Abstract

Wasserstein gradient flows provide a powerful means of understanding and solving many diffusion equations. Specifically, Fokker-Planck equations, which model the diffusion of probability measures, can be understood as gradient descent over entropy functionals in Wasserstein space. This equivalence, introduced by Jordan, Kinderlehrer and Otto, inspired the so-called JKO scheme to approximate these diffusion processes via an implicit discretization of the gradient flow in Wasserstein space. Solving the optimization problem associated to each JKO step, however, presents serious computational challenges. We introduce a scalable method to approximate Wasserstein gradient flows, targeted to machine learning applications. Our approach relies on input-convex neural networks (ICNNs) to discretize the JKO steps, which can be optimized by stochastic gradient descent. Unlike previous work, our method does not require domain discretization or particle simulation. As a result, we can sample from the measure at each time step of the diffusion and compute its probability density. We demonstrate our algorithm’s performance by computing diffusions following the Fokker-Planck equation and apply it to unnormalized density sampling as well as nonlinear filtering.

1 Introduction

Stochastic differential equations (SDEs) are used to model the evolution of random diffusion processes across time, with applications in physics [63], finance [22, 52], and population dynamics [35]. In machine learning, diffusion processes also arise in applications filtering [44, 21] and unnormalized posterior sampling via a discretization of the Langevin diffusion [70].

The time-evolving probability density $\rho_t$ of these diffusion processes is governed by the Fokker-Planck equation. Jordan, Kinderlehrer, and Otto [32] showed that the Fokker-Planck equation is
equivalent to following the gradient flow of an entropy functional in Wasserstein space, i.e., the space of probability measures with finite second order moment endowed with the Wasserstein distance. This inspired a simple minimization scheme called JKO scheme, which consists an implicit Euler discretization of the Wasserstein gradient flow. However, each step of the JKO scheme is costly as it requires solving a minimization problem involving the Wasserstein distance.

One way to compute the diffusion is to use a fixed discretization of the domain and apply standard numerical integration methods \cite{13, 49, 15, 17, 40} to get \( \rho_t \). For example, \cite{50} proposes a method to approximate the diffusion based on JKO stepping and entropy-regularized optimal transport. However, these methods are limited to small dimensions since the discretization of space grows exponentially.

Another way to avoid discretization is to parameterize the density of \( \rho \). An alternative to domain discretization is particle simulation. It involves drawing random samples \( \pi \) where the minimum is over measures \( \Pi(\mu, \nu) \). In particular, ICNNs \cite{37, 44, 38} gained attention for Wasserstein-2 transport since their gradients \( \nabla \psi \in \mathbb{R}^D \rightarrow \mathbb{R}^D \) can represent OT maps for the quadratic cost. These continuous solvers scale better to high dimension without discretizing the input measures, but they are too computationally expensive to be applied directly to JKO steps.

Recently, \cite{24} introduced a parametric method to compute JKO steps via entropy-regularized optimal transport. The authors regularize the Wasserstein distance in the JKO step to ensure strict convexity and solve the unconstrained dual problem via stochastic program on a finite linear subset of basis functions. The method yields unnormalized probability density without direct sample access.

Recent works propose scalable continuous optimal transport solvers, parametrizing the solutions by reproducing kernels \cite{10}, fully-connected neural networks \cite{62}, or Input Convex Neural Networks (ICNNs) \cite{37, 44, 38}. In particular, ICNNs gained attention for Wasserstein-2 transport since their gradients \( \nabla \psi : \mathbb{R}^D \rightarrow \mathbb{R}^D \) can represent OT maps for the quadratic cost. These continuous solvers scale better to high dimension without discretizing the input measures, but they are too computationally expensive to be applied directly to JKO steps.

Contributions. We propose a scalable parametric method to approximate Wasserstein gradient flows using JKO stepping and entropy-regularized optimal transport. The authors regularize the Wasserstein distance in the JKO step to ensure strict convexity and solve the unconstrained dual problem via stochastic program on a finite linear subset of basis functions. The method yields unnormalized probability density without direct sample access.

Notation. \( \mathcal{P}_2(\mathbb{R}^D) \) denotes the set of Borel probability measures on \( \mathbb{R}^D \) with finite second moment. \( \mathcal{P}_{2, \text{ac}}(\mathbb{R}^D) \) denotes its subset of probability measures absolutely continuous with respect to Lebesgue measure. For \( \rho \in \mathcal{P}_{2, \text{ac}}(\mathbb{R}^D) \), we denote by \( \frac{d\rho}{dx}(x) \) its density with respect to the Lebesgue measure. \( \Pi(\mu, \nu) \) denotes the set of probability measures on \( \mathbb{R}^D \times \mathbb{R}^D \) with marginals \( \mu \) and \( \nu \). For measurable \( T : \mathbb{R}^D \rightarrow \mathbb{R}^D \), we denote by \( T^\# \) the associated push-forward operator between measures.

