

Conditioning in SDEs

9 February 2024

R255 Lecture

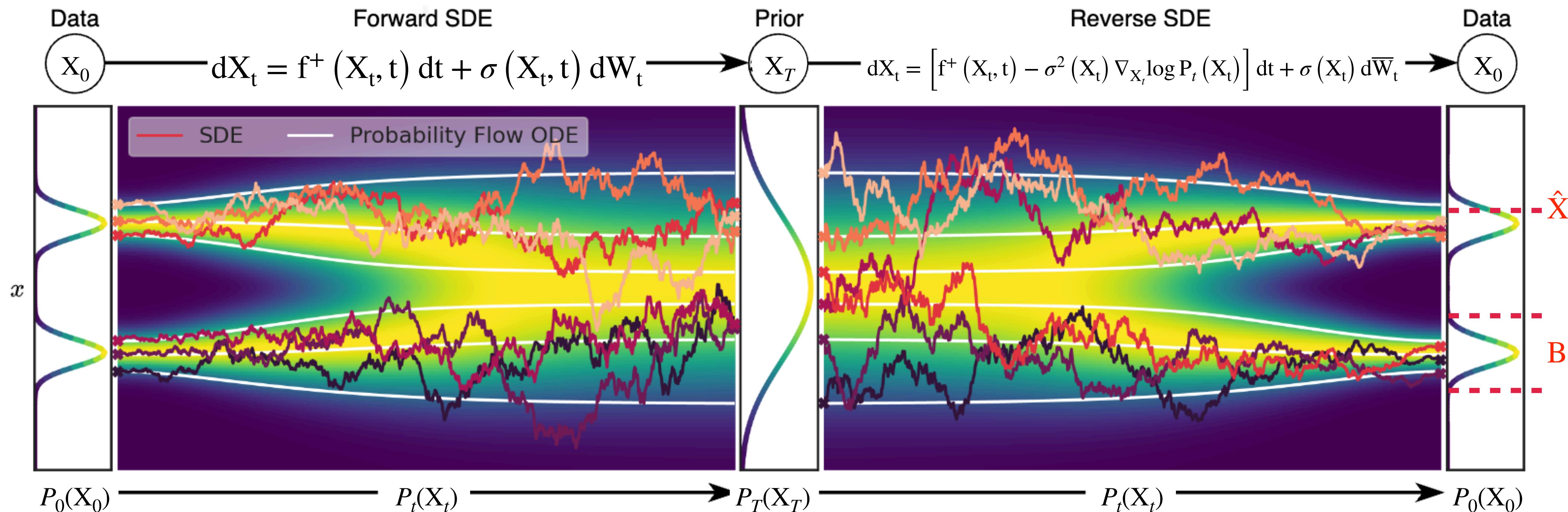
Shreyas Padhy

So far - Reversal of SDEs

- We have a forward SDE
- We can reverse the SDE

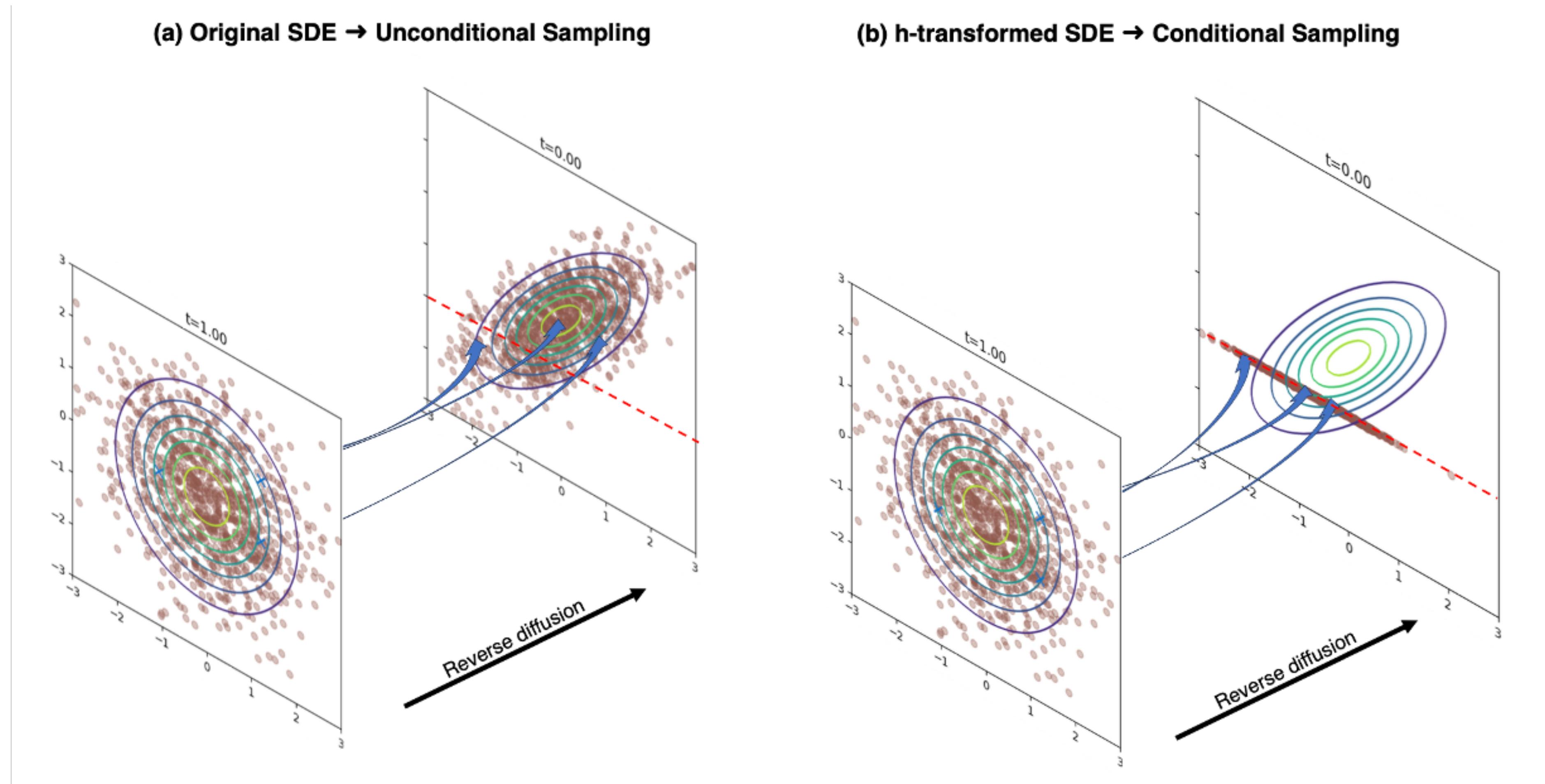
$$dX_t = f^+(X_t, t) dt + \sigma(X_t, t) dW_t$$

