A. Existence of Unified Flow Operator

Theorem 2.3. *For the optimal control problem in Eq. (13) and Eq. (14), there exists an open-loop control* $w^* = w^*(q(\boldsymbol{x},0),t)$ *such that the induced state* $q^*(\boldsymbol{x},t)$ *satisfies* $q^*(\boldsymbol{x},\infty) = p(\boldsymbol{x}|\mathcal{O}_{m+1})$. *Moreover,* w^* *has a fixed expression with respect to* $p(\boldsymbol{x}|\mathcal{O}_m)$ *and* $p(o_{m+1}|\boldsymbol{x})$ *across different* m.

Proof. By Theorem 2.2, $\tilde{w}^*(q(\boldsymbol{x},t),t) := \nabla_x \log q(\boldsymbol{x},t)$ can induce the optimal state $\tilde{q}^*(\boldsymbol{x},\infty) = p(\boldsymbol{x}|\mathcal{O}_{m+1})$ and achieve a zero loss, $d = 0$. Hence, $\tilde{w}^*$ is an optimal closed-loop control for this problem.

Although in general closed-loop control has a stronger characterization to the solution, in a deterministic system like Eq. (14), the optimal closed-loop control and the optimal open-loop control will give the same control law and thus the same optimality to the loss function(Dreyfus, 1964). Hence, there exists an optimal open-loop control $w^* = w^*(q(\boldsymbol{x},0),t)$ such that the induced optimal state also gives a zero loss and thus $q^*(\boldsymbol{x},\infty) = p(\boldsymbol{x}|\mathcal{O}_{m+1})$.

More specifically, when the system is deterministic, a state $q(\boldsymbol{x},t)$ is just a deterministic result of the initial state $q(\boldsymbol{x},0)$ and the dynamics. The optimal flow determined by $\tilde{w}^*(q(\boldsymbol{x},t),t)$ is

$$f = \nabla_x \log p(\boldsymbol{x}|\mathcal{O}_m)p(o_{m+1}|\boldsymbol{x}) - \nabla_x \log q(\boldsymbol{x},t).$$

The continuity equation gives

$$\begin{aligned}\frac{\partial q(\boldsymbol{x},t)}{\partial t} =& -\nabla_x \cdot (q\nabla_x \log p(\boldsymbol{x}|\mathcal{O}_m)p(o_{m+1}|\boldsymbol{x})) \\ &+ \Delta_x q(\boldsymbol{x},t) \\ :=& \, g(p(\boldsymbol{x}|\mathcal{O}_m)p(o_{m+1}|\boldsymbol{x}), q(\boldsymbol{x},t))\end{aligned}$$

Hence, for any $\boldsymbol{x}$,

$$q(\boldsymbol{x},t) = q(\boldsymbol{x},0) + \int_0^t g(p(\boldsymbol{x}|\mathcal{O}_m)p(o_{m+1}|\boldsymbol{x}), q(\boldsymbol{x},t))\, d\tau.$$

The dynamcis g is a fixed function of $p(\boldsymbol{x}|\mathcal{O}_m)$, $p(o_{m+1}|\boldsymbol{x})$ and $q(\boldsymbol{x},t)$, so the solution of this initial value problem(IVP) $q(\boldsymbol{x},t)$ is a fixed function of $p(\boldsymbol{x}|\mathcal{O}_m)$, $p(o_{m+1}|\boldsymbol{x})$, $q(\boldsymbol{x},0)$ and t, which can be written as

$$q(\boldsymbol{x},t) = \text{Solve-IVP}(p(\boldsymbol{x}|\mathcal{O}_m), p(o_{m+1}|\boldsymbol{x}), q(\boldsymbol{x},0), t).$$

Finally, we can write the optimal open-loop control as

$$\begin{aligned}&w^*(q(\boldsymbol{x},0),t) \\ =&\nabla_x \log(\text{Solve-IVP}(p(\boldsymbol{x}|\mathcal{O}_m), p(o_{m+1}|\boldsymbol{x}), q(\boldsymbol{x},0), t)).\end{aligned}$$

Hence, $w^*(q(\boldsymbol{x},0),t)$ has a fixed form across different m.

