N$
- Workflow:
 - Choose an easy-to-sample reference $\tilde{\pi}_0$
 - Design multiple intermediate targets $\tilde{\pi}_n$
 - Design two MCMC kernels with invariant measure as $\tilde{\pi}_0 \times \tilde{\pi}_1 \times \dots \times \tilde{\pi}_N$



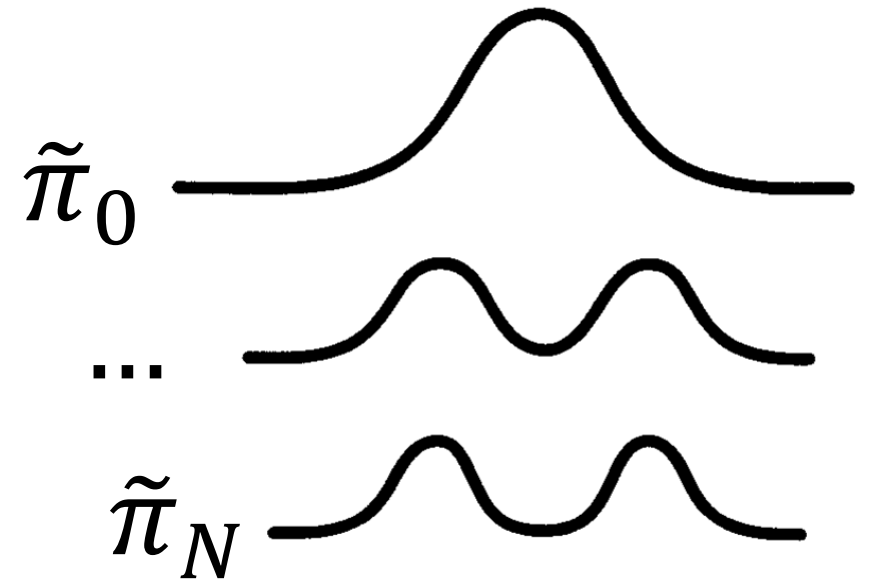
Parallel tempering

- An MCMC algorithm for target density $\tilde{\pi}_N$
 - Workflow:
 - Choose an easy-to-sample reference $\tilde{\pi}_0$
 - Design multiple intermediate targets $\tilde{\pi}_n$
 - Design two MCMC kernels with invariant measure as $\tilde{\pi}_0 \times \tilde{\pi}_1 \times \dots \times \tilde{\pi}_N$
1. Local exploration kernel: independent MCMC for each $\tilde{\pi}_n$

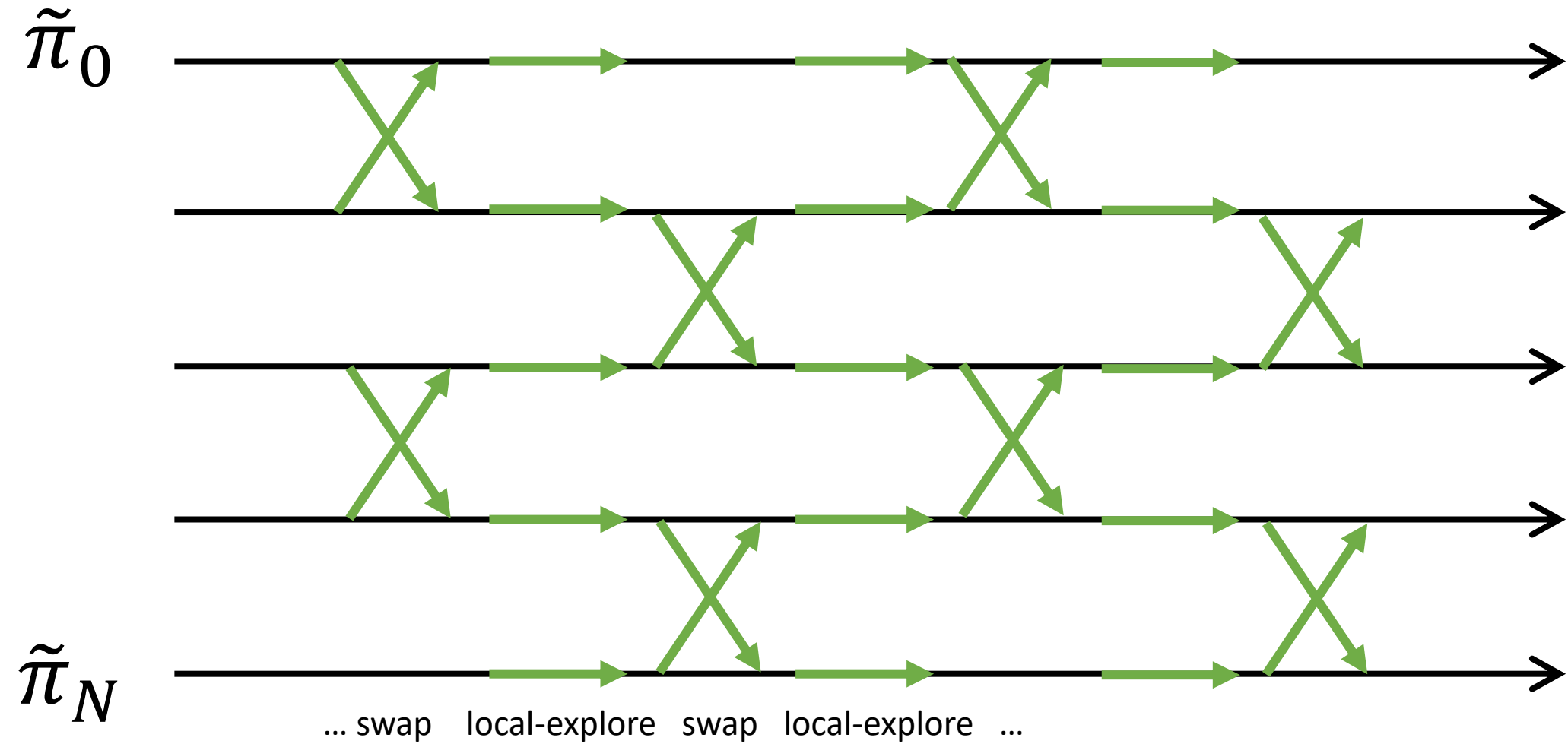


Parallel tempering

- An MCMC algorithm for target density $\tilde{\pi}_N$
 - Workflow:
 - Choose an easy-to-sample reference $\tilde{\pi}_0$
 - Design multiple intermediate targets $\tilde{\pi}_n$
 - Design two MCMC kernels with invariant measure as $\tilde{\pi}_0 \times \tilde{\pi}_1 \times \dots \times \tilde{\pi}_N$
1. Local exploration kernel: independent MCMC for each $\tilde{\pi}_n$
 2. Communication kernel: swap between all adjacent pairs $(\tilde{\pi}_n, \tilde{\pi}_{n+1})$



Parallel tempering



Density Ratio and where to find them

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

Density ratio: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$

- Communication in PT:

Density Ratio and where to find them

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

$$\text{Density ratio: } w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$$

- Communication in PT:

Assume replica m has density \tilde{p} , replica $m + 1$ has density \tilde{q} , **how to construct a MCMC “swap” kernel with invariant density $\tilde{p}(x) \times \tilde{q}(y)$?**

Density Ratio and where to find them

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

$$\text{Density ratio: } w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$$

Assume replica m has density \tilde{p} , replica $m + 1$ has density \tilde{q} , **how to construct a MCMC “swap” kernel with invariant density $\tilde{p}(x) \times \tilde{q}(y)$?**

- Communication in PT:

- 💡 current state $(x, y) \sim \tilde{p}(x)\tilde{q}(y)$
- 💡 Proposal $(x', y') \leftarrow (y, x)$
- 💡 next state $(x', y') \sim \tilde{p}(x)\tilde{q}(y)$

Density Ratio and where to find them

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

$$\text{Density ratio: } w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$$

Assume replica m has density \tilde{p} , replica $m + 1$ has density \tilde{q} , **how to construct a MCMC “swap” kernel with invariant density $\tilde{p}(x) \times \tilde{q}(y)$?**

- Communication in PT:

- 💡 current state $(x, y) \sim \tilde{p}(x)\tilde{q}(y)$

- 💡 Proposal $(x', y') \leftarrow (y, x)$

- 💡 next state $(x', y') \sim \tilde{p}(x)\tilde{q}(y)$

$$\alpha = \min\left\{1, \frac{\tilde{p}(x')\tilde{q}(y')\delta_{x,y}(x', y')}{\tilde{p}(x)\tilde{q}(y)\delta_{x',y'}(x, y)}\right\}$$

informally

Density Ratio and where to find them

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

$$\text{Density ratio: } w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$$

Assume replica m has density \tilde{p} , replica $m + 1$ has density \tilde{q} , **how to construct a MCMC “swap” kernel with invariant density $\tilde{p}(x) \times \tilde{q}(y)$?**

- Communication in PT:

- 💡 current state $(x, y) \sim \tilde{p}(x)\tilde{q}(y)$

- 💡 Proposal $(x', y') \leftarrow (y, x)$

- 💡 next state $(x', y') \sim \tilde{p}(x)\tilde{q}(y)$

$$\alpha = \min\left\{1, \frac{\tilde{p}(x')\tilde{q}(y')\delta_{x,y}(x', y')}{\tilde{p}(x)\tilde{q}(y)\delta_{x',y'}(x, y)}\right\}$$

informally

Requirement: proposal is involution $f(f(x)) = x$

Density Ratio and where to find them


Unnormalised density 1: \tilde{p}


Unnormalised density 2: \tilde{q}


$$\text{Density ratio: } w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$$

Assume replica m has density \tilde{p} , replica $m + 1$ has density \tilde{q} , **how to construct a MCMC “swap” kernel with invariant density $\tilde{p}(x) \times \tilde{q}(y)$?**

- Communication in PT:

-  current state $(x, y) \sim \tilde{p}(x)\tilde{q}(y)$

-  Proposal $(x', y') \leftarrow (y, x)$

-  next state $(x', y') \sim \tilde{p}(x)\tilde{q}(y)$

$$\alpha = \min\left\{1, \frac{\tilde{p}(x')\tilde{q}(y')}{\tilde{p}(x)\tilde{q}(y)}\right\}$$

Density Ratio and where to find them


Unnormalised density 1: \tilde{p}


Unnormalised density 2: \tilde{q}


$$\text{Density ratio: } w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$$

Assume replica m has density \tilde{p} , replica $m + 1$ has density \tilde{q} , **how to construct a MCMC “swap” kernel with invariant density $\tilde{p}(x) \times \tilde{q}(y)$?**

- Communication in PT:

-  current state $(x, y) \sim \tilde{p}(x)\tilde{q}(y)$

-  Proposal $(x', y') \leftarrow (y, x)$

-  next state $(x', y') \sim \tilde{p}(x)\tilde{q}(y)$

$$\begin{aligned} \alpha &= \min\left\{1, \frac{\tilde{p}(x')\tilde{q}(y')}{\tilde{p}(x)\tilde{q}(y)}\right\} \\ &= \min\left\{1, \frac{\tilde{p}(y)\tilde{q}(x)}{\tilde{p}(x)\tilde{q}(y)}\right\} \end{aligned}$$

Density Ratio and where to find them

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

$$\text{Density ratio: } w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$$

Assume replica m has density \tilde{p} , replica $m + 1$ has density \tilde{q} , **how to construct a MCMC “swap” kernel with invariant density $\tilde{p}(x) \times \tilde{q}(y)$?**

- Communication in PT:

- 💡 current state $(x, y) \sim \tilde{p}(x)\tilde{q}(y)$

- 💡 Proposal $(x', y') \leftarrow (y, x)$

- 💡 next state $(x', y') \sim \tilde{p}(x)\tilde{q}(y)$

$$\begin{aligned} \alpha &= \min\left\{1, \frac{\tilde{p}(x')\tilde{q}(y')}{\tilde{p}(x)\tilde{q}(y)}\right\} \\ &= \min\left\{1, \frac{\tilde{p}(y)\tilde{q}(x)}{\tilde{p}(x)\tilde{q}(y)}\right\} \end{aligned}$$

Density Ratio and where to find them

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

$$\text{Density ratio: } w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$$

Assume replica m has density \tilde{p} , replica $m + 1$ has density \tilde{q} , **how to construct a MCMC “swap” kernel with invariant density $\tilde{p}(x) \times \tilde{q}(y)$?**

- Communication in PT:

- 💡 current state $(x, y) \sim \tilde{p}(x)\tilde{q}(y)$

- 💡 Proposal $(x', y') \leftarrow (y, x)$

- 💡 next state $(x', y') \sim \tilde{p}(x)\tilde{q}(y)$

$$\alpha = \min\left\{1, \frac{\tilde{p}(x')\tilde{q}(y')}{\tilde{p}(x)\tilde{q}(y)}\right\}$$

$$= \min\left\{1, \frac{w(y)}{w(x)}\right\}$$

Wrap up

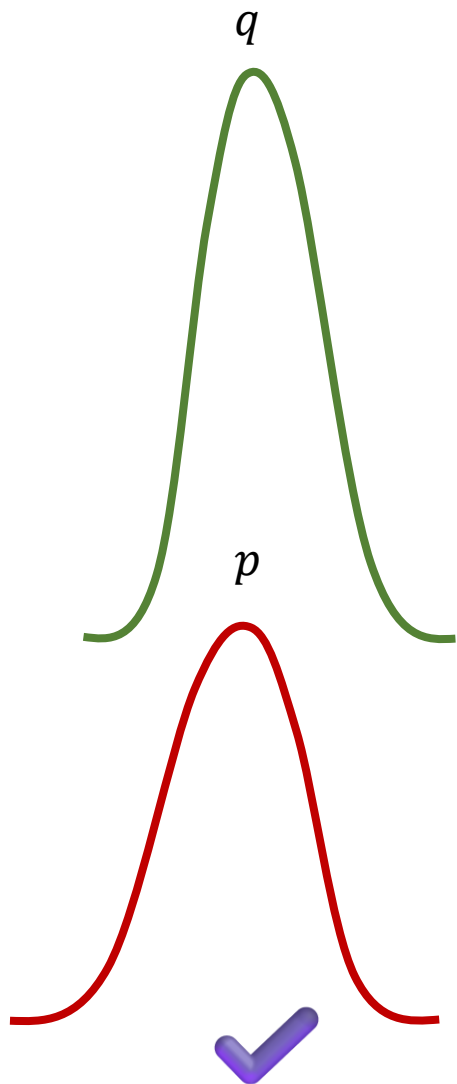
Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

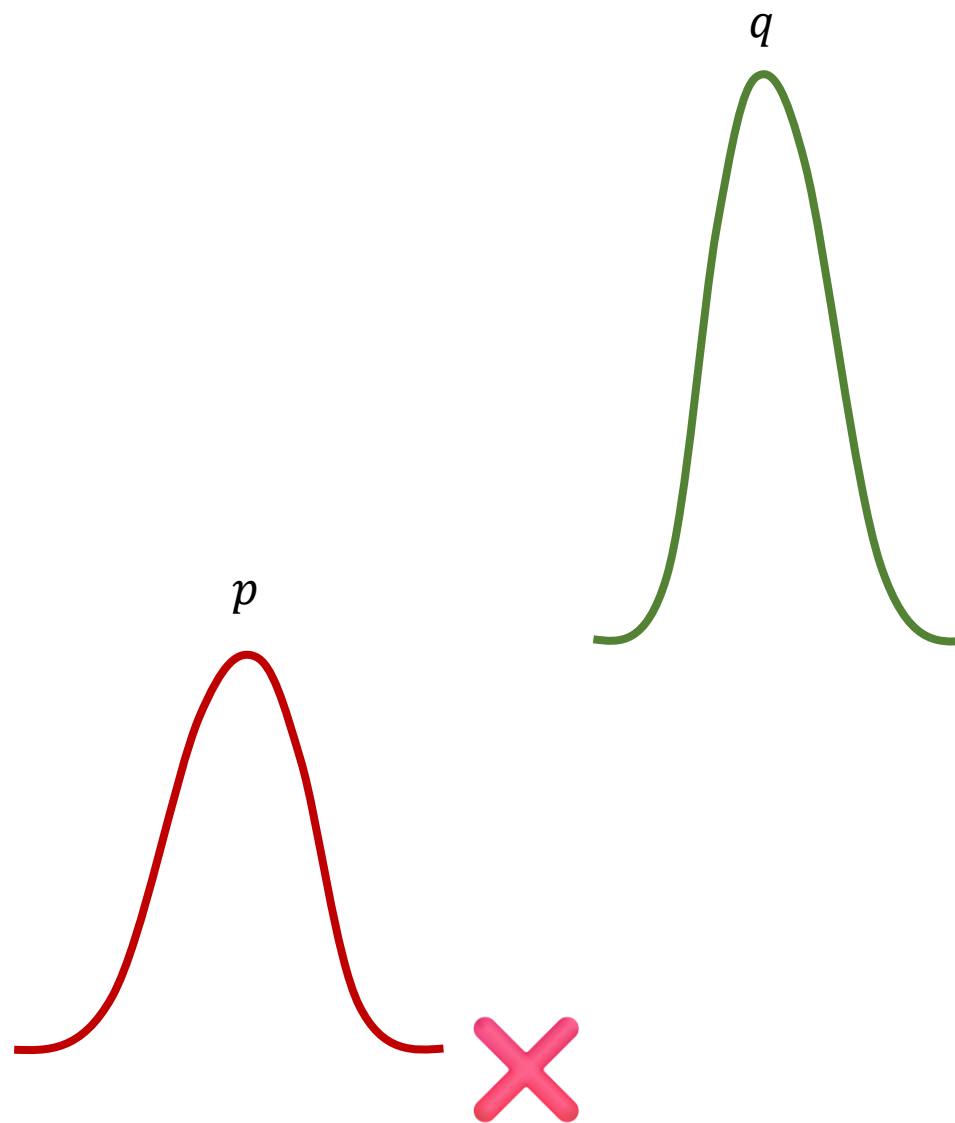
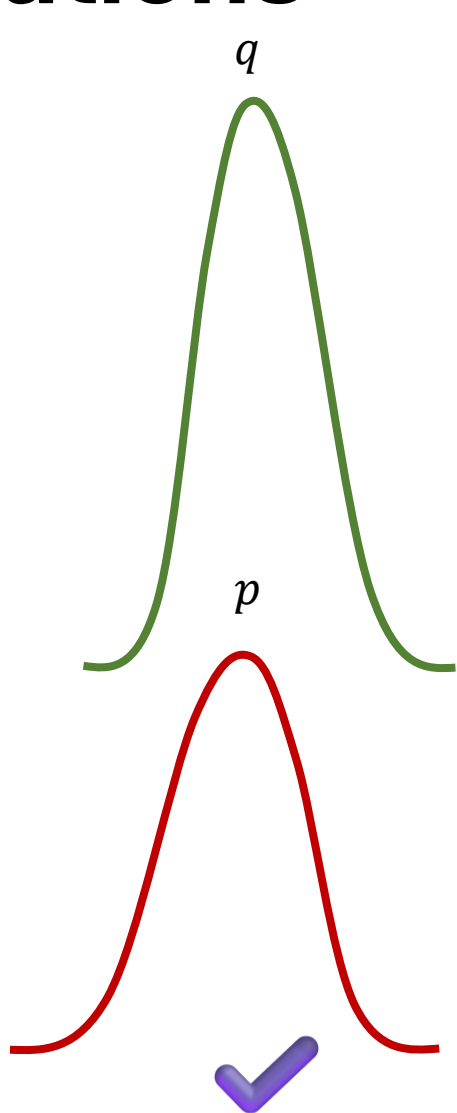
Density ratio: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$

- Importance sampling: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$
- FEP: $\Delta F = -\log(\int q(x)w(x) dx)$
- PT Swap: $\alpha = \min\{1, \frac{w(y)}{w(x)}\}$