$$dX_t = f^-(X_t, t) dt + \sigma(X_t, t) d\bar{W}_t$$



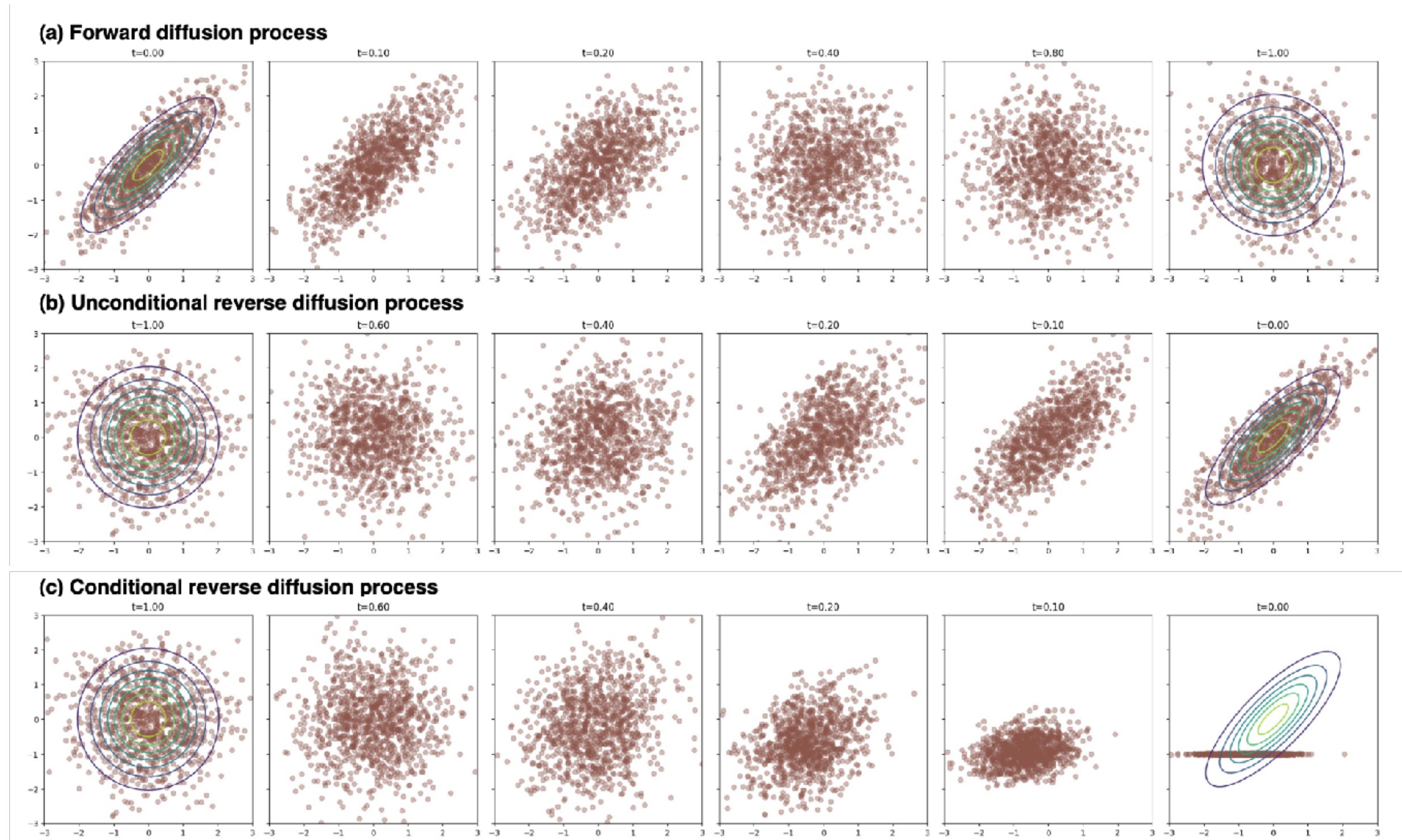
Conditioning of SDEs

- We want the reverse SDE to hit a certain constraint set $X_0 \in B$ at time $T = 0$