□

B. Adjoint Method

To explain it more clearly, let us denote the evolution of the n-th particles at the m-th stage by $\boldsymbol{x}_m^n(t)$ for $t \in [0,T]$. Note that $\boldsymbol{x}_m^n(T) = \boldsymbol{x}_{m+1}^n(0)$. (Then the notation $\boldsymbol{x}_m^n$ in the main text will become $\boldsymbol{x}_m^n(T)$.)

Recall the loss for each task:

$$\mathcal{L}(\mathcal{T}) = \frac{1}{MN}\sum_{m=1}^{M}\sum_{n=1}^{N}\left(\log q_m^n(\boldsymbol{x}_m^n(T),T) - \log p(\boldsymbol{x}_m^n(T),\mathcal{O}_m)\right).$$

The loss of one particle $\boldsymbol{x}^n$ is

$$L^n := \frac{1}{M}\sum_{m=1}^{M} L_m^n,$$

where

$$L_m^n := -y_m^n(T) - \log p(\boldsymbol{x}_m^n(T),\mathcal{O}_m)$$

and $y_m^n(t) := -\log q_m^n(x_m^n(t), t)$.

First, an adjoint process is defined as

$$\boldsymbol{p}_m(t) := \frac{\partial L^n}{\partial[\boldsymbol{x}_m^n(t), y_m^n(t)]}.$$

Denote $f_m(\boldsymbol{x}(t), \theta) = f_\theta(\mathcal{X}_m, o_{m+1}, \boldsymbol{x}(t), t)$. During the m-th stage, the adjoint process follows the following differential equation

$$\frac{d\boldsymbol{p}_m}{dt} = -\frac{\partial}{\partial[\boldsymbol{x}_m^n(t), y_m^n(t)]} \begin{bmatrix} f_m(\boldsymbol{x}_m^n(t), \theta) \\ \nabla_{\boldsymbol{x}} \cdot f_m(\boldsymbol{x}_m^n(t), \theta) \end{bmatrix}^\top \boldsymbol{p}_m(t). \tag{21}$$

Note that

$$\boldsymbol{p}_m(T) = \sum_{m' \geq m} \frac{1}{M} \frac{\partial L_{m'}^n}{\partial[\boldsymbol{x}_m^n(T), y_m^n(T)]}. \tag{22}$$

Claim: The gradient of the loss is the solution of a backward ODE. That is to say, $\frac{\partial L^n}{\partial \theta} = \boldsymbol{z}_1(0)$, if $\boldsymbol{z}_M(T) = \mathbf{0}$ and

$$\frac{d\boldsymbol{z}_m(t)}{dt} = -\begin{bmatrix} \frac{\partial f_m}{\partial \theta}(\boldsymbol{x}_m^n(t), \theta) \\ \frac{\partial}{\partial \theta}\left[\nabla_{\boldsymbol{x}} \cdot f_m(\boldsymbol{x}_m^n(t), \theta)\right] \end{bmatrix}^\top \boldsymbol{p}_m(t), \tag{23}$$

and $\boldsymbol{z}_m(T) = \boldsymbol{z}_{m+1}(0)$, for $m = 0, \cdots, M-1$.