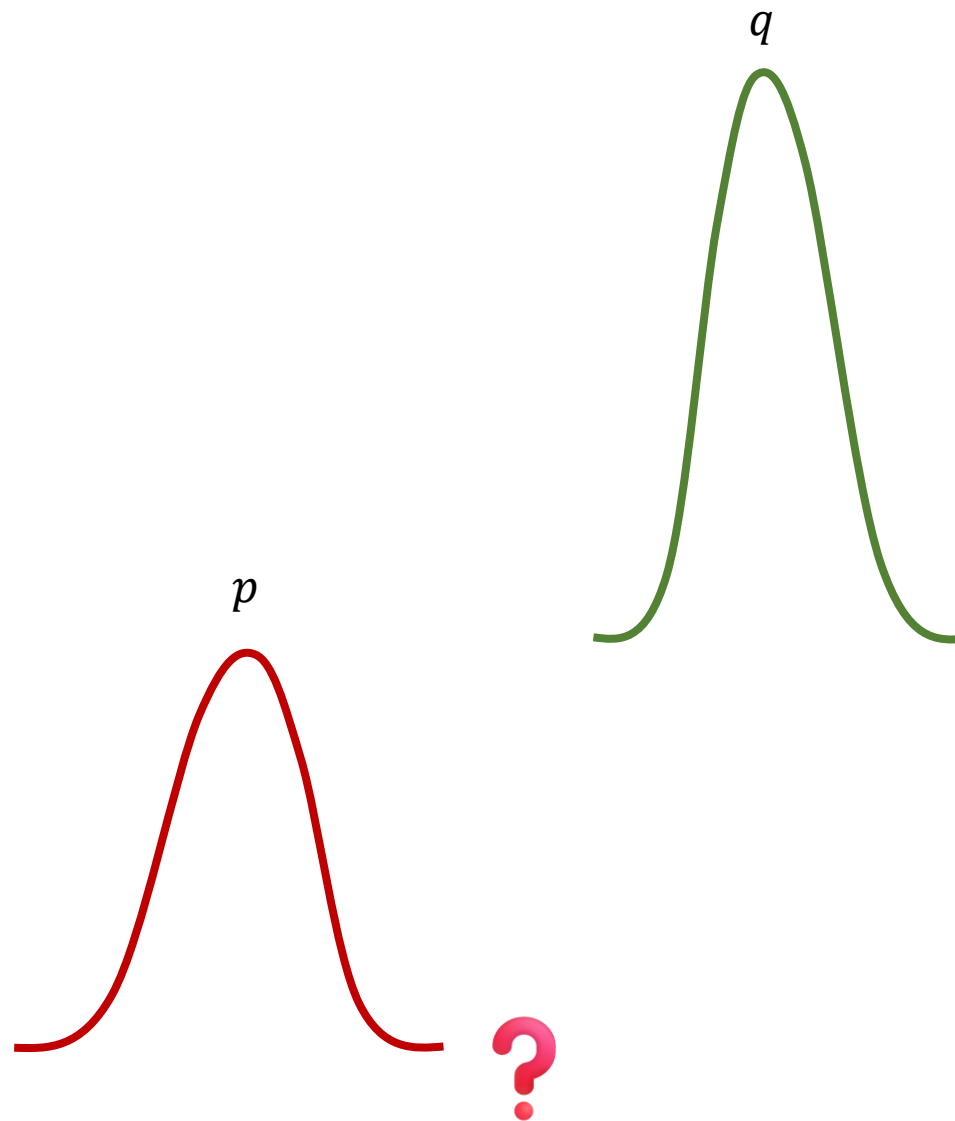
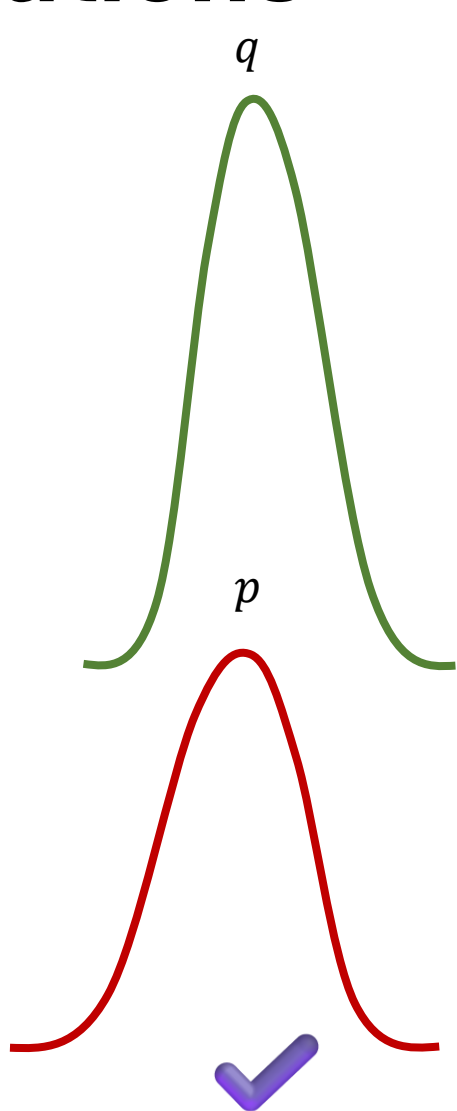
Limitations



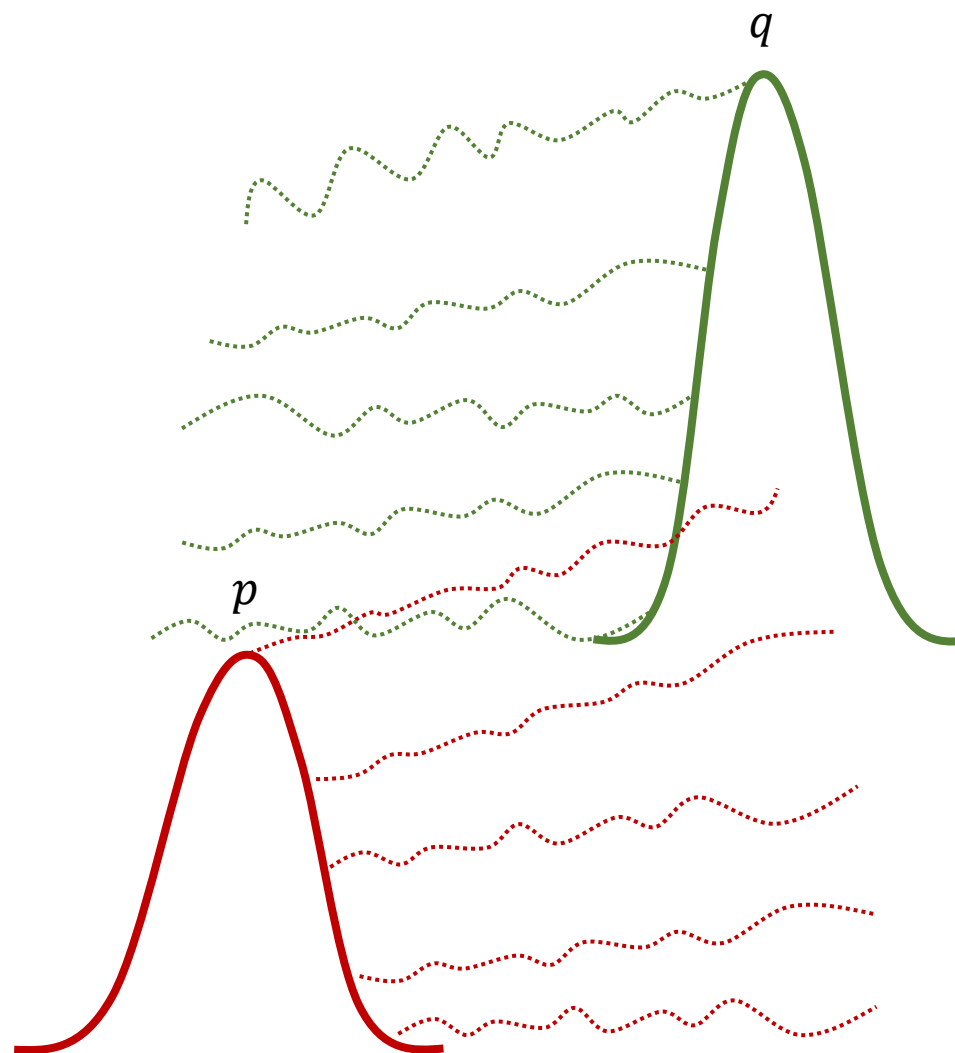
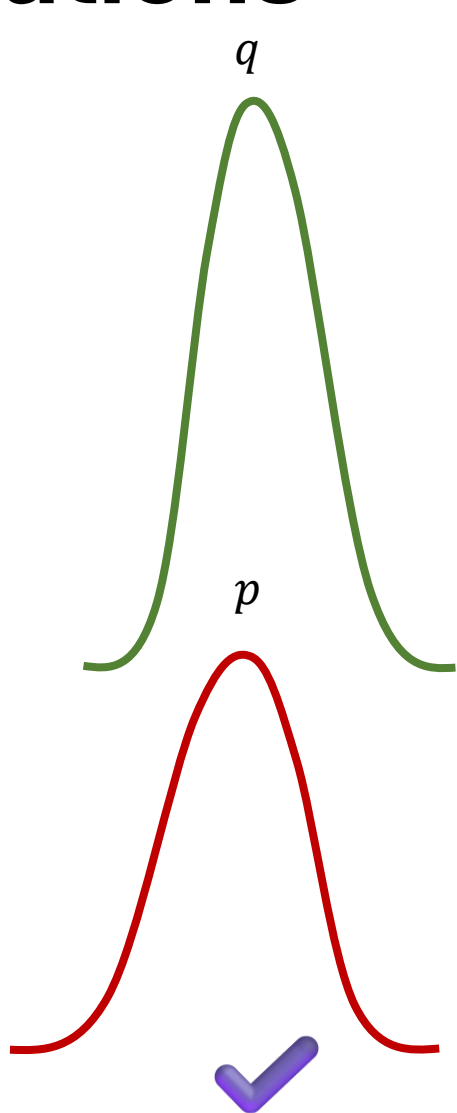
Limitations



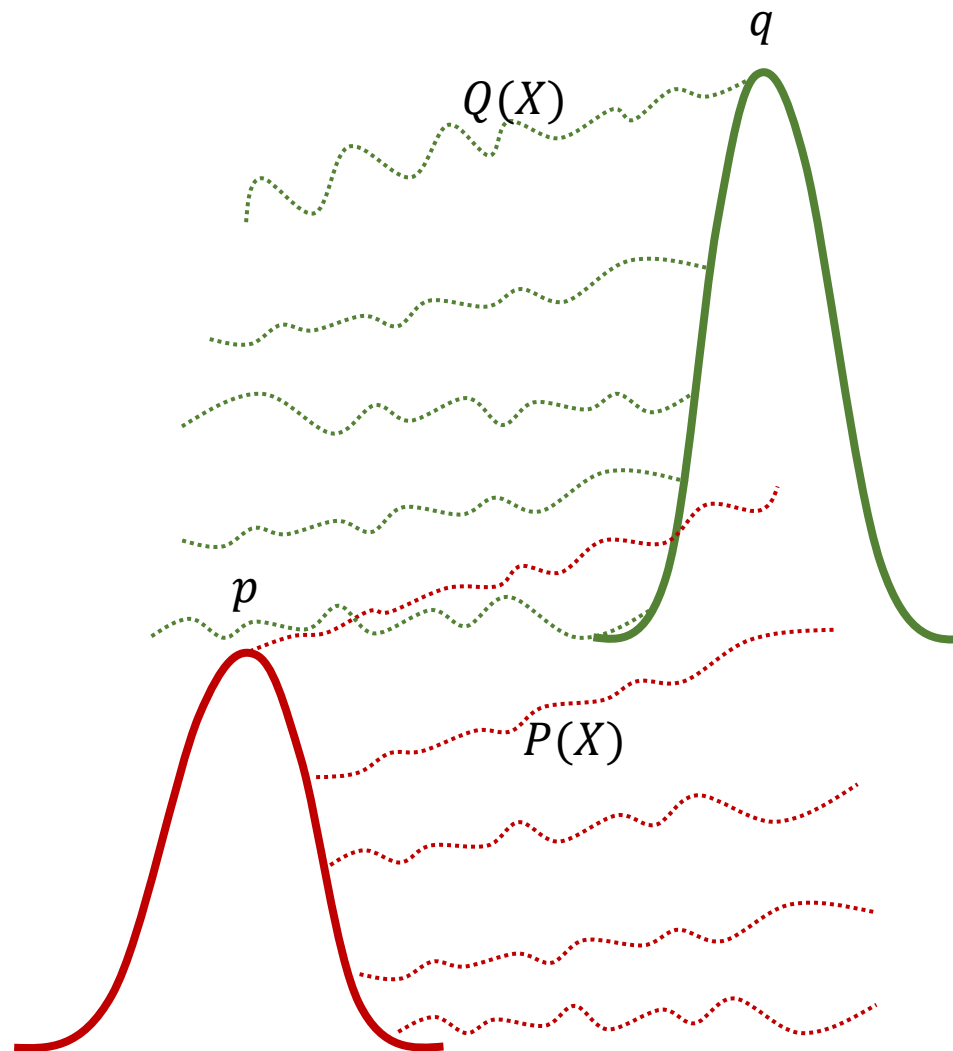
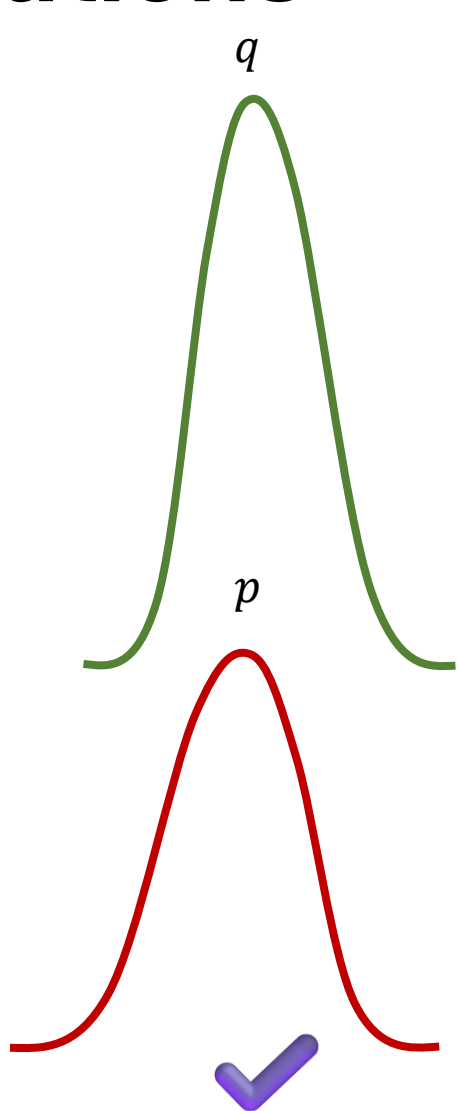
Limitations



Limitations



Limitations



From Density Ratio to Path RND

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

Density ratio: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$

Path measure 1: P

Path measure 2: Q

“Density” ratio: $\frac{dP}{dQ}(x)$

From Density Ratio to Path RND

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

Density ratio: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$

Path measure 1: P

Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

From Density Ratio to Path RND

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

$$\text{Density ratio: } w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$$

Path measure 1: P

Path measure 2: Q

$$\text{“Unnormalised” RND: } w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$$

- Importance sampling: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$
- FEP: $\Delta F = -\log(\int q(x)w(x) dx)$
- PT Swap: $\alpha = \min\{1, \frac{w(y)}{w(x)}\}$

From Density Ratio to Path RND

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

$$\text{Density ratio: } w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$$

- Importance sampling: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$
- FEP: $\Delta F = -\log(\int q(x)w(x) dx)$
- PT Swap: $\alpha = \min\{1, \frac{w(y)}{w(x)}\}$

Path measure 1: P

Path measure 2: Q

$$\text{“Unnormalised” RND: } w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$$

- Path Importance sampling: $w(X)$
- Path FEP: $\Delta F = -\log(\int dQ(X)w(X))$
- Path PT Swap: $\alpha = \min\{1, \frac{w(Y)}{w(X)}\}$

From Density Ratio to Path RND

Wait... WHY PATH?

Unnormalised density 1: \tilde{p}
Unnormalised density 2: \tilde{q}

$$\text{Density ratio: } w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$$

- Importance sampling: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$
- FEP: $\Delta F = -\log(\int q(x)w(x) dx)$
- PT Swap: $\alpha = \min\{1, \frac{w(y)}{w(x)}\}$

Path measure 1: P
Path measure 2: Q

$$\text{“Unnormalised” RND: } w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$$

- Path Importance sampling: $w(X)$
- Path FEP: $\Delta F = -\log(\int dQ(X)w(X))$
- Path PT Swap: $\alpha = \min\{1, \frac{w(Y)}{w(X)}\}$

From Density Ratio to Path RND

Wait...WHY PATH?

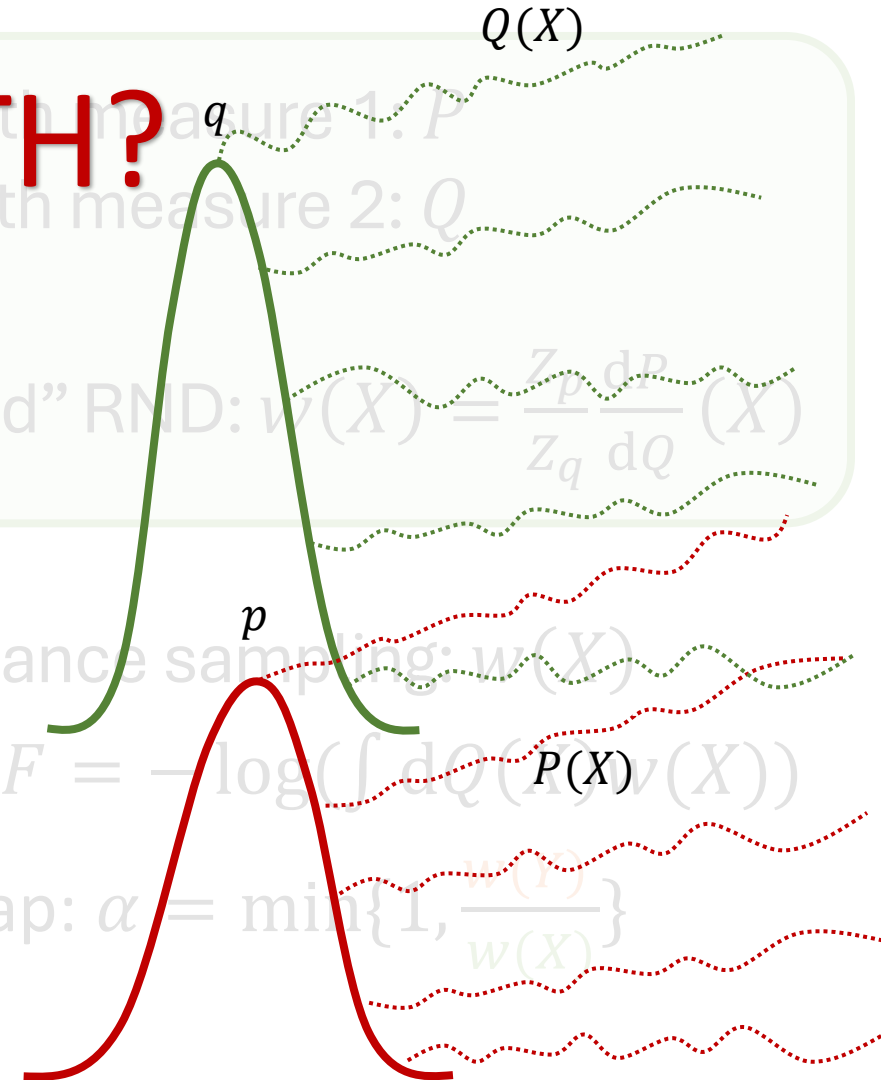
Unnormalised density 1: \tilde{p}
 Unnormalised density 2: \tilde{q}

Density ratio: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$

- Importance sampling: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$
- FEP: $\Delta F = -\log(\int q(x)w(x) dx)$
- PT Swap: $\alpha = \min\{1, \frac{w(y)}{w(x)}\}$

“Unnormalised” RND: $w(X) = \frac{Z_p \int dP}{Z_q \int dQ} (X)$

- Path Importance sampling: $w(X)$
- Path FEP: $\Delta F = -\log(\int dQ(X)w(X))$
- Path PT Swap: $\alpha = \min\{1, \frac{w(y)}{w(x)}\}$



From Density Ratio to Path RND

Wait...WHY PATH?



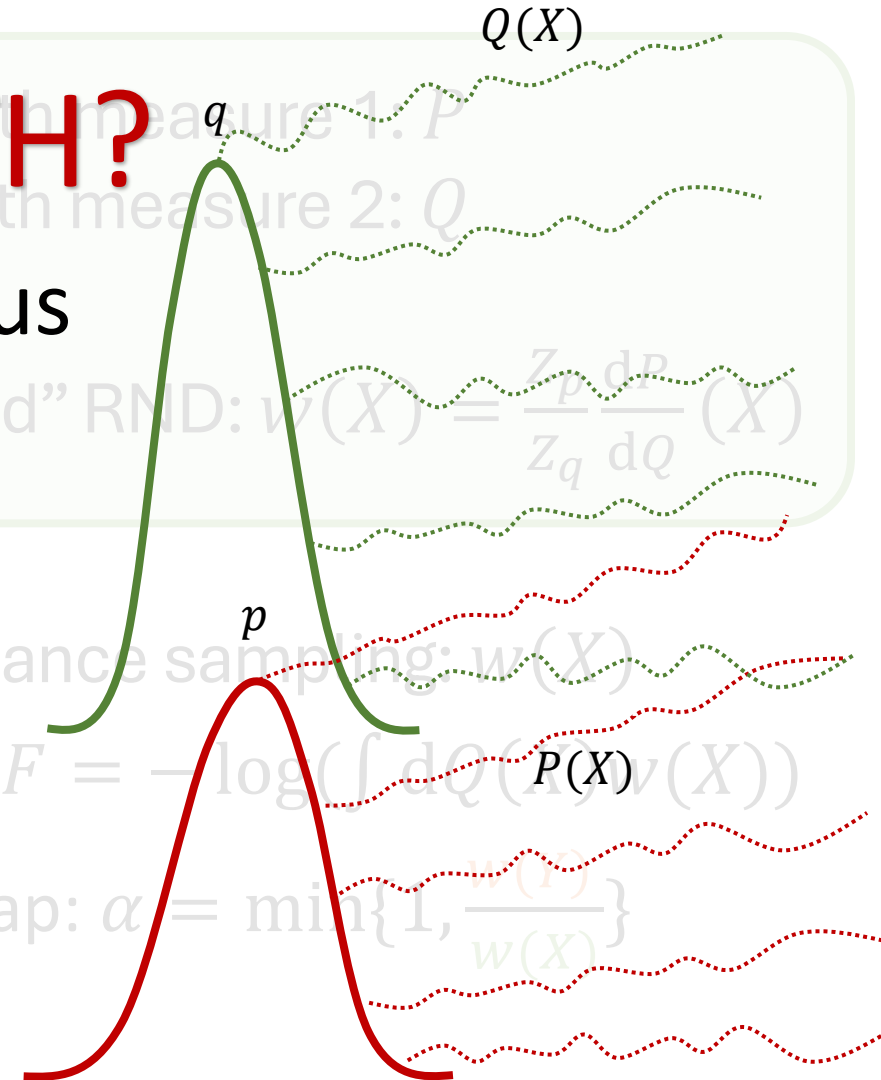
data processing inequality (DPI) told us

Density ratio: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$

- Importance sampling: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$
- FEP: $\Delta F = -\log(\int q(x)w(x) dx)$
- PT Swap: $\alpha = \min\{1, \frac{w(y)}{w(x)}\}$

“Unnormalised” RND: $w(X) = \frac{Z_p dP}{Z_q dQ}(X)$

- Path Importance sampling: $w(X)$
- Path FEP: $\Delta F = -\log(\int dQ(X)w(X))$
- Path PT Swap: $\alpha = \min\{1, \frac{w(y)}{w(x)}\}$



From Density Ratio to Path RND

Wait... WHY PATH?