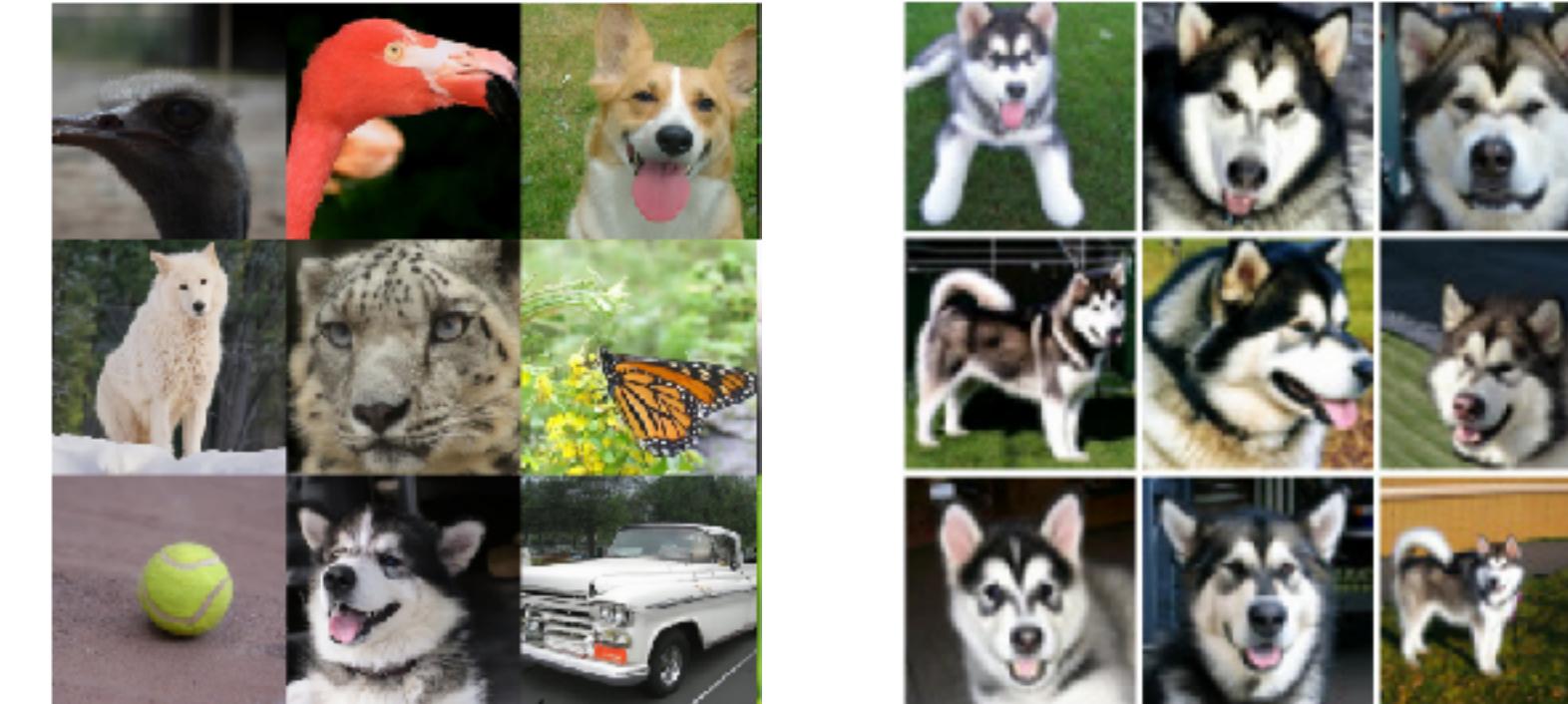
Conditioning of SDEs

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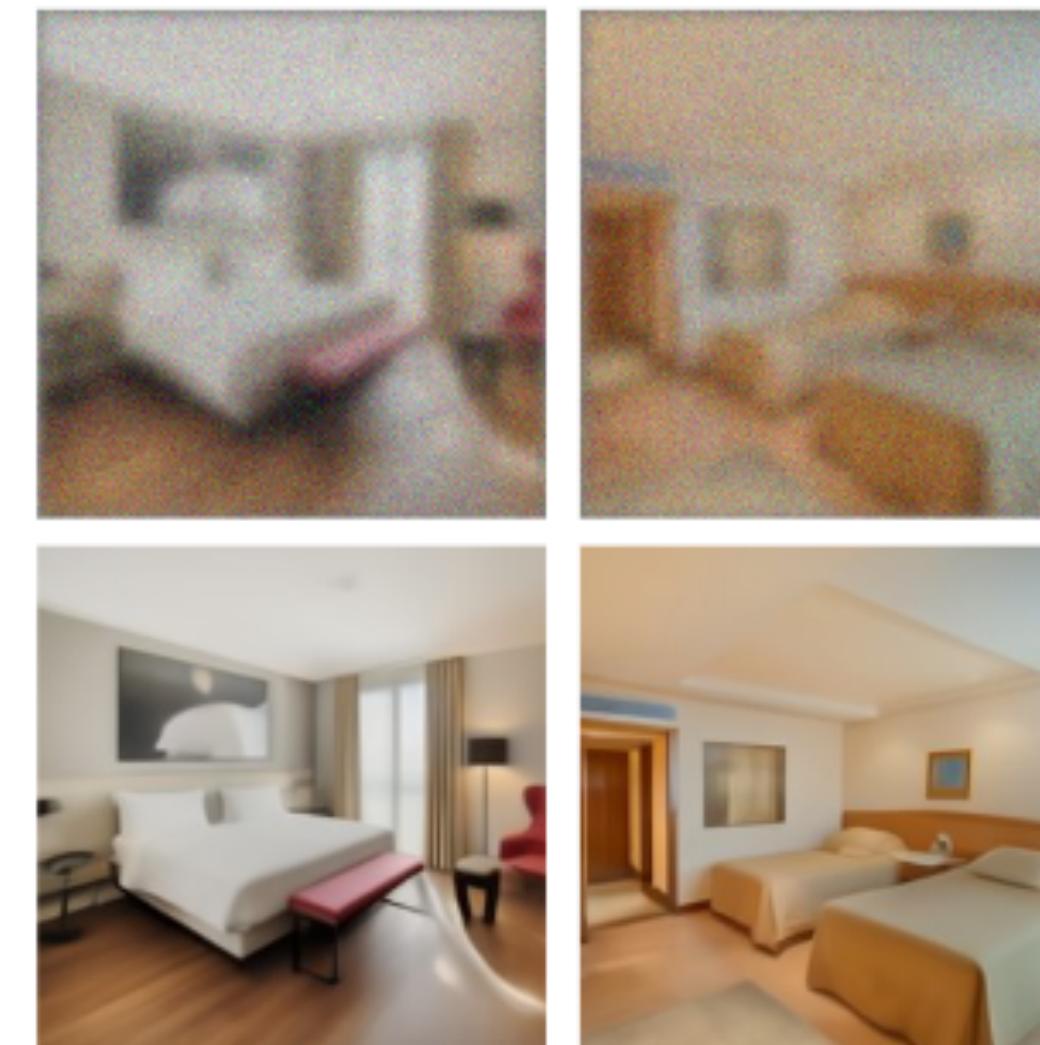


Conditioning of SDEs

- We want the reverse SDE to hit a certain constraint set $X_0 \in B$ at time $T = 0$
- Applications -
 - Class-conditional sampling
- Inverse modeling, where we rewrite $X_0 \in B$ to equivalently $\mathcal{A}(X_0) = y$



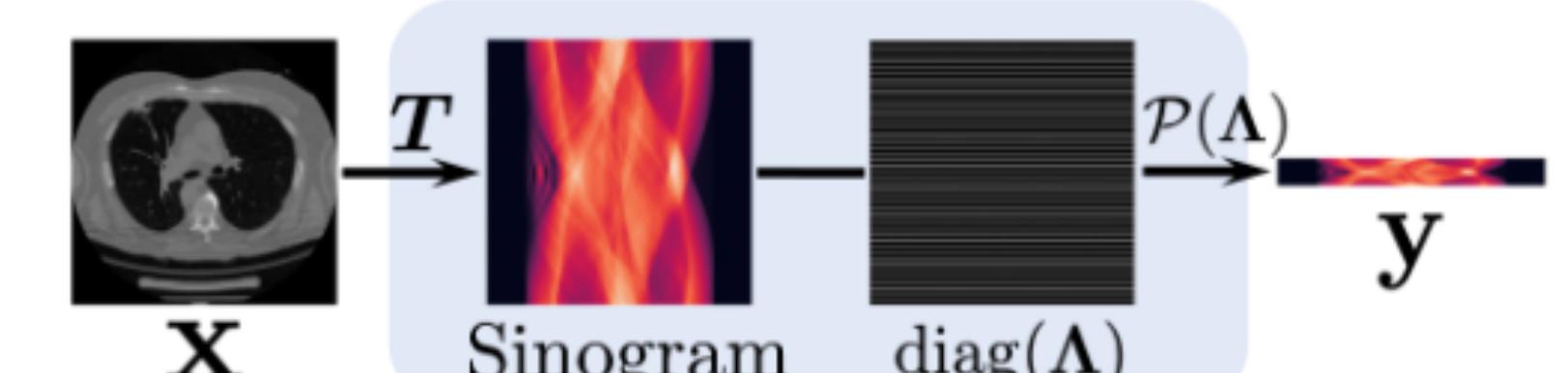
In-painting



Deblurring



Colorisation



Medical Imaging

Conditioning of SDEs - Doob's h -transform

[Rogers and Williams 2000] Consider the forward SDE:

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

where time flows forwards and with transition densities $p_{t|s}$. It then follows that the conditioned process $X_t | X_T \in B$ is a solution of

$$dH_t = \left(f_t^+(H_t, t) + \sigma_t^2 \nabla_{H_t} \ln P_{T|t}(X_T \in B | H_t) \right) dt + \sigma_t dW_t,$$

such that $\text{Law}(H_t | H_s) = \vec{p}_{t|s,T}(h_t | h_s, X_T \in B)$ and $\mathbb{P}(H_T \in B) = 1$.