2 Background on Wasserstein Gradient Flows

We consider gradient flows in Wasserstein space \( (\mathcal{P}_2(\mathbb{R}^D), \mathcal{W}_2) \), the space of probability measures with finite second moment on \( \mathbb{R}^D \) endowed with the Wasserstein-2 metric \( \mathcal{W}_2 \).

Wasserstein-2 distance. The (squared) Wasserstein-2 metric \( \mathcal{W}_2 \) between \( \mu, \nu \in \mathcal{P}_2(\mathbb{R}^D) \) is

\[
\mathcal{W}_2^2(\mu, \nu) \overset{\text{def}}{=} \min_{\pi \in \Pi(\mu, \nu)} \int_{\mathbb{R}^D \times \mathbb{R}^D} \|x - y\|^2 d\pi(x, y),
\]

where the minimum is over measures \( \pi \) on \( \mathbb{R}^D \times \mathbb{R}^D \) with marginals \( \mu \) and \( \nu \) respectively \cite{68}.
For $\mu \in \mathcal{P}_{2,ac}(\mathbb{R}^D)$, there exists a $\mu$-unique map $\nabla \psi^*: \mathbb{R}^D \to \mathbb{R}^D$ that is the gradient of a convex function $\psi^*: \mathbb{R}^D \to (-\infty, \infty]$ satisfying $\nabla \psi^* \sharp \mu = \nu$ [46]. From Brenier’s theorem [13], it follows that $\pi^* = [\text{id}_{\mathbb{R}^D}, \nabla \psi^*] \sharp \mu$ is the unique minimizer of (1), i.e.,

$$W_2^2(\mu, \nu) = \int_{\mathbb{R}^D} ||x - \nabla \psi^*(x)||^2_2 \, d\mu(x).$$

**Wasserstein Gradient Flows.** In the Euclidean case, gradient flows along a function $W$ follows the steepest descent direction, but this time the notion of gradient is more complex. We refer the reader to [4] for exposition of gradient flows in metric spaces, or [59] Chapter 8 for an accessible introduction.

A curve of measures $\{\rho_t\}_{t \in \mathbb{R}}$ following the Wasserstein gradient flow of a functional $F$ solves the continuity equation

$$\frac{\partial \rho_t}{\partial t} = \text{div}(\rho_t \nabla_x F'(\rho_t)), \quad \text{s.t. } \rho_0 = \rho^0, \quad (2)$$

where $F'()$ is the first variation of $F$ [4, Theorem 8.3.1]. The term on the right can be understood as the gradient of $F$ in Wasserstein space, a vector field perturbatively rearranging the mass in $\rho_t$ to yield the steepest possible local change of $F$.

Wasserstein gradient flows are used in various applied tasks. For example, gradient flows are applied in training [83] [43] [25] or refinement [2] of implicit generative models. In reinforcement learning, gradient flows facilitate policy optimization [55] [72]. Other tasks include crowd motion modelling [45] [58] [50], dataset optimization [2], and in-between animation [26].

Many applications come from the connection between Wasserstein gradient flows and SDEs. Consider an $\mathbb{R}^D$-valued stochastic process $\{X_t\}_{t \in \mathbb{R}}$ governed by the following Itô SDE:

$$dX_t = -\nabla \Phi(X_t) \, dt + \sqrt{2\beta^{-1}} \, dW_t, \quad \text{s.t. } X_0 \sim \rho^0 \quad (3)$$

where $\Phi: \mathbb{R}^D \to \mathbb{R}$ is the potential function, $W_t$ is the standard Wiener process, and $\beta > 0$ is the magnitude. The solution of (3) is called an advection-diffusion process. The marginal measure $\rho_t$ of $X_t$ at each time satisfies the Fokker-Planck equation with fixed diffusion coefficient:

$$\frac{\partial \rho_t}{\partial t} = \text{div}(\nabla \Phi(x) \rho_t) + \beta^{-1} \Delta \rho_t, \quad \text{s.t. } \rho_0 = \rho^0. \quad (4)$$

Equation (4) is the Wasserstein gradient flow [4] for $F$ given by the Fokker-Planck free energy functional [32]

$$FP_F(\rho) = U(\rho) - \beta^{-1} \mathcal{E}(\rho), \quad (5)$$

where $U(\rho) = \int_{\mathbb{R}^D} \Phi(x) \, d\rho(x)$ is the potential energy and $\mathcal{E}(\rho) = \int_{\mathbb{R}^D} \log \frac{d\rho}{d\mu}(x) \, d\rho(x)$ is the entropy. As the result, to solve the SDE (3), one may compute the Wasserstein gradient flow of the Fokker-Planck equation with the free-energy functional $FP_F$ given by (5).

