
FANTASTIC
PATH RND
AND WHERE
TO FIND THEM
JIAJUN HE
*generated by ChatGPT

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

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Free-energy Perturbation

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- 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 $\tilde{\pi}_0 \times \tilde{\pi}_1 \times \cdots \times \tilde{\pi}_N$

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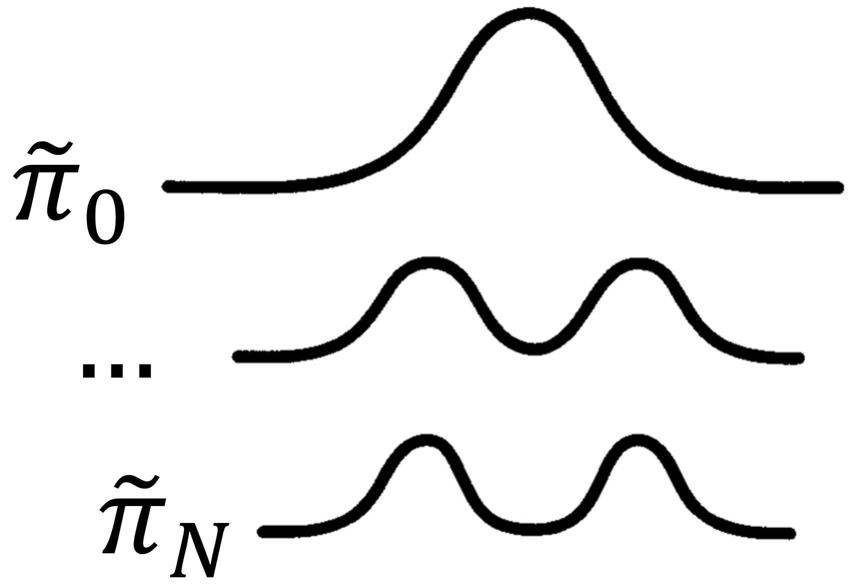

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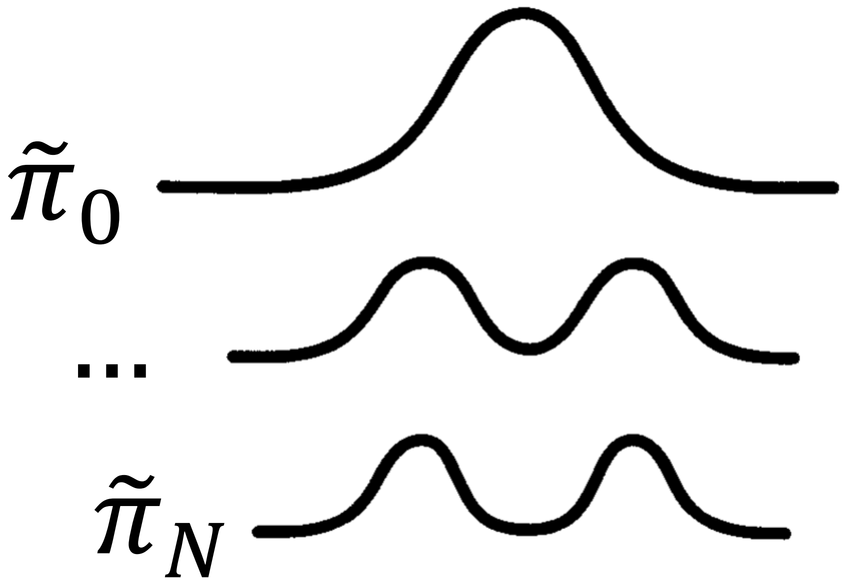

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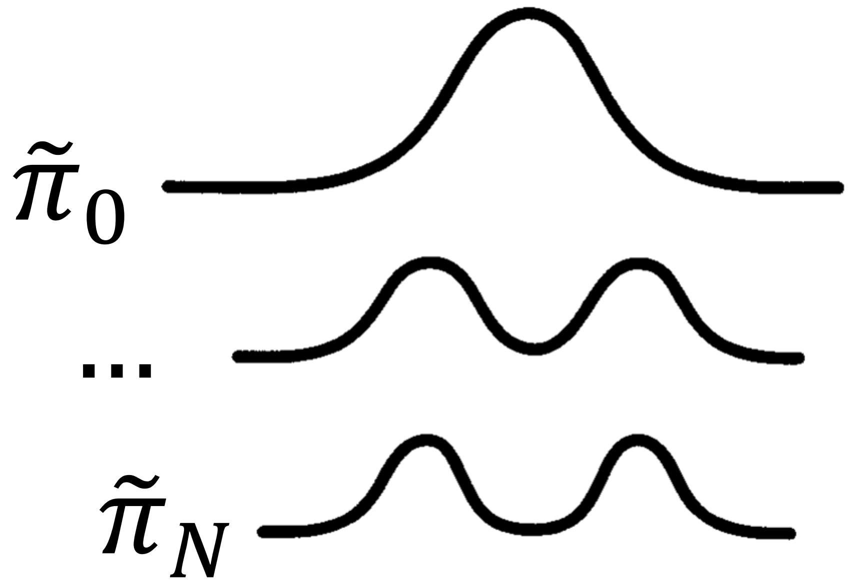

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1. Local exploration kernel: independent MCMC for each $\tilde{\pi}_n$
2. Communication kernel: swap between all adjacent pairs $(\tilde{\pi}_n, \tilde{\pi}_{n+1})$

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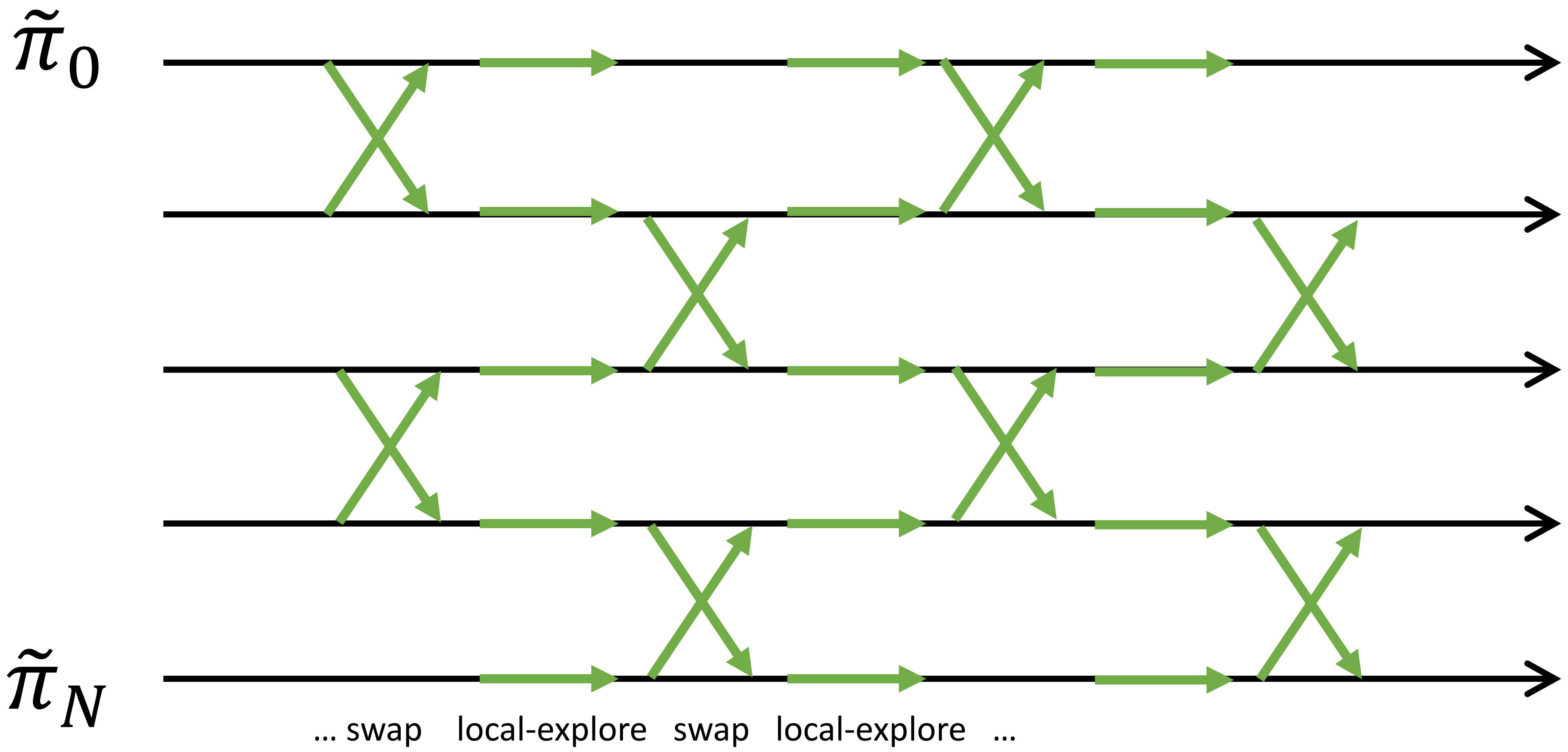

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Assume replica m has density $\tilde{p}$, replica $m+1$ has density $\tilde{q}$, **how to construct a MCMC "swap" kernel with invariant density $\tilde{p}(x) \times \tilde{q}(y)$?**

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informally

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

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

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

Wrap up

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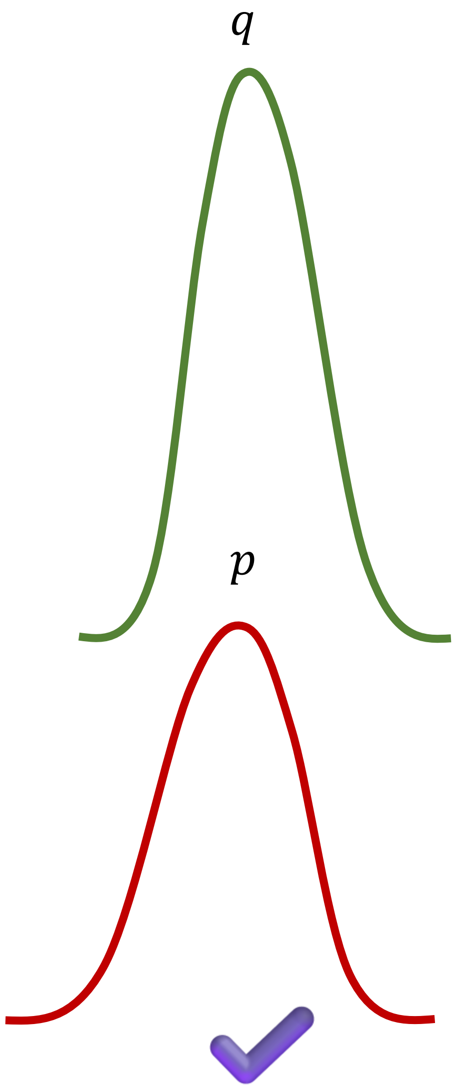
Density ratio: $w(x) = \frac{\tilde{p}(x)}{\tilde{q}(x)}$

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

Limitations



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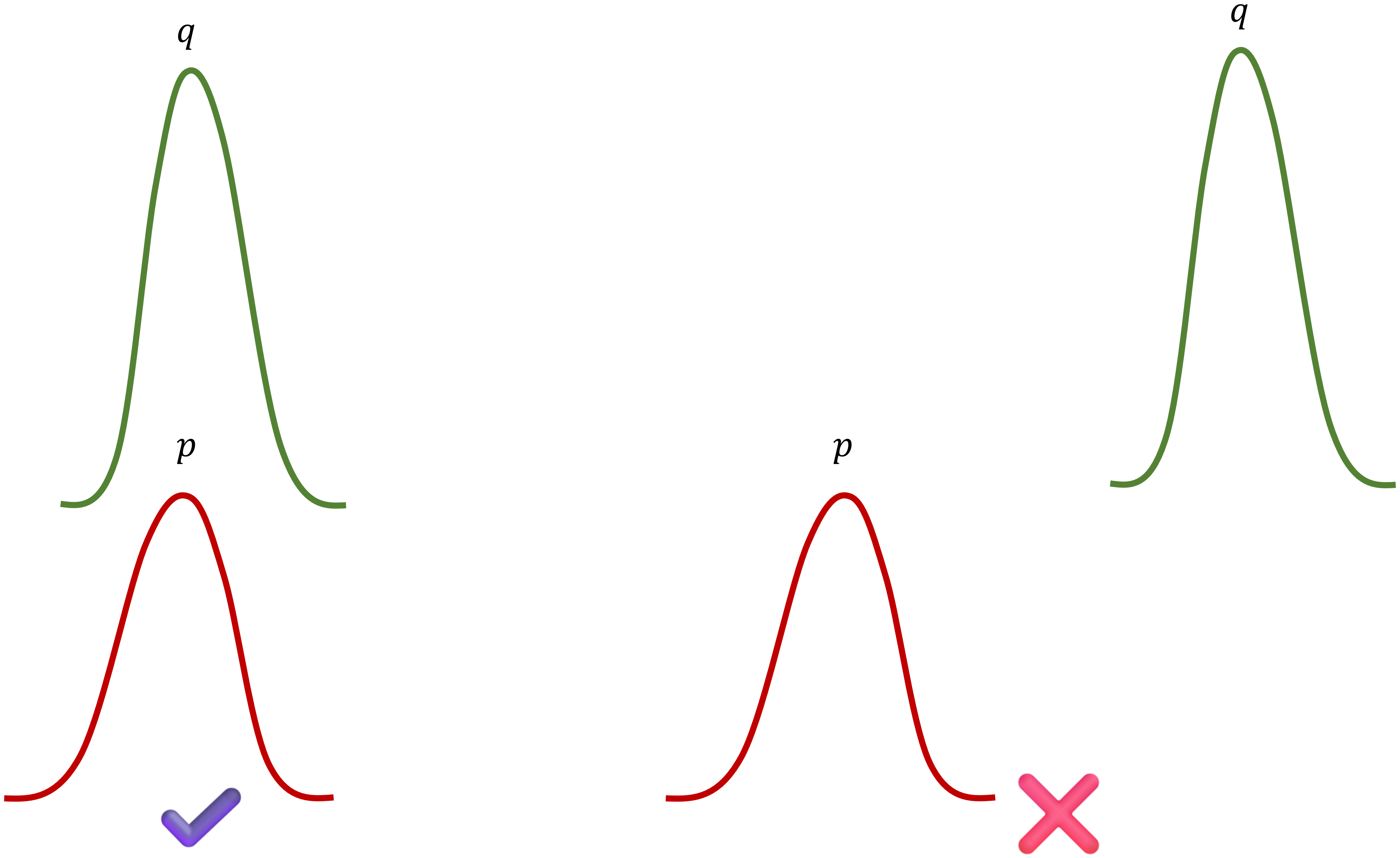

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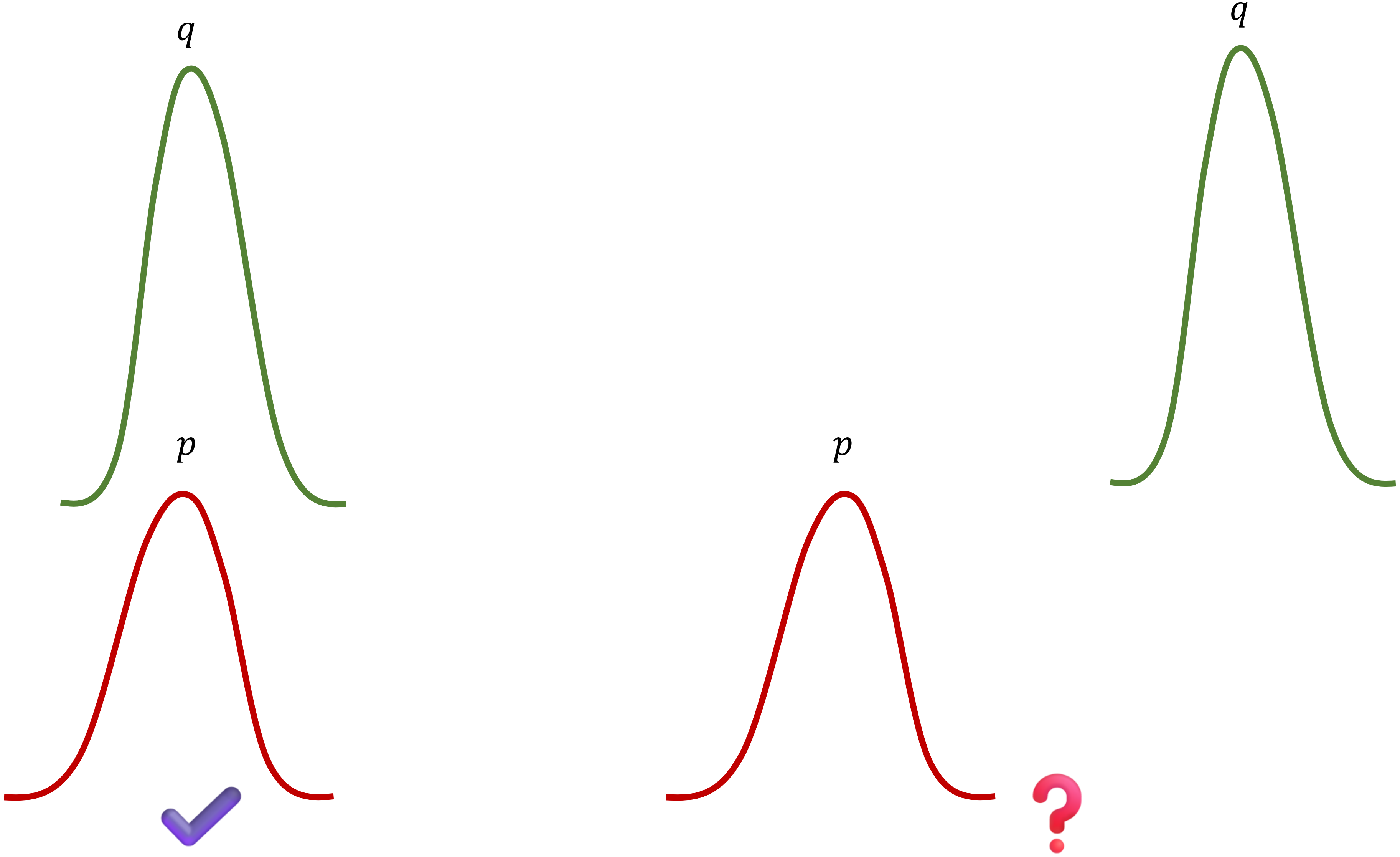

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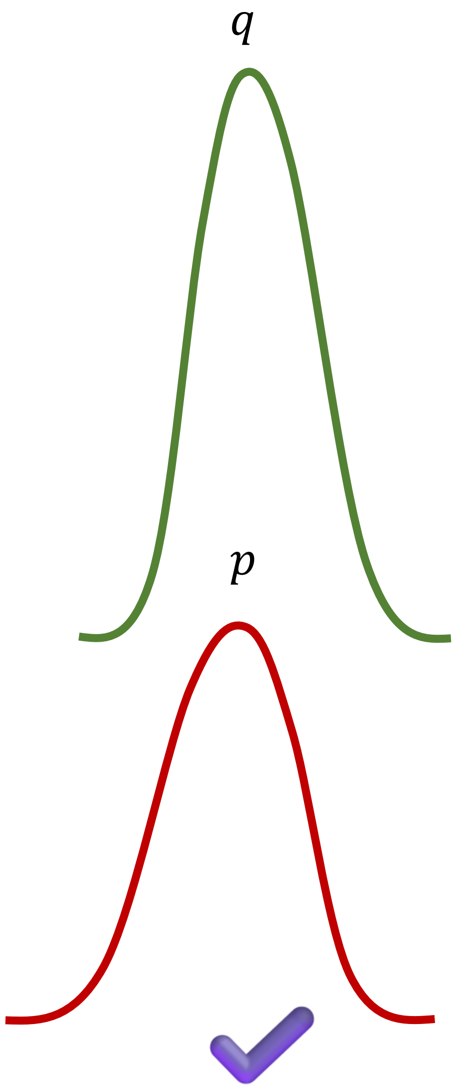