- By conditioning a diffusion process to hit a particular event $X_T \in B$, we get a resulting conditional process that is also an SDE with an additional drift term.
- $h(t, H_t) \triangleq P_{T|t}(X_T \in B | H_t)$ is known as the **h -transform**

Aside - FPK and Infinitesimal Generators

- The FPK, a PDE that describes the evolution of the probability density of an SDE
 - $dX_t = \mu(X_t, t) dt + \sigma(X_t, t) dW_t$
 - $\frac{\partial}{\partial t} p(x, t) = - \frac{\partial}{\partial x} [\mu(x, t)p(x, t)] + \frac{\partial^2}{\partial x^2} [D(x, t)p(x, t)]$
- Let us define an operator called the (infinitesimal) generator of a stochastic process
 - $\mathcal{A}\phi(x_t, t) = \lim_{s \rightarrow 0} \frac{\mathbb{E} [\phi(x_{t+s}, t+s)] - \phi(x_t, t)}{s}$
- Why is it called the generator?
 - $\mathbb{E} [\phi(x_{t+s}, t+s)] \simeq \phi(x_t, t) + s\mathcal{A}\phi(x_t, t)$

Aside - FPK and Infinitesimal Generators

$$\mathcal{A}\phi(x_t, t) = \lim_{s \rightarrow 0} \frac{\mathbb{E} [\phi(x_{t+s}, t+s)] - \phi(x_t, t)}{s}$$

- For the Ito process $dX_t = \mu(X_t, t) dt + \sigma(X_t, t) dW_t$, the generator is given by

$$\mathcal{A}(\bullet) = \sum_i \frac{\partial(\bullet)}{\partial x_i} f_i(x_t, t) + \frac{1}{2} \sum_{i,j} \left(\frac{\partial^2(\bullet)}{\partial x_i \partial x_j} \right) [\sigma^2(X_t, t)]_{ij}$$

- We can show that the transition densities of the SDE satisfy the backwards Kolmogorov equation defined by the generator acting on the transition density

$$-\frac{\partial p(x_{t+s}, t+s \mid x_t, t)}{\partial t} = \mathcal{A}p(x_{t+s}, t+s \mid x_t, t)$$

Doob's h -transform (Quick Proof)

- Given the SDE with transition density $p_{t|s}(x_t \mid x_s)$, where $t > s$,
- We wish to obtain the process after conditioning the SDE to hit a deterministic end point z at time T ,

$$p_{t|s,T}(x_t \mid x_s, x_T = z) = \frac{p_{t|s,T}(x_T = z \mid x_t) p_{t|s}(x_t \mid x_s)}{p(x_T = z \mid x_s)}$$

- Let us try to find the SDE that would have this transition density

Doob's h -transform (Quick Proof)

- Apply Bayes' rule

$$p_{t|s,T}(x_t | x_s, x_T = z) = \frac{p_{T|s,t}(x_T = z | x_s, x_t) p_{t|s}(x_t | x_s)}{p_{T|s}(x_T = z | x_s)}$$

- Now, apply the Markov property $p_{T|s,t}(x_T = z | x_s, x_t) \rightarrow p_{T|s,t}(x_T = z | x_t)$,

$$p_{t|s,T}(x_t | x_s, x_T = z) = \frac{p_{T|t}(x_T = z | x_t) p_{t|s}(x_t | x_s)}{p_{T|s}(x_T = z | x_s)}$$

- Now, define $h(x_t, t) = p_{T|t}(x_T = z | x_t)$, and replace above to get

$$p_{t|s,T}(x_t | x_s, x_T = z) = \frac{h(x_t, t) p_{t|s}(x_t | x_s)}{h(x_s, s)}$$

Doob's h -transform (Quick Proof)

- In order for this to be a valid Markov kernel, we require

$$\int_{x_t} p_{t|s,T}(x_t | x_s, x_T = z) dx_t = 1$$

$$\int_{x_t} \frac{h(x_t, t)p_{t|s}(x_t | x_s)}{h(x_s, s)} dx_t = 1$$

- Taking $h(x_s, s)$ to the RHS (independent of x_t), we get the following property that $h(x_s, s)$ satisfies

- $h(x_s, s) = \int_{x_t} h(x_t, t)p_{t|s}(x_t | x_s) = \mathbb{E}[h(x_t, t)]$

- From the definition for infinitesimal generator \mathcal{A} , we have (assuming $(t, t + s)$ instead of (s, t))

- $\mathcal{A}\phi(\mathbf{x}, t) = \lim_{s \downarrow 0} \frac{\mathbb{E}[\phi(\mathbf{x}(t + s), t + s)] - \phi(\mathbf{x}(t), t)}{s}$

- Therefore, $\mathcal{A}h(x_t, t) = 0$

Doob's h -transform (Quick Proof)

- $\mathcal{A}h(x_t, t) = 0$, and the new transition probability $p^h = p \frac{h(x_{t+s}, t+s)}{h(x_t, t)}$
- Writing down the infinitesimal generator for some arbitrary ϕ , \mathbb{E} w.r.t p^h , we get

$$\mathcal{A}\phi = \lim_{s \rightarrow 0} \frac{\mathbb{E}^h[\phi(x_{t+s}, t+s)] - \phi(x_t, t)}{s}$$

- Noting that $\mathbb{E}^h[\phi] = \mathbb{E} \left[\phi \frac{h(x_{t+s}, t+s)}{h(x_t, t)} \right]$, we have

$$\mathcal{A}^h\phi = \lim_{s \downarrow 0} \frac{\mathbb{E}[\phi(x_{t+s})h(x_{t+s}, t+s)] - \phi(x_t)h(x_t, t)}{sh(x_t, t)}$$

$$= \frac{1}{h(x_t, t)} \mathcal{A}\{h(x_t, t)\}\phi(x_t)$$

- Now, remember the form of \mathcal{A} below, and apply the product rule to $h(\cdot)\phi(\cdot)$

$$\mathcal{A}(\cdot) = \sum_i \frac{\partial(\cdot)}{\partial x_i} f_i(x_t, t) + \frac{1}{2} \sum_{i,j} \left(\frac{\partial^2(\cdot)}{\partial x_i \partial x_j} \right) [\sigma^2(X_t, t)]_{ij}$$

Doob's h -transform (Quick Proof)

- Now, remember the form of \mathcal{A} below, and apply the product rule to $h(\cdot)\phi(\cdot)$

$$\mathcal{A}(\cdot) = \sum_i \frac{\partial(\cdot)}{\partial x_i} f_i(x_t, t) + \frac{1}{2} \sum_{i,j} \left(\frac{\partial^2(\cdot)}{\partial x_i \partial x_j} \right) [\sigma^2(X_t, t)]_{ij}$$

- We get this behemoth

$$\begin{aligned} & \frac{1}{h(t, x_t)} \left\{ \frac{\partial h(t, x_t)}{\partial t} \phi + \sum_i \left[\frac{\partial h(t, x_t)}{\partial x_i} \phi(x_t) + h(t, x_t) \frac{\partial \phi(x_t)}{\partial x_i} \right] f_i(x_t, t) \right. \\ \mathcal{A}^h \phi = & \left. + \frac{1}{2} \sum_{i,j} \frac{\partial^2 [h(t, x_t) \phi(x_t)]}{\partial x_i \partial x_j} [\sigma^2(x_t, t)]_{ij} \right\} \end{aligned}$$