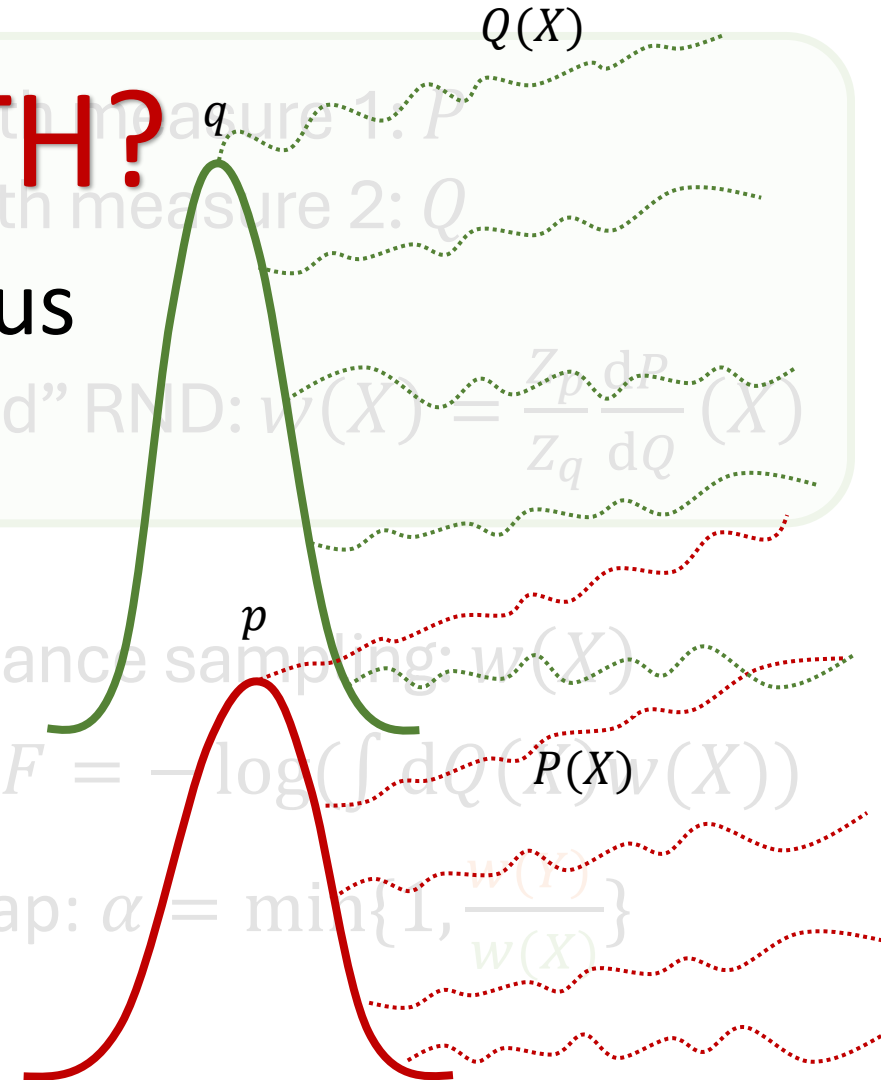


data processing inequality (DPI) told us

😞 $D_f[q||p] \leq D_f[Q||P]$

- Importance sampling: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$
- FEP: $\Delta F = -\log(\int q(x)w(x) dx)$
- PT Swap: $\alpha = \min\{1, \frac{w(y)}{w(x)}\}$

- Path Importance sampling: $w(X) = \frac{Z_p dP}{Z_q dQ}(X)$
- Path FEP: $\Delta F = -\log(\int dQ(X)w(X))$
- Path PT Swap: $\alpha = \min\{1, \frac{w(y)}{w(x)}\}$



From Density Ratio to Path RND

Wait...WHY PATH?

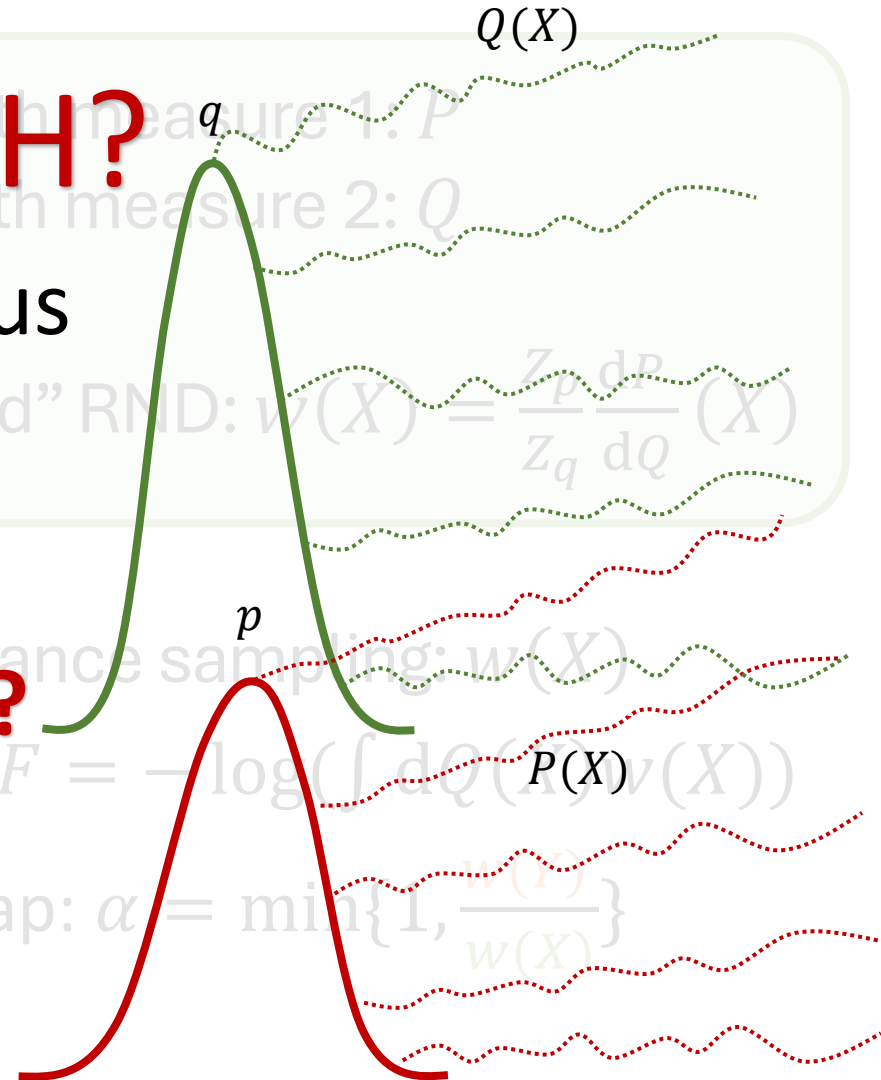


data processing inequality (DPI) told us

🤔 $D_f[q||p] \leq D_f[Q||P]$

- Importance sampling: $w(x) = \frac{\tilde{p}(x)}{q(x)}$
- FEP: $\Delta F = -\log(\int q(x)w(x) dx)$
- PT Swap: $\alpha = \min\{1, \frac{w(y)}{w(x)}\}$

- Path Importance sampling: $w(X) = \frac{\tilde{p}(X)}{Q(X)}$
- Path FEP: $\Delta F = -\log(\int dQ(X)w(X))$
- Path PT Swap: $\alpha = \min\{1, \frac{w(Y)}{w(X)}\}$



From Density Ratio to Path RND

Path weight always has **larger variance?**

Path measure 1: P

Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

- Importance sampling: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$
- FEP: $\Delta F = -\log(\int q(x)w(x) dx)$
- PT Swap: $\alpha = \min\{1, \frac{w(y)}{w(x)}\}$

- Path Importance sampling: $w(X)$
- Path FEP: $\Delta F = -\log(\int dQ(X)w(X))$
- Path PT Swap: $\alpha = \min\{1, \frac{w(Y)}{w(X)}\}$

From Density Ratio to Path RND

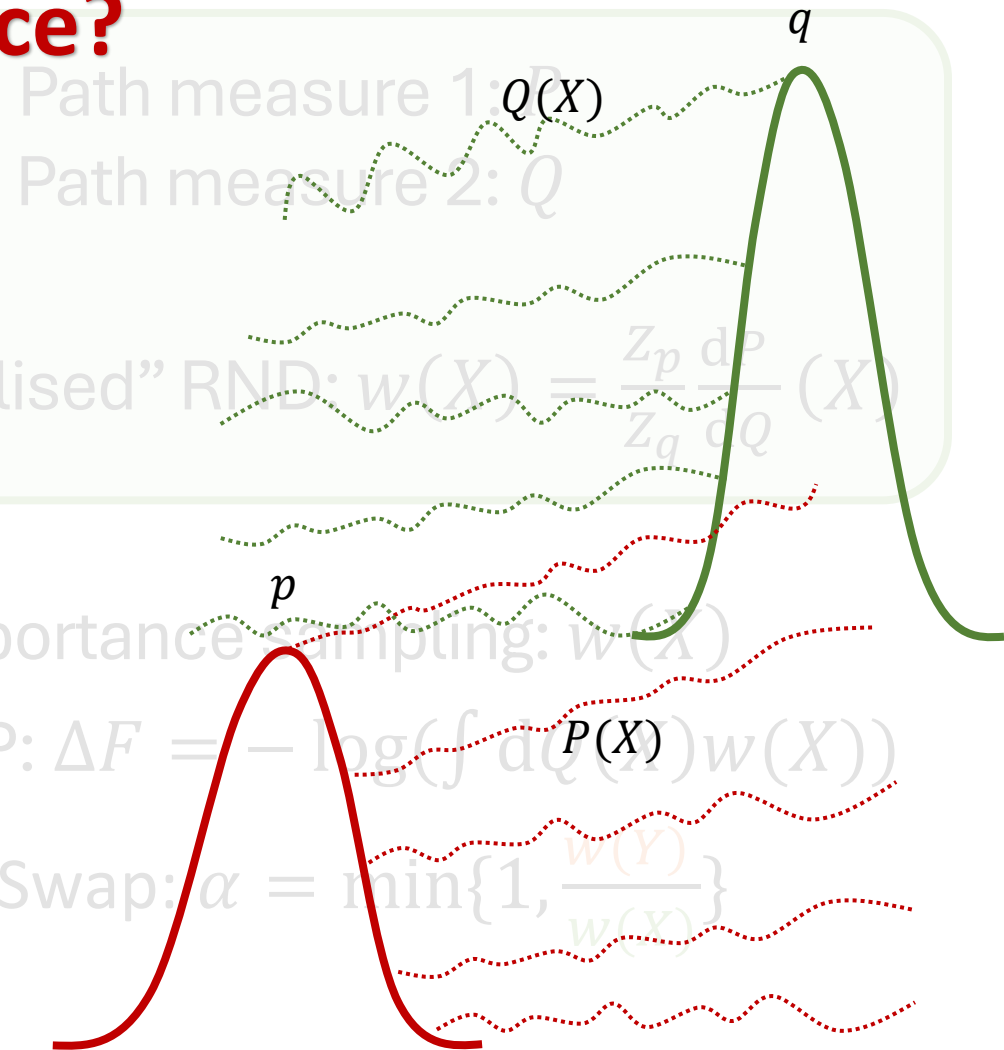
Path weight always has larger variance?

💡 **Not for FB RND!**

- Importance sampling: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$
- FEP: $\Delta F = -\log(\int q(x)w(x) dx)$
- PT Swap: $\alpha = \min\{1, \frac{w(y)}{w(x)}\}$

“Unnormalised” RND: $w(X) = \frac{Z_p dP}{Z_q dQ}(X)$

- Path Importance sampling: $w(X)$
- Path FEP: $\Delta F = -\log(\int dQ(X)w(X))$
- Path PT Swap: $\alpha = \min\{1, \frac{w(Y)}{w(X)}\}$



From Density Ratio to Path RND

Path weight always has larger variance?

💡 **Not for FB RND!**

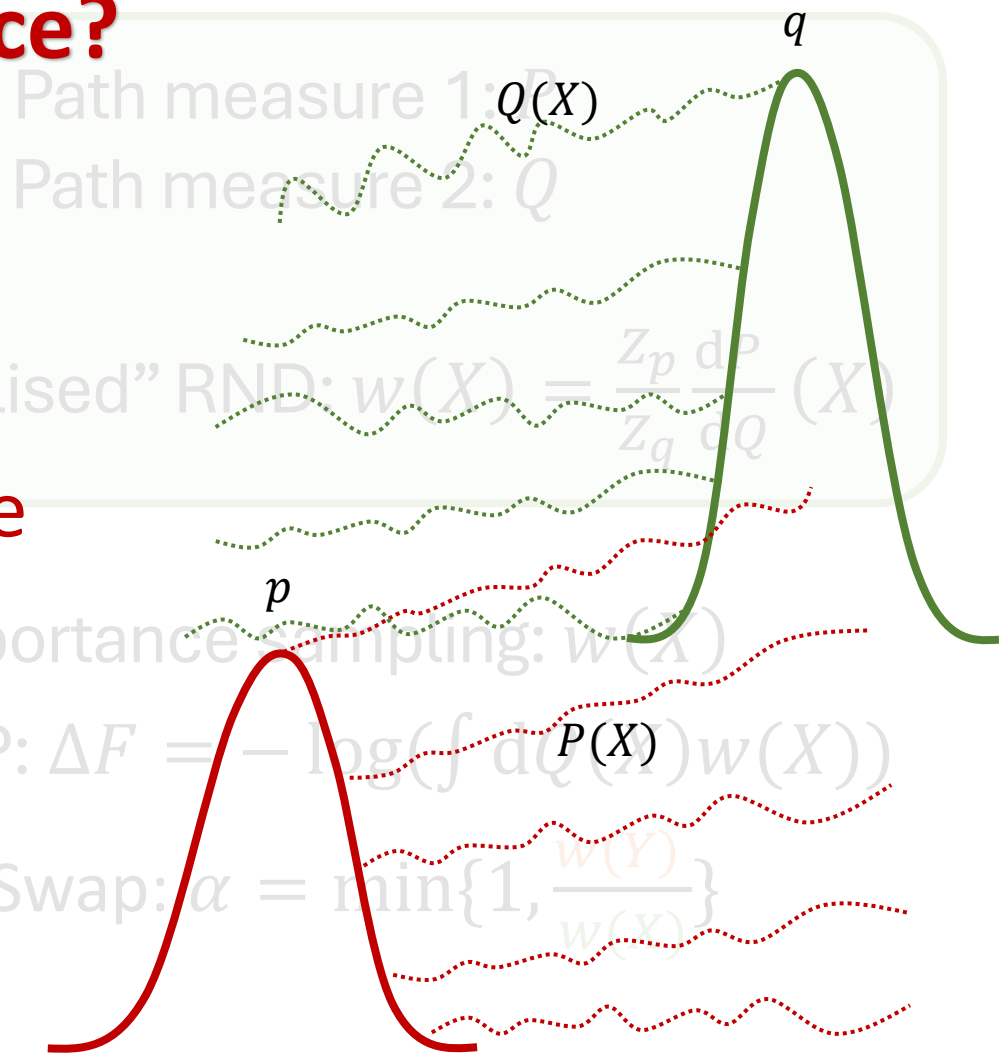
If $\bar{Q} = P$ (time-reversal)

The path weight will have 0 variance

- Importance sampling: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$
- FEP: $\Delta F = -\log(\int q(x)w(x) dx)$
- PT Swap: $\alpha = \min\{1, \frac{w(y)}{w(x)}\}$

“Unnormalised” RND: $w(X) = \frac{Z_p dP}{Z_q dQ}(X)$

- Path Importance sampling: $w(X)$
- Path FEP: $\Delta F = -\log(\int dQ(X)w(X))$
- Path PT Swap: $\alpha = \min\{1, \frac{w(Y)}{w(X)}\}$



Time-reversal and Nelson's relation

$$P : dX_t = f(X_t, t)dt + \sigma_t dW_t, X_0 \sim p_0$$
$$\bar{Q} : dX_t = g(X_t, t)dt + \sigma_t \overleftarrow{dW}_t, X_1 \sim p_1$$

“time-reversal” $\bar{Q} = P, \text{ i. e., } \frac{\overleftarrow{dQ}}{dP} = 1$

Iff

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

From Density Ratio to Path RND

Path measure 1: P

Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

- Path Importance sampling: $w(X)$
- Path FEP: $\Delta F = -\log(\int dQ(X)w(X))$
- Path PT Swap: $\alpha = \min\{1, \frac{w(Y)}{w(X)}\}$

From Density Ratio to Path RND

Path measure 1: P

Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

- Path Importance sampling: $w(X)$
- Path FEP: $\Delta F = -\log(\int dQ(X)w(X)) \longrightarrow$ (escorted) Jarzynski/Crooks
- Path PT Swap: $\alpha = \min\{1, \frac{w(Y)}{w(X)}\} \longrightarrow$ Replica exchange with nonequilibrium switches [1] / Accelerated PT [2]

[1] Ballard, Andrew J., and Christopher Jarzynski. "Replica exchange with nonequilibrium switches." *Proceedings of the National Academy of Sciences* 106.30 (2009): 12224-12229.

[2] Zhang, Leo, et al. "Accelerated Parallel Tempering via Neural Transports." *arXiv preprint arXiv:2502.10328* (2025).

From Density Ratio to Path RND

Path measure 1: P

Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

Equilibrium method and nonequilibrium ones are not too different:

One use *Marginal space RND*

One use *Path space RND*

- Path Importance sampling: $w(X)$
- Path FEP: $\Delta F = -\log(\int dQ(X)w(X))$ \longrightarrow (escorted) Jarzynski/Crooks
- Path PT Swap: $\alpha = \min\{1, \frac{w(Y)}{w(X)}\}$ \longrightarrow Replica exchange with nonequilibrium switches [1] / Accelerated PT [2]

[1] Ballard, Andrew J., and Christopher Jarzynski. "Replica exchange with nonequilibrium switches." *Proceedings of the National Academy of Sciences* 106.30 (2009): 12224-12229.

[2] Zhang, Leo, et al. "Accelerated Parallel Tempering via Neural Transports." *arXiv preprint arXiv:2502.10328* (2025).

Example: Path RND to Jarzynski Equality

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

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

Example: Path RND to Jarzynski Equality

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

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

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

Example: Path RND to Jarzynski Equality

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

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

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

Example: Path RND to Jarzynski Equality

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

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

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

 conversion rule

Example: Path RND to Jarzynski Equality

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

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

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

$$= \frac{p(X_1)}{q(X_0)} \exp \left(\int \frac{\nabla U_t}{2} \cdot dX_t + \int \frac{\nabla U_t}{2} \cdot \overleftarrow{dX}_t \right)$$

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

 conversion rule

Example: Path RND to Jarzynski Equality

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

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

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

Example: Path RND to Jarzynski Equality

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

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

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

 Ito's lemma

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

Example: Path RND to Jarzynski Equality

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

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

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



Ito's lemma

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

Example: Path RND to Jarzynski Equality

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

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

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

$$= \frac{p(X_1)}{q(X_0)} \exp \left(\int dU_t(X_t) - \partial_t U_t(X_t) dt \right)$$

 Ito's lemma

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

$$= \frac{p(X_1)}{q(X_0)} \exp \left(U_1(X_1) - U_0(X_0) + \int -\partial_t U_t(X_t) dt \right)$$

Example: Path RND to Jarzynski Equality

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

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

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

$$= \frac{p(X_1)}{q(X_0)} \exp \left(\int dU_t(X_t) - \partial_t U_t(X_t) dt \right)$$

 Ito's lemma

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

$$= \frac{Z_0 \exp(-U_1(X_1))}{Z_1 \exp(-U_0(X_0))} \exp \left(U_1(X_1) - U_0(X_0) + \int -\partial_t U_t(X_t) dt \right)$$

Example: Path RND to Jarzynski Equality

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

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

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

Example: Path RND to Jarzynski Equality

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

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

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

Example: Path RND to Jarzynski Equality

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

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

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

💡 Crooks Fluctuation Theorem

Example: Path RND to Jarzynski Equality

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

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

$$\frac{\overleftarrow{dP}}{dQ} = \frac{Z_0}{Z_1} \exp\left(\int -\partial_t U_t(X_t) dt\right) \quad \text{💡 Crooks Fluctuation Theorem}$$

$$\mathbf{E}_Q \left[\frac{\overleftarrow{dP}}{dQ} \right] = \mathbf{E}_Q \left[\frac{Z_0}{Z_1} \exp\left(\int -\partial_t U_t(X_t) dt\right) \right] = 1 \quad \text{💡 Jarzynski Equation}$$

From Jarzynski to Escorted Jarzynski

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

$$X_1 \sim p \quad dX_t = [\sigma^2 \nabla U_t(X_t) + u_t(X_t)]dt + \sigma\sqrt{2} \overleftarrow{dW}_t,$$

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

💡 Controlled Crooks Fluctuation Theorem

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

💡 Escorted Jarzynski Equation

From Jarzynski to Escorted Jarzynski

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

$$X_1 \sim p \quad dX_t = [\sigma^2 \nabla U_t(X_t) + u_t(X_t)]dt + \sigma\sqrt{2} \overleftarrow{dW}_t,$$

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

💡 Controlled Crooks Fluctuation Theorem

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

💡 Escorted Jarzynski Equation

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*.