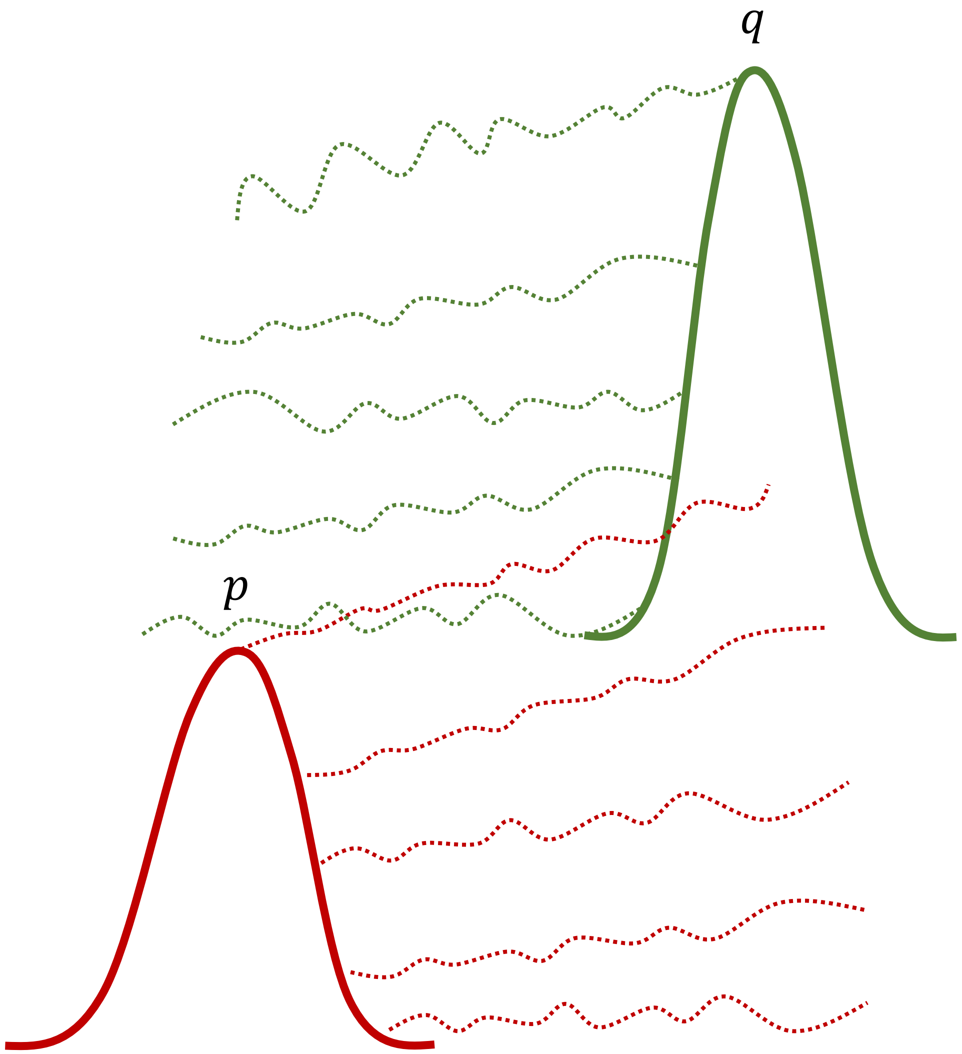

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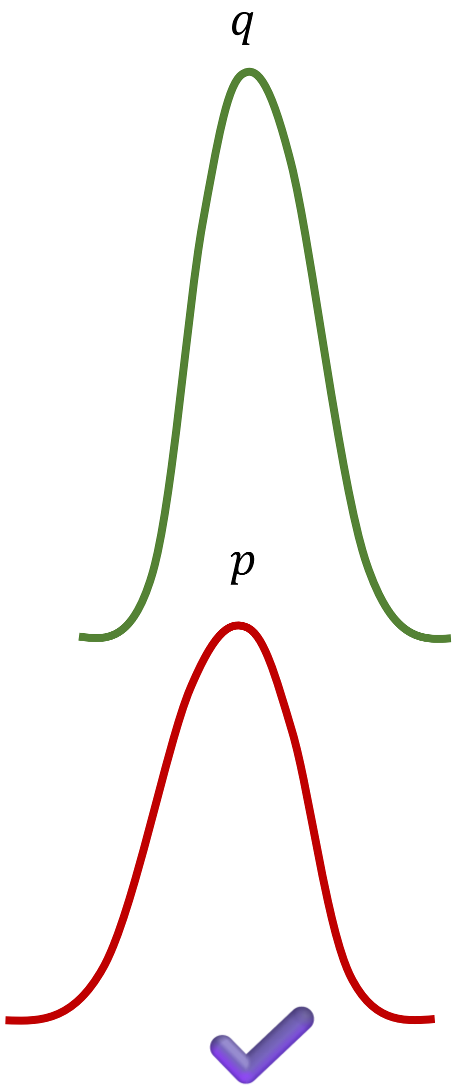

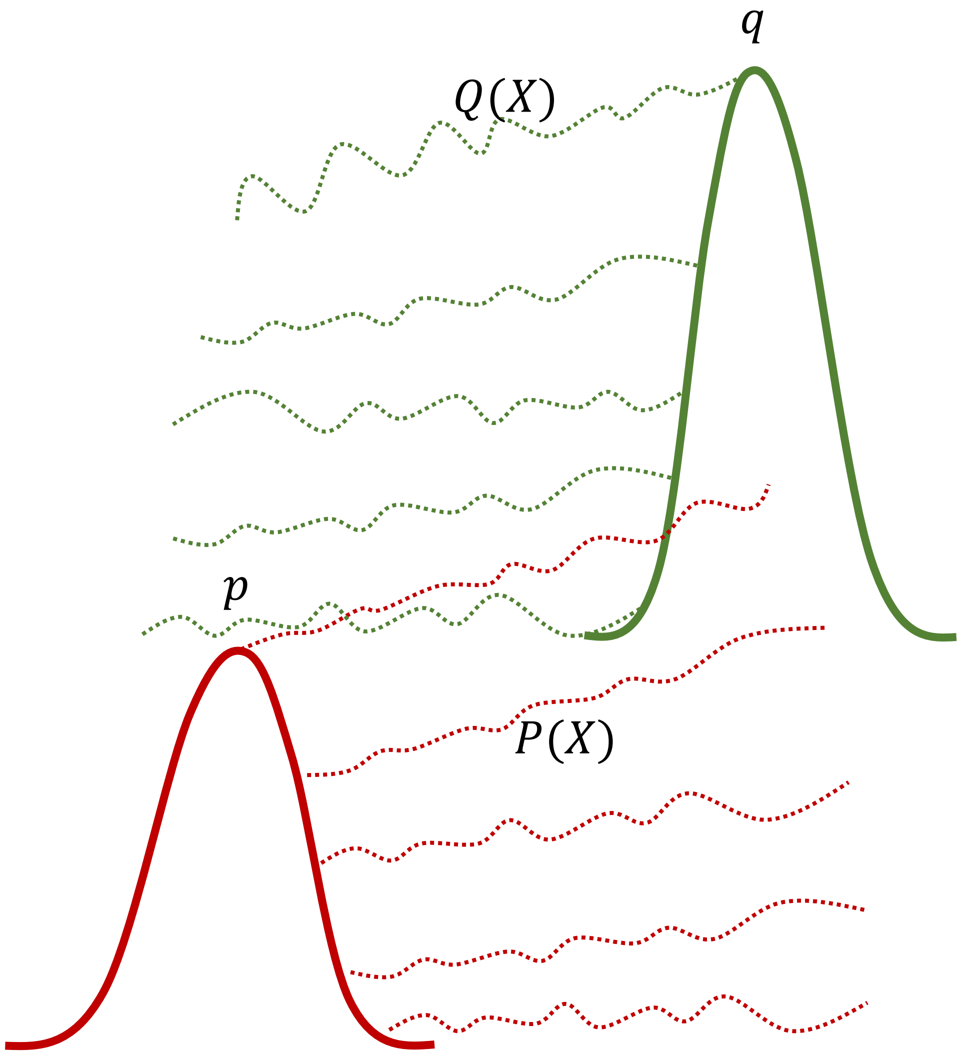

From Density Ratio to Path RND

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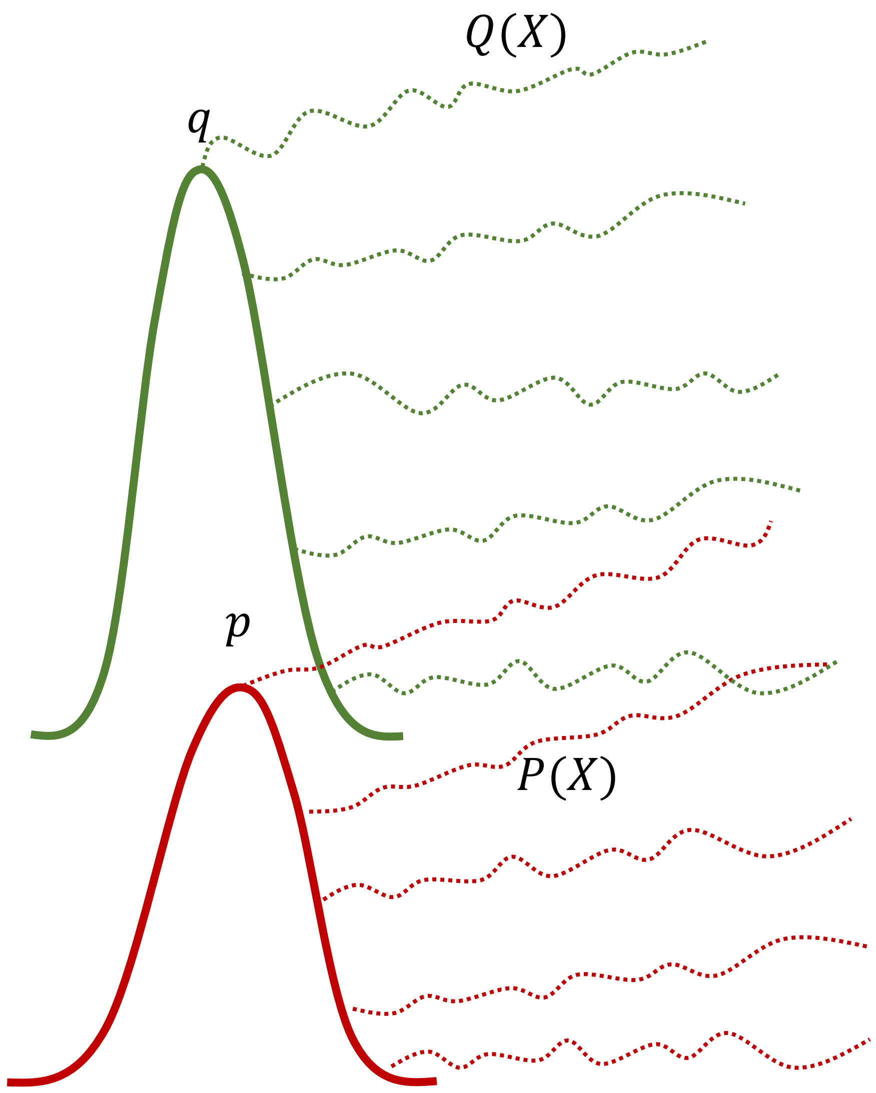
Path measure 1: P
Path measure 2: Q

"Density" ratio: $\frac{\mathrm{d}P}{\mathrm{d}Q}(x)$

Forward-forward RND (FF-RND) and Girsanov

$P: \mathrm{d}X_t = f(X_t, t)\mathrm{d}t + \sigma_t \mathrm{d}W_t, X_0 \sim p_0 = p$
$Q: \mathrm{d}X_t = g(X_t, t)\mathrm{d}t + \sigma_t \mathrm{d}W_t, X_0 \sim q_0 = q$



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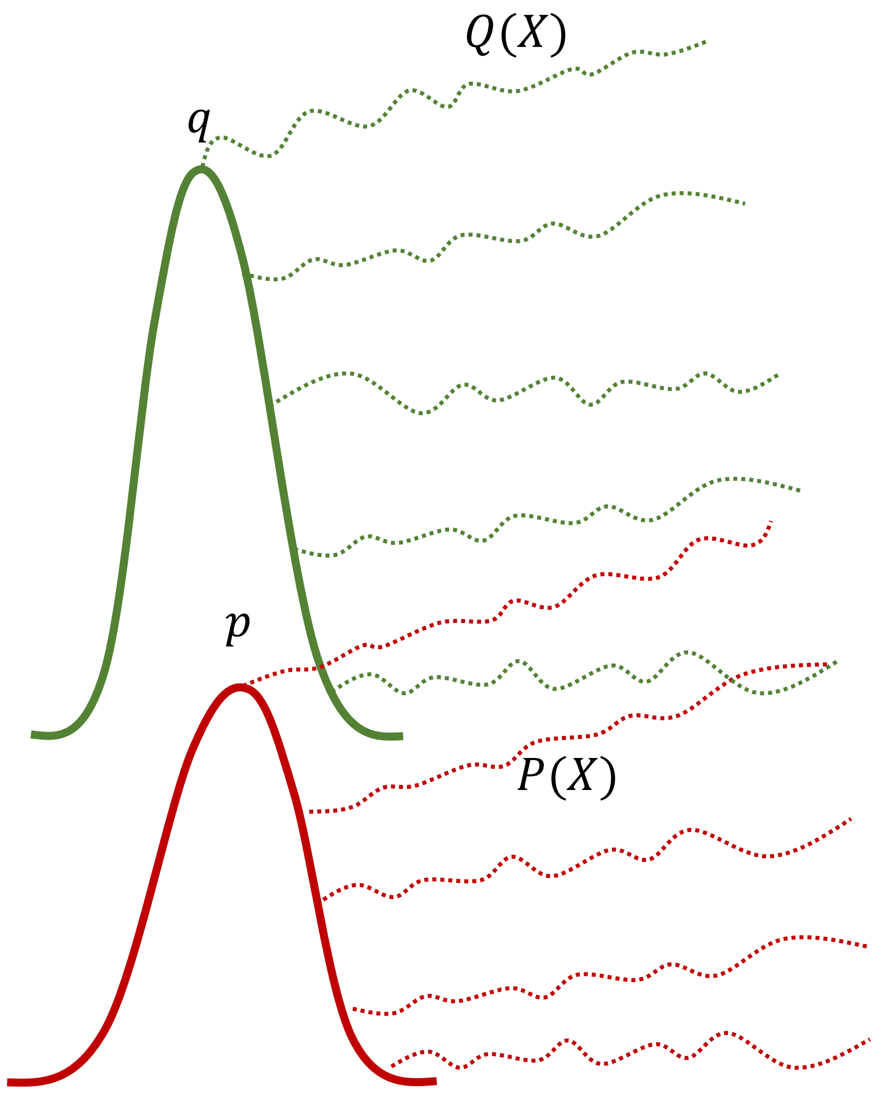
$$\frac{\mathrm{d}P}{\mathrm{d}Q}(X) = \lim \frac{p(X_0) \prod N_1(X_{n+1} | X_n)}{q(X_0) \prod N_2(X_{n+1} | X_n)}$$

Initial density ratio

Transition kernel ratio



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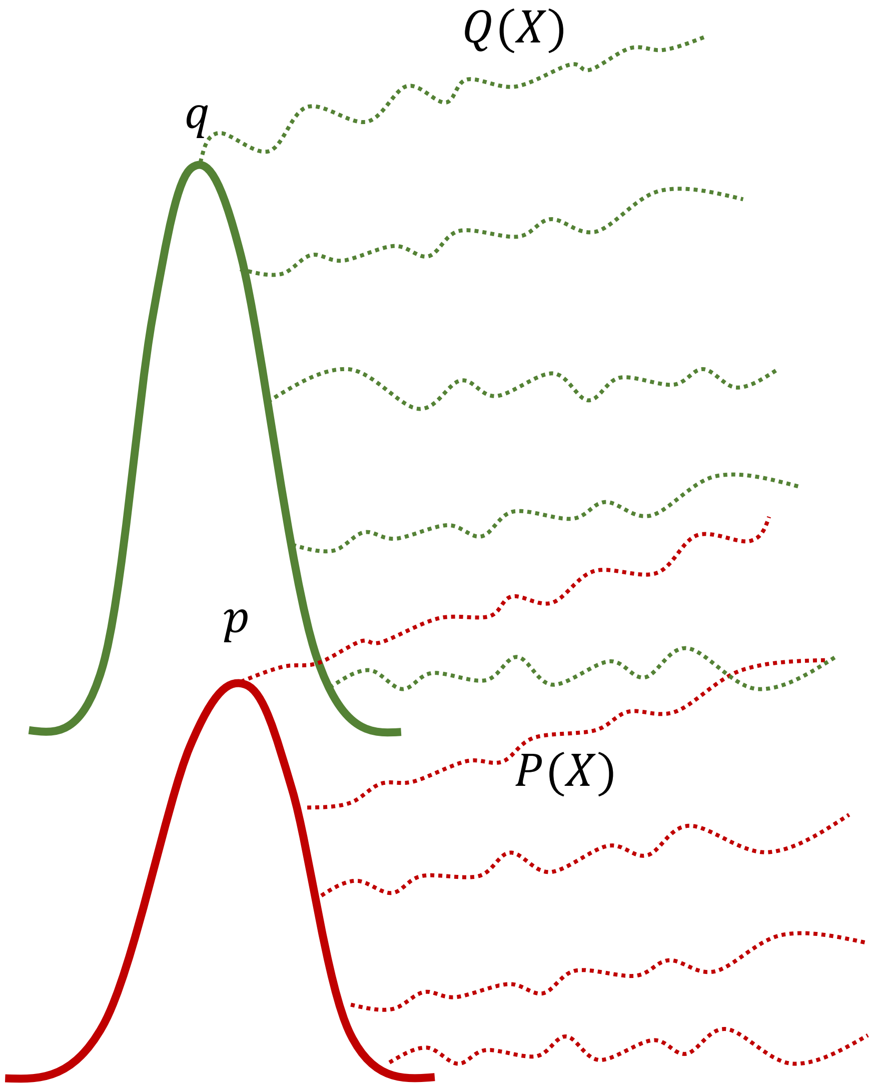

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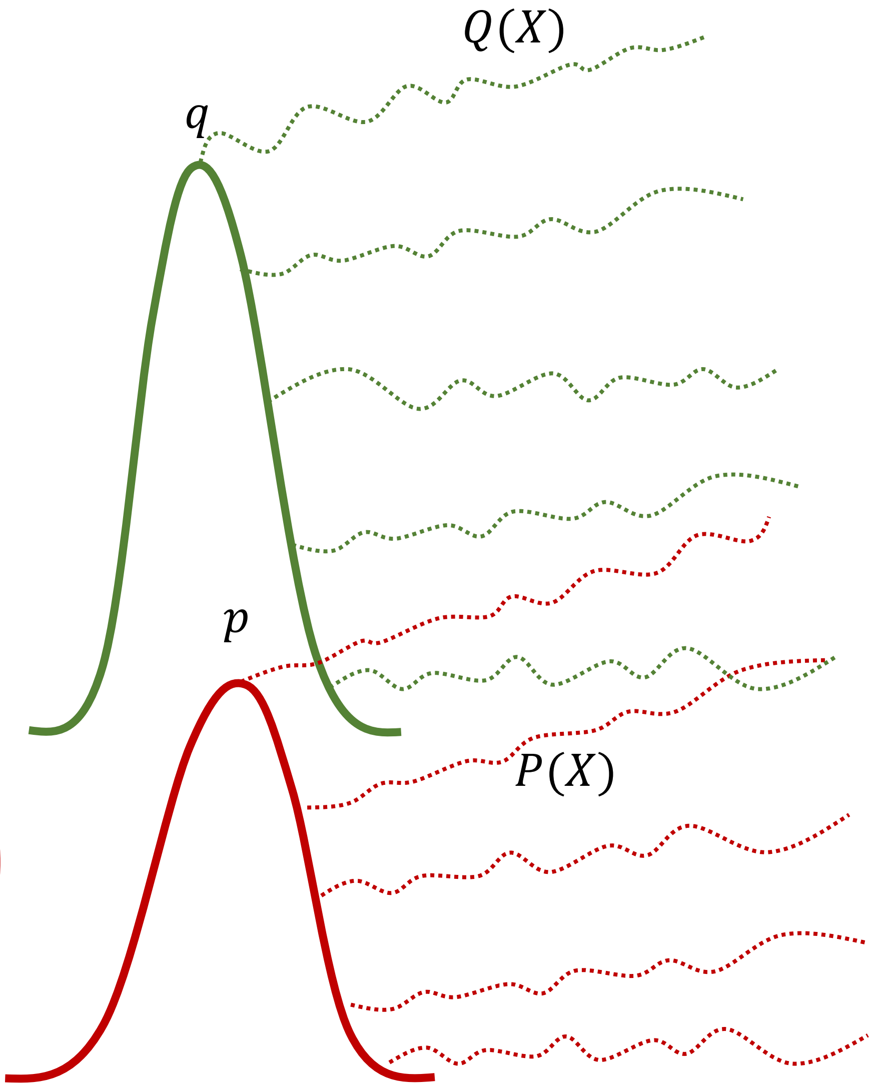
$$\frac{\mathrm{d}P}{\mathrm{d}Q}(X) = \lim \underbrace{\frac{p(X_0)}{q(X_0)}}_{\text{Initial density ratio}} \underbrace{\frac{\prod N_1(X_{n+1}|X_n)}{\prod N_2(X_{n+1}|X_n)}}_{\text{Transition kernel ratio}}$$

Initial density ratio

Transition kernel ratio

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

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



Forward-forward RND (FF-RND) and Girsanov

Unnormalised density?