- This gives us an even bigger behemoth

$$\mathcal{A}h = 0$$

$$\begin{aligned} & = \frac{1}{h(t, x_t)} \left\{ \left[\frac{\partial h(t, x_t)}{\partial t} + \sum_i \frac{\partial h(t, x_t)}{\partial x_i} f_i(x_t, t) + \frac{1}{2} \sum_{i,j} \frac{\partial^2 h(t, x_t)}{\partial x_i \partial x_j} [\sigma^2(x_t, t)]_{ij} \right] \phi(x_t) + \sum_i h(t, x_t) \frac{\partial \phi(x_t)}{\partial x_i} f_i(x_t, t) + \right. \\ & \left. + \frac{1}{2} \sum_{i,j} \left[\frac{\partial h(t, x_t)}{\partial x_j} \frac{\partial \phi(x_t)}{\partial x_i} + \frac{\partial h(t, x_t)}{\partial x_i} \frac{\partial \phi(x_t)}{\partial x_j} + h(t, x_t) \frac{\partial^2 \phi(x_t)}{\partial x_i \partial x_j} \right] [\sigma^2(x_t, t)]_{ij} \right\} \end{aligned}$$

Doob's h -transform (Quick Proof)

- Finally, arranging terms we get

$$= \sum_i \left[f_i(x_t, t) + \sigma^2(x_t, t) \frac{\nabla h(t, x_t)}{h(t, x_t)} \right] \frac{\partial \phi(x_t)}{\partial x_i} + \frac{1}{2} \sum_{i,j} \frac{\partial^2 \phi(x_t)}{\partial x_i \partial x_j} [\sigma^2(x_t, t)]_{ij}$$

- Comparing to $\mathcal{A}(\bullet) = \sum_i \frac{\partial(\bullet)}{\partial x_i} f_i(x_t, t) + \frac{1}{2} \sum_{i,j} \left(\frac{\partial^2(\bullet)}{\partial x_i \partial x_j} \right) [\sigma^2(x_t, t)]_{ij}$

- The new drift is $f_i(x_t, t) + \sigma^2(x_t, t) \frac{\nabla h(t, x_t)}{h(t, x_t)} = f_i(x_t, t) + \sigma^2(x_t, t) \nabla \log h(x_t, t)$

Example: Pinned Brownian Motion

- Consider a Brownian motion starting from arbitrary $X_0 \sim p_{\text{data}}$, and $dX_t = \sigma dW_t$
- Let us condition this Brownian motion to hit $X_T = 0$ at time T,
 - Therefore $h(x_t, t) = P(X_T = 0 | X_t) = \mathcal{N}(X_t, \sigma(T-t))$
 - Which gives us $\nabla_{X_t} \log h(X_t, t) = \nabla_{X_t} \left(C - \frac{(X_t - 0)^2}{2\sigma^2(T-t)} \right) = -\frac{X_t}{\sigma^2(T-t)}$
- Plugging into the conditioned process formula, we get
 - $dH_t = \left(f_t^+ (H_t, t) + \sigma_t^2 \nabla_{H_t} \ln P_{T|t} (X_T \in B | H_t) \right) dt + \sigma_t dW_t,$
 - $dH_t = -\frac{X_t}{T-t} + \sigma dW_t$

Doob's h -transform on the reverse SDE

[Rogers and Williams 2000] Consider the reverse SDE:

$$dX_t = f^-(X_t, t) dt + \sigma_t d\bar{W}_t$$

where time flows backwards and with transition densities $\bar{p}_{t|s}$. It then follows that the conditioned process $X_t \mid X_0 \in B$ is a solution of

$$dH_t = \left(f_t^-(H_t, t) - \sigma_t^2 \nabla_{H_t} \ln \bar{P}_{0|t}(X_0 \in B \mid H_t) \right) dt + \sigma_t \bar{d}_t \bar{W}_t,$$

such that $\text{Law}(H_s \mid H_t) = \vec{p}_{s|t,0}(h_s \mid h_t, x_0 \in B)$ and $\mathbb{P}(H_0 \in B) = 1$.

Specifying hard constraints

- We consider events of the form $X_0 \in B$ that can be described by

- An equality constraint $\mathcal{A}(X_0) = y$

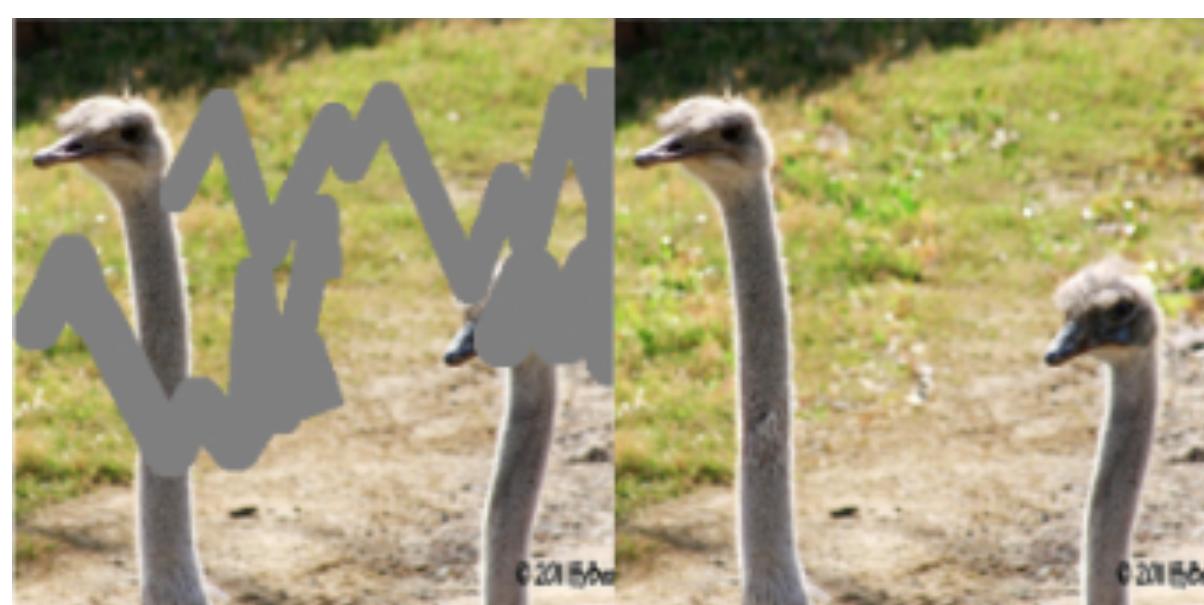
- Consider Doob's h -transform with hard constraints

- $dH_t = \left(f_t^- (H_t, t) - \sigma_t^2 \nabla_{H_t} \ln \bar{P}_{0|t} (\mathcal{A}(X_0) = y | H_t) \right) dt + \sigma_t \bar{d}_t \bar{W}_t,$