From Density Ratio to Path RND

Path measure 1: P

Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

Equilibrium method and nonequilibrium ones are not too different:

One use *Marginal space RND*

One use *Path space RND*

✓ Path Importance sampling: $w(X)$

✓ Path FEP: $\Delta F = -\log(\int dQ(X)w(X))$ → (escorted) Jarzynski/Crooks

• Path PT Swap: $\alpha = \min\{1, \frac{w(Y)}{w(X)}\}$ → Replica exchange with nonequilibrium switches [1] / Accelerated PT [2]

[1] Ballard, Andrew J., and Christopher Jarzynski. "Replica exchange with nonequilibrium switches." *Proceedings of the National Academy of Sciences* 106.30 (2009): 12224-12229.

[2] Zhang, Leo, et al. "Accelerated Parallel Tempering via Neural Transports." *arXiv preprint arXiv:2502.10328* (2025).

From Density Ratio to Path RND

Path measure 1: P

Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

Equilibrium method and nonequilibrium ones are not too different:

One use *Marginal space RND*

One use *Path space RND*

✓ Path Importance sampling: $w(X)$

✓ Path FEP: $\Delta F = -\log(\int dQ(X)w(X))$ → (escorted) Jarzynski/Crooks

• Path PT Swap: $\alpha = \min\left\{1, \frac{w(Y)}{w(X)}\right\}$ → Replica exchange with nonequilibrium switches [1] / Accelerated PT [2]

[1] Ballard, Andrew J., and Christopher Jarzynski. "Replica exchange with nonequilibrium switches." *Proceedings of the National Academy of Sciences* 106.30 (2009): 12224-12229.

[2] Zhang, Leo, et al. "Accelerated Parallel Tempering via Neural Transports." *arXiv preprint arXiv:2502.10328* (2025).

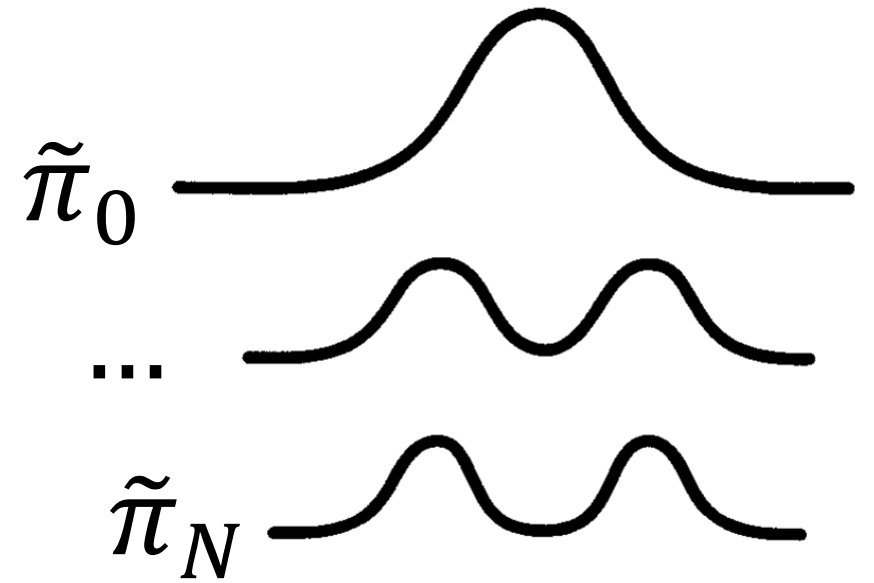
Parallel tempering

- An MCMC algorithm for target density $\tilde{\pi}_N$

- Workflow:

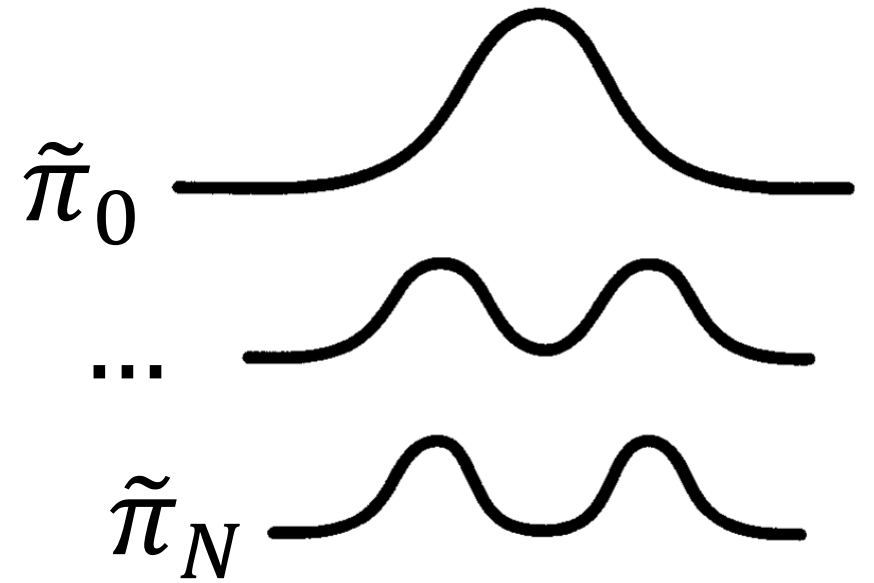
- Choose an easy-to-sample reference $\tilde{\pi}_0$
- Design multiple intermediate targets $\tilde{\pi}_n$
- Design two MCMC kernels with invariant measure as $\tilde{\pi}_0 \times \tilde{\pi}_1 \times \dots \times \tilde{\pi}_N$

1. Local exploration kernel: independent MCMC for each $\tilde{\pi}_n$
2. Communication kernel: swap between all adjacent pairs $(\tilde{\pi}_n, \tilde{\pi}_{n+1})$



Parallel tempering

- An MCMC algorithm for target density $\tilde{\pi}_N$
- Workflow:
 - Choose an easy-to-sample reference $\tilde{\pi}_0$
 - Design multiple intermediate targets $\tilde{\pi}_n$
 - Design two MCMC kernels with invariant measure as $\tilde{\pi}_0 \times \tilde{\pi}_1 \times \dots \times \tilde{\pi}_N$



Unchanged!

1. Local exploration kernel: independent MCMC for each $\tilde{\pi}_n$
2. Communication kernel: swap between all adjacent pairs $(\tilde{\pi}_n, \tilde{\pi}_{n+1})$

Extend to path!

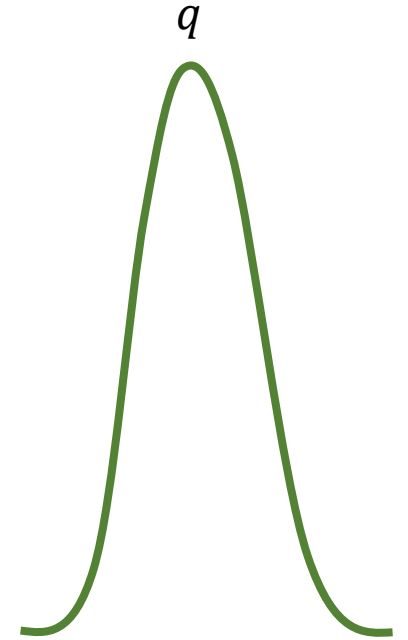
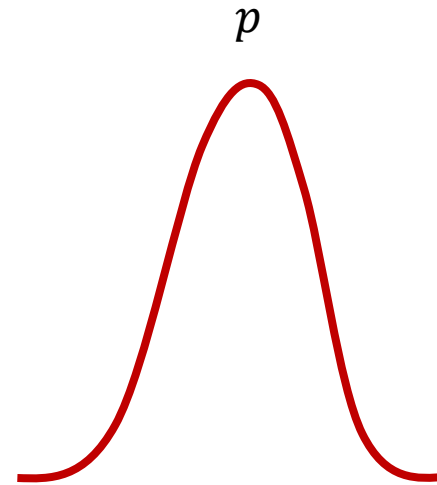
Parallel tempering Swap in Path Space

Path measure 1: P

Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

(1) Current state $(x, y) \sim p(x) \times q(y)$



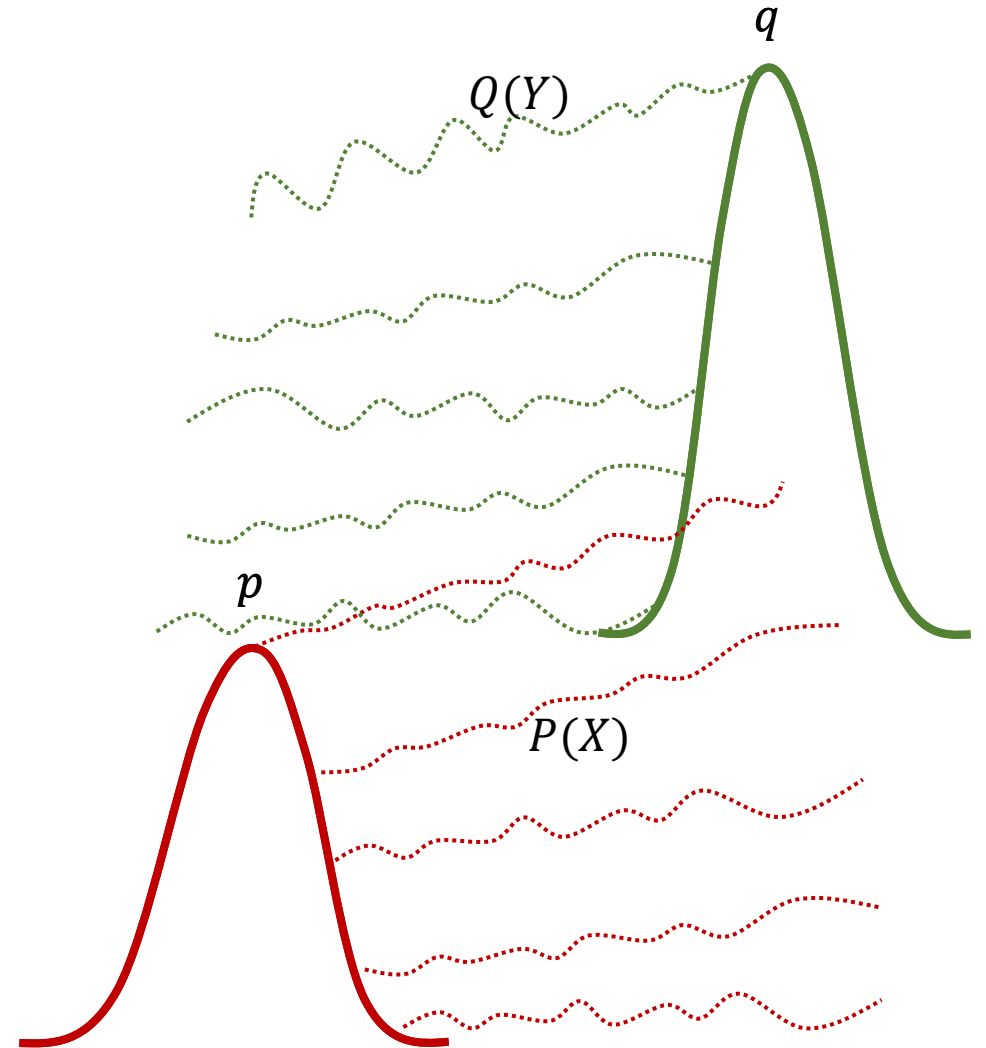
Parallel tempering Swap in Path Space

Path measure 1: P

Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

(2) Extend current states with path
 $(X, Y) \sim P(X) \times Q(Y)$



Parallel tempering Swap in Path Space

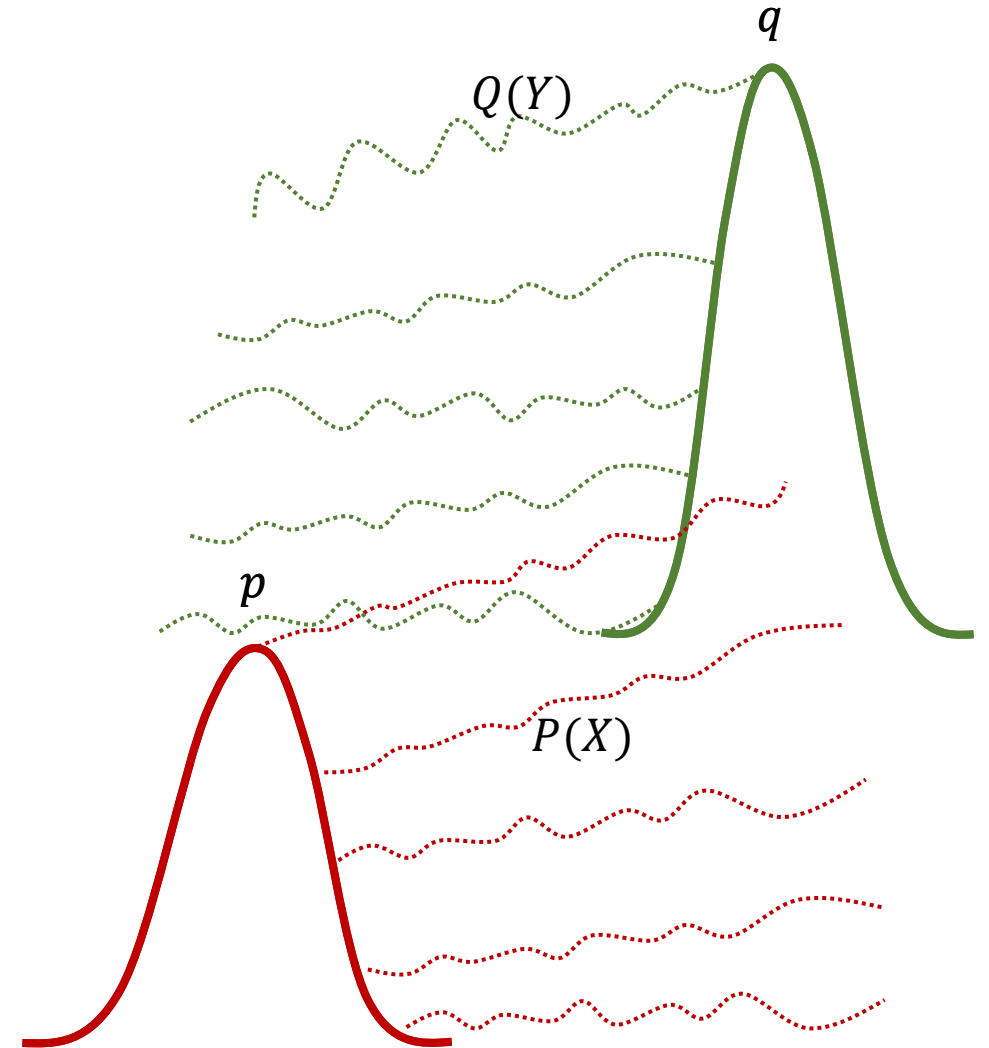
Path measure 1: P

Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

(3) Swap the Paths

$(X', Y') \leftarrow (Y, X)$



*Note that this proposal function is still involution

Parallel tempering Swap in Path Space

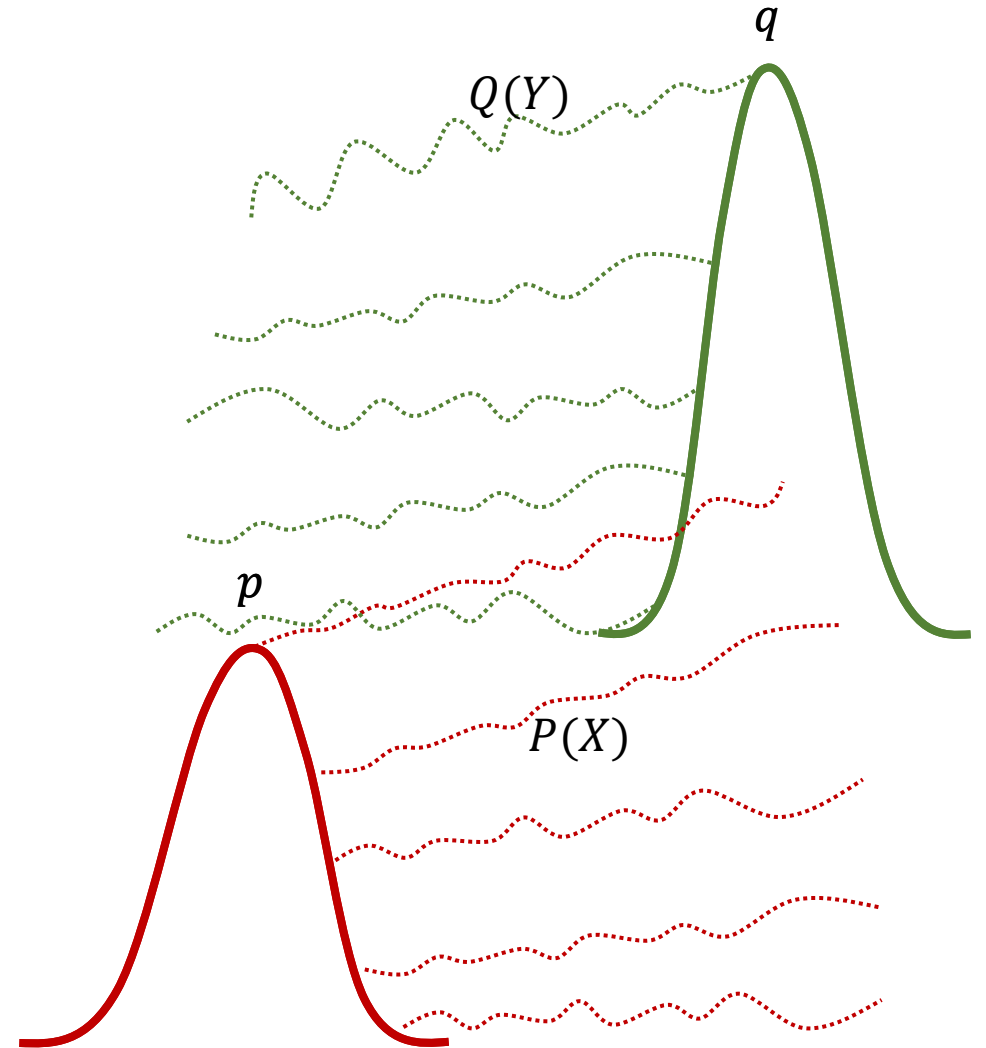
Path measure 1: P

Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

(4) Calculate MH correction

$$\alpha = \min\left\{1, \frac{d P(X') \times Q(Y')}{d P(X) \times Q(Y)}\right\}$$