Proof. First, we can compute $\frac{d}{dt}\frac{\partial L^n}{\partial \theta}$:

$$\begin{aligned}
\frac{d}{dt}\frac{\partial L^n}{\partial \theta} &= \frac{\partial}{\partial \theta} \sum_{m=1}^{M} \left(\frac{\partial L^n}{\partial \boldsymbol{x}_m^n(t)}^\top \frac{d\boldsymbol{x}_m^n(t)}{dt} + \frac{\partial L^n}{\partial y_m^n(t)} \frac{dy_m^n(t)}{dt} \right) \\
&= \frac{\partial}{\partial \theta} \sum_{m=1}^{M} \left[\boldsymbol{p}_m(t)^\top \begin{bmatrix} f_m(\boldsymbol{x}_m^n(t), \theta) \\ \nabla_{\boldsymbol{x}} \cdot f_m(\boldsymbol{x}_m^n(t), \theta) \end{bmatrix} \right] \\
&= \sum_{m=1}^{M} \begin{bmatrix} \frac{\partial f_m}{\partial \theta}(\boldsymbol{x}_m^n(t), \theta) \\ \frac{\partial}{\partial \theta}\left[\nabla_{\boldsymbol{x}} \cdot f_m(\boldsymbol{x}_m^n(t), \theta)\right] \end{bmatrix}^\top \boldsymbol{p}_m(t)
\end{aligned}$$

Next, we have

$$0 - \frac{\partial L^n}{\partial \theta} = -\int_{t=0}^{T} \frac{d}{dt}\frac{\partial L^n}{\partial \theta} = \sum_{m=1}^{M} \int_{t=0}^{T} -\begin{bmatrix} \frac{\partial f_m}{\partial \theta}(\boldsymbol{x}_m^n(t), \theta) \\ \frac{\partial}{\partial \theta}\left[\nabla_{\boldsymbol{x}} \cdot f_m(\boldsymbol{x}_m^n(t), \theta)\right] \end{bmatrix}^\top \boldsymbol{p}_m(t) = \boldsymbol{z}_M(T) - \boldsymbol{z}_1(0).$$

Hence, $\frac{\partial L^n}{\partial \theta} = \boldsymbol{z}_1(0)$ if $\boldsymbol{z}_M(T) = \mathbf{0}$. □

An algorithm for computing $\frac{\partial L}{\partial \theta}$ is summarized in Algorithm 2. A nice python package of realizing this algorithm is provided by Chen et al. (2018).

Algorithm 2 Adjoint Method of Computing the Gradient

Function `Grad`$(\theta, \mathcal{X}_0, p(o|\boldsymbol{x}), \mathcal{O}_M)$**:**
  Denote $f_\theta^m = f_\theta(\mathcal{X}_m, o_{m+1}, \boldsymbol{x}(t), t)$ ▷ notation
  Set $y_0^n = -\log p(\boldsymbol{x}_0^n)$ for each $\boldsymbol{x}_0^n \in \mathcal{X}_0$
  For all $n = 1$ *to* N **do**
    For $m = 0$ *to* $M-1$ **do**
      $\begin{bmatrix} \boldsymbol{x}_{m+1}^n \\ y_{m+1}^n \end{bmatrix} \leftarrow \begin{bmatrix} \boldsymbol{x}_m^n \\ y_m^n \end{bmatrix} + \int_0^T \begin{bmatrix} f_\theta^m \\ \nabla \cdot f_\theta^m \end{bmatrix} dt$
    Set $\boldsymbol{p}_M^n(T) = \mathbf{0}$ and $\boldsymbol{z}_M^n(T) = \mathbf{0}$
    For $m = M$ *to* 1 **do**
      $\boldsymbol{p}_m^n(T) \leftarrow \boldsymbol{p}_m^n(T) + \frac{1}{M} \frac{\partial L_m^n}{\partial [\boldsymbol{x}_m^n, y_m^n]}$
      Solve ODEs in Eq. (4), Eq. (8), Eq. (21) and Eq. (23) for $\boldsymbol{x}_m^n(t)$, $\boldsymbol{p}_m^n(t)$ and $\boldsymbol{z}_m^n(t)$ backwardly from T to 0
      Set $\boldsymbol{x}_{m-1}^n(T) = \boldsymbol{x}_m^n(0)$, $\boldsymbol{p}_{m-1}^n(T) = \boldsymbol{p}_m^n(0)$ and $\boldsymbol{z}_{m-1}^n(T) = \boldsymbol{z}_m^n(0)$
  return $\frac{1}{N}\sum_{n=1}^N \frac{\partial L^n}{\partial \theta} = \frac{1}{N}\sum_{n=1}^N \boldsymbol{z}_1^n(0)$