- Replacing $f_t^-(H_t, t) = f^+(H_t, t) - \sigma^2 \nabla_{H_t} \ln P_t(H_t)$, we get

- $dH_t = f_t^+ (H_t, t) - \sigma_t^2 \left(\nabla_{H_t} \ln P_t(H_t) + \nabla_{H_t} \ln \bar{P}_{0|t} (\mathcal{A}(X_0) = y | H_t) \right) dt + \sigma_t \bar{d}_t \bar{W}_t,$

- Sampling from this SDE gives us $x \sim p_{\text{data}}$ that satisfy $\mathcal{A}(x) = y$



In-painting

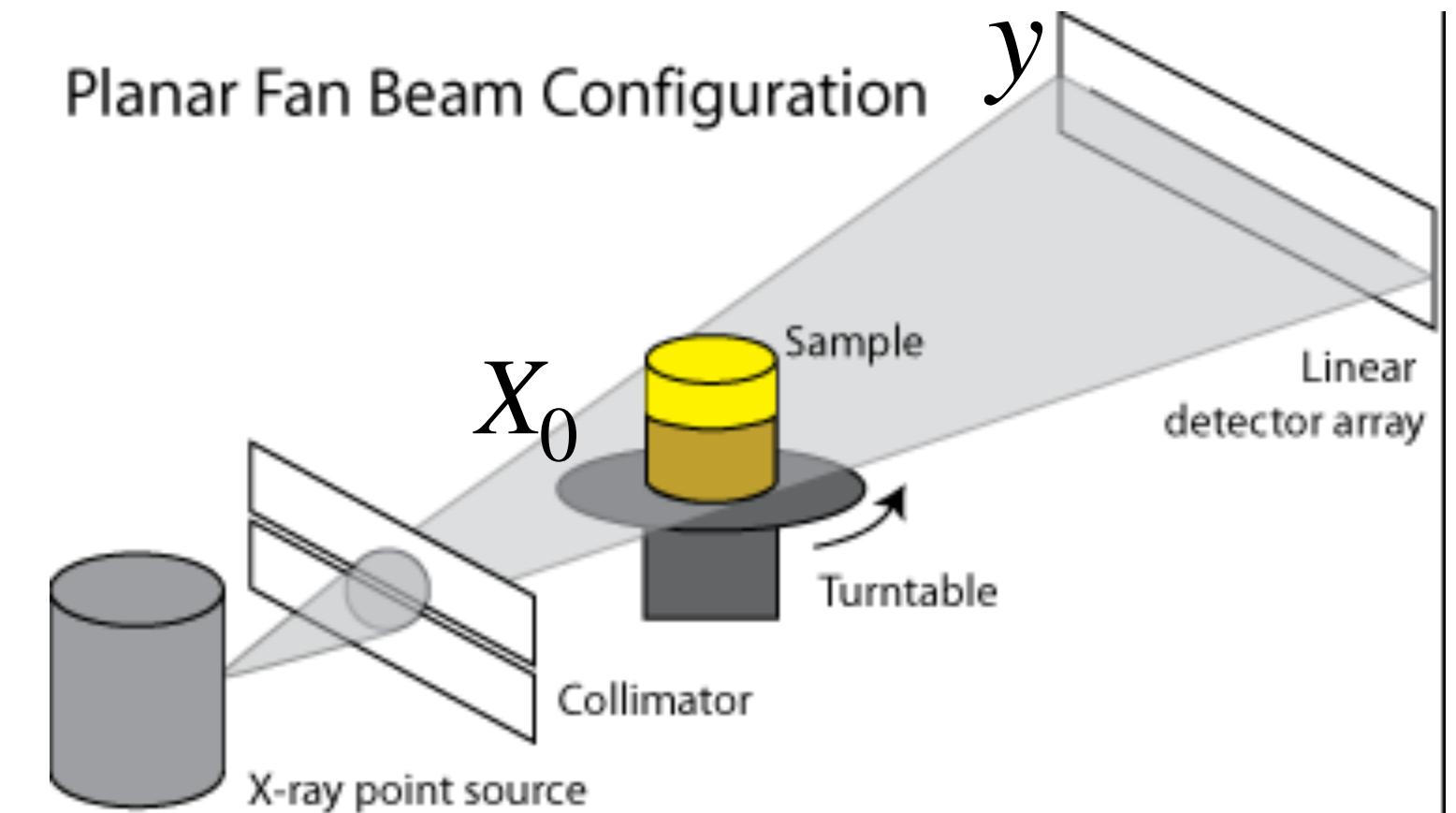
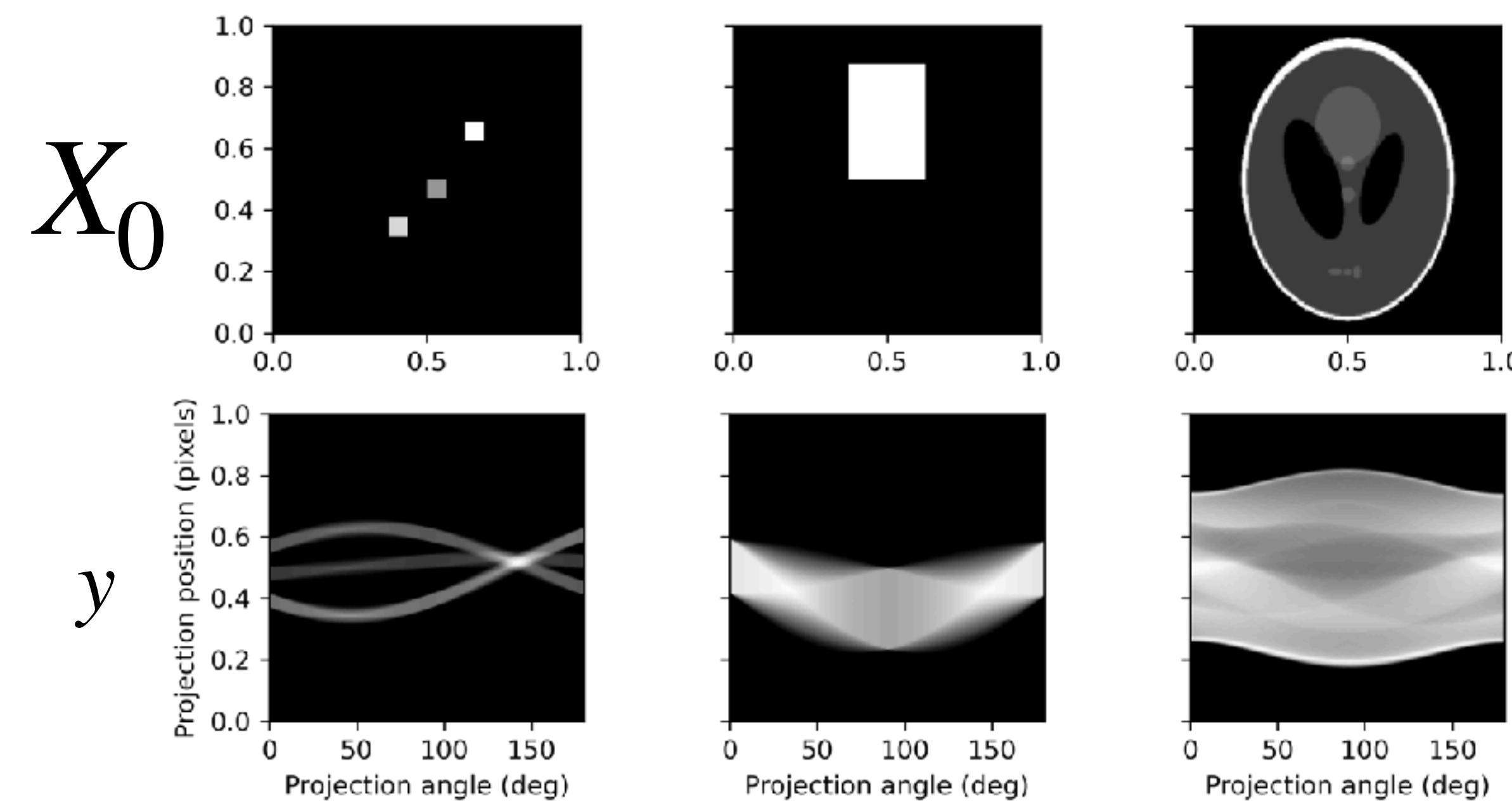
$$\mathcal{A} = \{0,1\}^{H \times W \times C}$$