Parallel tempering Swap in Path Space

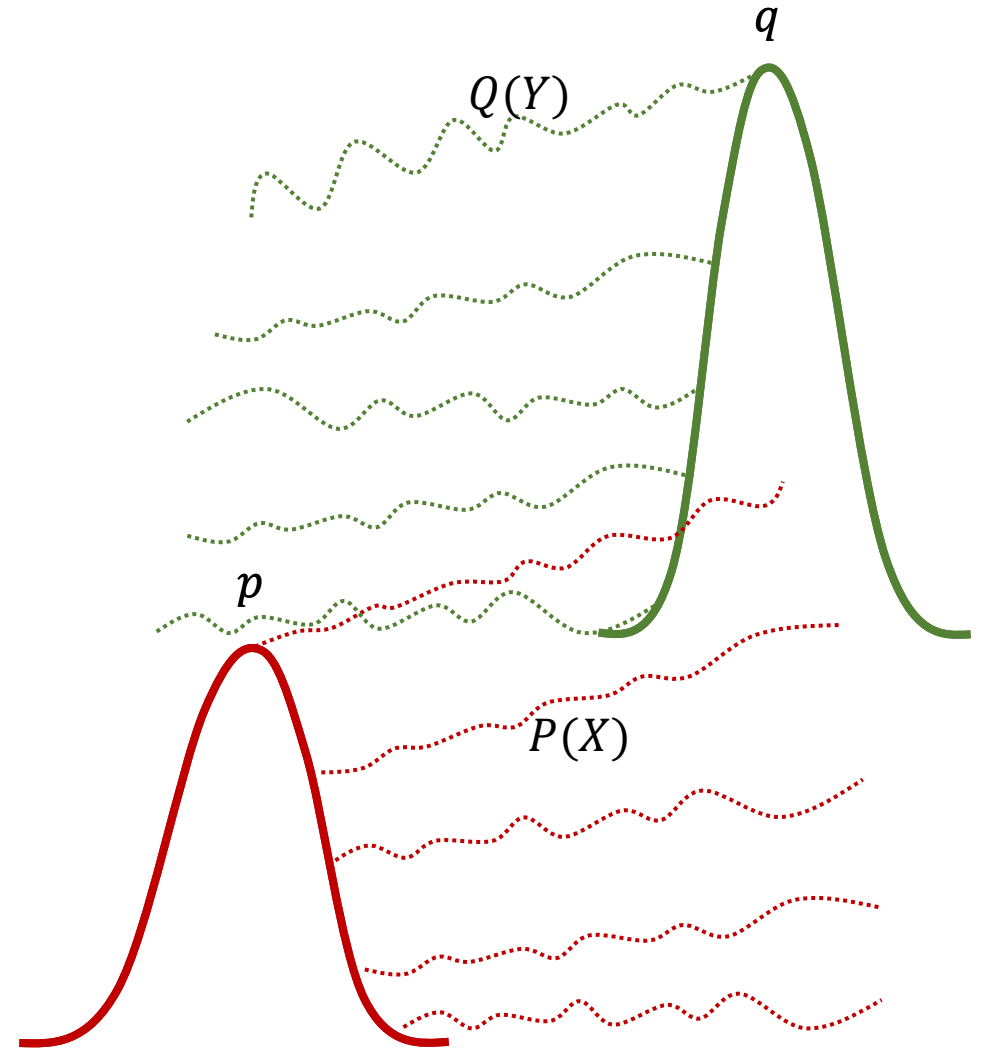
Path measure 1: P

Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

(4) Calculate MH correction

$$\alpha = \min\left\{1, \frac{d P(Y) \times Q(X)}{d P(X) \times Q(Y)}\right\}$$



Parallel tempering Swap in Path Space

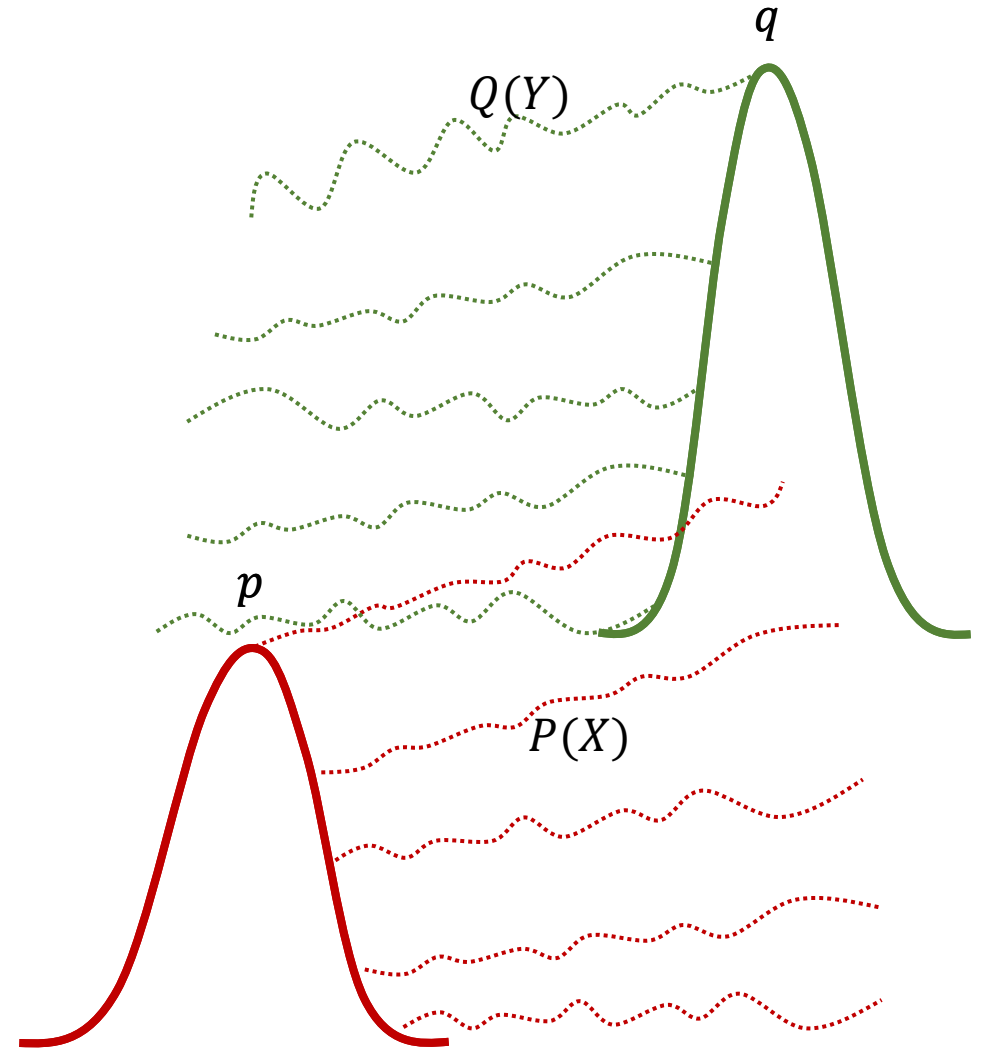
Path measure 1: P

Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

(4) Calculate MH correction

$$\alpha = \min\left\{1, \frac{d P(Y) \times Q(X)}{d P(X) \times Q(Y)}\right\}$$



Parallel tempering Swap in Path Space

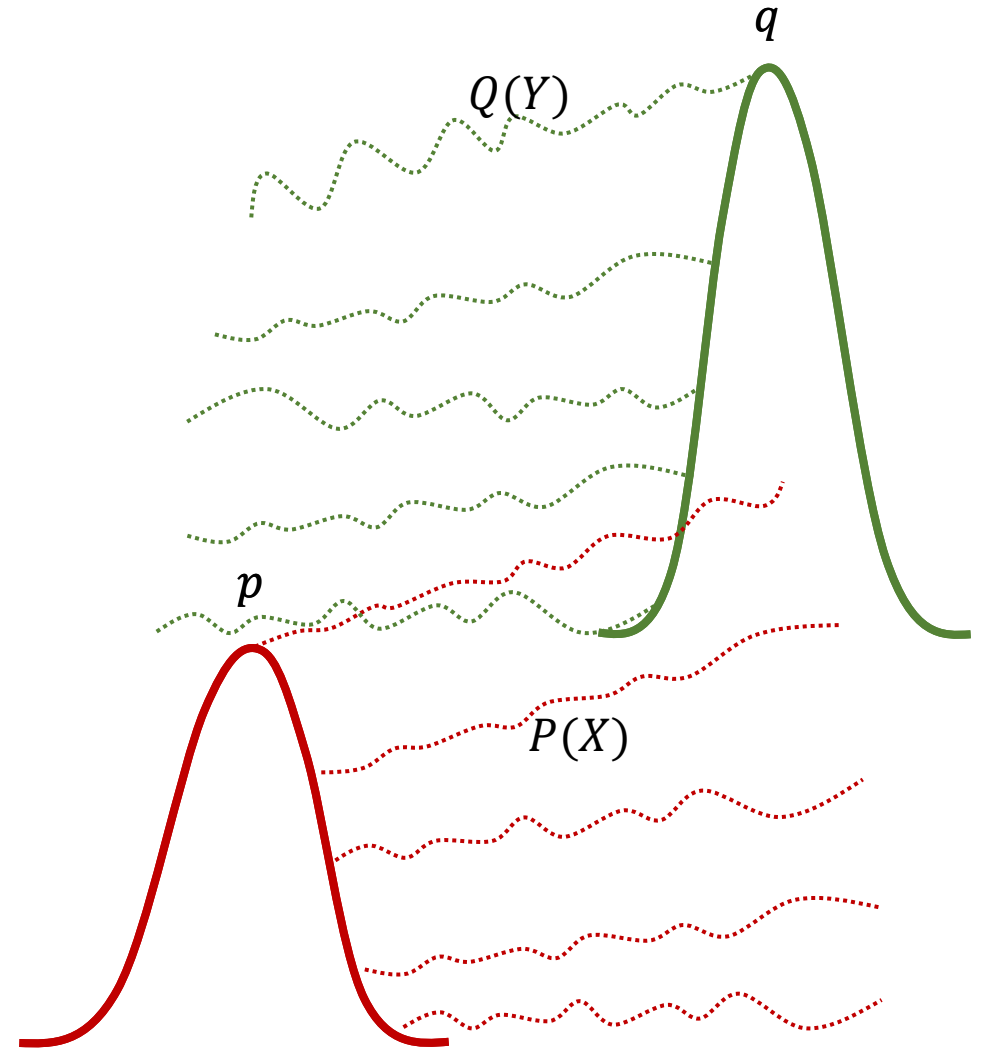
Path measure 1: P

Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

(4) Calculate MH correction

$$\alpha = \min\left\{1, \frac{dP}{dQ}(Y) \frac{dQ}{dP}(X)\right\}$$



Parallel tempering Swap in Path Space

Path measure 1: P

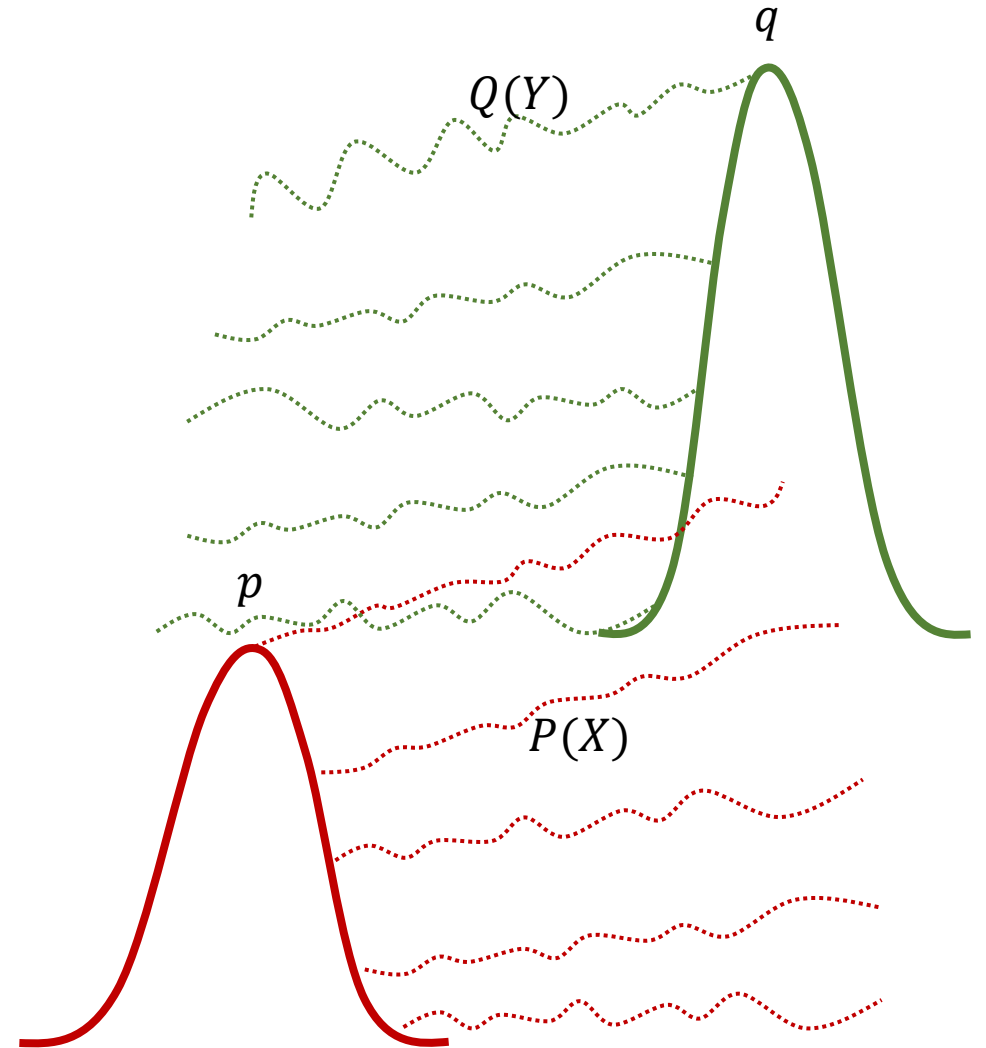
Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

(4) Calculate MH correction

$$\alpha = \min\left\{1, \frac{dP}{dQ}(Y) \frac{dQ}{dP}(X)\right\}$$

if $P \approx Q$, $\alpha \approx 1$ 🥳



Parallel tempering Swap in Path Space

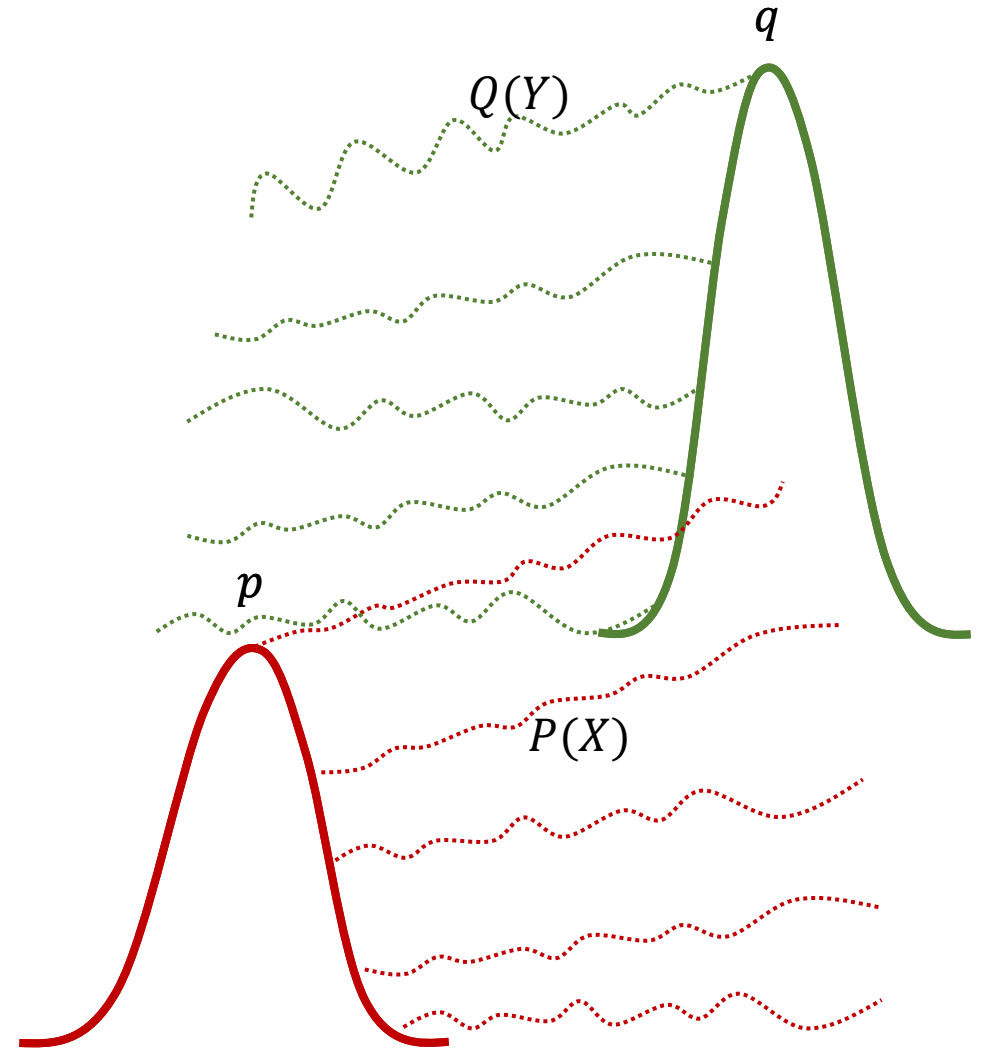
Path measure 1: P

Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

(4) Calculate MH correction

$$\alpha = \min\left\{1, \frac{Z_p}{Z_q} \frac{dP}{dQ}(Y) \frac{Z_q}{Z_p} \frac{dQ}{dP}(X)\right\}$$



Parallel tempering Swap in Path Space

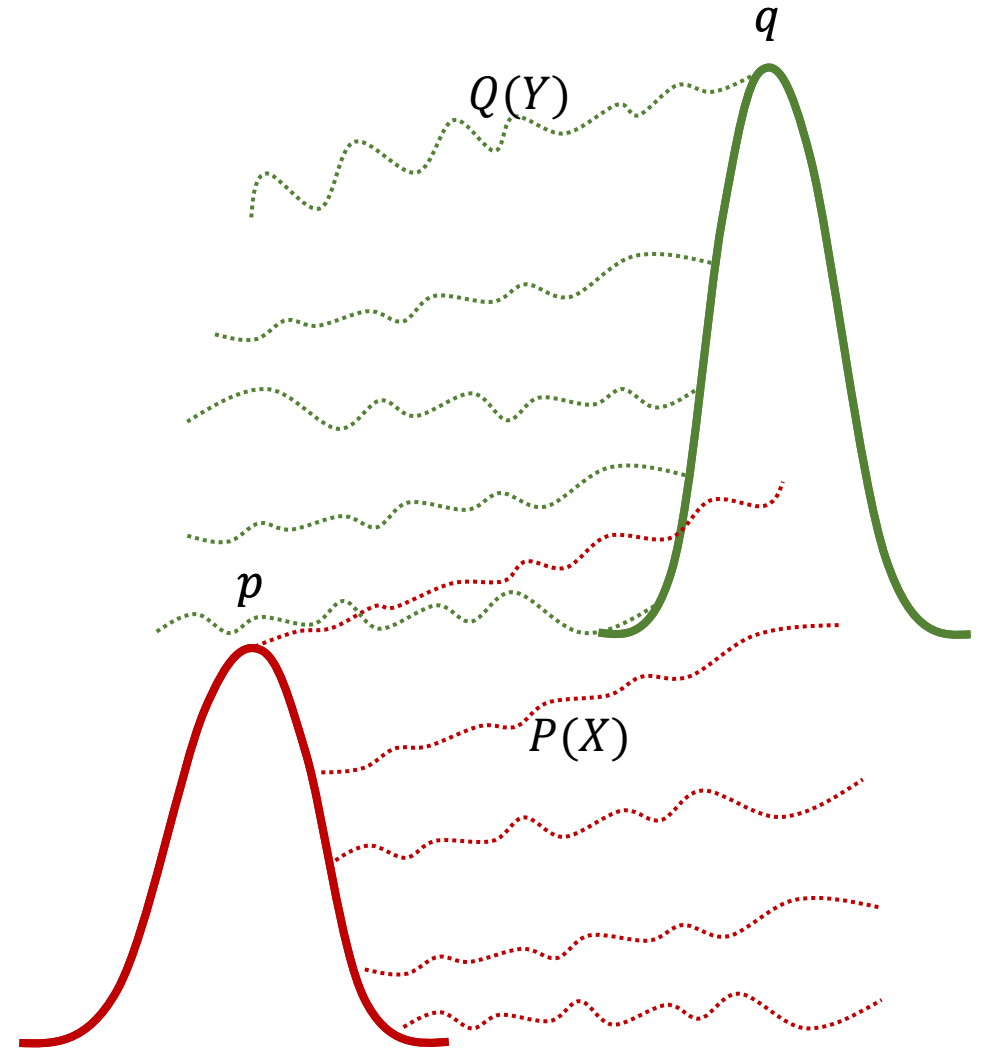
Path measure 1: P

Path measure 2: Q

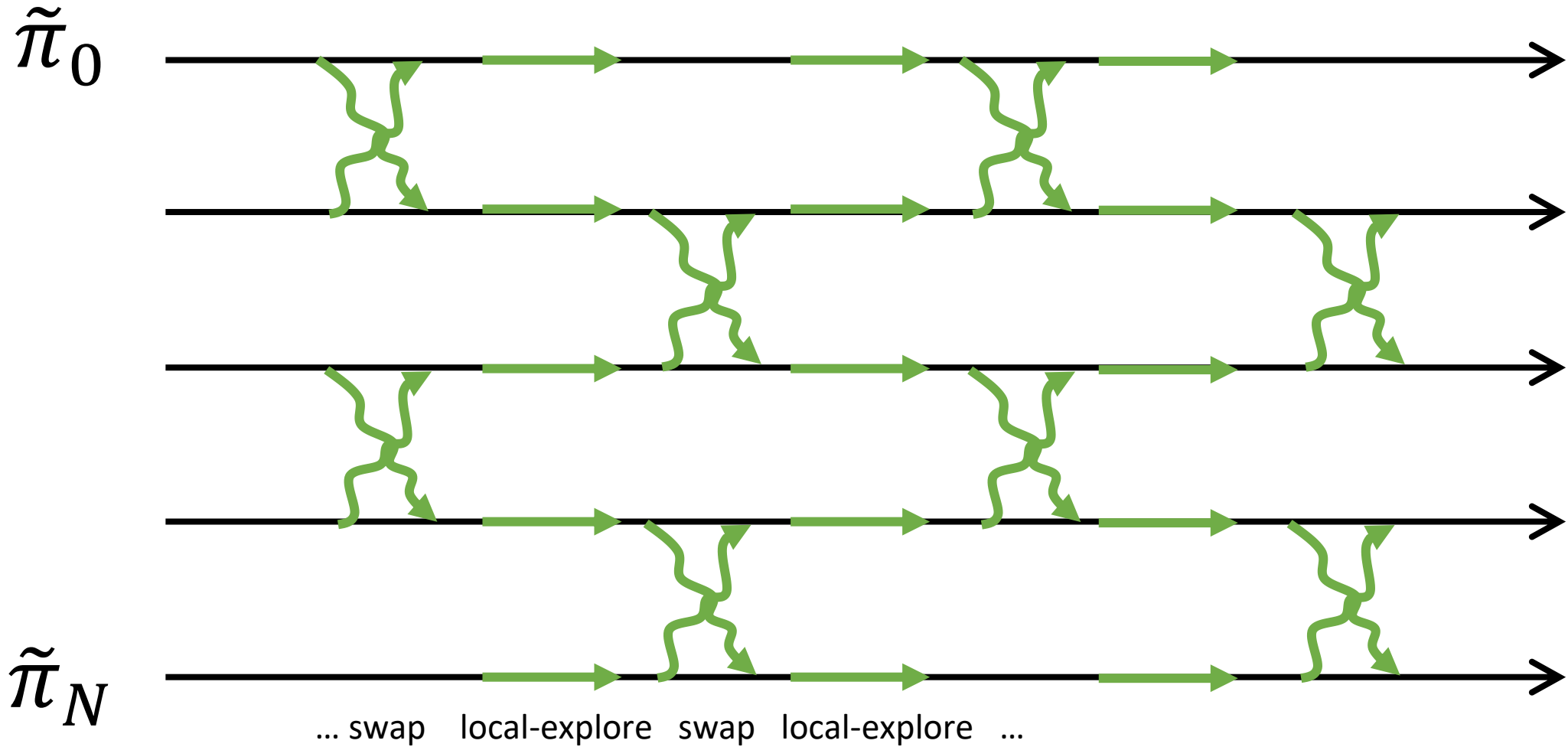
“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$

How to realise the path?