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Initial density ratio

Transition kernel ratio

$$= \frac{p(X_0)}{q(X_0)} \exp\left(\int \frac{f_t(X_t)}{\sigma_t^2}\cdot \mathrm{d}X_t - \frac{f_t^2(X_t)}{2\sigma_t^2}\mathrm{d}t - \int \frac{g_t(X_t)}{\sigma_t^2}\cdot \mathrm{d}X_t + \frac{g_t^2(X_t)}{2\sigma_t^2}\mathrm{d}t\right)$$

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Initial density ratio

Transition kernel ratio

$$= \frac{p(X_0)}{q(X_0)} \exp\left(\int \frac{f_t(X_t)}{\sigma_t^2}\cdot \mathrm{d}X_t - \frac{f_t^2(X_t)}{2\sigma_t^2}\mathrm{d}t - \int \frac{g_t(X_t)}{\sigma_t^2}\cdot \mathrm{d}X_t + \frac{g_t^2(X_t)}{2\sigma_t^2}\mathrm{d}t\right)$$

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

Forward-forward RND (FF-RND) and Girsanov

Unnormalised density?

$$P:\ \mathrm{d}X_t = f(X_t,t)\mathrm{d}t + \sigma_t \mathrm{d}W_t, X_0 \sim \tilde{p}_0 = \tilde{p}$$
$$Q:\ \mathrm{d}X_t = g(X_t,t)\mathrm{d}t + \sigma_t \mathrm{d}W_t, X_0 \sim \tilde{q}_0 = \tilde{q}$$

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

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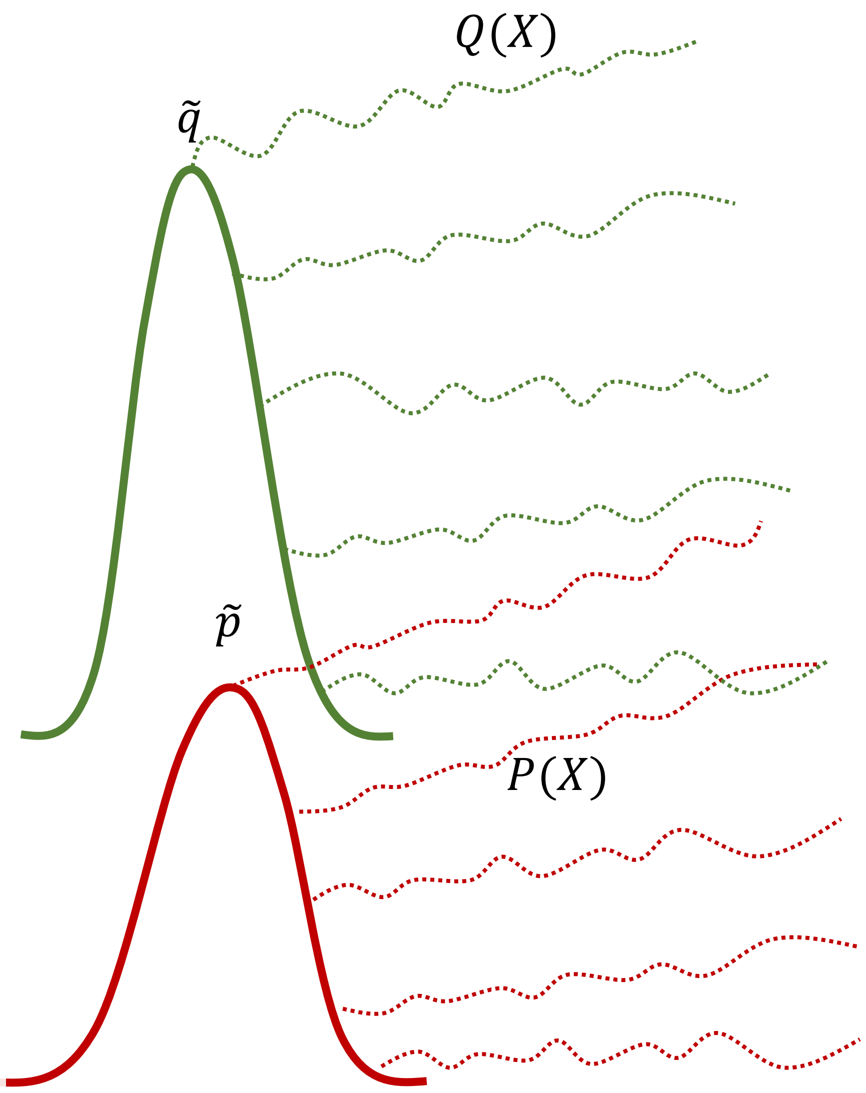

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$$w(X) = \frac{Z_p}{Z_q}\frac{\mathrm{d}P}{\mathrm{d}Q}(X) = \lim \frac{\tilde{p}(X_0)\prod N_1(X_{n+1}|X_n)}{\underbrace{\tilde{q}(X_0)}_{\text{Initial density ratio}}\underbrace{\prod N_2(X_{n+1}|X_n)}_{\text{Transition kernel ratio}}}$$

Initial density ratio

Transition kernel ratio

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

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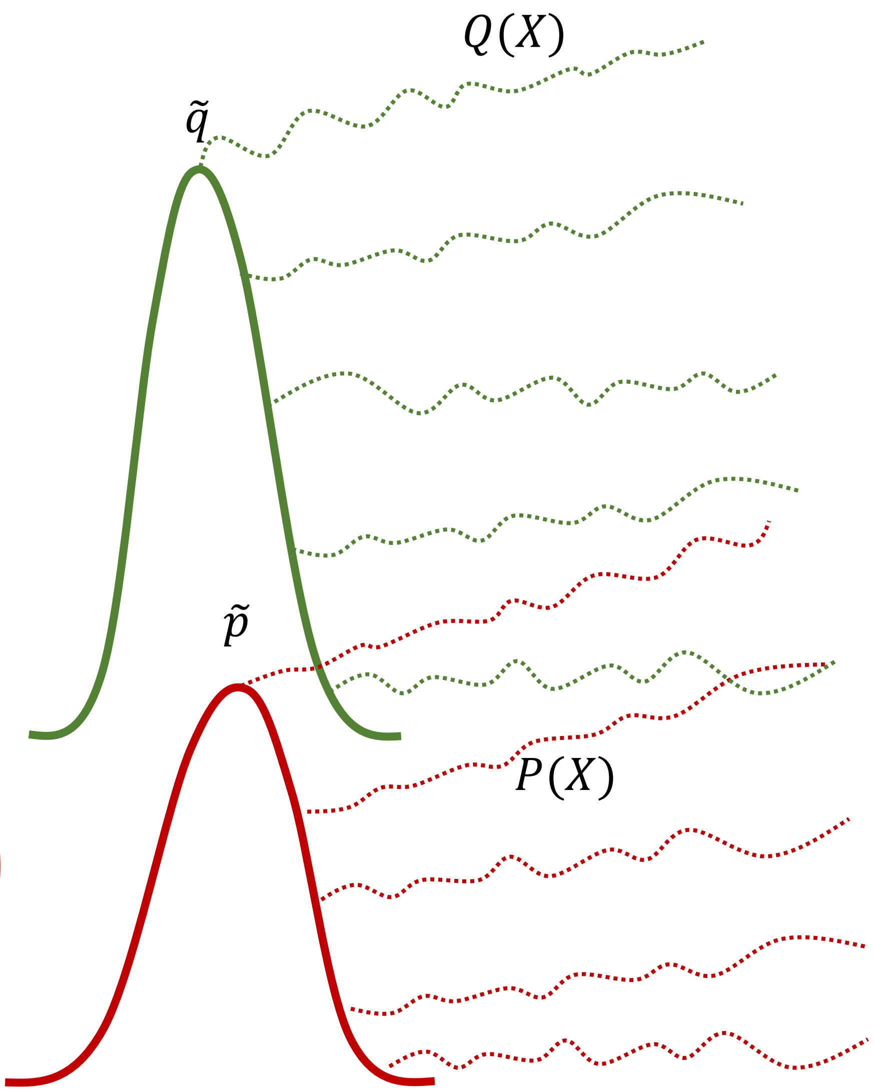

Forward-backward RND (FB-RND)

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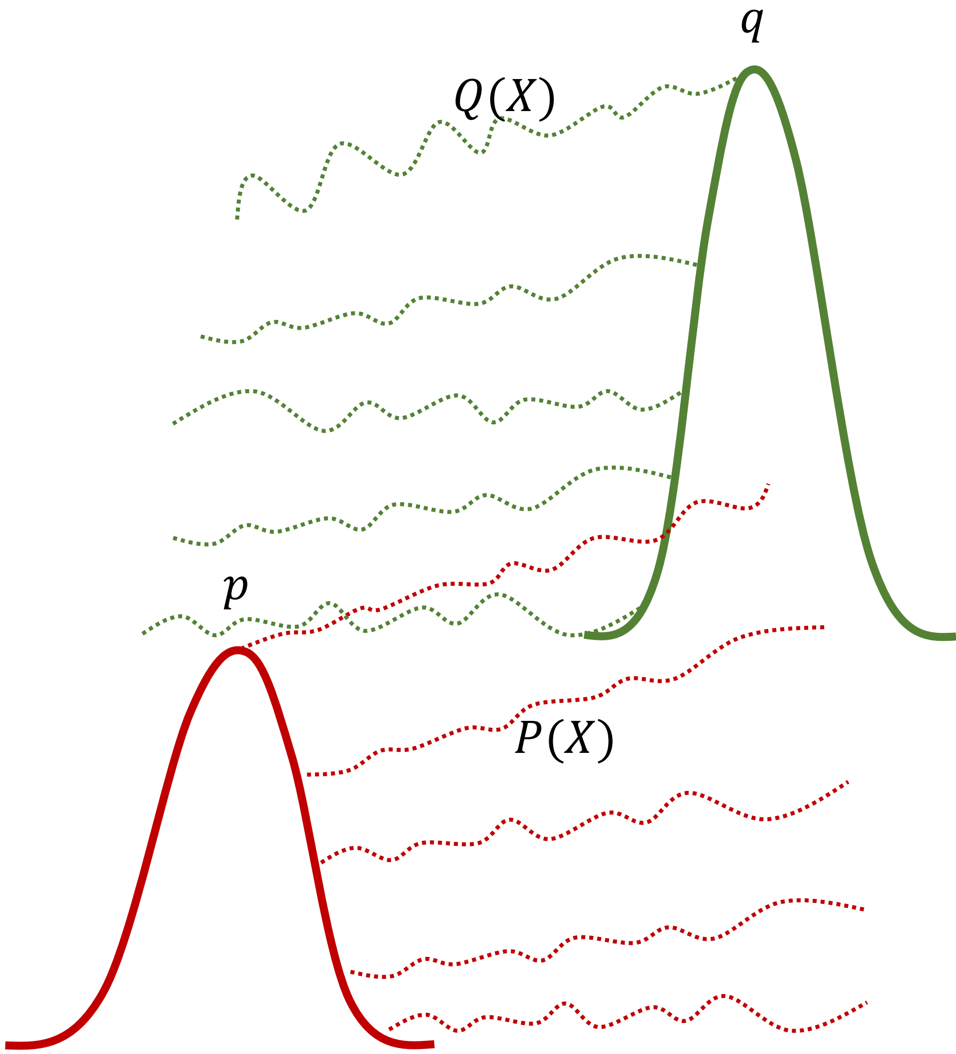

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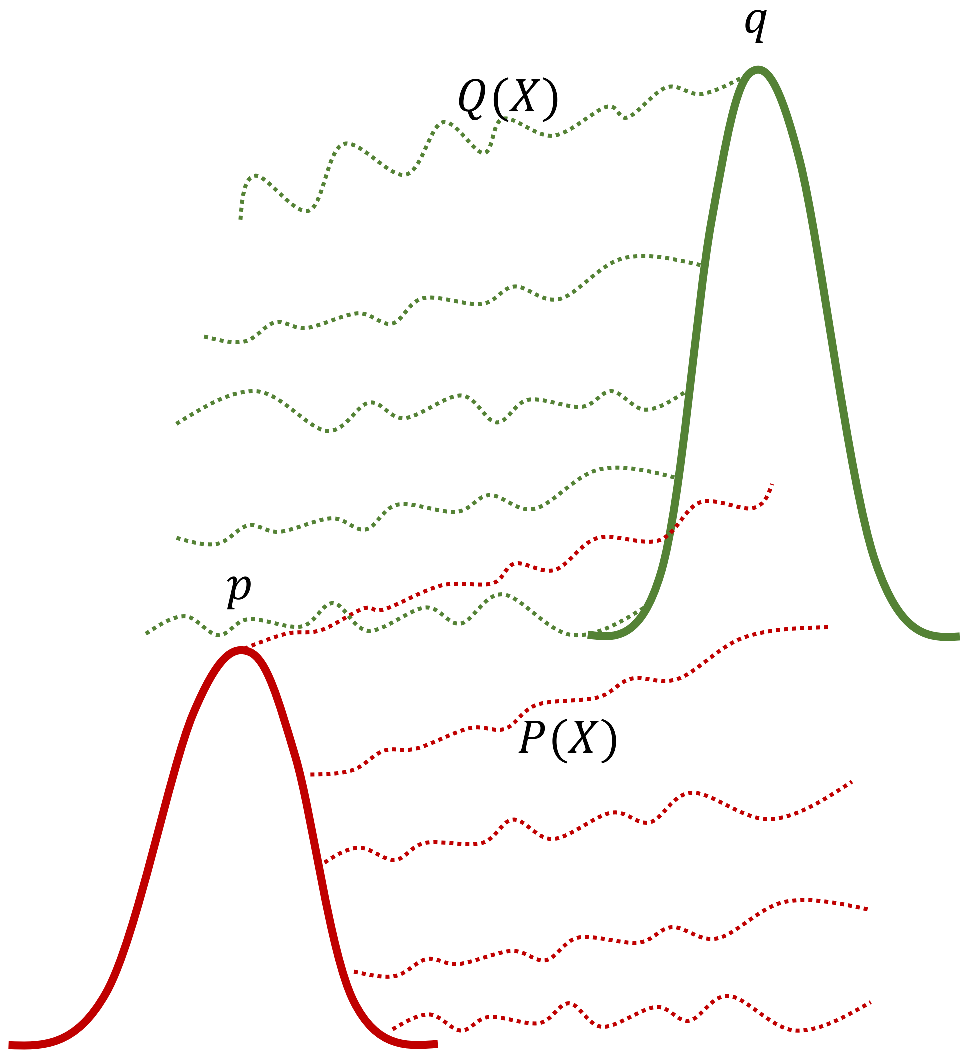
Initial density ratio

Transition kernel ratio



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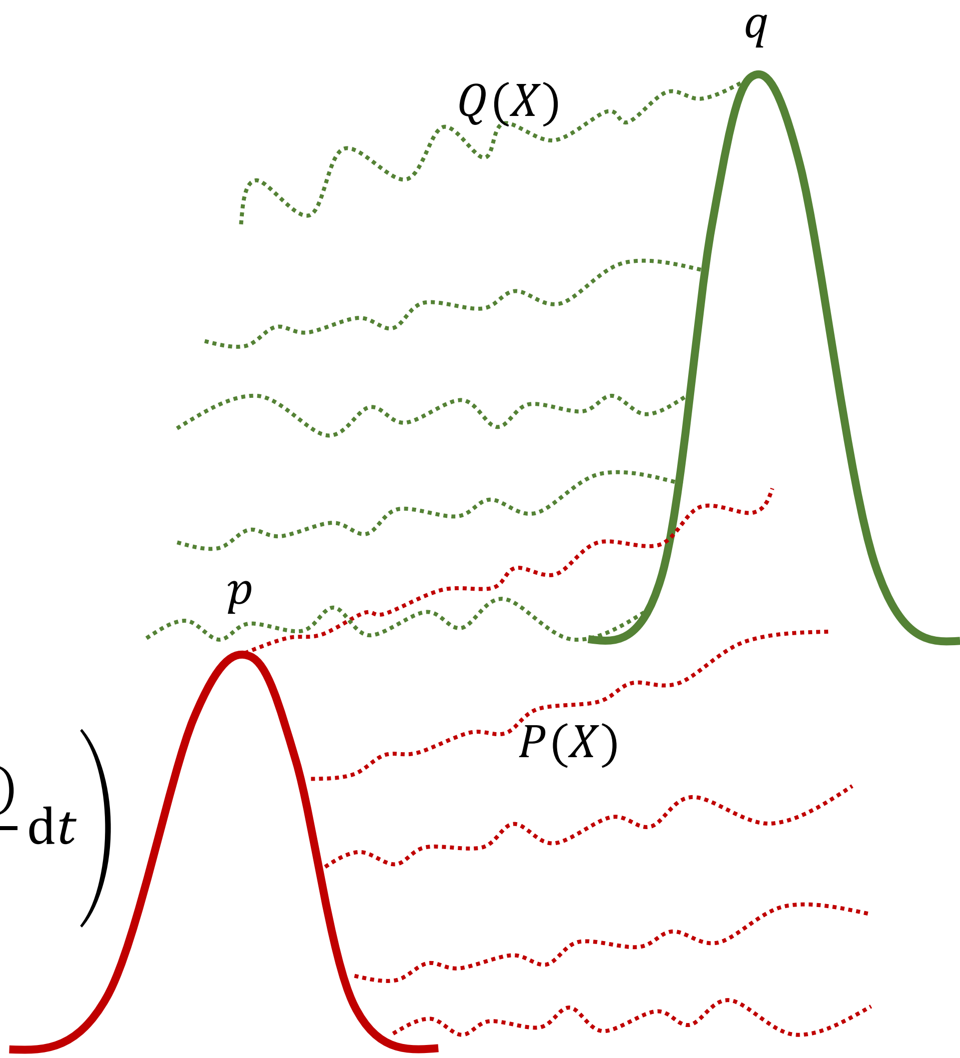
Initial density ratio

Transition kernel ratio

$$= \frac{\tilde{p}_0\,(X_0)}{\tilde{q}_1(X_1)} \exp\left(\int \frac{f_t(X_t)}{\sigma_t^2} \cdot \mathrm{d}X_t - \frac{f_t^2(X_t)}{2\sigma_t^2}\mathrm{d}t - \underbrace{\int \frac{g_t(X_t)}{\sigma_t^2} \cdot \overleftarrow{\mathrm{d}X_t}} + \frac{g_t^2(X_t)}{2\sigma_t^2}\mathrm{d}t \right)$$

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



A Side Note on Stochastic Intergrals

Ito forward integral

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

Ito backward integral

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

Conversion rule:

$$\int a_t(X_t) \cdot \mathrm{d}X_t - \int a_t(X_t) \cdot \overleftarrow{\mathrm{d}X_t} = -\int \sigma_t^2 \nabla \cdot a_t \mathrm{d}t$$

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: $w(X) = \frac{Z_p}{Z_q} \frac{\mathrm{d}P}{\mathrm{d}Q}(X)$

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From Density Ratio to Path RND

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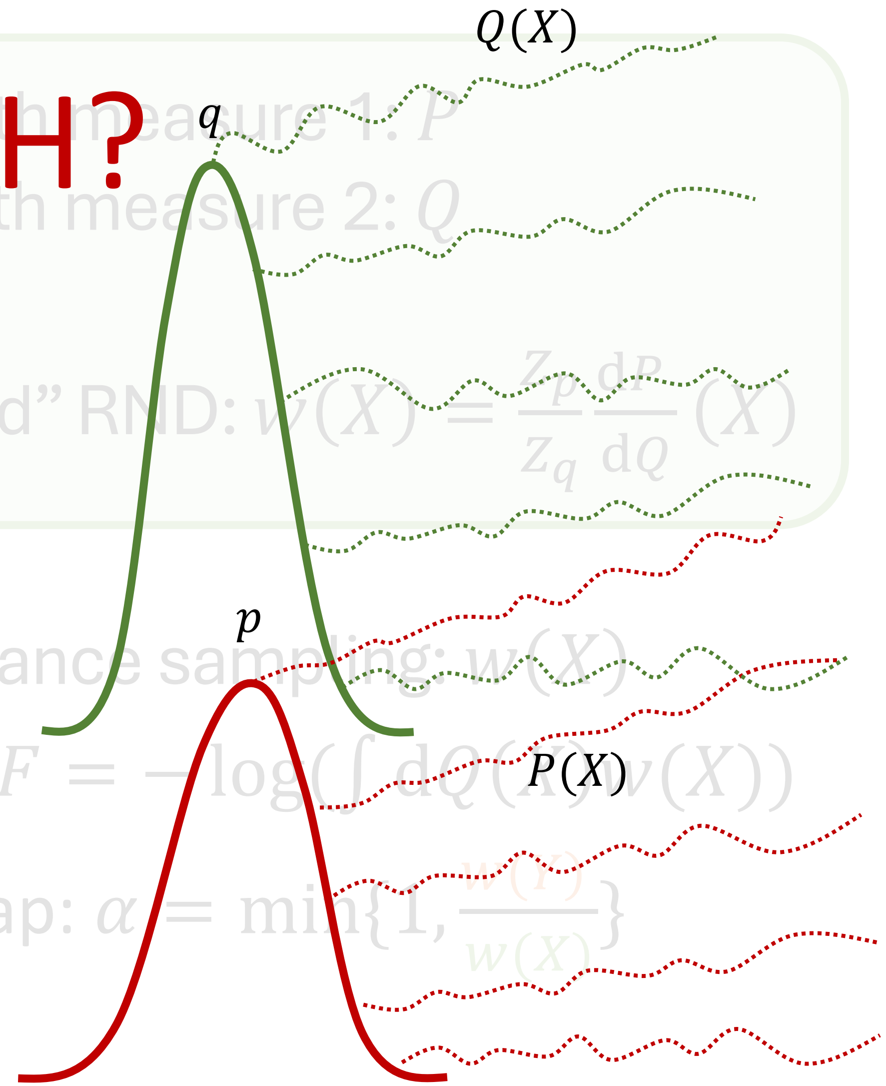

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😳 data processing inequality (DPI) told us

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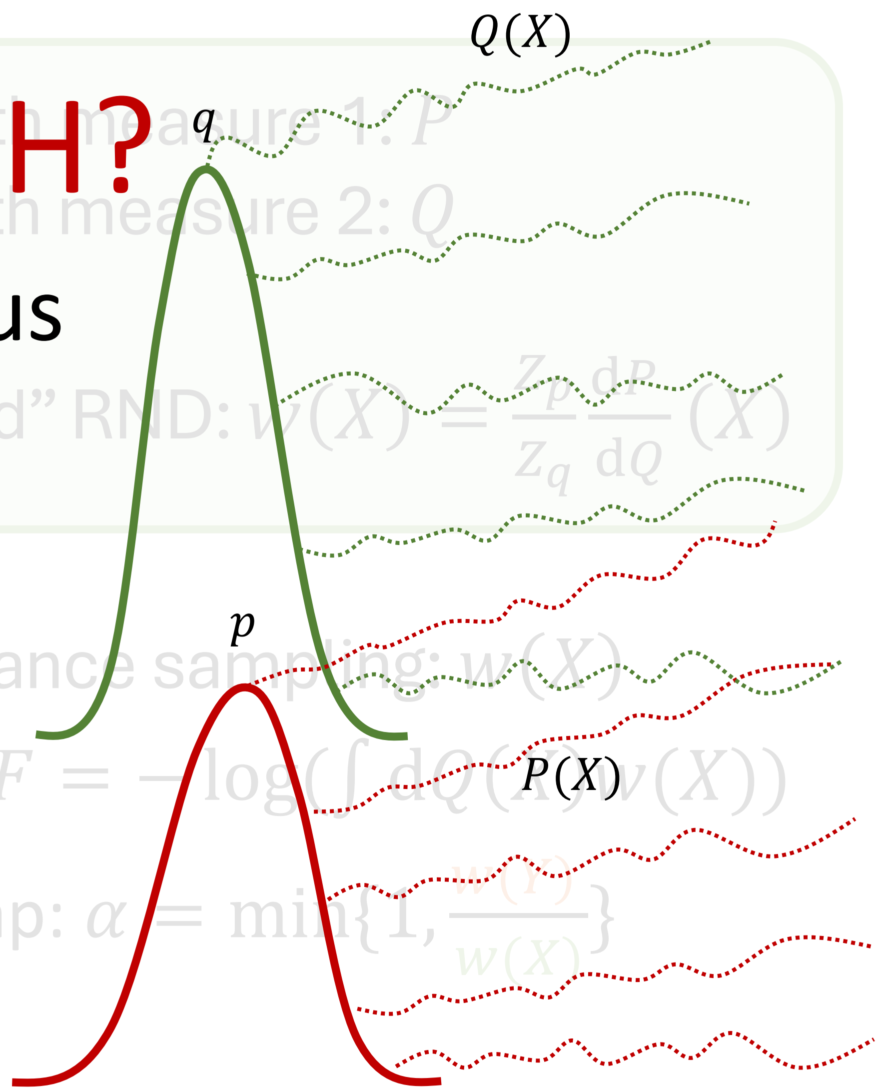