Known
unconditional
score

Unknown
conditional
score

Specifying soft constraints

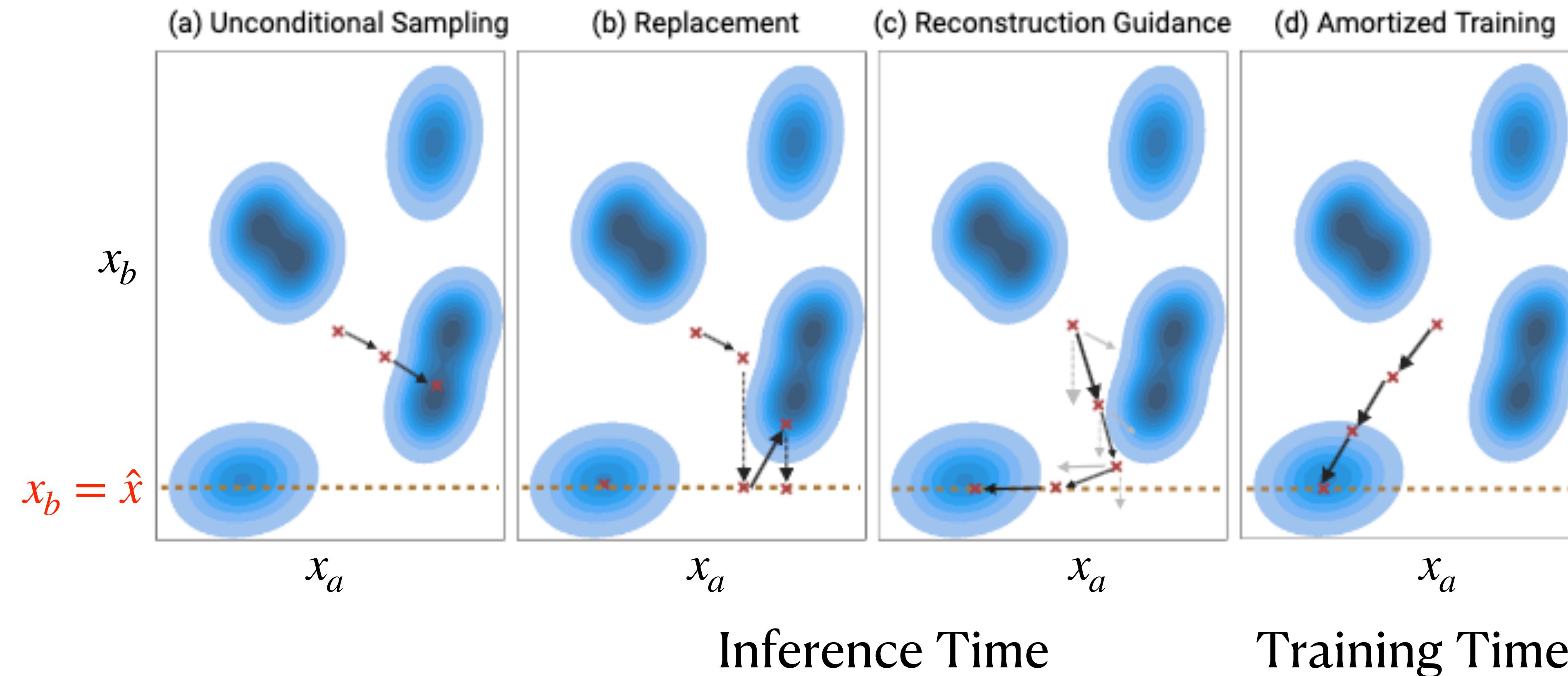
- We consider events of the form $X_0 \in B$ that can be described by
 - Noisy observations $y = \mathcal{A}(X_0) + \eta$, and a density $p(y | X_0)$
 - We wish to recover the posterior $p(X_0 | y)$



Specifying soft constraints

- We consider events of the form $X_0 \in B$ that can be described by
 - Noisy observations $y = \mathcal{A}(X_0) + \eta$, and a density $p(y | X_0)$
 - We wish to recover the posterior $p(X_0 | y)$
- Consider Doob's h -transform with soft constraints
 - $dH_t = \left(f_t^- (H_t, t) - \sigma_t^2 \nabla_{H_t} \ln \bar{P}_{y|t} (Y = y | H_t) \right) dt + \sigma_t \bar{d}_t \bar{W}_t,$
 - Again, replacing $f_t^-(H_t, t) = f_t^+(H_t, t) - \sigma_t^2 \nabla_{H_t} \ln P_t(H_t)$, we get
 - $dH_t = f_t^+ (H_t, t) - \sigma_t^2 \left(\nabla_{H_t} \ln P_t(H_t) + \nabla_{H_t} \ln \bar{P}_{y|t} (Y = y | H_t) \right) dt + \sigma_t \bar{d}_t \bar{W}_t,$
- Sampling from this SDE gives us $x \sim p(x_0 | Y = y) = \frac{p(y | x_0) p_{\text{data}}(x_0)}{p(y)}$

Different approaches for conditioning



How do we sample from conditioned SDE?

- We have

$$dH_t = f_t^+ (H_t, t) - \sigma_t^2 \left(\nabla_{H_t} \ln P_t(H_t) + \nabla_{H_t} \ln \bar{P}_{y|t} (Y = y | H_t) \right) dt + \sigma_t \bar{d}_t \bar{W}_t,$$

- The challenge is $\bar{P}_{y|t} (Y = y | H_t) = \int p(y | x_0) \bar{p}_{0|t} (x_0 | H_t) dx_0$
- We can sample from the reverse SDE to obtain samples from $p(x_0 | H_t)$
- We cannot estimate the integral without *many* samples, or evaluate at fixed x_0
- Can we approximate $p(x_0 | H_t)$?