CMCD Path / Diffusion Path / etc...



Accelerated Parallel tempering in Path Space



Extensions

Diffusion Inference-time control with Path RND

Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control

- Our setup so far:
 - Given unnormalised density, generated samples from it
- Diffusion test-time control:
 - Given a pretrained diffusion, steer distribution of generated samples

Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control

- Our setup so far:
 - Given unnormalised density, generated samples from it
- Diffusion test-time control:
 - Given a pretrained diffusion, steer distribution of generated samples

tempering:

$\pi_0(x) \propto p_0^j(x)^\beta$ with inverse-temperature $\beta > 0$;

reward-tilting/posterior sampling:

$\pi_0(x) \propto p_0^j(x) \exp(r_0(x))$ with reward/likelihood $r_0(x)$;

model composition:

$\pi_0(x) \propto \prod_j p_0^j(x)$ composing J diffusions $p_0^j, j = 1, \dots, J$.

Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control

tempering:

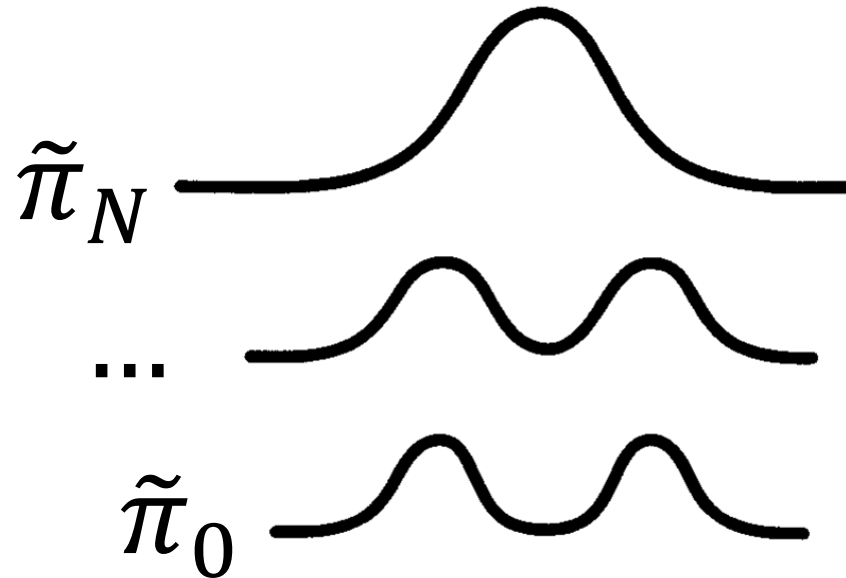
$\pi_0(x) \propto p_0^j(x)^\beta$ with inverse-temperature $\beta > 0$;

reward-tilting/posterior sampling:

$\pi_0(x) \propto p_0^j(x) \exp(r_0(x))$ with reward/likelihood $r_0(x)$;

model composition:

$\pi_0(x) \propto \prod_j p_0^j(x)$ composing J diffusions $p_0^j, j = 1, \dots, J$.



Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control

tempering:

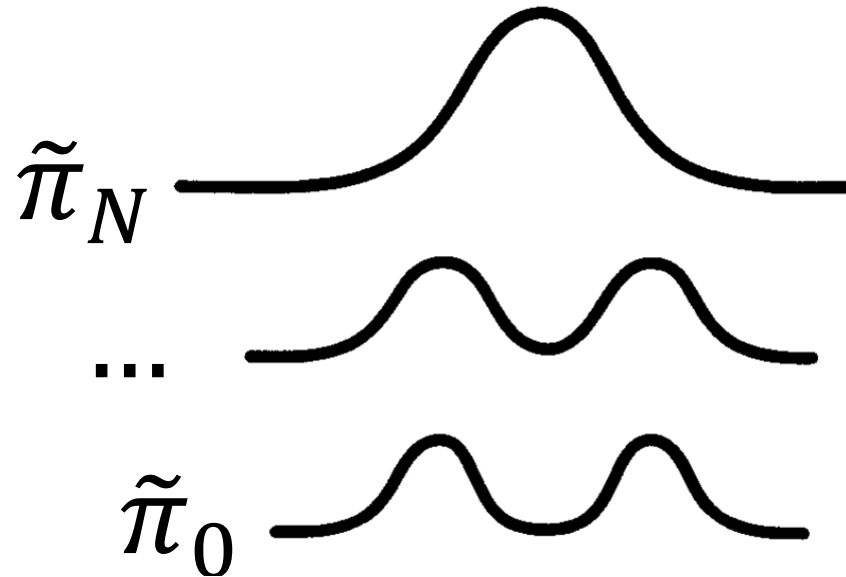
$$\pi_0(x) \propto p_0^j(x)^\beta \text{ with inverse-temperature } \beta > 0;$$

reward-tilting/posterior sampling:

$$\pi_0(x) \propto p_0^j(x) \exp(r_0(x)) \text{ with reward/likelihood } r_0(x);$$

model composition:

$$\pi_0(x) \propto \prod_j p_0^j(x) \text{ composing } J \text{ diffusions } p_0^j, j = 1, \dots, J.$$



tempering:

$$\pi_t(x) \propto p_t^j(x)^\beta \text{ with inverse-temperature } \beta > 0;$$

reward-tilting/posterior sampling:

$$\pi_t(x) \propto p_t^j(x) \exp(r_t(x)) \text{ with reward/likelihood } r_t(x);$$

model composition:

$$\pi_t(x) \propto \prod_j p_t^j(x) \text{ composing } J \text{ diffusions } p_t^j, j = 1, \dots, J.$$

Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control

tempering:

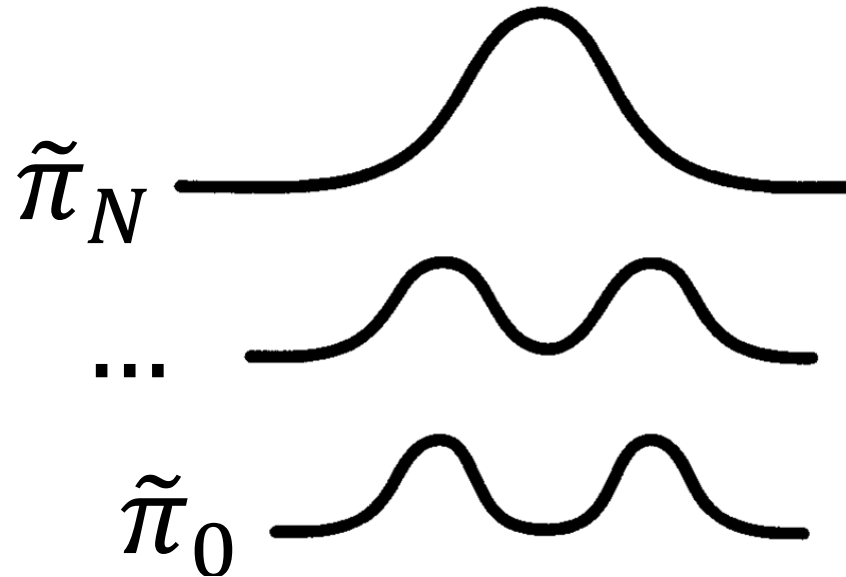
$$\pi_0(x) \propto p_0^j(x)^\beta \text{ with inverse-temperature } \beta > 0;$$

reward-tilting/posterior sampling:

$$\pi_0(x) \propto p_0^j(x) \exp(r_0(x)) \text{ with reward/likelihood } r_0(x);$$

model composition:

$$\pi_0(x) \propto \prod_j p_0^j(x) \text{ composing } J \text{ diffusions } p_0^j, j = 1, \dots, J.$$



tempering:

$$\pi_t(x) \propto p_t^j(x)^\beta \text{ with inverse-temperature } \beta > 0;$$

In short, control the marginal of each denoising step using APT

model composition:

$$\pi_t(x) \propto \prod_j p_t^j(x) \text{ composing } J \text{ diffusions } p_t^j, j = 1, \dots, J.$$

Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control (reward-tilting as example)

Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control (reward-tilting as example)



$$\tilde{\pi}_N \propto p_N \exp(r_N)$$



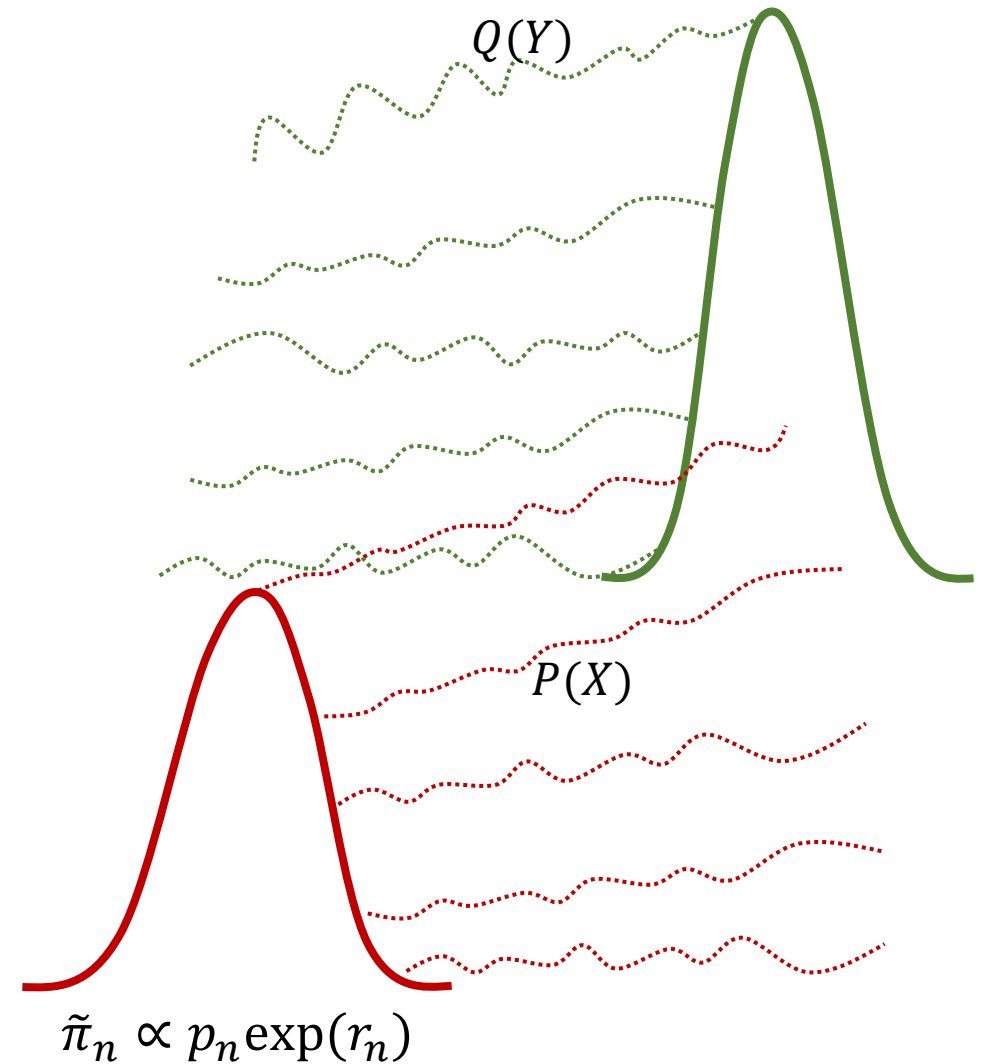
...



$$\tilde{\pi}_0 \propto p_0 \exp(r)$$

Accelerated Parallel tempering in Path Space

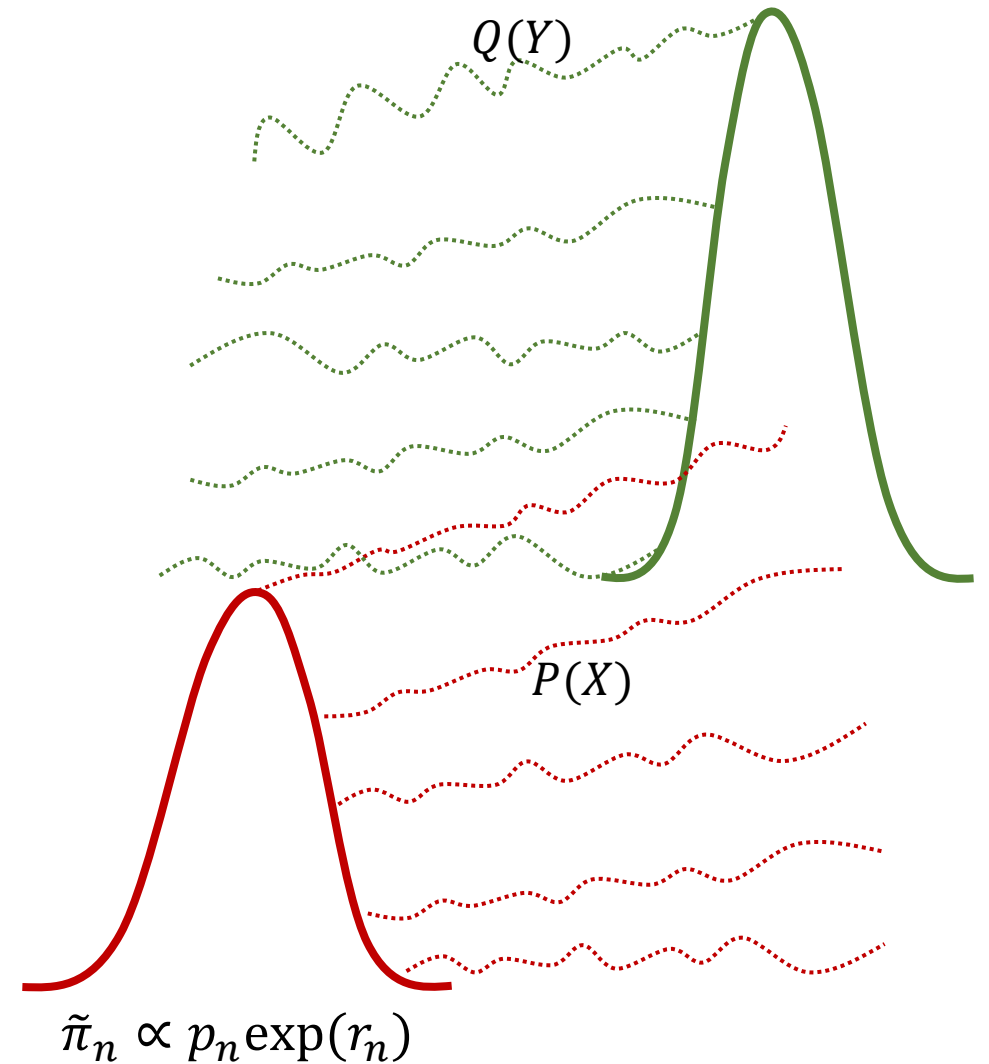
For Diffusion Test-time Control (reward-tilting as example) $\tilde{\pi}_{n+1} \propto p_{n+1} \exp(r_{n+1})$



Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control (reward-tilting as example) $\tilde{\pi}_{n+1} \propto p_{n+1} \exp(r_{n+1})$

$$\alpha = \min\left\{1, \frac{dP}{dQ}(Y) \frac{dQ}{dP}(X)\right\}$$

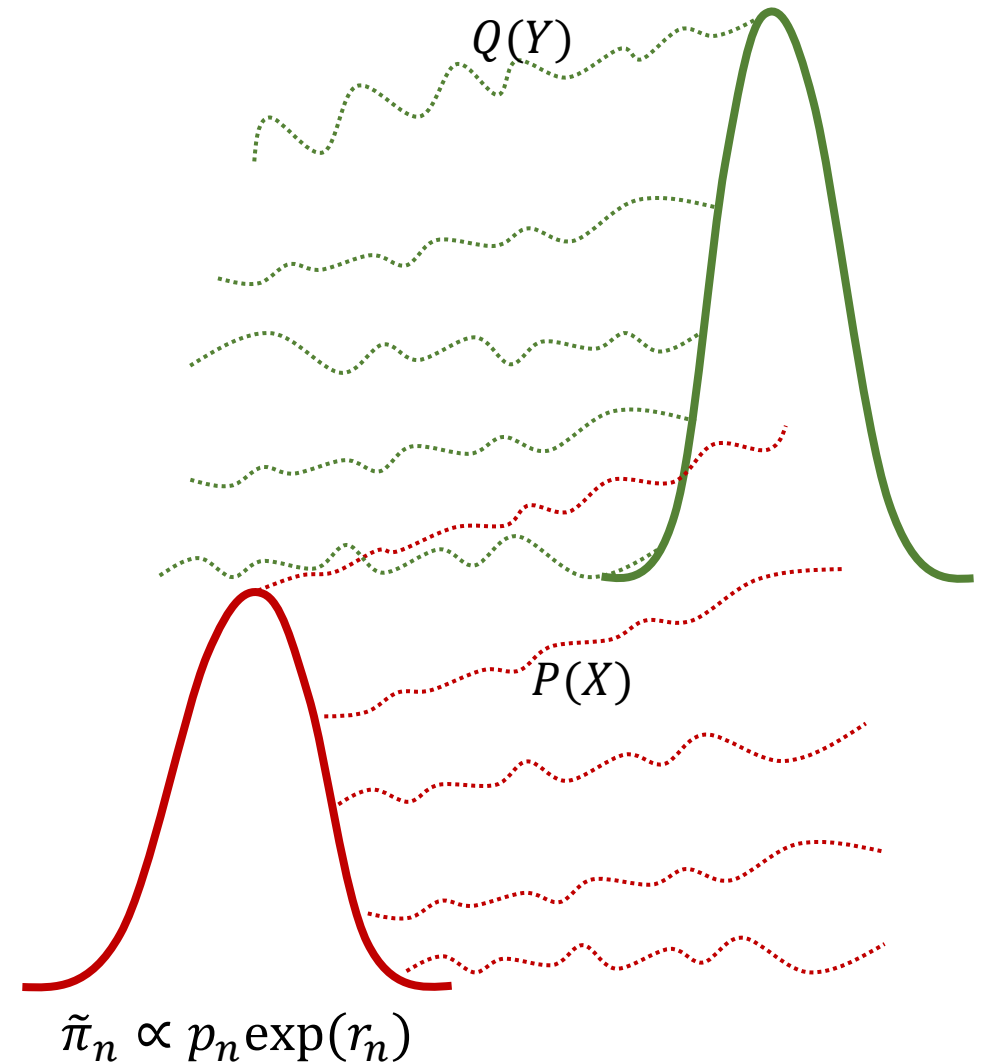


Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control (reward-tilting as example) $\tilde{\pi}_{n+1} \propto p_{n+1} \exp(r_{n+1})$

$$\alpha = \min\left\{1, \frac{dP}{dQ}(Y) \frac{dQ}{dP}(X)\right\}$$

$$\frac{dP}{dQ} \propto \frac{\tilde{\pi}_n(X_0)}{\tilde{\pi}_{n+1}(X_1)} \lim \frac{\prod N_1(X_{k+1}|X_k)}{\prod N_2(X_k|X_{k+1})}$$