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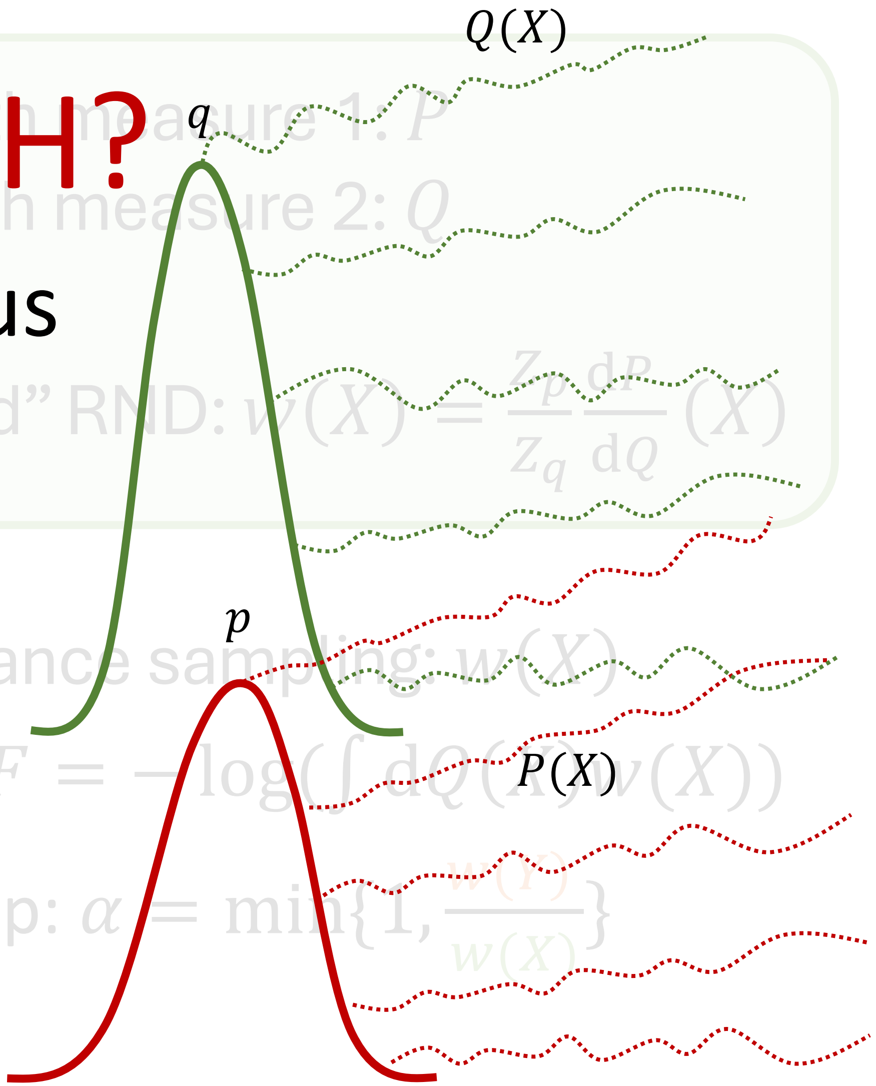
😵 $D_f[q||p] \leq D_f[Q||P]$



From Density Ratio to Path RND

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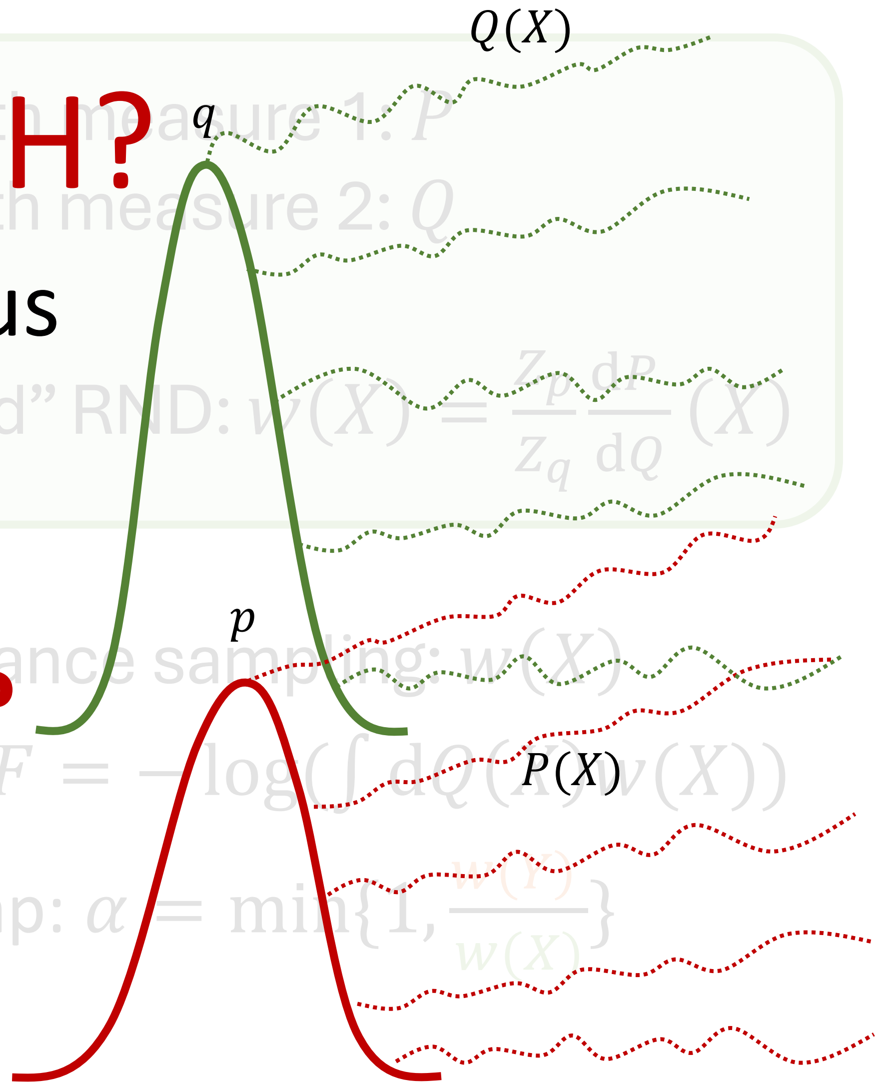
Path weight always has **larger variance?**



From Density Ratio to Path RND

Path weight always has **larger variance?**

Path measure 1: P

Path measure 2: Q

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From Density Ratio to Path RND

Path weight always has **larger variance?**

💡 **Not for FB RND!**

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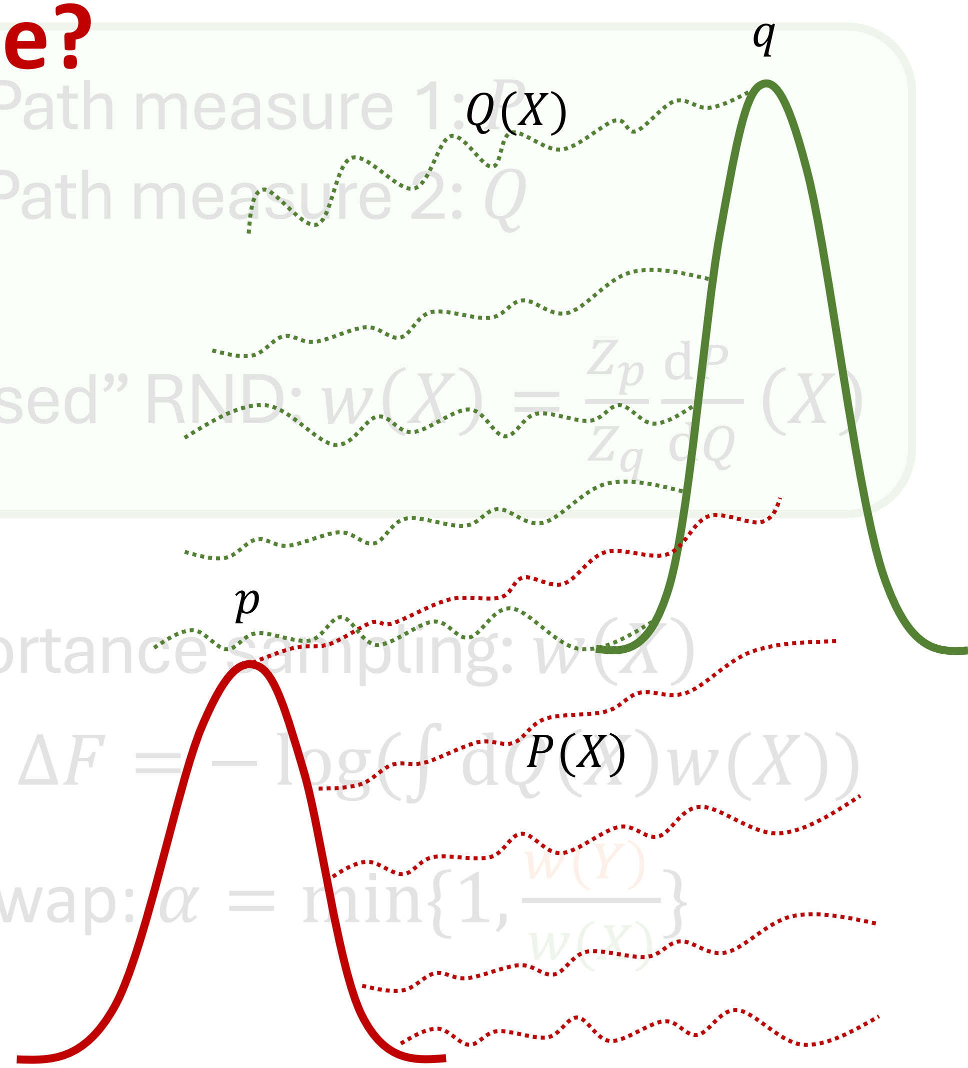

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- Path Importance Sampling: $w(X)$
- Path FEP: $\Delta F = -\log(\int \mathrm{d}Q(X)\,w(X))$
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From Density Ratio to Path RND

Path weight always has **larger variance?**

💡 **Not for FB RND!**

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

The path weight will have 0 variance

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

Path measure 1: P

Path measure 2: Q

“Unnormalised” RND: $w(X) = \frac{Z_p}{Z_q} \frac{\mathrm{d}P}{\mathrm{d}Q}(X)$

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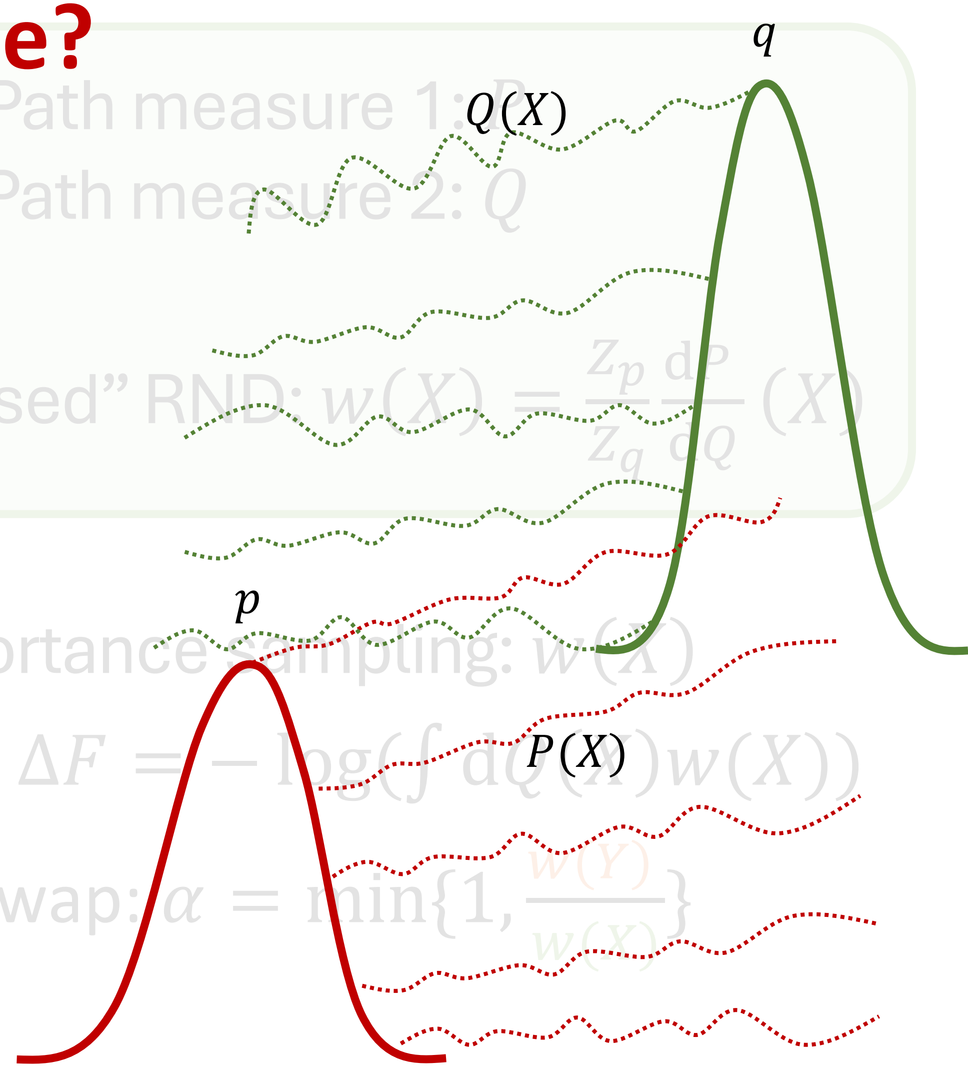

Time-reversal and Nelson's relation

$$P : \ \mathrm{d}X_t = f(X_t, t)\mathrm{d}t + \sigma_t \mathrm{d}W_t, X_0 \sim p_0$$
$$\overleftarrow{Q} : \ \mathrm{d}X_t = g(X_t, t)\mathrm{d}t + \sigma_t \overleftarrow{\mathrm{d}W_t}, X_1 \sim p_1$$

"time-reversal"

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

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: $w(X) = \frac{Z_p}{Z_q} \frac{\mathrm{d}P}{\mathrm{d}Q}(X)$

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- Path FEP: $\Delta F = -\log(\int \mathrm{d}Q(X) w(X))$ → (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

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Path measure 2: Q

"Unnormalised" RND: $w(X) = \frac{Z_p}{Z_q}\frac{\mathrm{d}P}{\mathrm{d}Q}(X)$

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: $\Delta F = -\log(\int \mathrm{d}Q(X) w(X))$ → (escorted) Jarzynski/Crooks
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Example: Path RND to Jarzynski Equality

$X_0 \sim q \qquad \mathrm{d}X_t = -\sigma^2 \nabla U_t(X_t)\mathrm{d}t + \sigma\sqrt{2}\,\overrightarrow{\mathrm{d}W_t},$

$X_1 \sim p \qquad \mathrm{d}X_t = \sigma^2 \nabla U_t(X_t)\mathrm{d}t + \sigma\sqrt{2}\,\overleftarrow{\mathrm{d}W_t},$

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$$X_1 \sim p \qquad \mathrm{d}X_t = \sigma^2 \nabla U_t(X_t)\mathrm{d}t + \sigma\sqrt{2}\,\overleftarrow{\mathrm{d}W_t},$$

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

Example: Path RND to Jarzynski Equality

$$X_0 \sim q \qquad \mathrm{d}X_t = -\sigma^2 \nabla U_t(X_t)\mathrm{d}t + \sigma\sqrt{2}\,\overrightarrow{\mathrm{d}W_t},$$

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$$= \frac{p(X_1)}{q(X_0)} \exp\left(\int \frac{\nabla U_t}{2} \cdot \mathrm{d}X_t + \int \frac{\nabla U_t}{2} \cdot \overleftarrow{\mathrm{d}X_t} \right)$$

Example: Path RND to Jarzynski Equality

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

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👉 conversion rule

Example: Path RND to Jarzynski Equality

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

$$= \frac{p(X_1)}{q(X_0)} \exp\left(\int \frac{\nabla U_t}{2} \cdot \mathrm{d}X_t + \int \frac{\nabla U_t}{2} \cdot \overleftarrow{\mathrm{d}X_t} \right)$$

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

👉 conversion rule

Example: Path RND to Jarzynski Equality

$$X_0 \sim q \qquad \mathrm{d}X_t = -\sigma^2 \nabla U_t(X_t)\mathrm{d}t + \sigma\sqrt{2}\,\overrightarrow{\mathrm{d}W_t},$$

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Ito's lemma

$$\mathrm{d}f_t(X_t) = (\partial_t f(X_t) + \sigma_t^2 \Delta f)\mathrm{d}t + \nabla U_t \cdot \mathrm{d}X_t$$

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💡 Crooks Fluctuation Theorem

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$$\mathbf{E}_{\mathbf{Q}}\left[\frac{\overleftarrow{\mathrm{dP}}}{\mathrm{dQ}}\right] = \mathbf{E}_{\mathbf{Q}}\left[\frac{Z_0}{Z_1}\exp\left(\int -\partial_t U_t(X_t)\mathrm{d}t\right)\right] = 1$$

💡 Jarzynski Equation

From Jarzynski to Escorted Jarzynski

$$X_0 \sim q \qquad \mathrm{d}X_t = [-\sigma^2 \nabla U_t(X_t) + u_t(X_t)]\mathrm{d}t + \sigma\sqrt{2}\,\overrightarrow{\mathrm{d}W_t},$$

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💡 Controlled Crooks Fluctuation Theorem

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

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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: $w(X) = \frac{Z_p}{Z_q}\frac{\mathrm{d}P}{\mathrm{d}Q}(X)$

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: $\Delta F = -\log(\int \mathrm{d}Q(X)w(X))$ → (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).

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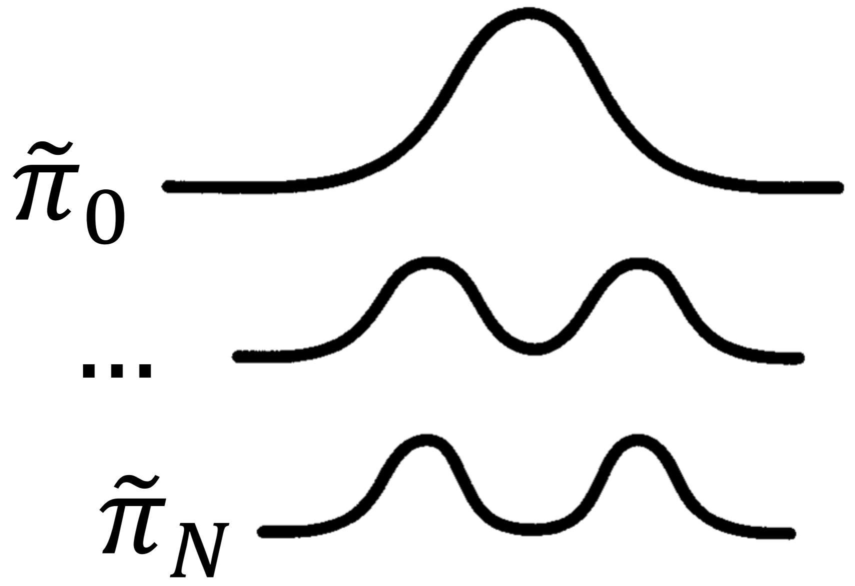
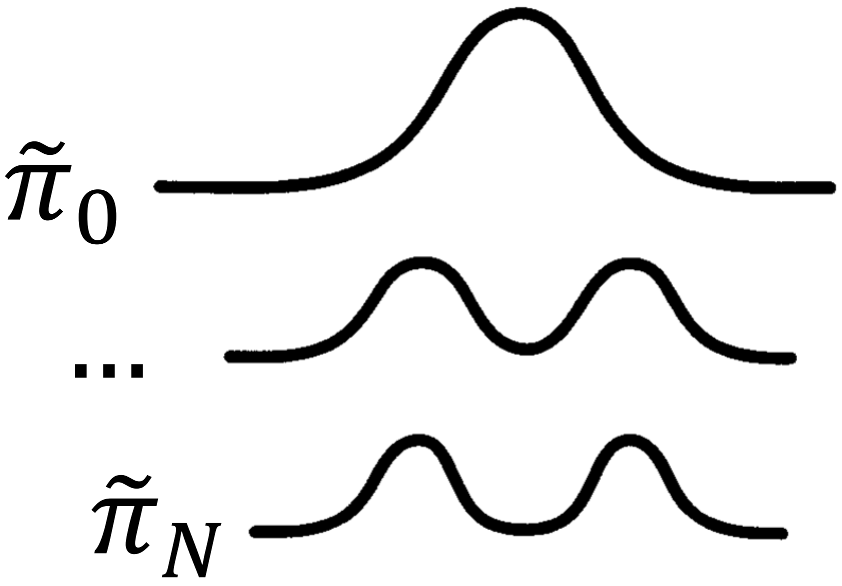
Parallel tempering



- **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 $\tilde{\pi}_0 \times \tilde{\pi}_1 \times \cdots \times \tilde{\pi}_N$

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



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Unchanged!

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

Extend to path!