C. Experiment Details

C.1. Parameterization

Overall we parameterize the flow velocity as

$$f = \boldsymbol{h}\left(\tfrac{1}{N}\textstyle\sum_{n=1}^N \boldsymbol{\phi}(\boldsymbol{x}_m^n), o_{m+1}, \boldsymbol{x}(t), t\right),$$

where both $\boldsymbol{\phi}$ and $\boldsymbol{h}$ are neural networks. For instance, let $\text{ctx} = [\frac{1}{N}\sum_{n=1}^N \boldsymbol{\phi}(\boldsymbol{x}_m^n)^\top, o_{m+1}^\top]$ be the context of this conditional flow, where $\boldsymbol{\phi}$ is a dense feed-forward neural network, a specific neural architecture we use in the experiment is

$$f = \text{Gated}_k\left(\cdots[\text{ctx}, \text{Gated}_2\left([\text{ctx}, \text{Gated}_1\left([\text{ctx}, \boldsymbol{x}(t)^\top]^\top, t\right)]^\top, t\right)]^\top \cdots, t\right), \tag{24}$$

$$\text{where Gated}_j(\boldsymbol{y}, t) = (W_j\boldsymbol{y} + \boldsymbol{b}_j) * \sigma(t\boldsymbol{v}_j + \boldsymbol{c}_j) + t\boldsymbol{c}_j, \tag{25}$$

where $*$ is element-wise multiplication. The number of layers k can be tuned, but in general $\boldsymbol{h}$ is a shallow network.

C.2. Evaluation Metric

MMD^2 The maximum mean discrepancy (MMD) of the true posterior p and the estimated posterior q is defined as

$$\text{MMD}[\mathcal{F}, p, q] := \sup_{f\in\mathcal{F}}(\mathbb{E}_{x\sim p}[f(x)] - \mathbb{E}_{y\sim q}[f(y)]).$$

When $\mathcal{F}$ is a unit ball in a characteristic RKHS, Gretton et al. (2012) showed that the squared MMD is

$$\text{MMD}^2[\mathcal{F}, p, q] = \mathbb{E}[k(x, x')] - 2\mathbb{E}[k(x, y)] + \mathbb{E}[k(y, y')],$$

where $x, x' \sim p$ and $y, y' \sim q$.

Cross-entropy Evaluating the KL divergence is equivalent to evaluating the cross-entropy.

$$\mathbb{E}_{x\sim p} - \log q(x) \approx \frac{1}{n}\sum_{n=1}^N (-\log q(x^n)), \tag{26}$$

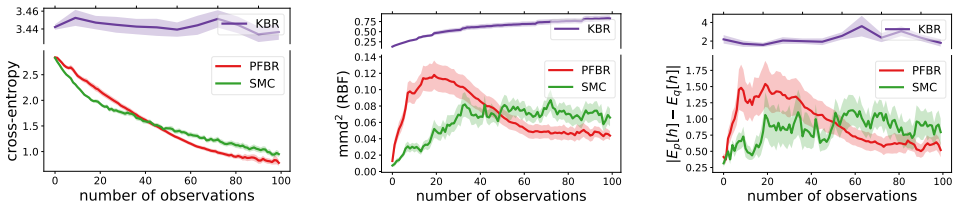
where $q(x)$ is approximated by kernel density estimation on the set of particles obtained from different sampling methods.

Integral Evaluation When the true posterior is a Gaussian distribution $\mathcal{N}(\mu, \Sigma)$, the expectation of the following test functions have closed-form expressions.