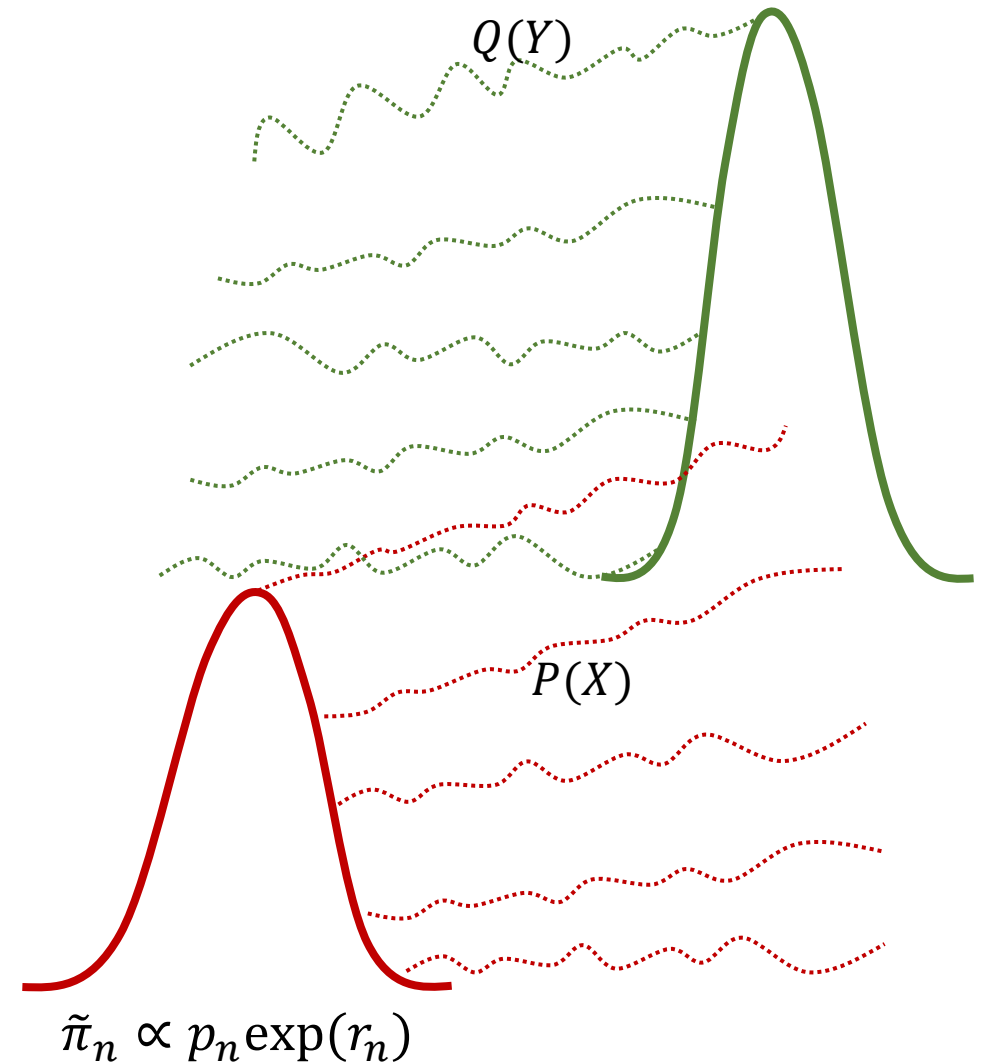


Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control (reward-tilting as example) $\tilde{\pi}_{n+1} \propto p_{n+1} \exp(r_{n+1})$

$$\alpha = \min\left\{1, \frac{dP}{dQ}(Y) \frac{dQ}{dP}(X)\right\}$$

$$\frac{dP}{dQ} \propto \frac{\tilde{\pi}_n(X_0) N_1(X_1|X_0)}{\tilde{\pi}_{n+1}(X_1) N_2(X_0|X_1)}$$

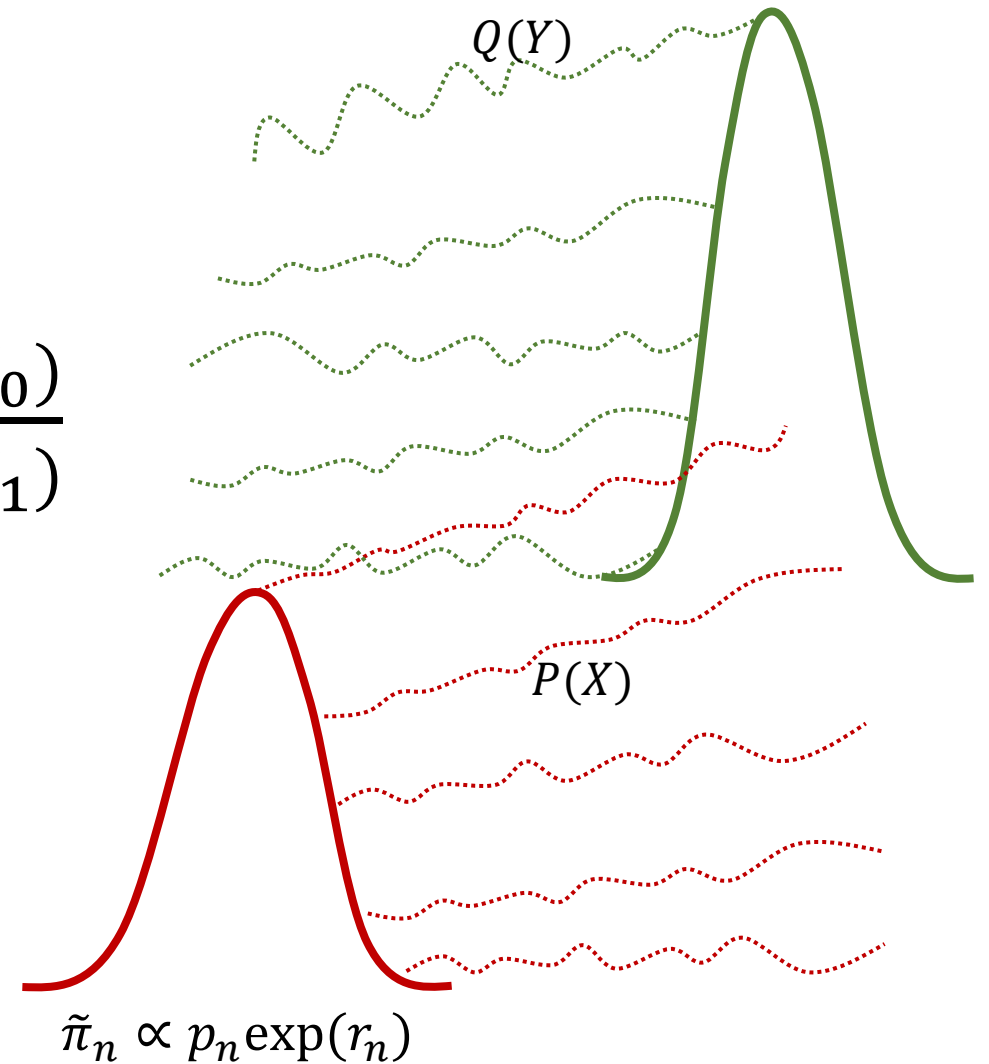


Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control (reward-tilting as example) $\tilde{\pi}_{n+1} \propto p_{n+1} \exp(r_{n+1})$

$$\alpha = \min\left\{1, \frac{dP}{dQ}(Y) \frac{dQ}{dP}(X)\right\}$$

$$\frac{dP}{dQ} \propto \frac{p_n(X_0)}{p_{n+1}(X_1)} \frac{\exp(r_n(X_0))}{\exp(r_{n+1}(X_0))} \frac{N_1(X_1|X_0)}{N_2(X_0|X_1)}$$

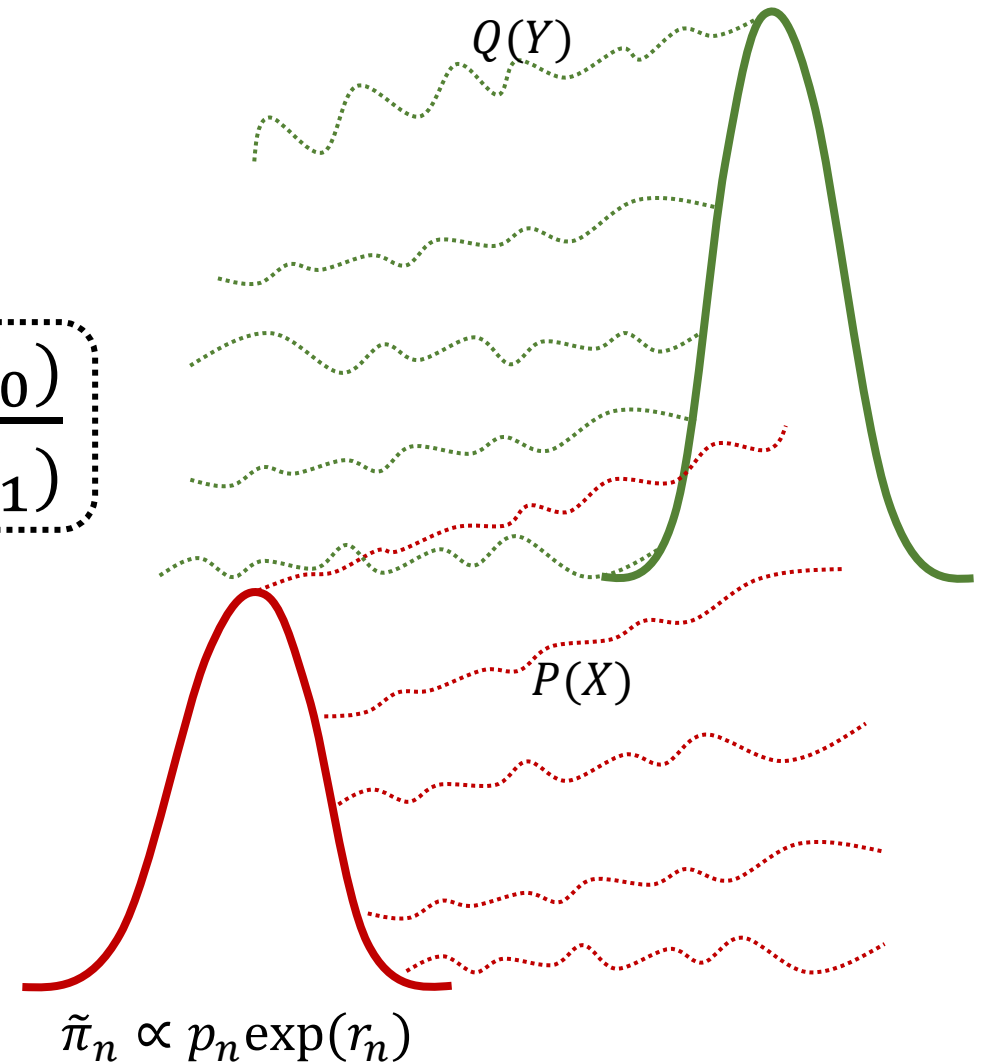


Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control (reward-tilting as example) $\tilde{\pi}_{n+1} \propto p_{n+1} \exp(r_{n+1})$

$$\alpha = \min\left\{1, \frac{dP}{dQ}(Y) \frac{dQ}{dP}(X)\right\}$$

$$\frac{dP}{dQ} \propto \frac{p_n(X_0)}{p_{n+1}(X_1)} \underbrace{\frac{\exp(r_n(X_0))}{\exp(r_{n+1}(X_0))} \frac{N_1(X_1|X_0)}{N_2(X_0|X_1)}}_{\text{known}}$$



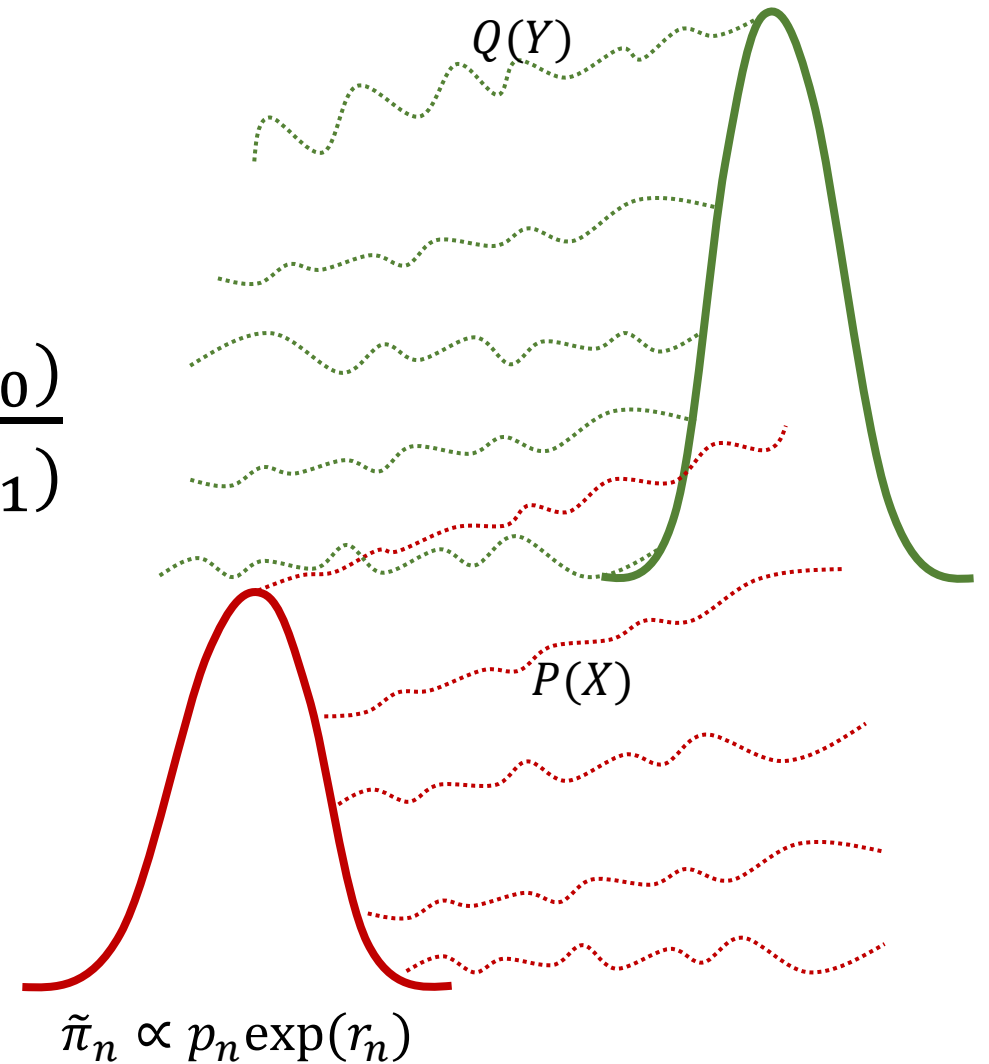
Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control (reward-tilting as example) $\tilde{\pi}_{n+1} \propto p_{n+1} \exp(r_{n+1})$

$$\alpha = \min\left\{1, \frac{dP}{dQ}(Y) \frac{dQ}{dP}(X)\right\}$$

$$\frac{dP}{dQ} \propto \frac{p_n(X_0)}{p_{n+1}(X_1)} \frac{\exp(r_n(X_0))}{\exp(r_{n+1}(X_0))} \frac{N_1(X_1|X_0)}{N_2(X_0|X_1)}$$

unknown



Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control (reward-tilting as example)

$$\bar{P}: dX_t = \text{diffusion denoising drift } dt + \sigma_t \overleftarrow{dW}_t \quad X_1 \sim p_{n+1}$$

$$P: dX_t = \text{diffusion noising drift } dt + \sigma_t dW_t \quad X_0 \sim p_n$$

$$\frac{p_n(X_0)}{p_{n+1}(X_1)} = ?$$

Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control (reward-tilting as example)

$$\begin{array}{ll} \overleftarrow{P}: dX_t = \text{diffusion denoising drift } dt + \sigma_t \overleftarrow{dW}_t & X_1 \sim p_{n+1} \\ P: dX_t = \text{diffusion noising drift } dt + \sigma_t dW_t & X_0 \sim p_n \end{array} \quad \rightarrow \quad \frac{\overleftarrow{dP}}{dP} = 1$$

$$\frac{p_n(X_0)}{p_{n+1}(X_1)} = ?$$

Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control (reward-tilting as example)

$$\begin{array}{ll} \overleftarrow{P}: dX_t = \text{diffusion denoising drift } dt + \sigma_t \overleftarrow{dW}_t & X_1 \sim p_{n+1} \\ P: dX_t = \text{diffusion noising drift } dt + \sigma_t dW_t & X_0 \sim p_n \end{array} \quad \longrightarrow \quad \frac{\overleftarrow{dP}}{dP} = 1$$

$$\frac{p_n(X_0)}{p_{n+1}(X_1)} \frac{N_{\text{noise}}(X_1|X_0)}{N_{\text{denoise}}(X_0|X_1)} \approx 1$$

Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control (reward-tilting as example)

$$\begin{array}{ll} \overleftarrow{P}: dX_t = \text{diffusion denoising drift } dt + \sigma_t \overleftarrow{dW}_t & X_1 \sim p_{n+1} \\ P: dX_t = \text{diffusion noising drift } dt + \sigma_t dW_t & X_0 \sim p_n \end{array} \quad \rightarrow \quad \frac{\overleftarrow{dP}}{dP} = 1$$

$$\frac{p_n(X_0)}{p_{n+1}(X_1)} \approx \frac{N_{\text{denoise}}(X_0|X_1)}{N_{\text{noise}}(X_1|X_0)}$$

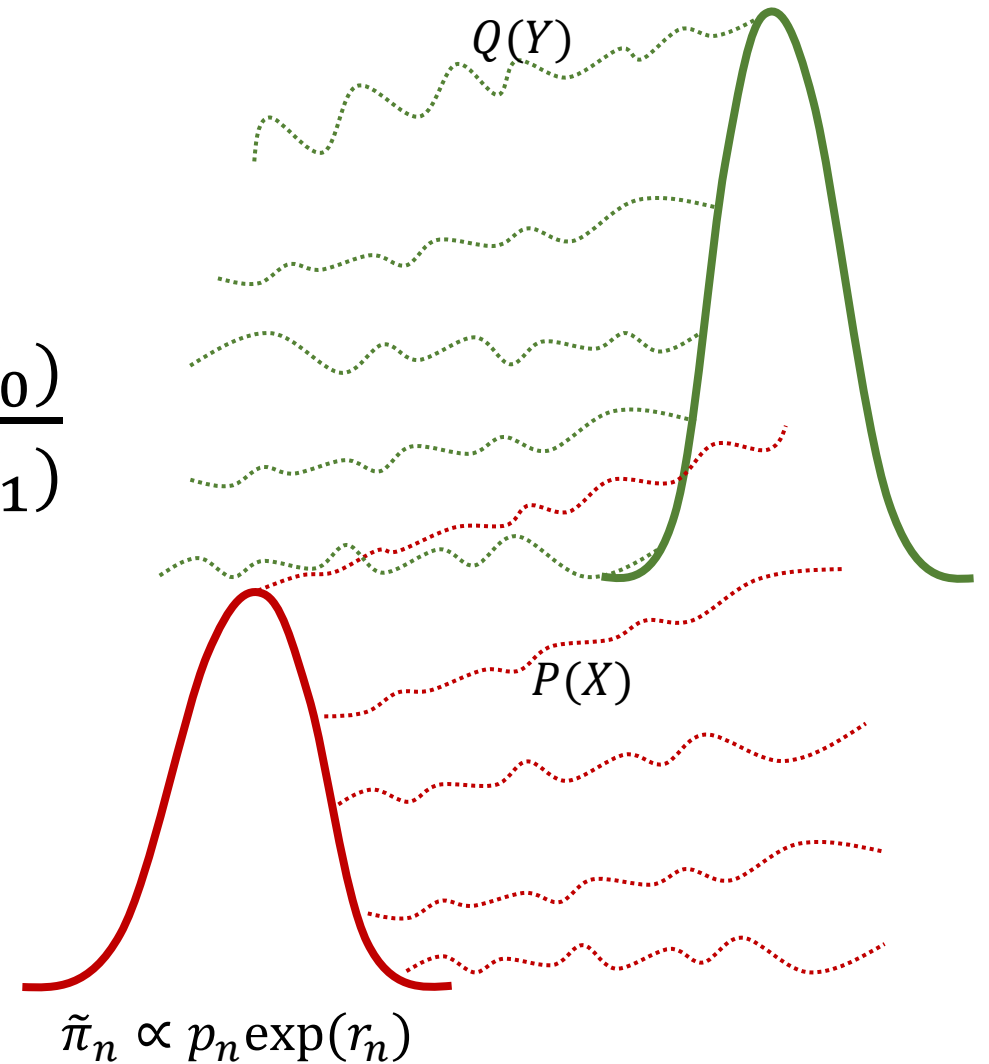
Accelerated Parallel tempering in Path Space

For Diffusion Test-time Control (reward-tilting as example) $\tilde{\pi}_{n+1} \propto p_{n+1} \exp(r_{n+1})$

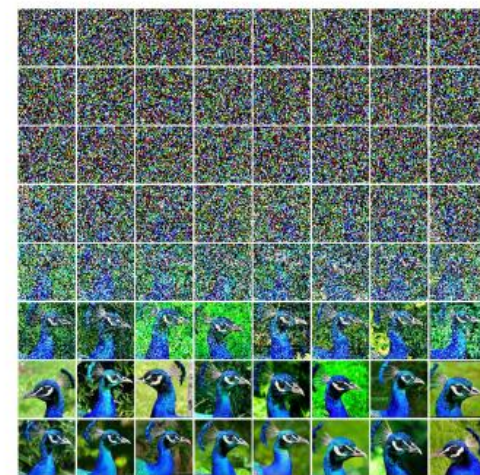
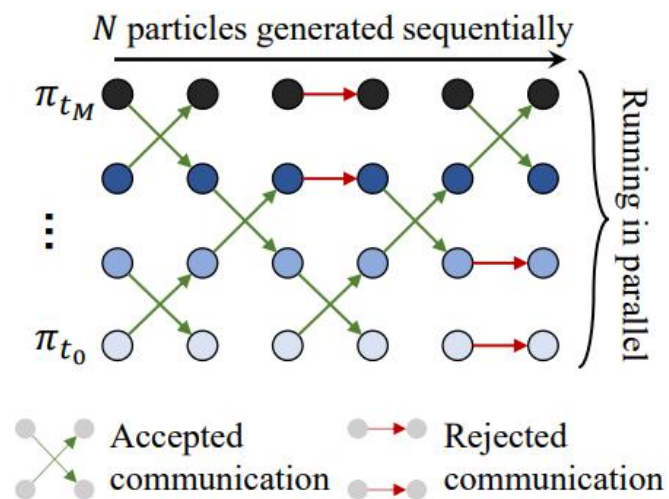
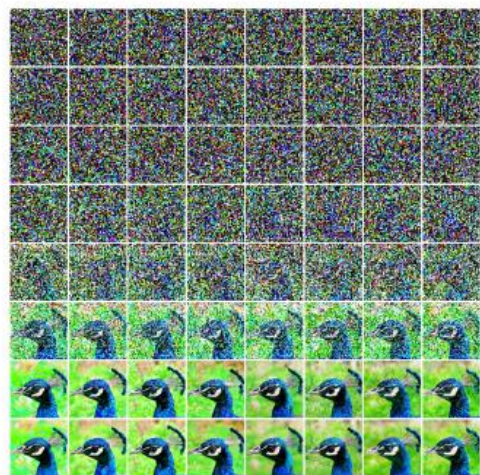
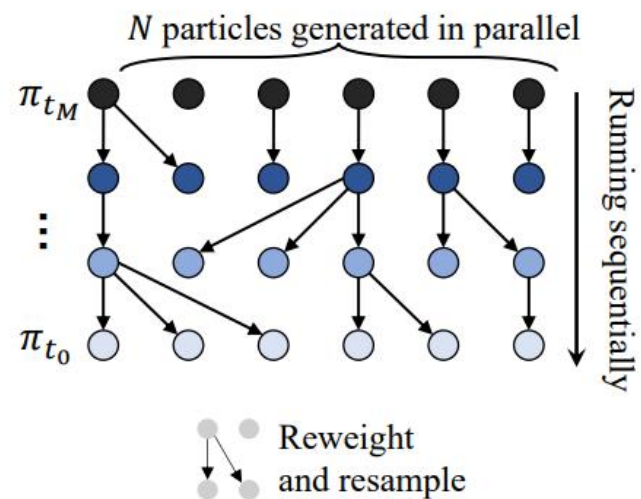
$$\alpha = \min\left\{1, \frac{dP}{dQ}(Y) \frac{dQ}{dP}(X)\right\}$$

$$\frac{dP}{dQ} \propto \frac{p_n(X_0)}{p_{n+1}(X_1)} \frac{\exp(r_n(X_0))}{\exp(r_{n+1}(X_0))} \frac{N_1(X_1|X_0)}{N_2(X_0|X_1)}$$

unknown



CREPE: Controlling Diffusion with Replica Exchange



CREPE: Controlling Diffusion with Replica Exchange

class condition: *balloon*; **prompt:** *a blue balloon*



class condition: *pinwheel*; **prompt:** *a colorful pinwheel*



class condition: *Christmas stocking*; **prompt:** *a green Christmas stocking*



class condition: *cab*; **prompt:** *a yellow cab with dark background*



CREPE iteration →

Figure 1: Trajectory of images generated using CREPE for prompted reward-tilting on ImageNet-512, thinned every 8 iterations. After burn-in, the samples align closely with the prompt.