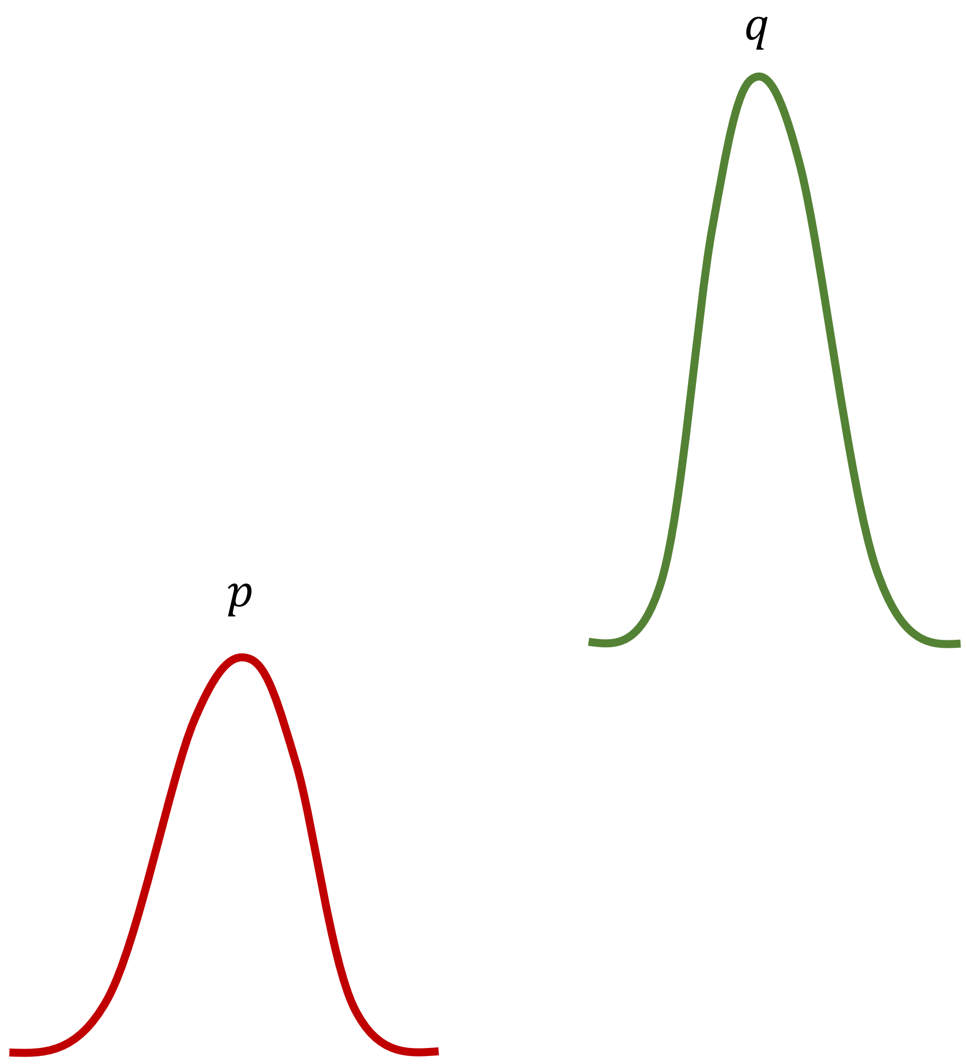
Parallel tempering Swap in Path Space

Path measure 1: P

Path measure 2: Q

"Unnormalised" RND: $w(X) = \frac{Z_p}{Z_q} \frac{\mathrm{d}P}{\mathrm{d}Q}(X)$

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



Parallel tempering Swap in Path Space

Path measure 1: P

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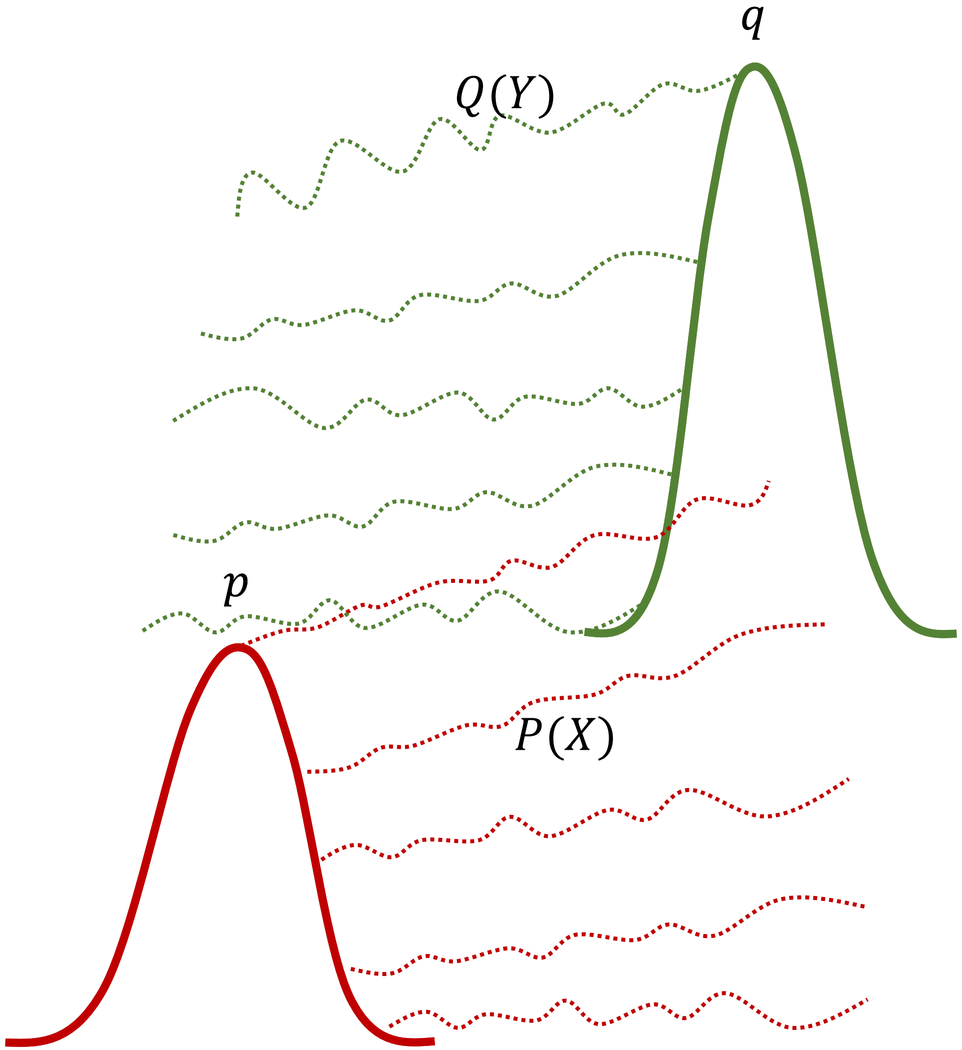
"Unnormalised" RND: $w(X) = \frac{Z_p}{Z_q}\frac{\mathrm{d}P}{\mathrm{d}Q}(X)$

(2) Extend current states with path

$$(X, Y) \sim P(X) \times Q(Y)$$



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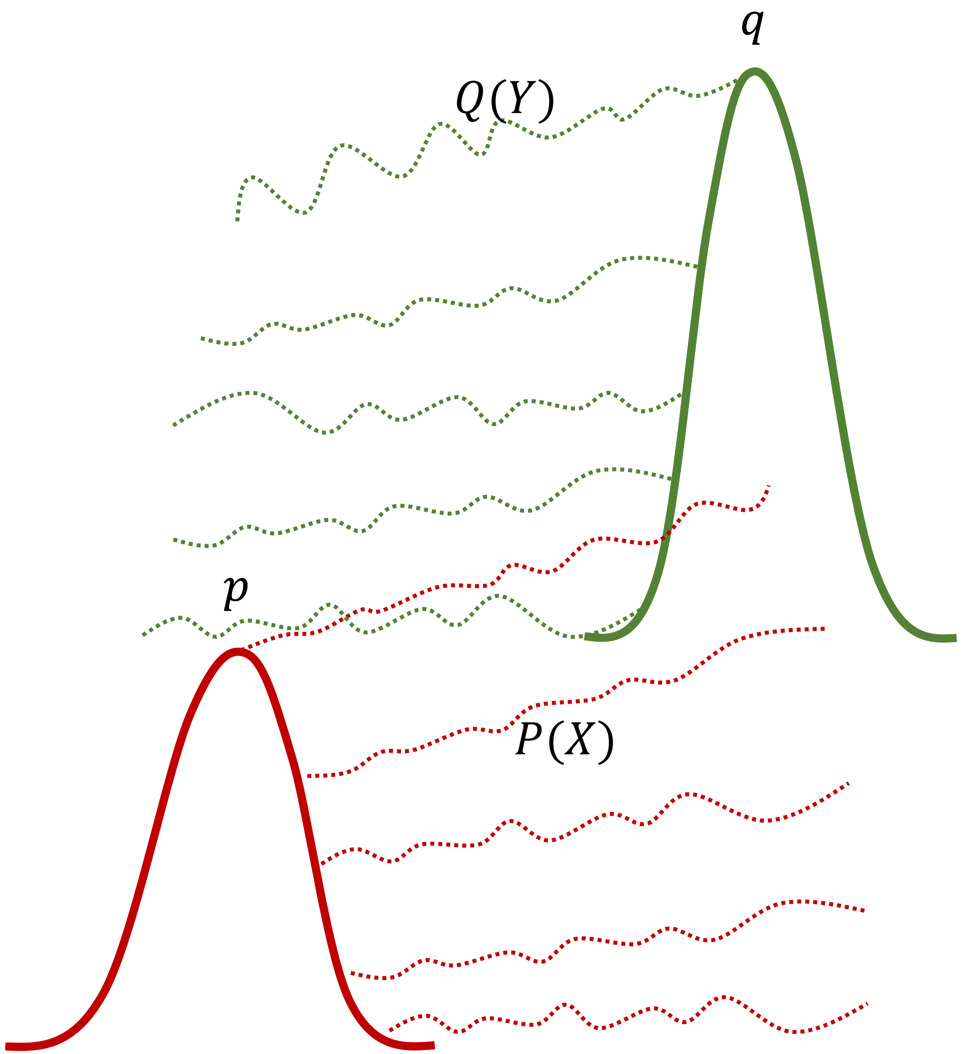
"Unnormalised" RND: $w(X) = \frac{Z_p}{Z_q}\frac{\mathrm{d}P}{\mathrm{d}Q}(X)$

(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
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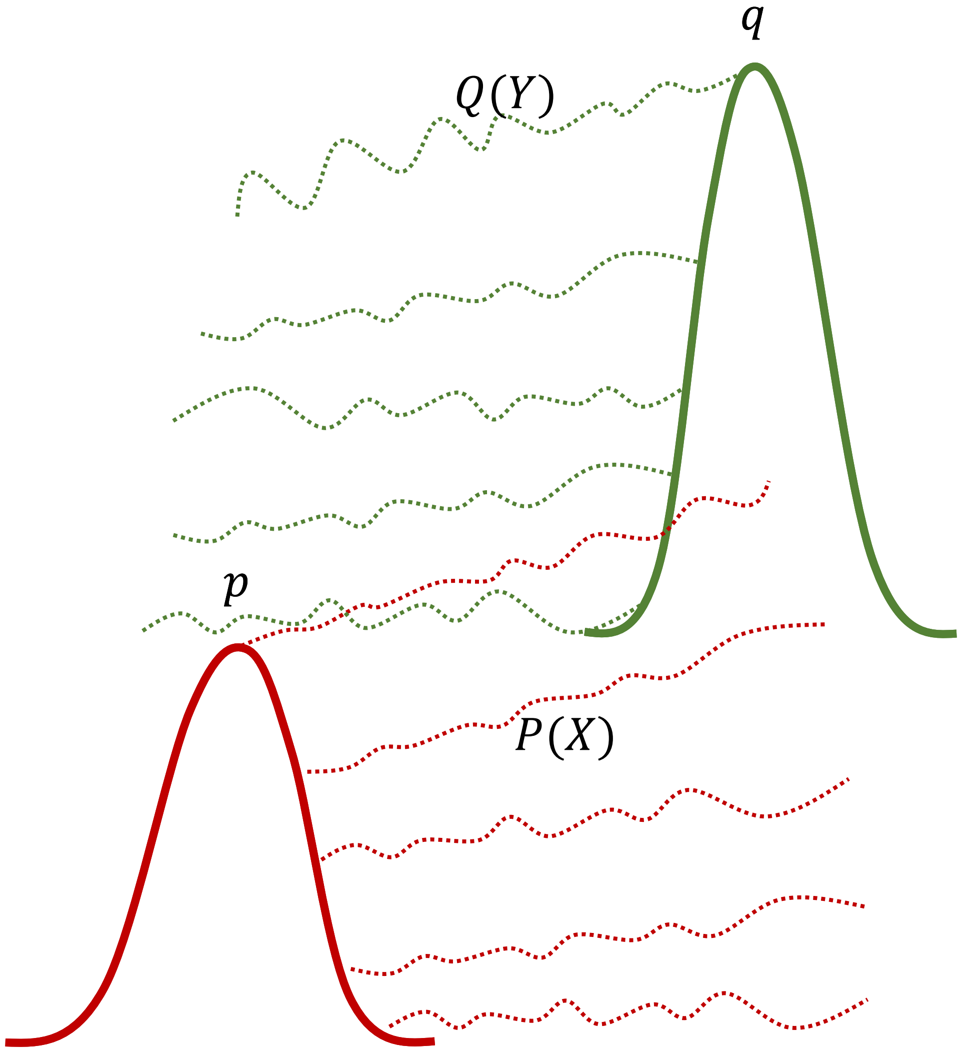
"Unnormalised" RND: $w(X) = \frac{Z_p}{Z_q} \frac{\mathrm{d}P}{\mathrm{d}Q}(X)$

(4) Calculate MH correction

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



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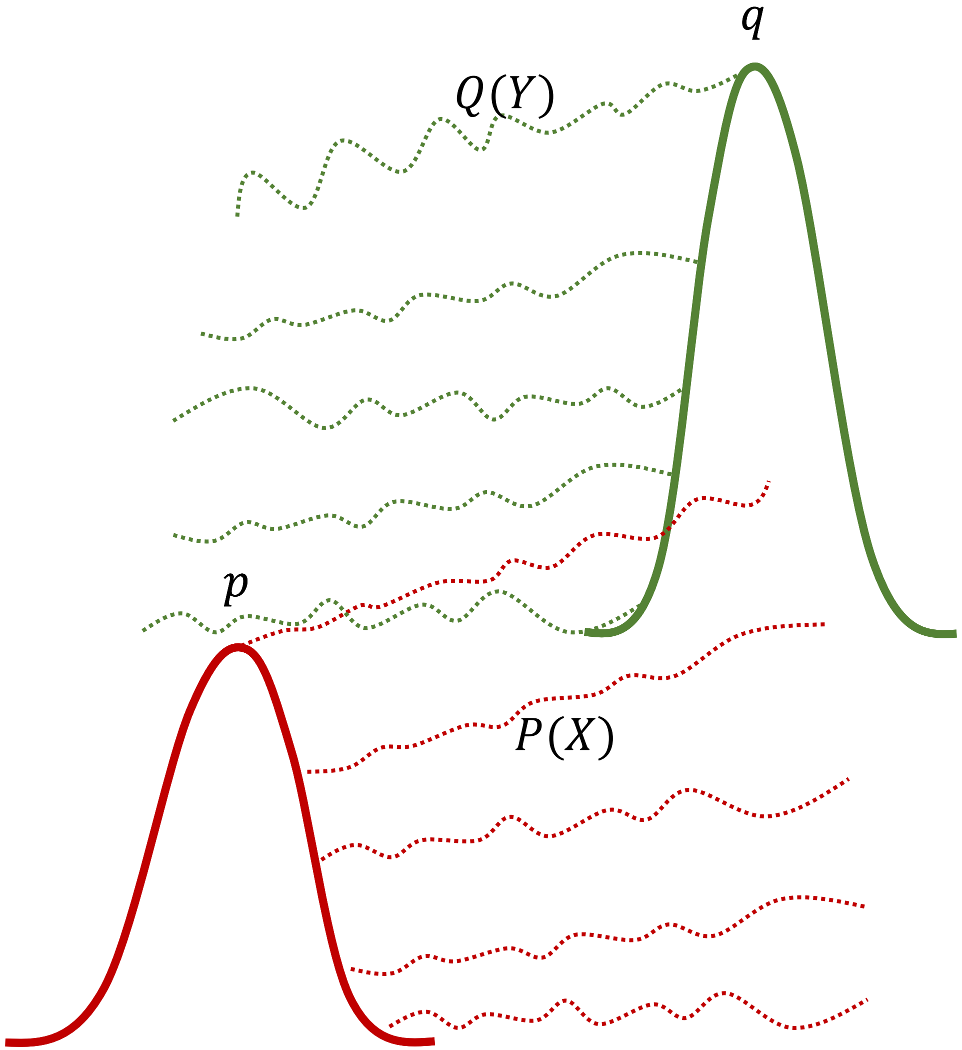

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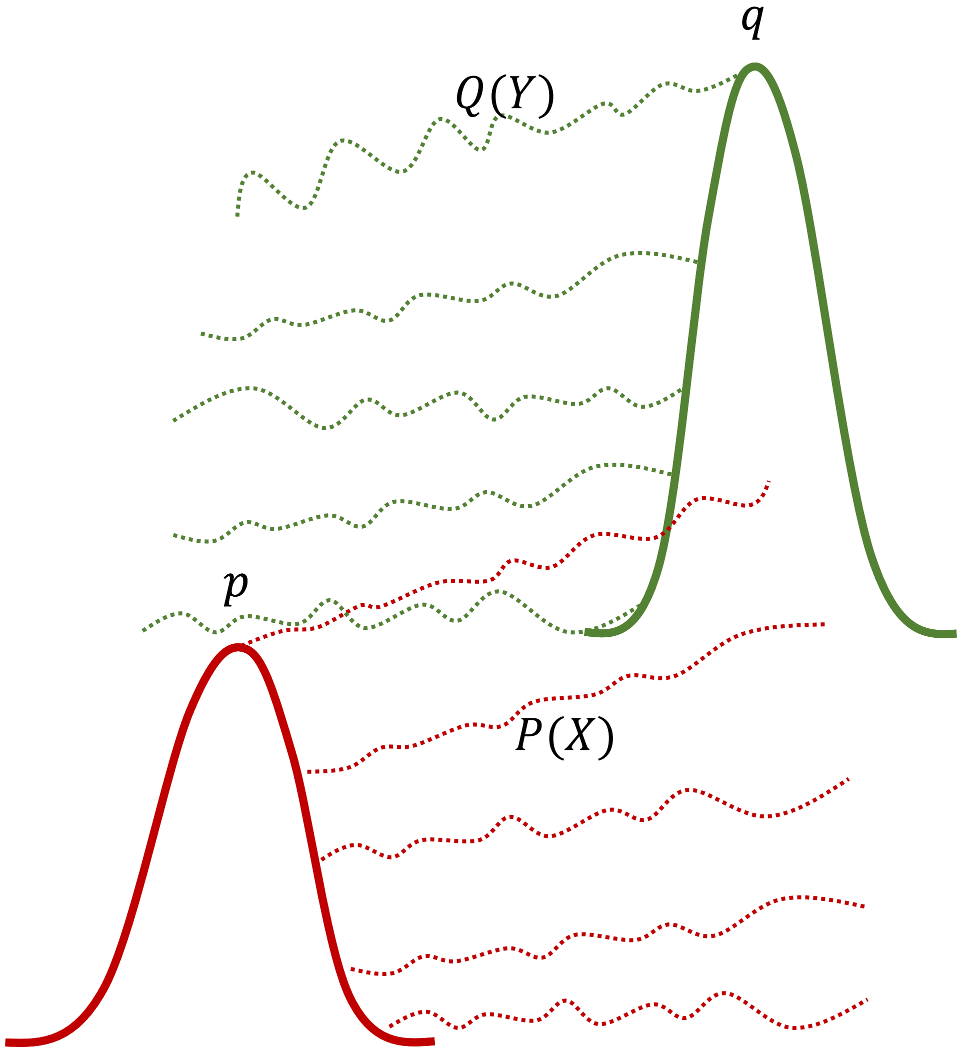

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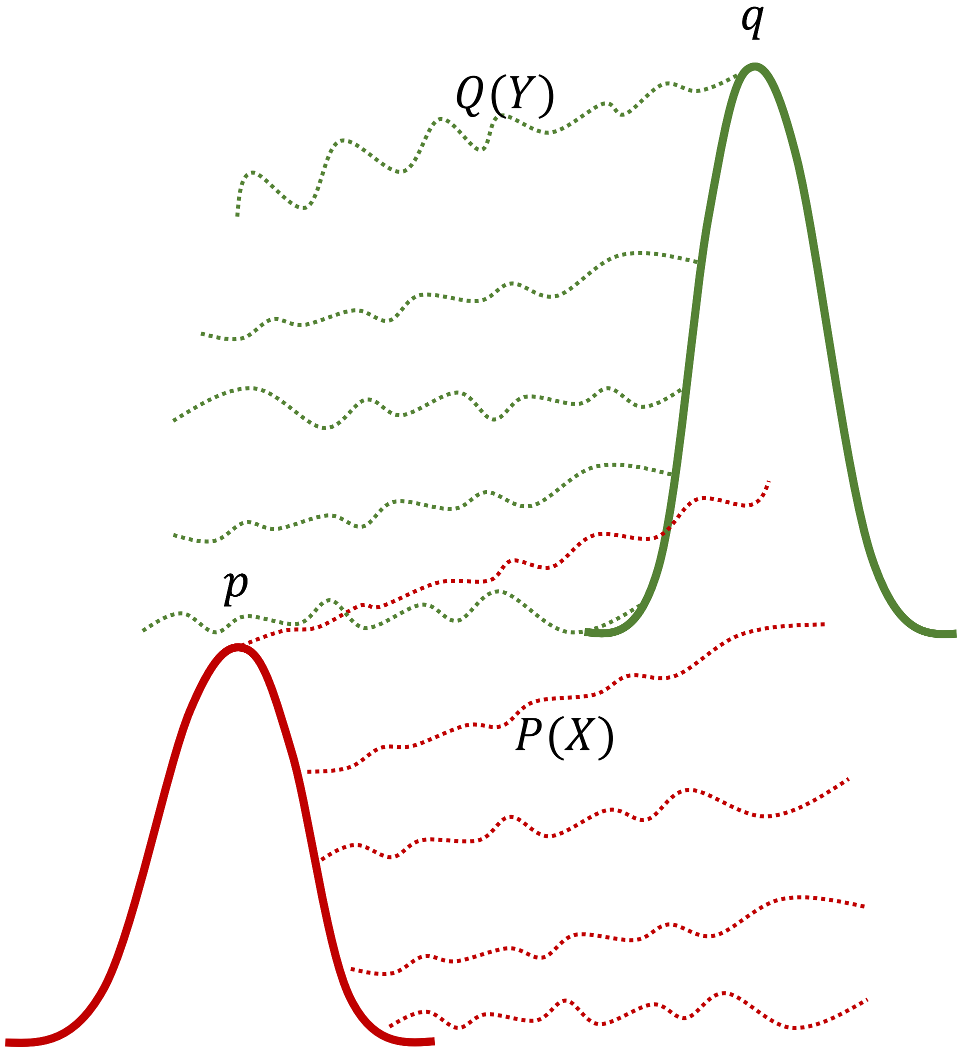