Reconstruction Guidance

- Approximate $p(x_0 \mid x_t)$ with a Gaussian approximation using **Tweedie's formula**

[Tweedie's formula]. Let $p(a \mid b) = p_0(a)\exp(b^\top T(a) - \psi(b))$. Then the posterior mean $\hat{b} = \mathbb{E}[b \mid a]$ should satisfy

$$(\nabla_a T(a))^\top \hat{b} = \nabla_a \log p(a) - \nabla_a \log p_0(a)$$

- Diffusion Posterior Sampling** [Chung et al 2023]: Forward process is VP-SDE or DDPM sampling, approximate posterior mean using Tweedie's formula:

$$\hat{x}_0 = \mathbb{E}[x_0 \mid x_t] = \frac{1}{\sqrt{\bar{\alpha}(t)}} \left(x_t + (1 - \bar{\alpha}(t)) \nabla_{x_t} \log p_t(x_t) \right)$$

- Then approximate

$$\bar{P}_{y|t}(Y = y \mid x_t) = \int p(y \mid x_0) \bar{p}_{0|t}(x_0 \mid x_t) dx_0 \simeq p(y \mid \hat{x}_0)$$

- Simulate the following reverse SDE

$$dH_t = f_t^+(H_t, t) - \sigma_t^2 \left(\boxed{\nabla_{H_t} \ln P_t(H_t)} + \boxed{\nabla_{H_t} \ln p(y \mid \hat{x}_0)} \right) dt + \sigma_t d\bar{W}_t,$$

Known unconditional score

Extra backprop through score network

Classifier Guidance

- When we have external labels to guide diffusion
- Consider $d\mathbf{X}_t = f_t^+ (\mathbf{X}_t, t) - \sigma_t^2 \left(\nabla_{\mathbf{X}_t} \ln P_t(\mathbf{X}_t) + \nabla_{\mathbf{X}_t} \ln P(Y=y | \mathbf{X}_t) \right) dt + \sigma_t d\bar{\mathbf{W}}_t$,
 - We can train a time-dependent classifier by creating training data
 - Sample (x_0, y) from dataset, then sample $x_t \sim \text{SDE}$ to obtain (x_t, y)
 - Using trained $p(y | x_t)$ classifier, we backprop to get $\nabla_{x_t} \ln p(y | x_t)$
 - $\nabla_{x_t} \ln p(x_t)$ is unconditional score model
 - We can overweight “guidance”, $\nabla_{\mathbf{X}_t} \ln P_t(\mathbf{X}_t) + \gamma \nabla_{\mathbf{X}_t} \ln P(Y=y | \mathbf{X}_t)$



Classifier Free Guidance

- What if we don't want to train a separate classifier model?
- Consider $dX_t = f_t^+ (X_t, t) - \sigma_t^2 \left(\nabla_{X_t} \ln P_t(X_t) + \nabla_{X_t} \ln P(Y = y | X_t) \right) dt + \sigma_t d\bar{W}_t$,
 - From Bayes' rule, $\nabla_{X_t} \ln p(X_t | y) = \nabla_{X_t} \ln p(X_t) + \nabla_{X_t} \ln p(y | X_t)$
 - Train a single model to approximate both $p(X_t | y)$ and $p(X_t)$ on (X_0, y) inputs
 - Occasionally, 10-20% of the time, drop y to learn $p(X_t)$, otherwise $p(X_t | y)$
 - At inference time, $\nabla_x \log p_\gamma(x | y) = \nabla_x \log p(x) + \gamma (\nabla_x \log p(x | y) - \nabla_x \log p(x))$



Amortised training of h -transform

- Can we learn a score model for the h -transform directly?
- Consider $dX_t = f_t^+ (X_t, t) - \sigma_t^2 \left(\nabla_{X_t} \ln P(X_t | y) \right) dt + \sigma_t d\bar{W}_t$,
- Let us learn a score model $f(t, X_t, y, \mathcal{A})$ to approximate $\nabla_{X_t} \ln p(X_t | y)$

$$f^* = \arg \min_f \mathbb{E}_{Y \sim p_{|\mathcal{A}, X_0}, \mathcal{A} \sim p, X_0 \sim p_{\text{data}}} \left[\int_0^T \left\| f(t, X_t, y, \mathcal{A}) - \nabla_{X_t} \ln \vec{p}_{t|0}(X_t | X_0) \right\|^2 dt \right]$$

- Sample $X_0 \sim p_{\text{data}}$, sample an operator \mathcal{A} , sample $y \sim p(y | X_0, \mathcal{A})$
- We “amortise” the score model over y and \mathcal{A}
- The minimiser is given by the conditional score

$$f^*(t, X_t, y, A) = \nabla_{x_t} \ln p_{t|0}(X_t | Y = y, \mathcal{A} = A)$$

Proof of minimiser of loss function

$$\begin{aligned} f(x_t, y, A) &= \mathbb{E}_{X_0|X_t=x_t, Y=y, \mathcal{A}=A} \left[\nabla_{X_t} \ln p_{t|0}(X_t | X_0) \right] \\ &= \int \nabla_{x_t} \ln p_{t|0}(x_t | X_0) p_{0|t}(X_0 | x_t, y, A) dX_0 && \text{(Write expectation as integral)} \\ &= \int \nabla_{x_t} \ln p_{t|0}(x_t | X_0) \frac{p_{t|0}(x_t | X_0) p_0(X_0)}{p_t(x_t | y, A)} dX_0 && \text{(Bayes' rule)} \\ &= \int \frac{\nabla_{x_t} p_{t|0}(x_t | X_0)}{p_{t|0}(x_t | X_0)} \frac{p_{t|0}(x_t | X_0) p_0(X_0)}{p_t(x_t | y, A)} dX_0 && \text{(Expand the gradient of log)} \\ &= \frac{1}{p_t(x_t | y, A)} \int \frac{\nabla_{x_t} p_{t|0}(x_t | X_0)}{p_{t|0}(x_t | X_0)} p_{t|0}(x_t | X_0) p_0(X_0) dX_0 && \text{(Cancel terms)} \\ &= \frac{1}{p_t(x_t | y, A)} \int \nabla_{x_t} \left[p_{t|0}(x_t | X_0) \right] p_t(x_t | y, A) dX_0 && \text{(Swap integral derivative - Dominated Convergence Theorem)} \\ &= \frac{1}{p_t(x_t | y, A)} \nabla_{x_t} \int \left[p_{t|0}(x_t | x_0) \right] p_t(x_t | y, A) dX_0 && \text{(Marginalise over } X_0\text{)} \\ &= \frac{1}{p_t(x_t | y, A)} \nabla_{x_t} p_t(x_t | y, A) \\ &= \nabla_{x_t} \ln p_t(x_t | y, A) \end{aligned}$$