CREPE: Controlling Diffusion with Replica Exchange

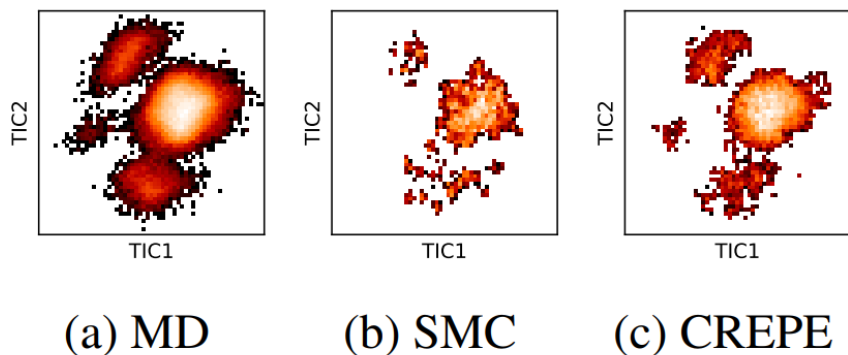
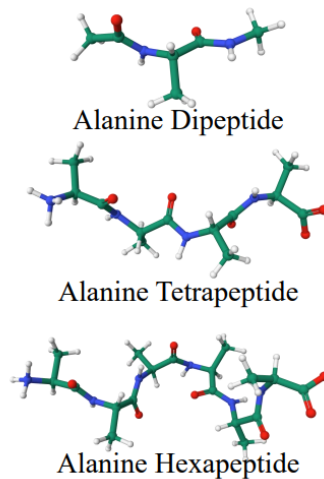


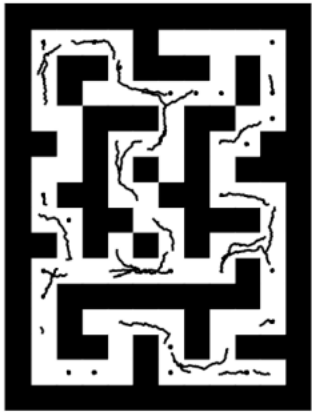
Figure 3: TICA of Alanine Hexapeptide annealed to 600K by SMC and CREPE. CREPE maintains more diversity.

Table 1: Inference-time tempering performance for Alanine Dipeptide, Tetrapeptide and Hexapeptide.

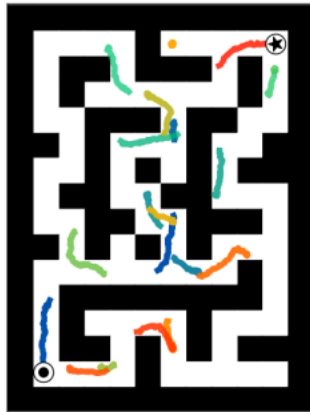


		FKC		RNE	CREPE (Ours)
		Anneal Score	Anneal Noise		
ALA Dipeptide (800K → 300K)	Energy TVD	0.345 ± 0.010	0.894 ± 0.002	0.391 ± 0.006	0.224 ± 0.005
	Distance TVD	0.023 ± 0.001	0.036 ± 0.001	0.024 ± 0.001	0.019 ± 0.000
	Sample W2	0.293 ± 0.001	0.282 ± 0.001	0.282 ± 0.001	0.264 ± 0.001
	TICA MMD	0.116 ± 0.003	0.108 ± 0.004	0.168 ± 0.007	0.096 ± 0.014
ALA Tetrapeptide (800K → 500K)	Energy TVD	0.122 ± 0.012	0.436 ± 0.007	0.154 ± 0.006	0.122 ± 0.004
	Distance TVD	0.014 ± 0.000	0.015 ± 0.000	0.013 ± 0.001	0.013 ± 0.001
	Sample W2	0.923 ± 0.008	0.892 ± 0.001	0.893 ± 0.005	0.856 ± 0.004
	TICA MMD	0.183 ± 0.020	0.138 ± 0.017	0.155 ± 0.009	0.035 ± 0.002
ALA Hexapeptide (800K → 600K)	Energy TVD	0.091 ± 0.006	0.206 ± 0.005	0.087 ± 0.003	0.398 ± 0.001
	Distance TVD	0.018 ± 0.000	0.020 ± 0.001	0.010 ± 0.001	0.009 ± 0.001
	Sample W2	1.585 ± 0.001	1.652 ± 0.012	1.618 ± 0.001	1.299 ± 0.004
	TICA MMD	0.088 ± 0.004	0.068 ± 0.010	0.042 ± 0.004	0.009 ± 0.001

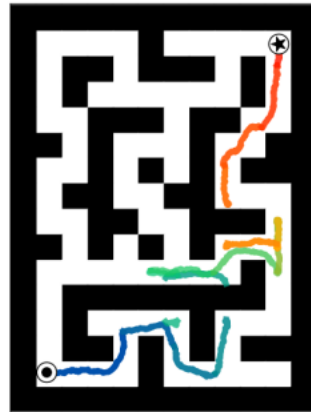
CREPE: Controlling Diffusion with Replica Exchange



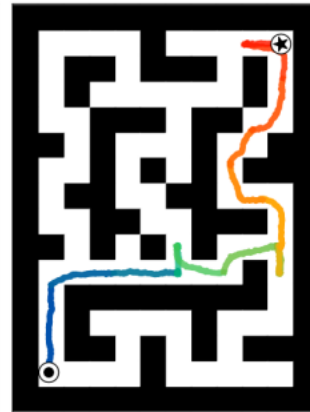
Example of training trajectories.



Trajectory after 1 PT iteration.



Trajectory after 10k PT iterations.



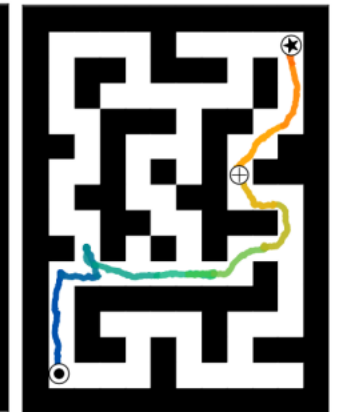
Trajectory after 50k PT iterations.



Trajectory after 100k PT iterations.



Trajectory after 101k PT iteration.



Trajectory after 150k PT iterations.

CREPE:

Controlling Diffusion with Replica Exchange

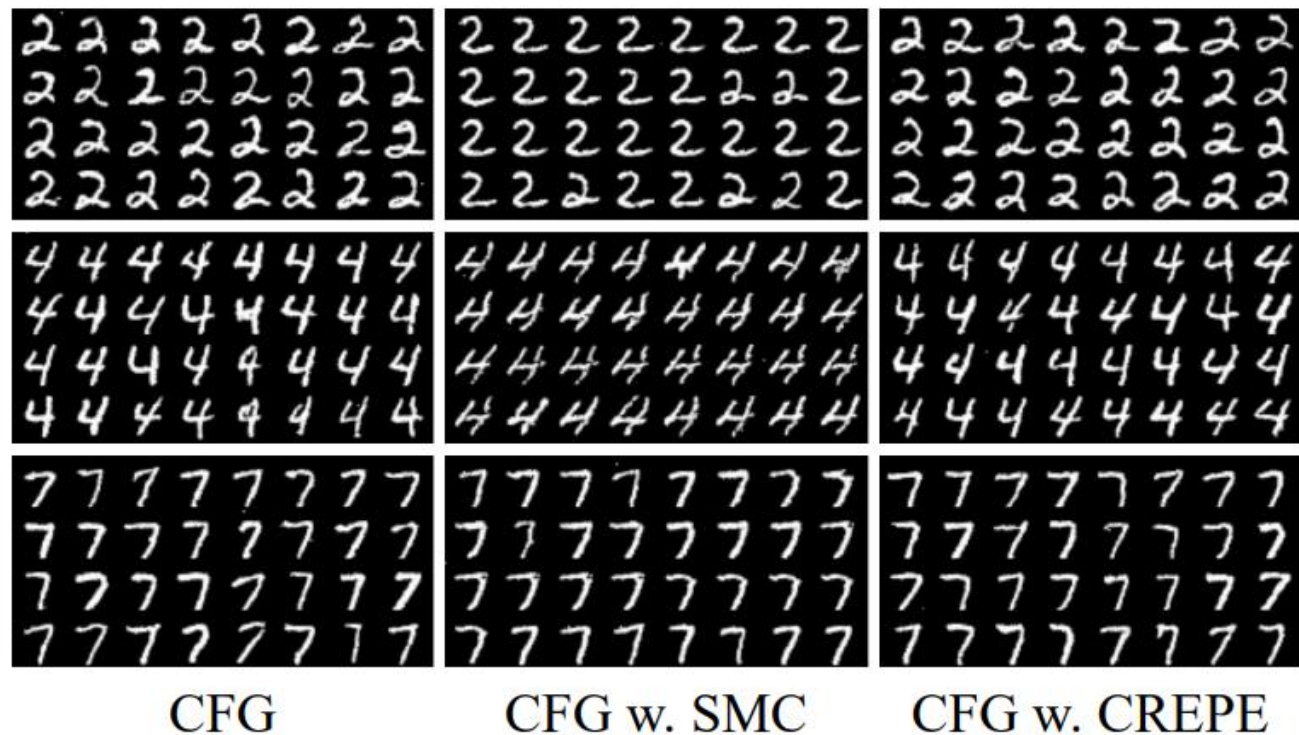
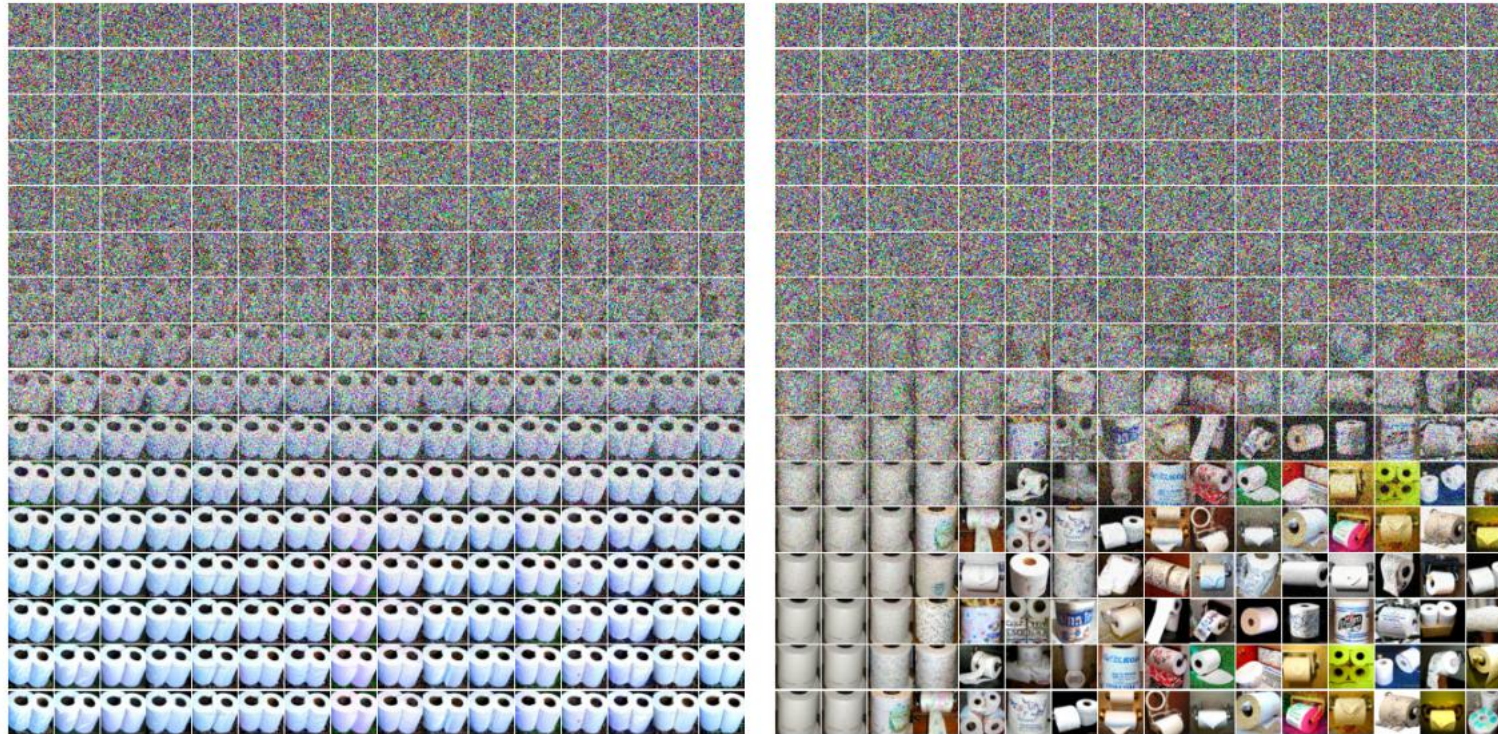


Figure 7: MNIST samples generated by CFG, and debiased by SMC and CREPE.

CREPE: Controlling Diffusion with Replica Exchange



(a) FKC

(b) CREPE

Figure 11: CFG Debiasing with FKC and CREPE for class “toilet tissue” (idx 999).

From Density Ratio to Path RND

Unnormalised density 1: \tilde{p}

Unnormalised density 2: \tilde{q}

$$\text{Density ratio: } w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$$

- Importance sampling: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$
- FEP: $\Delta F = -\log(\int q(x)w(x) dx)$
- PT Swap: $\alpha = \min\{1, \frac{w(y)}{w(x)}\}$

Path measure 1: P

Path measure 2: Q

$$\text{“Unnormalised” RND: } w(X) = \frac{Z_p}{Z_q} \frac{dP}{dQ}(X)$$

- Path Importance sampling: $w(X)$
- Path FEP: $\Delta F = -\log(\int dQ(X)w(X))$
- Path PT Swap: $\alpha = \min\{1, \frac{w(Y)}{w(X)}\}$

Variational Inference with Path RND

Let's first recap importance sampling...

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:

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

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 $f > 0$?

Importance Sampling in Path space:

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

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 $f > 0$?

$$q \propto pf$$

Importance Sampling in Path space:

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

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

Importance Sampling with Path RND

Likelihood

Importance Sampling:

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

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

$$q \propto pL$$

Importance Sampling in Path space:

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

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

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:

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

Variational Inference:

$$q^* \propto pL$$
$$q = \min D[q, q^*]$$

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:

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

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

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:

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

$$Q = \min \text{KL}[Q||Q^*]$$

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

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

Variational Inference with Path RND

Variational Inference in Path space:

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

$$\mathbf{Q} = \min \mathbf{E}_{\mathbf{Q}} \left[\log \frac{d\mathbf{Q}}{d\mathbf{Q}^*} \right]$$

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

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

Variational Inference with Path RND

Variational Inference in Path space:

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

$$\mathbf{Q} = \min \mathbf{E}_{\mathbf{Q}} \left[\log \frac{d\mathbf{Q}}{d\mathbf{Q}^*} \right] = \min \mathbf{E}_{\mathbf{Q}} \left[\log \frac{d\mathbf{Q}}{d\mathbf{P}} + \log \frac{d\mathbf{P}}{d\mathbf{Q}^*} \right]$$

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

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

Variational Inference with Path RND

Variational Inference in Path space:

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

$$\mathbf{Q} = \min \mathbf{E}_{\mathbf{Q}} \left[\log \frac{d\mathbf{Q}}{d\mathbf{Q}^*} \right] = \min \mathbf{E}_{\mathbf{Q}} \left[\log \frac{d\mathbf{Q}}{d\mathbf{P}} - \log L \right]$$

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

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

Variational Inference with Path RND

Variational Inference in Path space:

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

$$Q = \min \mathbf{E}_Q \left[\log \frac{dQ}{dQ^*} \right] = \min \mathbf{E}_Q \left[\log \frac{dQ}{dP} - \log L \right]$$

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

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

Forward-forward RND and Girsanov

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

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

Initial density ratio 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:

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

$$\mathbf{Q} = \min \mathbf{E}_{\mathbf{Q}} \left[\log \frac{d\mathbf{Q}}{d\mathbf{Q}^*} \right] = \min \mathbf{E}_{\mathbf{Q}} \left[\int \frac{1}{2} \|u_t\|^2 dt - \log L \right]$$

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

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

Variational Inference with Path RND

Variational Inference in Path space:

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

$$\mathbf{Q} = \min \mathbf{E}_{\mathbf{Q}} \left[\log \frac{d\mathbf{Q}}{d\mathbf{Q}^*} \right] = \min \mathbf{E}_{\mathbf{Q}} \left[\int \frac{1}{2} \|u_t\|^2 dt - \log L \right]$$

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

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

stochastic optimal control

Variational Inference with Path RND

Variational Inference in Path space:

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

$$\mathbf{Q} = \min \mathbf{E}_{\mathbf{Q}} \left[\log \frac{d\mathbf{Q}}{d\mathbf{Q}^*} \right] = \min \mathbf{E}_{\mathbf{Q}} \left[\int \frac{1}{2} \|u_t\|^2 dt - \log L \right]$$

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

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

stochastic optimal control

👉 **fine-tune diffusion models [1]**

👉 **neural samplers [2,3,4...]**

[1] Domingo-Enrich, C., Drozdal, 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 (random order): Free-energy estimator with adaptive transport



Collaborators (random order): Accelerated parallel tempering



Collaborators (random order): RNE: plug-and-play diffusion inference-time control and energy-based training



Collaborators (random order): Controlling diffusion with Replica Exchange



References

(1) Free energy estimation on Path:

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. *NeurIPS 2025*.

(2) Parallel Tempering on Path:

Zhang*, L., Potapchik*, P., He*, J., Du, Y., Doucet, A., Vargas, F., ... & Syed, S. (2025). Accelerated Parallel Tempering via Neural Transports. *ICLR 2026*.

(2) Diffusion Control / Energy-based training / Density estimation with FB Path RND:

He, J., Hernández-Lobato, J. M., Du, Y., & Vargas, F. (2025). RNE: plug-and-play diffusion inference-time control and energy-based training. *ICLR 2026*.

(3) Parallel Tempering for Diffusion Control:

He, J., Jeha, P., Potapchik, P., Zhang, L., Hernández-Lobato, J. M., Du, Y., ... & Vargas, F. (2025). CREPE: Controlling Diffusion with Replica Exchange. *ICLR 2026*.