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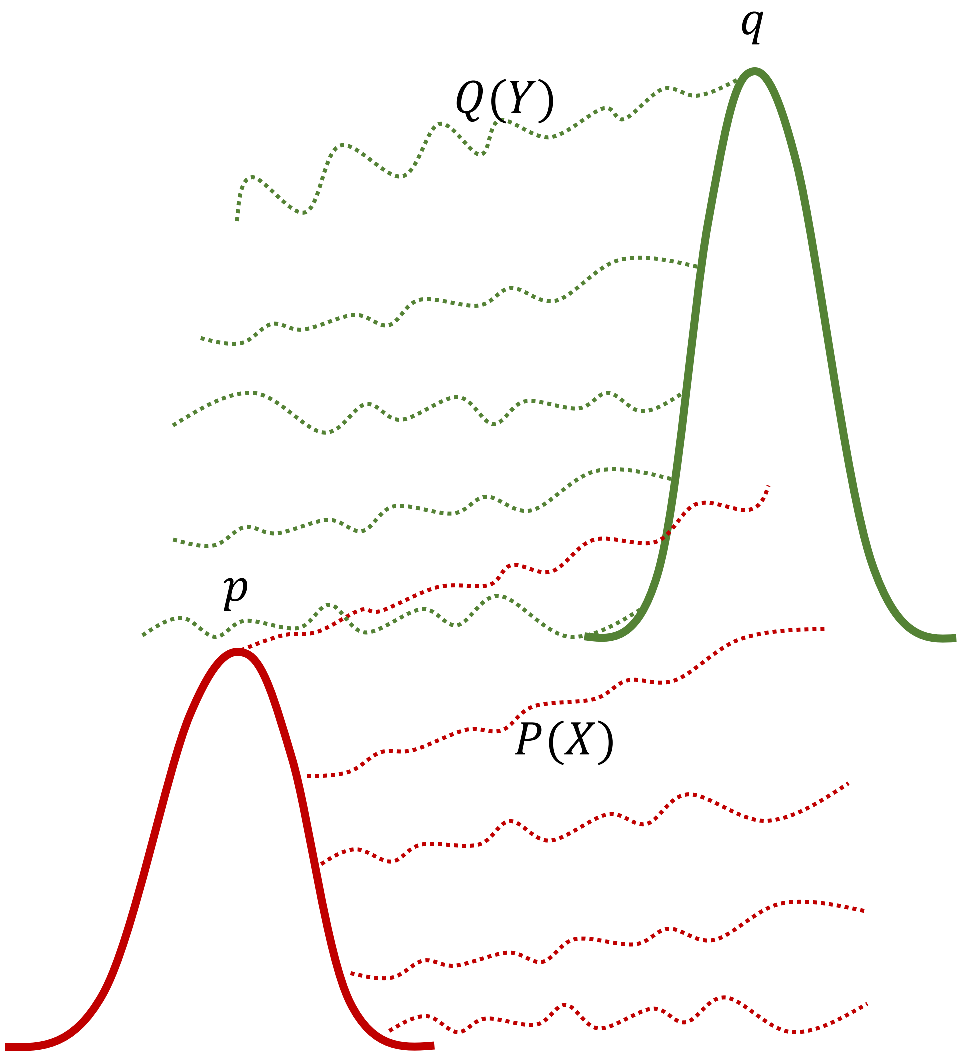
if $P \approx Q, \alpha \approx 1$ 🥳



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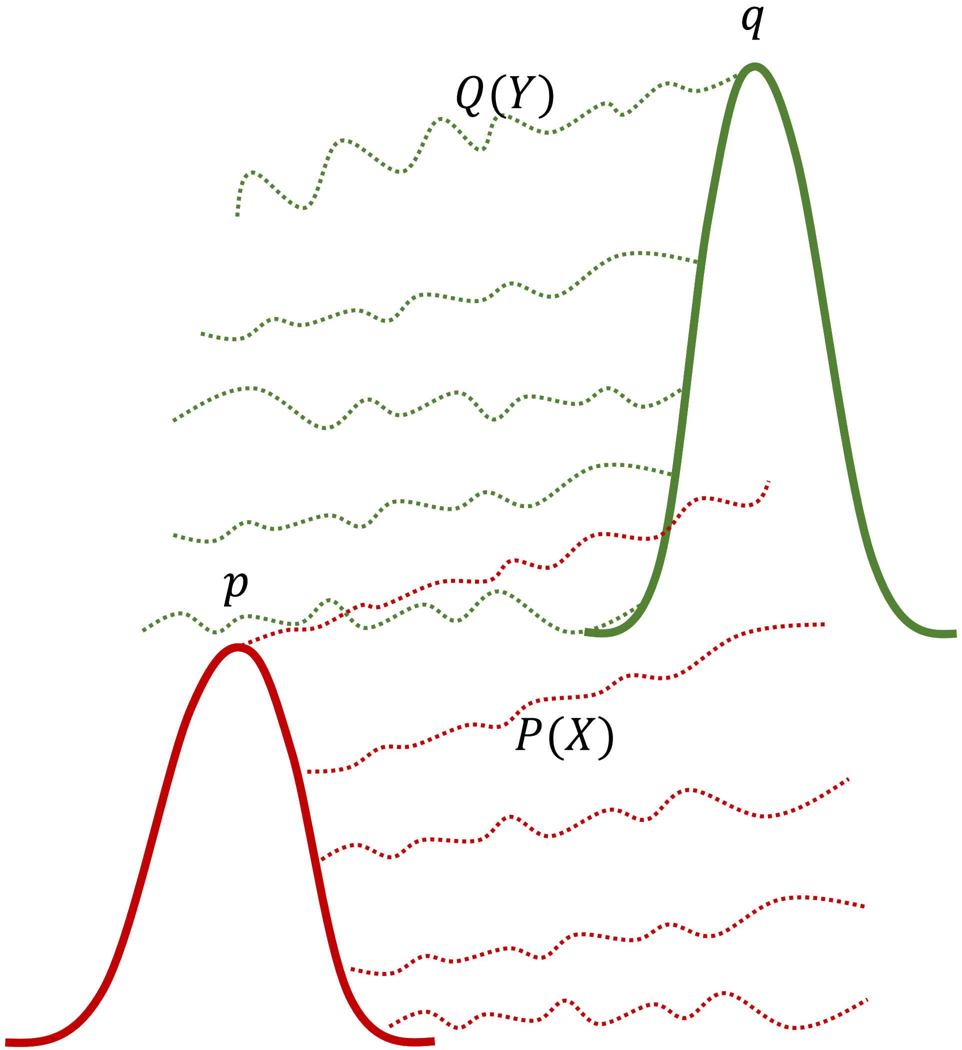

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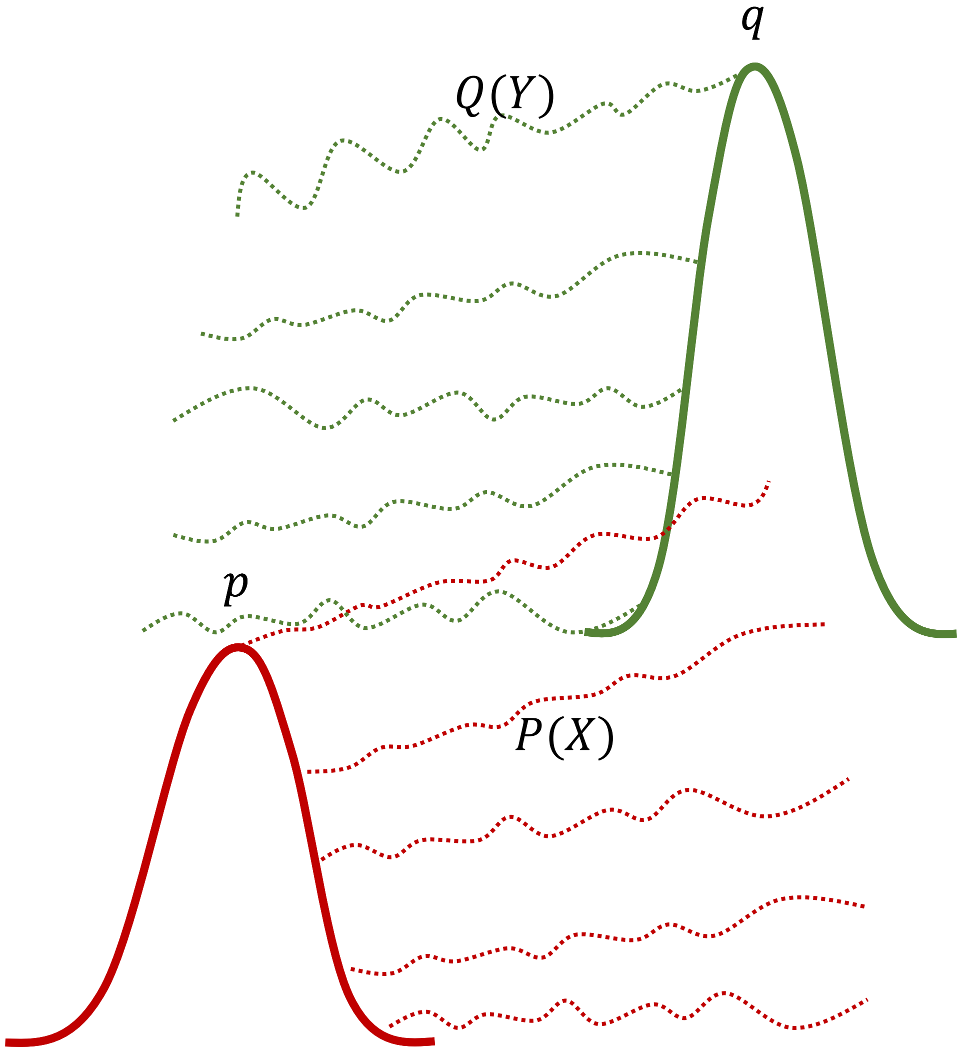
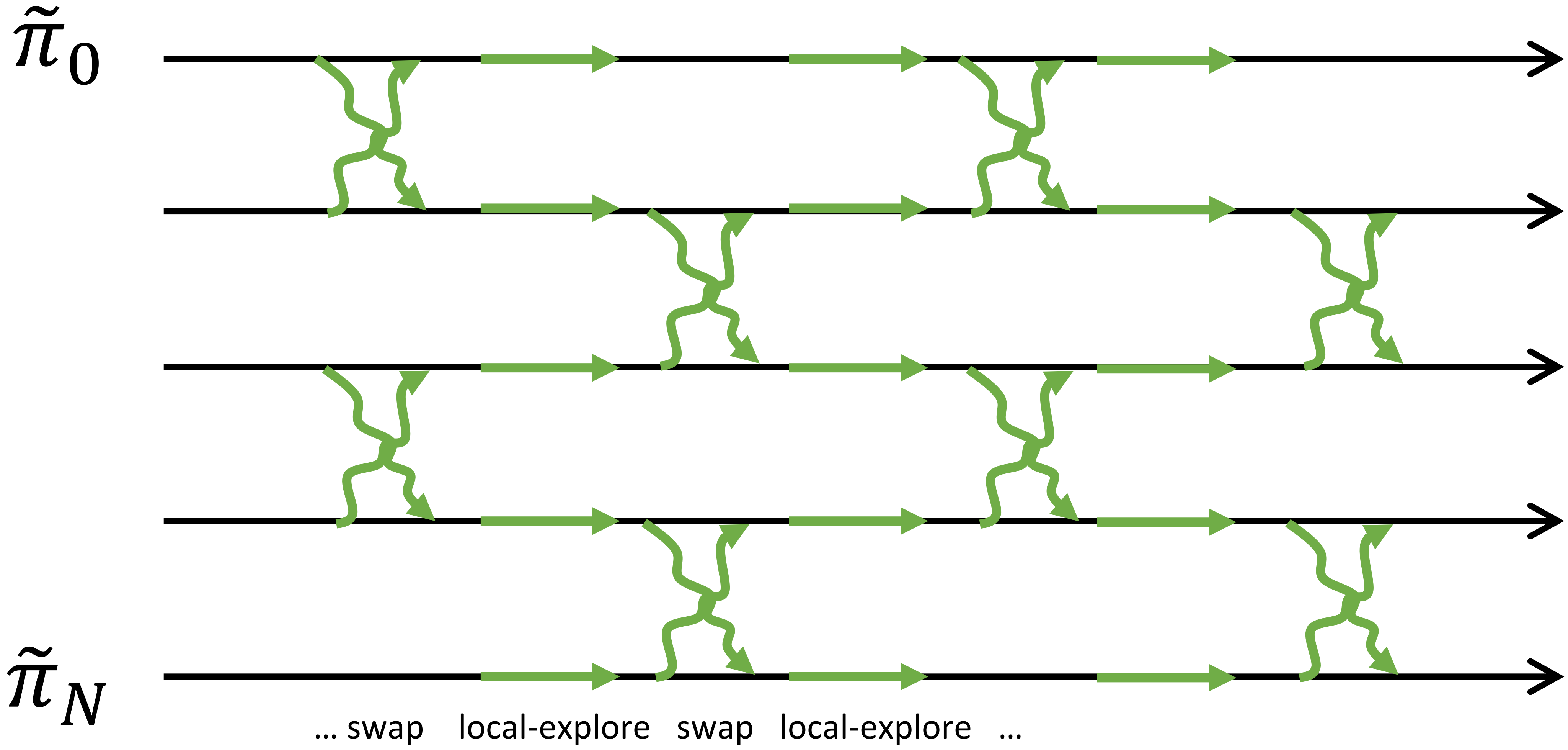


How to realise the path?

CMCD Path / Diffusion Path / etc…

Accelerated Parallel tempering in Path Space



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

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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 $p_0^j, j = 1, \cdots, J$.

Accelerated Parallel tempering in Path Space

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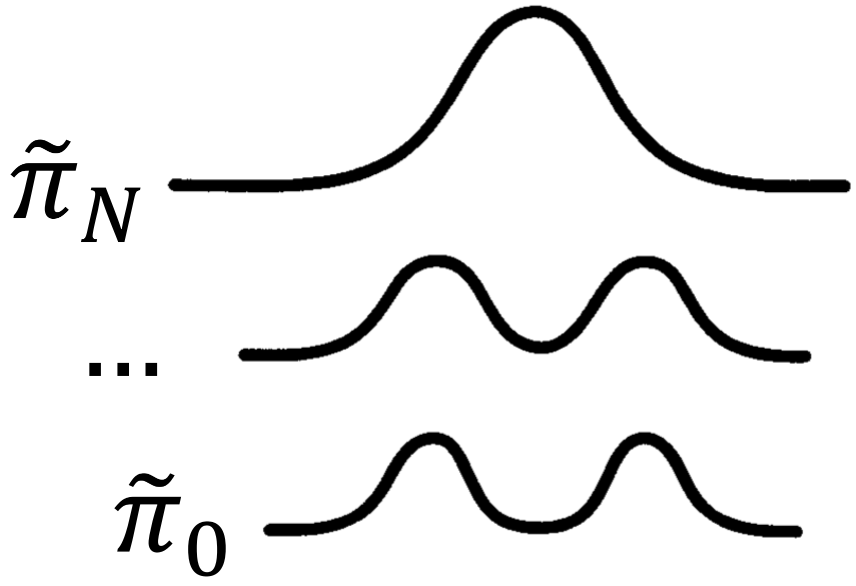

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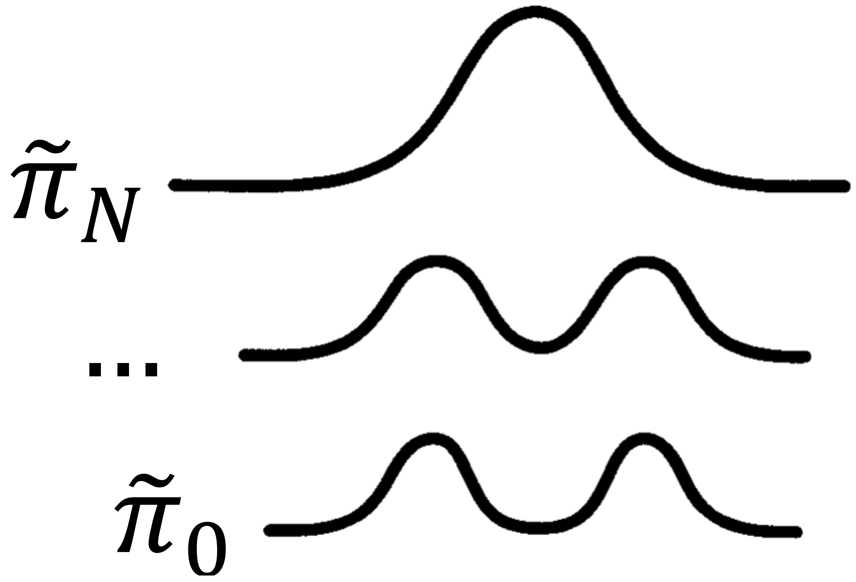


tempering: $\pi_t(x) \propto p_t^j(x)^\beta$ with inverse-temperature $\beta > 0$;

reward-tilting/posterior sampling: $\pi_t(x) \propto p_t^j(x)\exp(r_t(x))$ with reward/likelihood $r_t(x)$;

model composition: $\pi_t(x) \propto \prod_j p_t^j(x)$ composing J diffusions $p_t^j, j = 1, \cdots, J$.

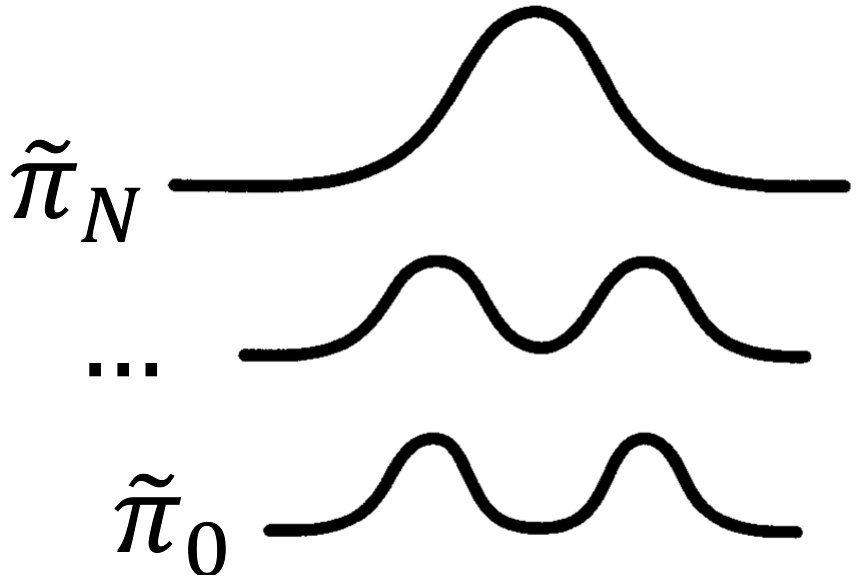
Accelerated Parallel tempering in Path Space

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 $p_0^j, j = 1, \cdots, J$.



tempering: $\pi_t(x) \propto p_t^j(x)^\beta$ with inverse-temperature $\beta > 0$;

model composition: $\pi_t(x) \propto \prod_j p_t^j(x)$ composing J diffusions $p_t^j, j = 1, \cdots, J$.