- $\mathbb{E}[\boldsymbol{x}] = \mu$
- $\mathbb{E}[\boldsymbol{x}^\top A\boldsymbol{x}] = tr(A\Sigma) + \mu^\top A\mu$
- $\mathbb{E}[(A\boldsymbol{x} + \boldsymbol{a})^\top(B\boldsymbol{x} + \boldsymbol{b})] = tr(A\Sigma B^\top) + (A\mu + \boldsymbol{a})^\top(B\mu + \boldsymbol{b})$

D. More Experimental Results

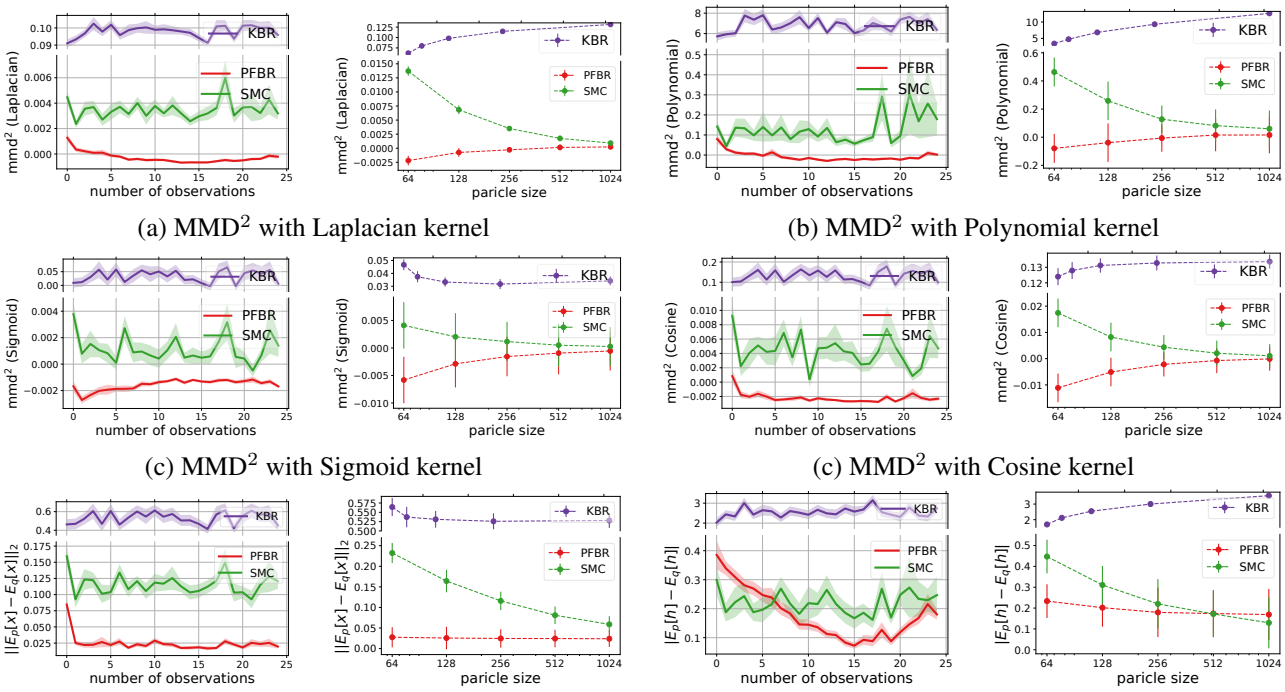
D.1. Multivariate Guassian Model



(a) cross-entropy (b) MMD^2 with RBF kernel (c) Integral estimation

Figure 7: Experimental results on 2 dimensional multivariate Gaussian model.

D.2. LDS Model



(a) MMD^2 with Laplacian kernel (b) MMD^2 with Polynomial kernel

(c) MMD^2 with Sigmoid kernel (c) MMD^2 with Cosine kernel

(d) Integral estimation on $h(\boldsymbol{x}) = \boldsymbol{x}$ (e) Integral estimation on $h(\boldsymbol{x}) = (A\boldsymbol{x} + \boldsymbol{a})^\top (B\boldsymbol{x} + \boldsymbol{b})$

Figure 8: Experimental results on LDS model.