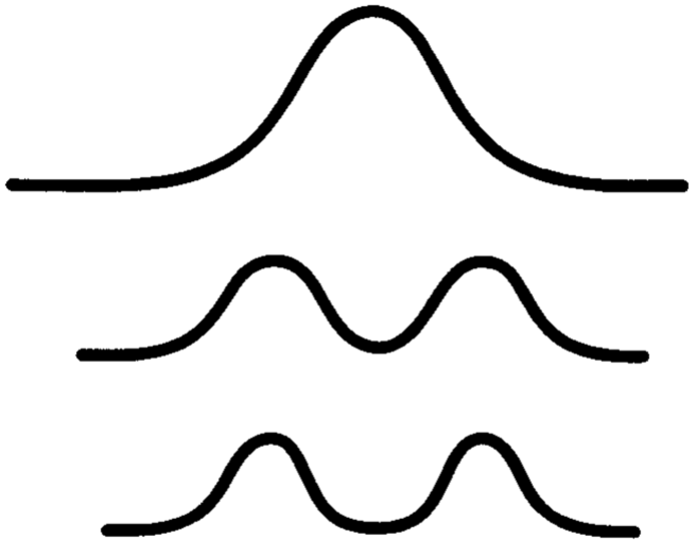
In short, control the marginal of each denoising step using APT

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)



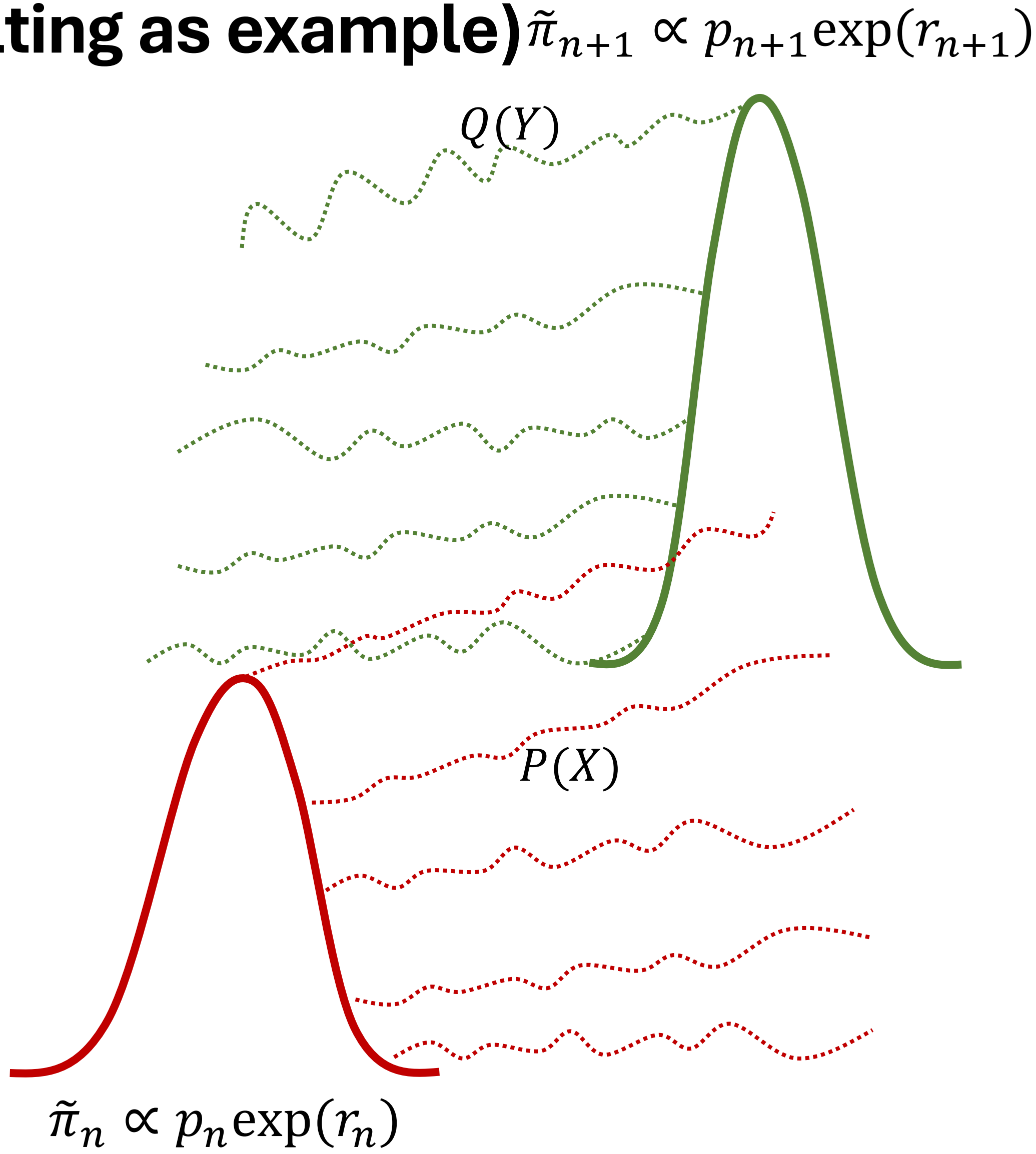
$$\tilde{\pi}_N \propto p_N \exp(r_N)$$

...

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

Accelerated Parallel tempering in Path Space

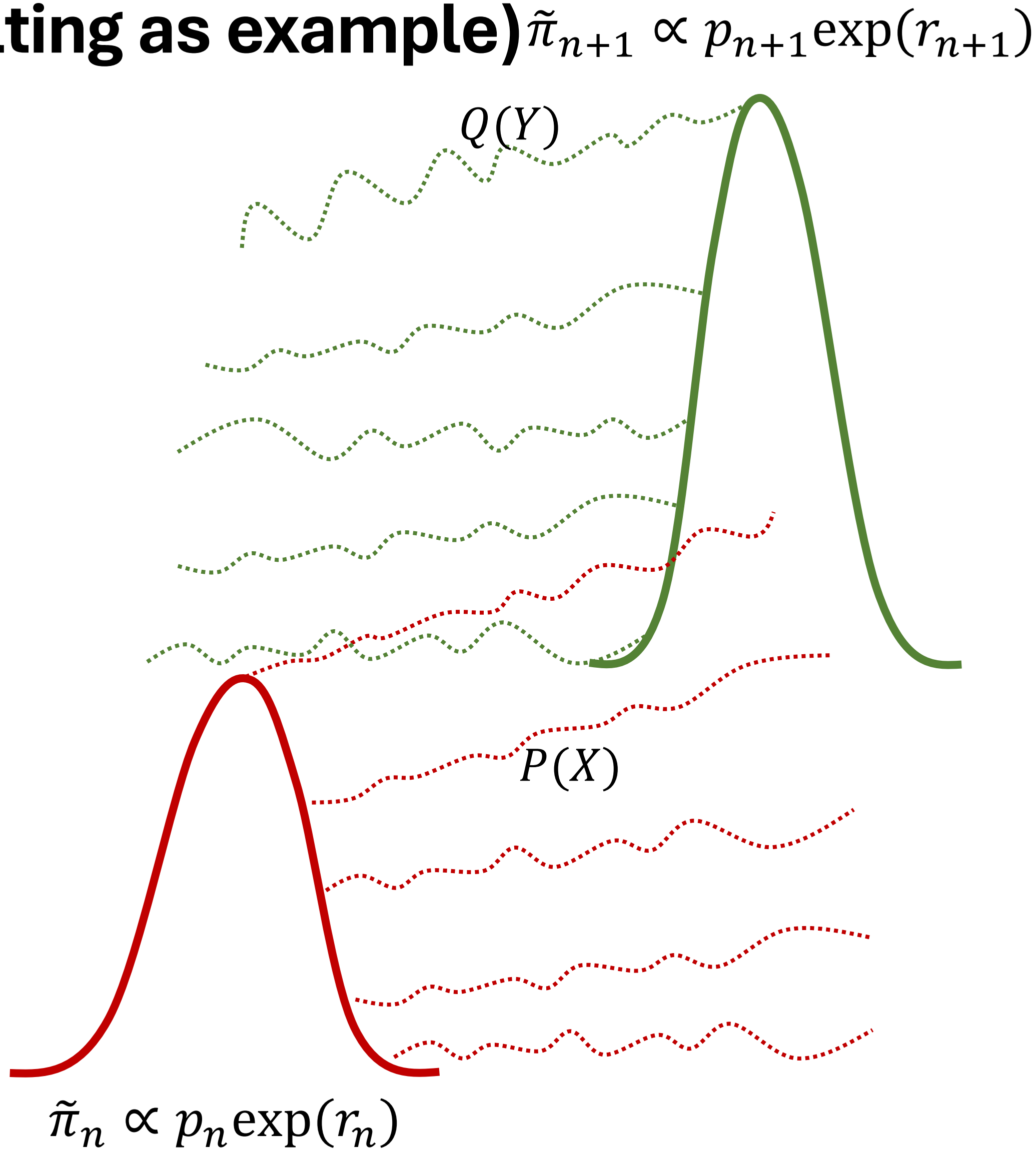
For Diffusion Test-time Control (reward-tilting as example)



Accelerated Parallel tempering in Path Space

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

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

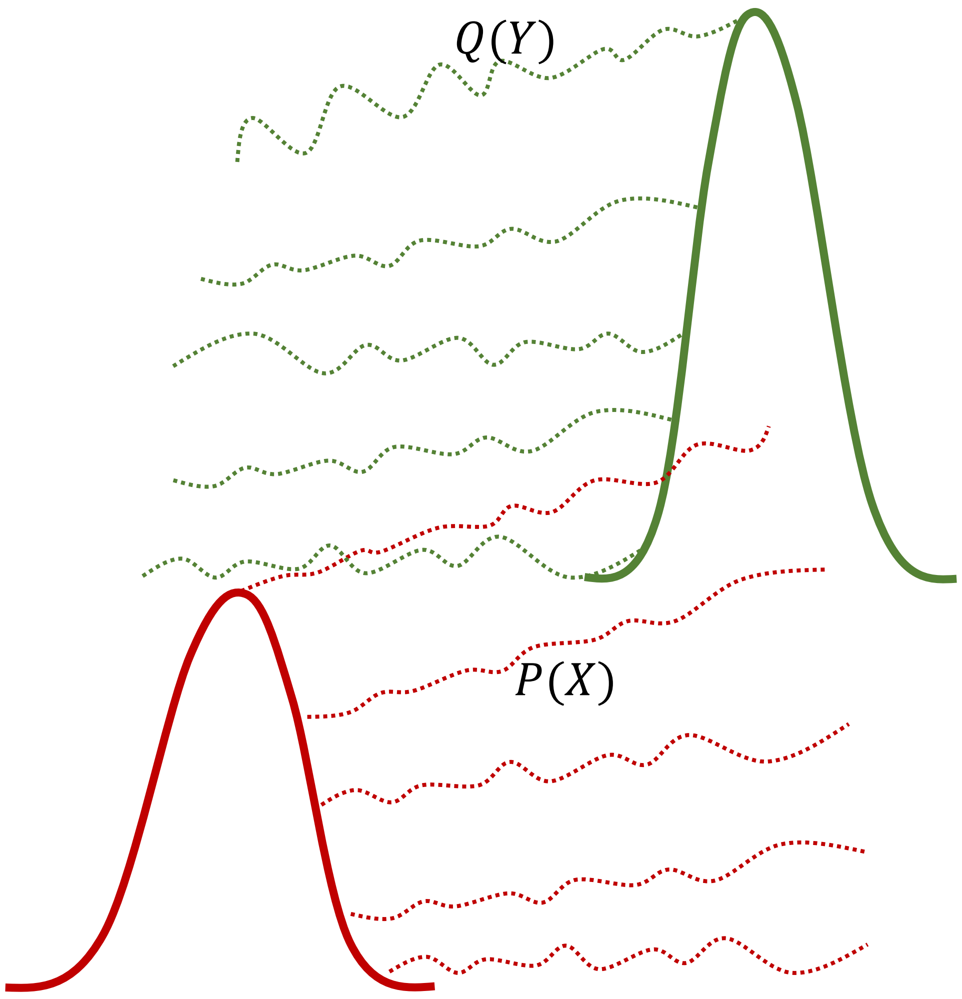


Accelerated Parallel tempering in Path Space

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

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

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

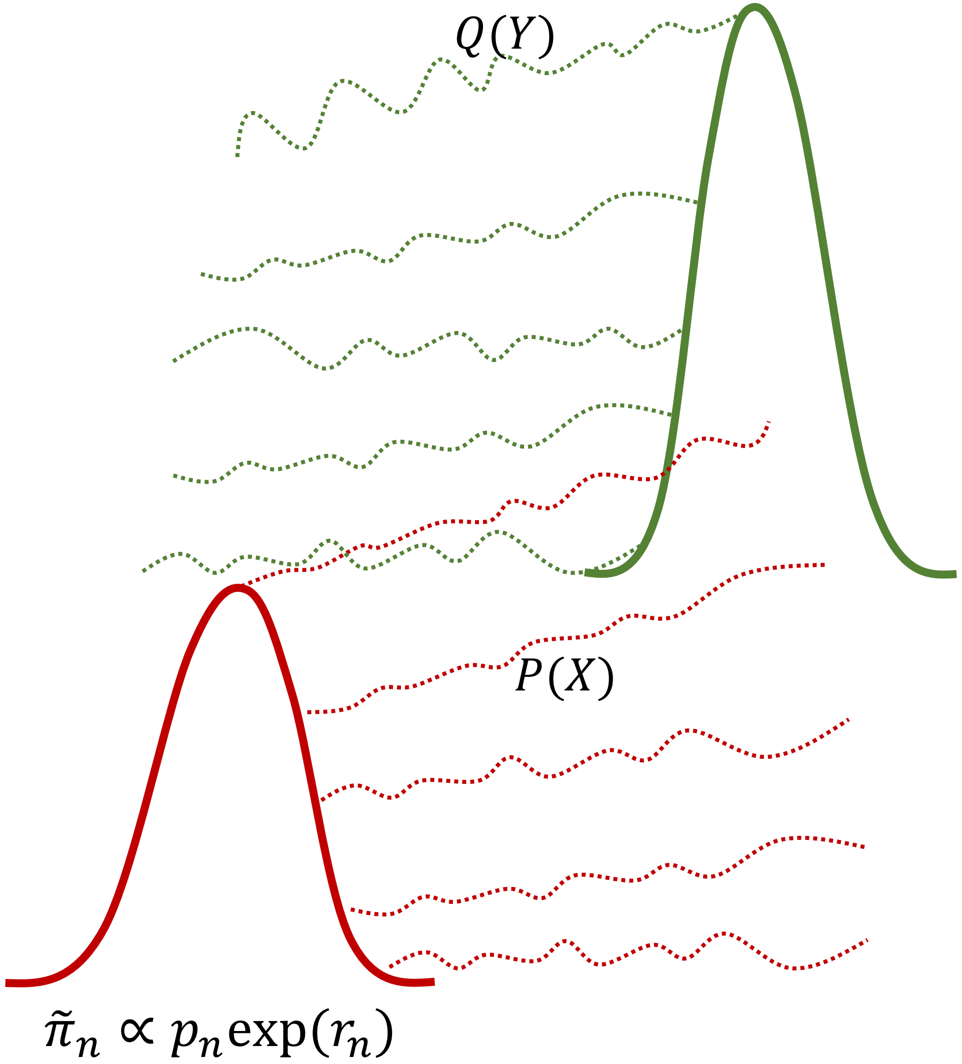


Accelerated Parallel tempering in Path Space

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

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

$$\frac{\mathrm{d}P}{\mathrm{d}Q} \propto \frac{\tilde{\pi}_n(X_0)}{\tilde{\pi}_{n+1}(X_1)} \frac{N_1(X_1|X_0)}{N_2(X_0|X_1)}$$

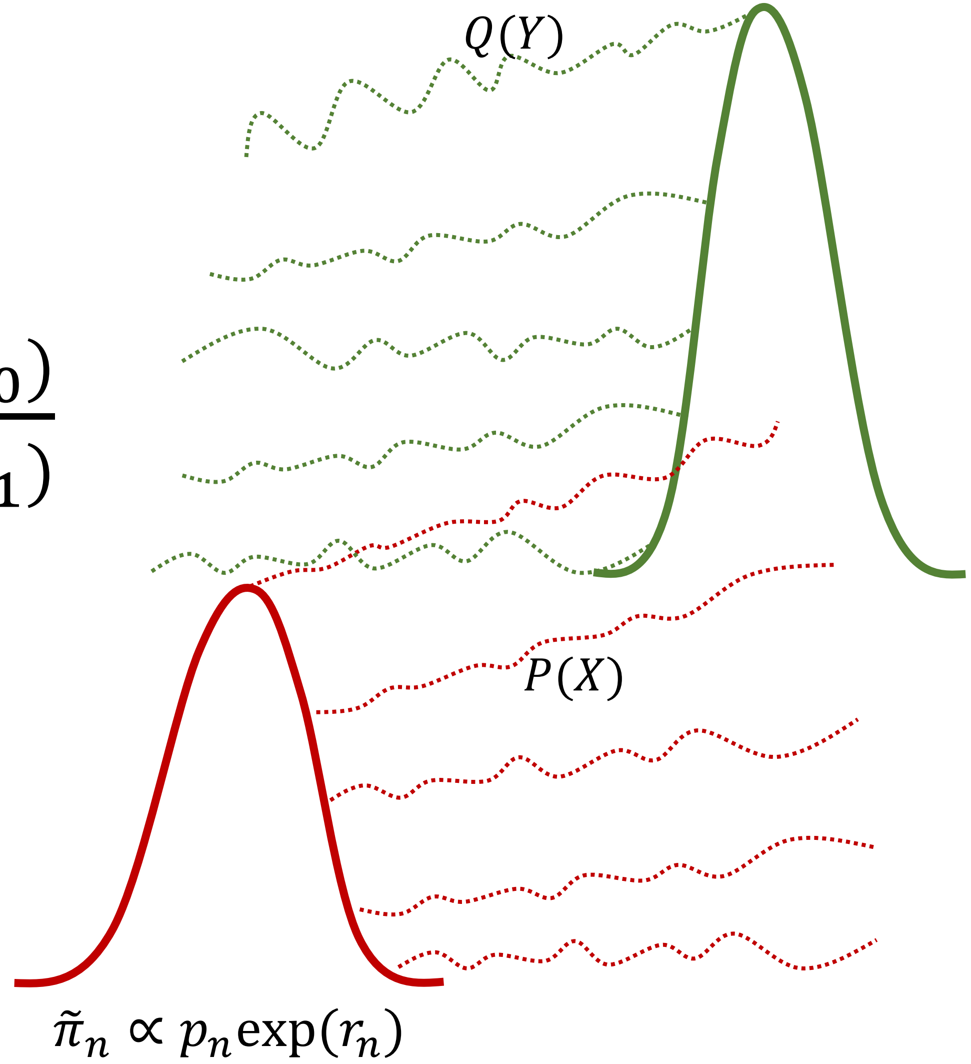


Accelerated Parallel tempering in Path Space

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

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

$$\frac{\mathrm{d}P}{\mathrm{d}Q} \propto \frac{p_n(X_0)}{p_{n+1}(X_1)} \frac{\exp(r_n(X_0))}{\exp(r_{n+1}(X_0))} \frac{N_1(X_1|X_0)}{N_2(X_0|X_1)}$$



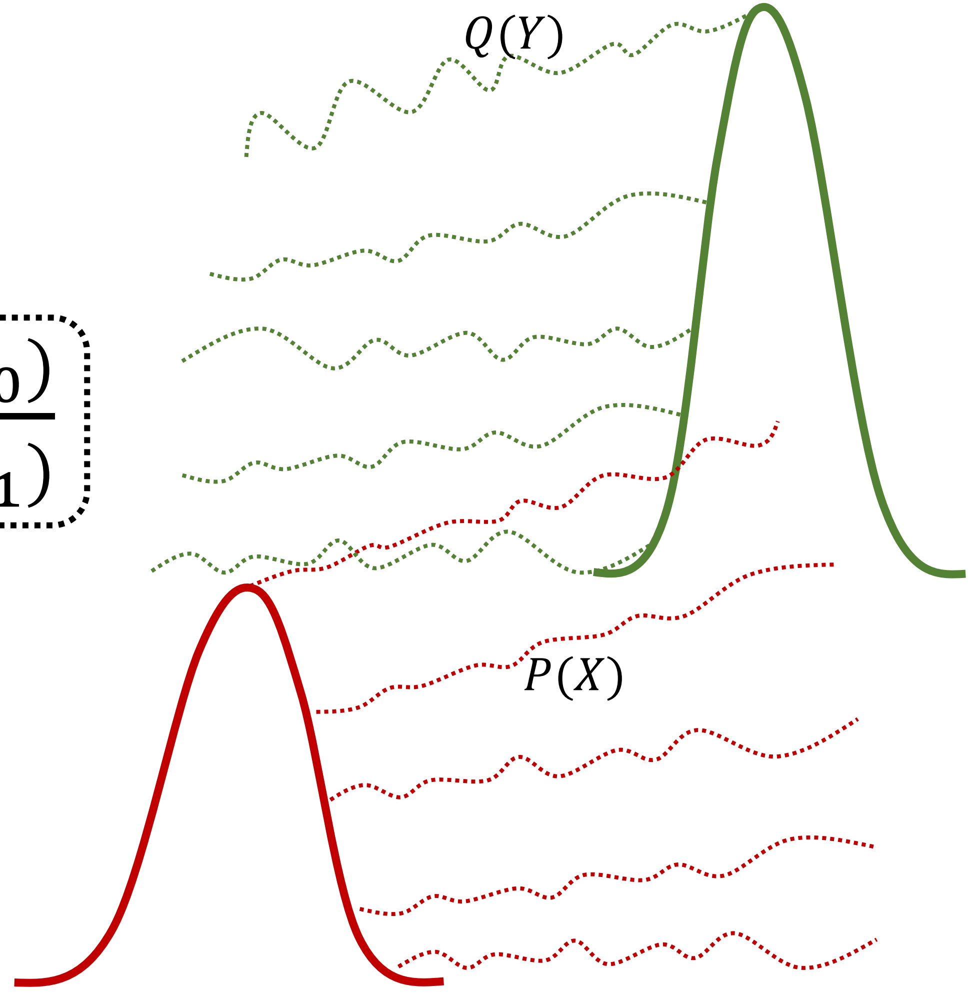
Accelerated Parallel tempering in Path Space

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

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

$$\frac{\mathrm{d}P}{\mathrm{d}Q} \propto \frac{p_n(X_0)}{p_{n+1}(X_1)}\frac{\exp(r_n(X_0))}{\exp(r_{n+1}(X_0))}\frac{N_1(X_1|X_0)}{N_2(X_0|X_1)}$$

known



$\tilde{\pi}_n \propto p_n\exp(r_n)$

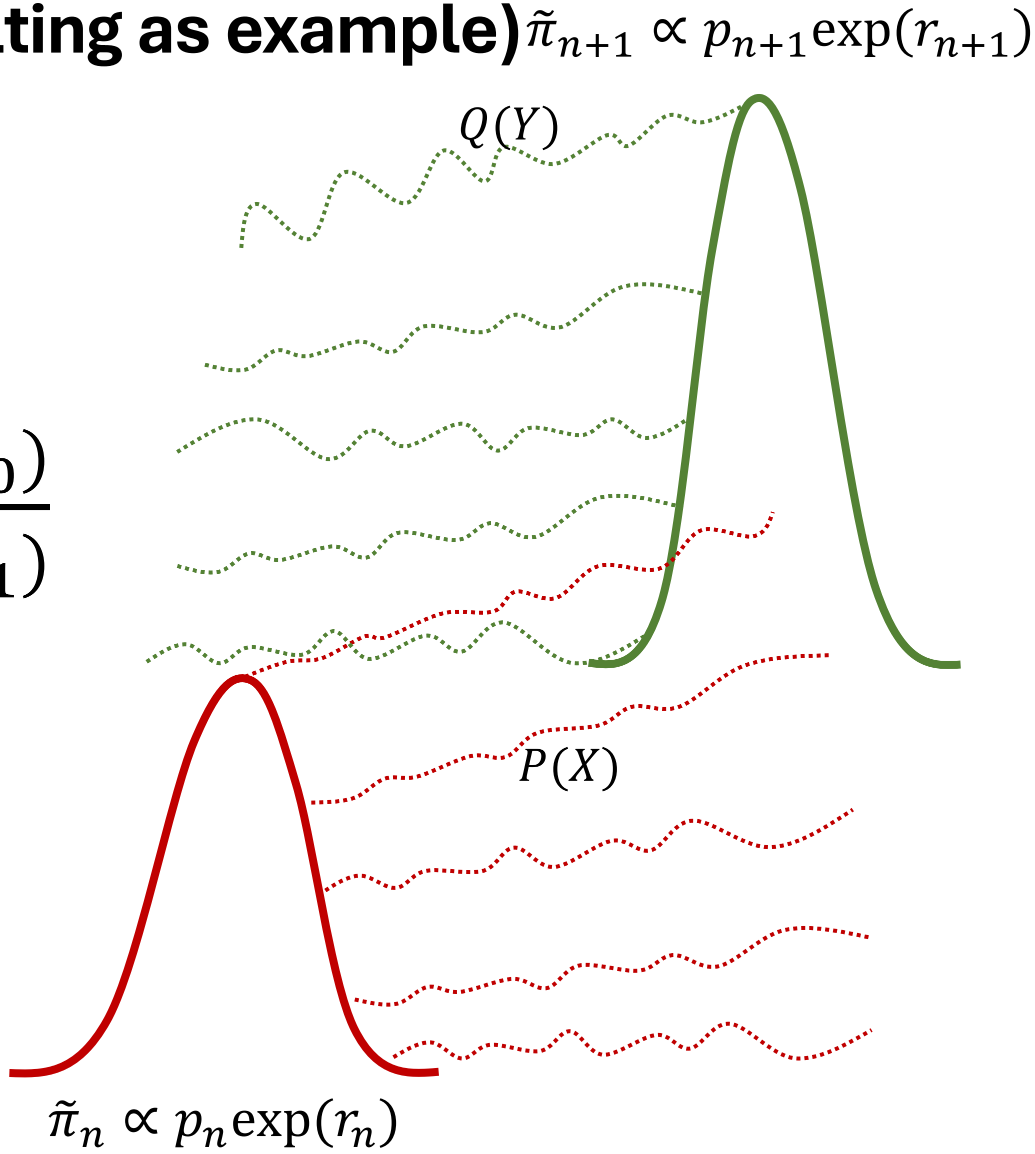
Accelerated Parallel tempering in Path Space

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

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

$$\frac{\mathrm{d}P}{\mathrm{d}Q} \propto \frac{p_n(X_0)}{p_{n+1}(X_1)} \frac{\exp(r_n(X_0))}{\exp(r_{n+1}(X_0))} \frac{N_1(X_1|X_0)}{N_2(X_0|X_1)}$$

unknown



Accelerated Parallel tempering in Path Space

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

$$\overleftarrow{P}: \; \mathrm{d}X_t = \text{diffusion denoising drift}\,\mathrm{d}t + \sigma_t \overleftarrow{\mathrm{d}W_t} \qquad X_1 \sim p_{n+1}$$

$$P: \; \mathrm{d}X_t = \text{diffusion noising drift}\,\mathrm{d}t + \sigma_t \mathrm{d}W_t \qquad X_0 \sim p_n$$

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

Accelerated Parallel tempering in Path Space

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

$$\overleftarrow{P}:\ \mathrm{d}X_t = \text{diffusion denoising drift}\,\mathrm{d}t + \sigma_t \overleftarrow{\mathrm{d}W_t} \qquad X_1 \sim p_{n+1}$$

$$P:\ \mathrm{d}X_t = \text{diffusion noising drift}\,\mathrm{d}t + \sigma_t \mathrm{d}W_t \qquad X_0 \sim p_n$$

$$\Rightarrow \quad \frac{\overleftarrow{dP}}{dP} = 1$$

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

Accelerated Parallel tempering in Path Space

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

$\overleftarrow{P}$: $\mathrm{d}X_t = \text{diffusion denoising drift}\,\mathrm{d}t + \sigma_t \overleftarrow{\mathrm{d}W_t}$ $\quad X_1 \sim p_{n+1}$

P: $\mathrm{d}X_t = \text{diffusion noising drift}\,\mathrm{d}t + \sigma_t \mathrm{d}W_t$ $\quad X_0 \sim p_n$

$$\Rightarrow \quad \frac{\overleftarrow{dP}}{dP} = 1$$

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

Accelerated Parallel tempering in Path Space

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

$$\overleftarrow{P}: \ \mathrm{d}X_t = \text{diffusion denoising drift } \mathrm{d}t + \sigma_t \overleftarrow{\mathrm{d}W_t} \qquad X_1 \sim p_{n+1}$$

$$P: \ \mathrm{d}X_t = \text{diffusion noising drift } \mathrm{d}t + \sigma_t \mathrm{d}W_t \qquad X_0 \sim p_n$$

$$\Rightarrow \quad \frac{\overleftarrow{dP}}{dP} = 1$$

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

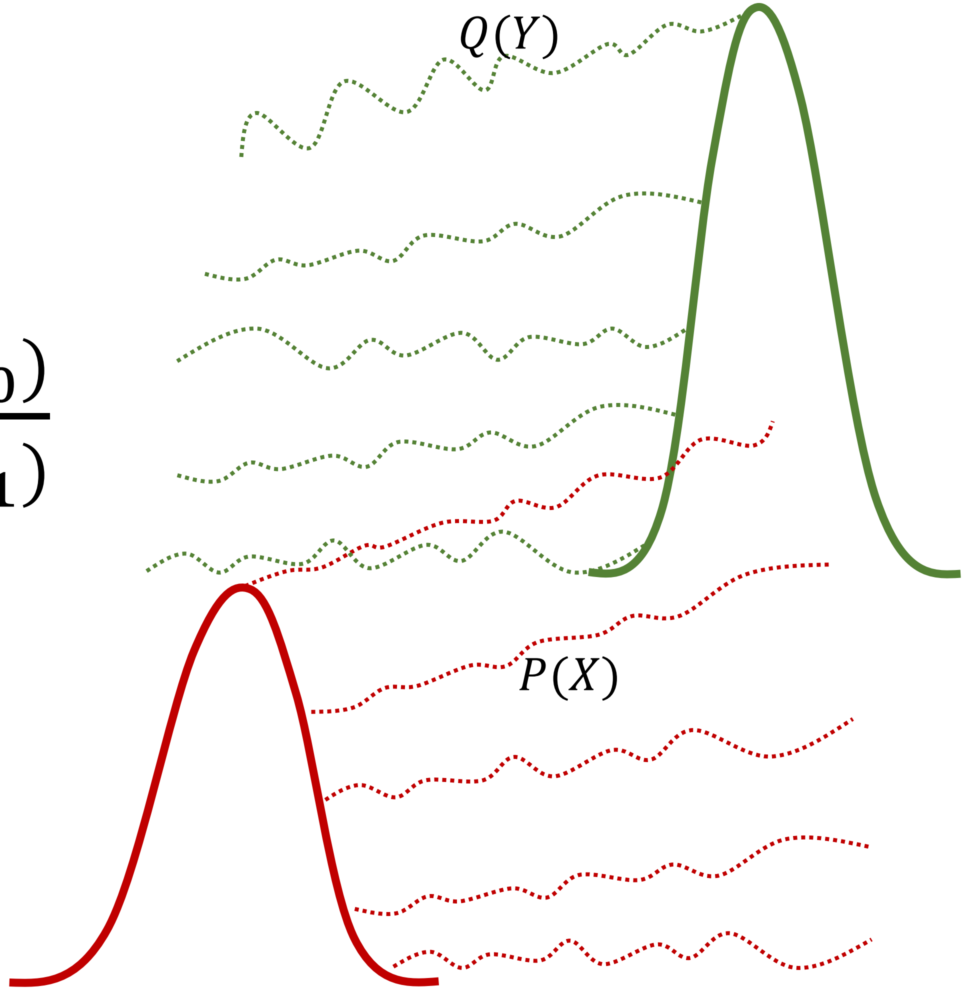
Accelerated Parallel tempering in Path Space

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

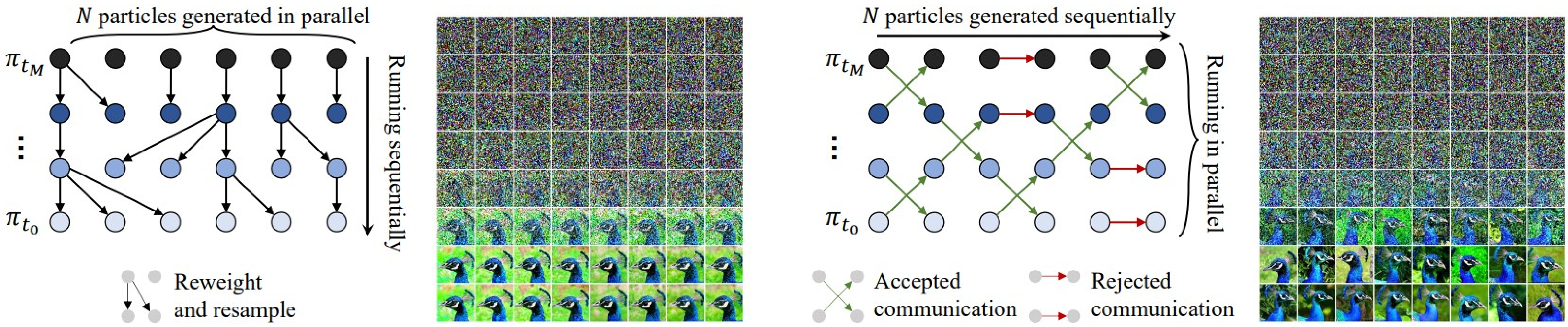
$$\alpha = \min\{1, \frac{\mathrm{d}P}{\mathrm{d}Q}(Y)\frac{\mathrm{d}Q}{\mathrm{d}P}(X)\}$$

$$\frac{\mathrm{d}P}{\mathrm{d}Q} \propto \frac{p_n(X_0)}{p_{n+1}(X_1)} \frac{\exp(r_n(X_0))}{\exp(r_{n+1}(X_0))} \frac{N_1(X_1|X_0)}{N_2(X_0|X_1)}$$

unknown



CREPE:
Controlling Diffusion with Replica Exchange



CREPE:
Controlling Diffusion with Replica Exchange

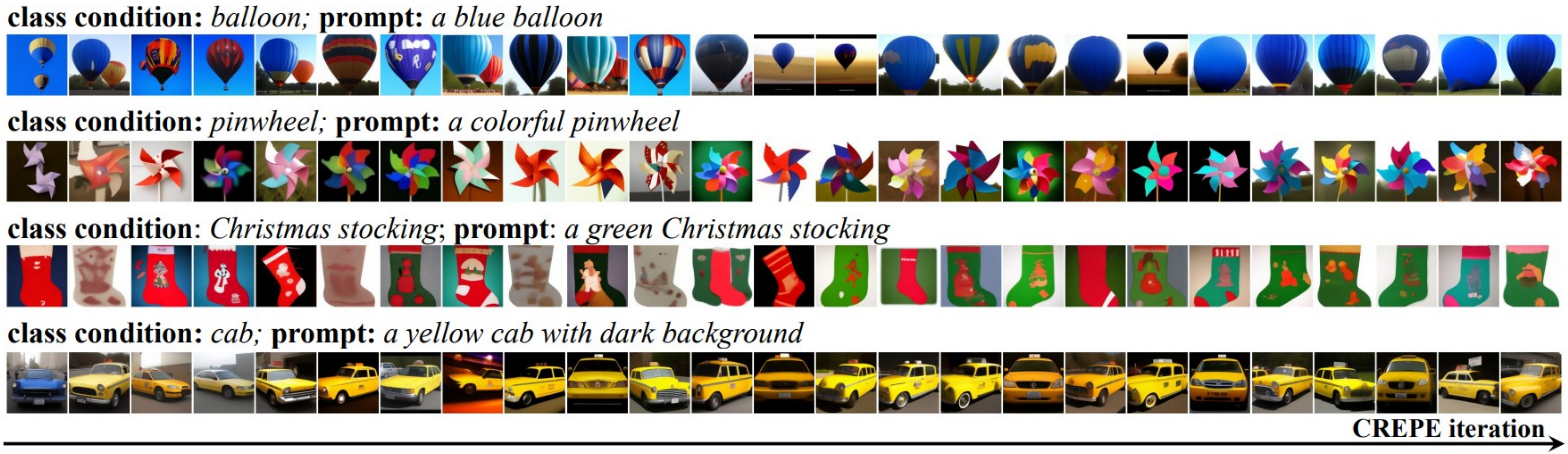
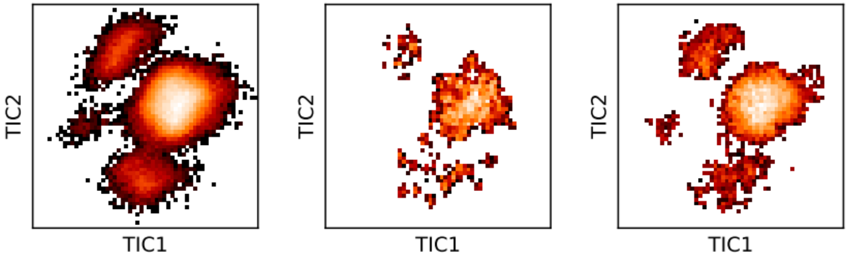


Figure 1: Trajectory of images generated using CREPE for prompted reward-tilting on ImageNet-512, thinned every 8 iterations. After burn-in, the samples align closely with the prompt.

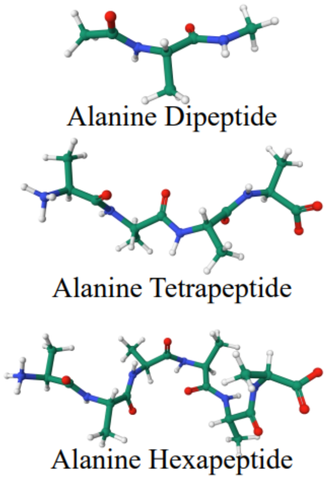
CREPE:
Controlling Diffusion with Replica Exchange



(a) MD (b) SMC (c) CREPE

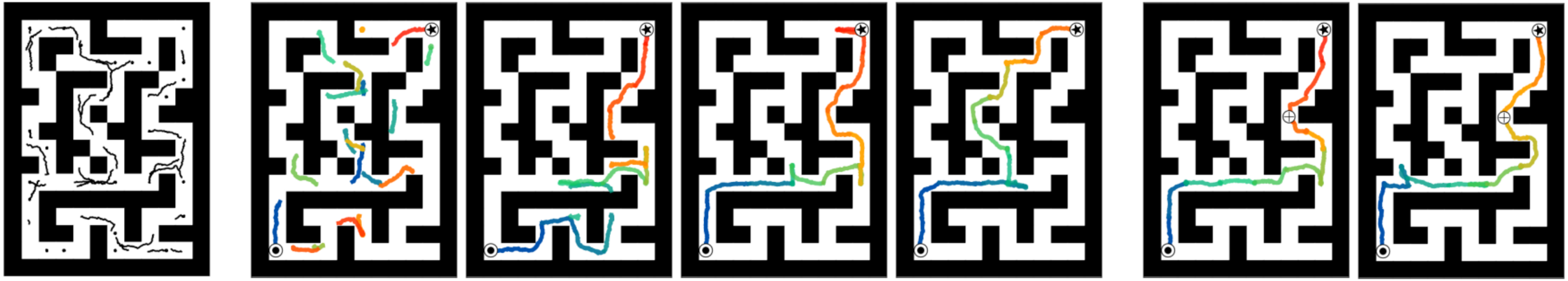
Figure 3: TICA of Alanine Hexapeptide annealed to 600K by SMC and CREPE. CREPE maintains more diversity.

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

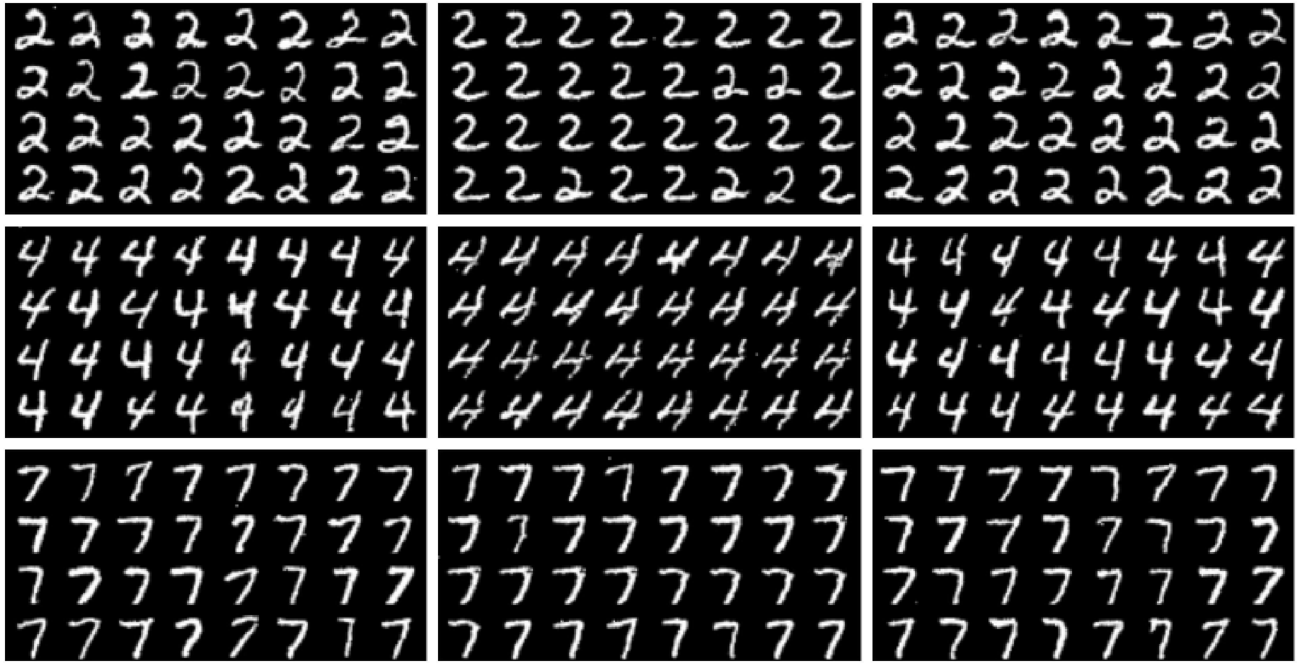
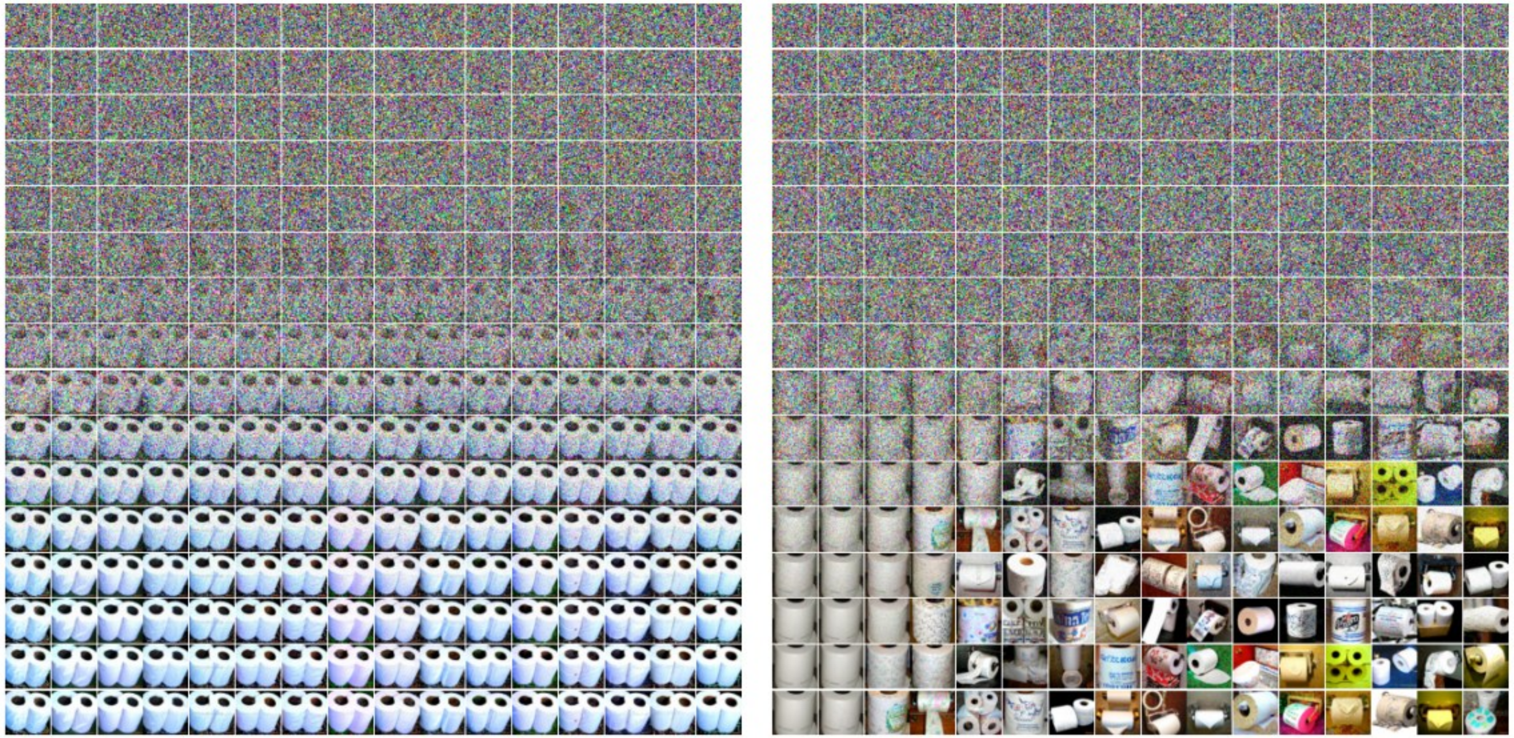


Figure 7: MNIST samples generated by CFG, and debiased by SMC and CREPE.

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: $\tilde{q}$

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

Path measure 1: P
Path measure 2: Q

"Unnormalised" RND: $w(X) = \frac{Z_p}{Z_q}\frac{\mathrm{d}P}{\mathrm{d}Q}(X)$

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

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

Collaborators (random order): Free-energy estimator with adaptive transport






Collaborators (random order):
Accelerated parallel tempering







Collaborators (random order):
Controlling diffusion with Replica Exchange