**JKO Scheme.** Computing Wasserstein gradient flows is challenging. The closed form solution is typically unknown, necessitating numerical approximation techniques. Jordan, Kinderlehrer, and Otto proposed a method—later abbreviated as JKO integration—to approximate the dynamics of $\rho_t$ in [9] [32]. It consists of a time-discretization update of the continuous flow given by:

$$\rho^{(k)} \leftarrow \arg \min_{\rho \in \mathcal{P}_a(\mathbb{R}^n)} \left[ F(\rho) + \frac{1}{2h} W_2^2(\rho^{(k-1)}, \rho) \right], \quad (6)$$

where $\rho^{(0)} = \rho^0$ is the initial condition and $h > 0$ is the time-discretization step size. The discrete time gradient flow converges to the continuous one as $h \to 0$, i.e., $\rho^{(k)} \approx \rho_{kh}$. The method was further developed in [4] [60], but performing JKO iterations remains challenging thanks to the minimization with respect to $W_2$.

A common approach to perform JKO steps is to discretize the spatial domain. For support size $\lesssim 10^6$, (6) can be solved by standard optimal transport algorithms [51]. In dimensions $D \geq 3$, discrete supports can hardly approximate continuous distributions and hence the dynamics of gradient flows. To tackle this issue, [24] propose a stochastic parametric method to approximate the density of $\rho_t$. Their method uses entropy-regularized optimal transport (OT), which is biased.
We propose to parametrize the search space using input convex neural networks (ICNNs) \cite{20}. Thanks to Brenier’s theorem, for any \( \rho \in \mathcal{P}_{2,ac} \) there exists a unique \( \rho^{(k-1)} \)-measurable gradient \( \nabla \psi : \mathbb{R}^D \rightarrow \mathbb{R}^D \) of a convex function \( \psi \) satisfying \( \rho = \nabla \psi \rho^{(k-1)} \). We set \( \rho = \nabla \psi \rho^{(k-1)} \) and rewrite \( 6 \) as an optimization over convex \( \psi \):

\[
\psi^{(k)} \leftarrow \arg \min_{\text{Convex } \psi} \left[ F(\nabla \psi \rho^{(k-1)}) + \frac{1}{2h} \mathcal{W}_2^2(\rho^{(k-1)}, \nabla \psi \rho^{(k-1)}) \right]. 
\]

To proceed to the next step of JKO scheme, we define \( \rho^{(k)} \equiv \nabla \psi^{(k)} \rho^{(k-1)} \).

Since \( \rho \) is the pushforward of \( \rho^{(k-1)} \) by the gradient of a convex function \( \nabla \psi \), the \( \mathcal{W}_2^2 \) term in \( 7 \) can be evaluated explicitly, simplifying the Wasserstein-2 distance term in \( 7 \):

\[
\psi^{(k)} \leftarrow \arg \min_{\text{Convex } \psi} \left[ F(\nabla \psi \rho^{(k-1)}) + \frac{2h}{2} \int_{\mathbb{R}^D} \|x - \nabla \psi(x)\|_2^2 d\rho^{(k-1)}(x) \right]. 
\]

This formulation avoids the difficulty of computing Wasserstein-2 distances. An additional advantage is that we can sample from \( \psi^{(k)} \). Since \( \rho^{(k)} = [\nabla \psi(0) \circ \cdots \circ \nabla \psi(1)]_{\#} \rho^0 \), one may sample \( x_0 \sim \rho^0 \), and then \( \nabla \psi(0) \circ \cdots \circ \nabla \psi(1)(x_0) \) gives a sample from \( \rho^{(k)} \). Moreover, if functions \( \psi^{(i)} \) are strictly convex, then gradients \( \nabla \psi^{(i)} \) are invertible. In this case, the density \( \frac{d\rho^{(k)}}{dx}(x_k) = [\det \nabla^2 \psi^{(k)}(x_{k-1})]^{-1} \cdots [\det \nabla^2 \psi^{(1)}(x_0)]^{-1} \frac{d\rho^{(0)}}{dx}(x_0) \),

where \( x_i = \nabla \psi^{(i)}(x_{i-1}) \) for \( i = 1, \ldots, k \) and \( \frac{d\rho^{(0)}}{dx} \) is the density of \( \rho^0 \).

We now describe our approach to compute Wasserstein gradient flows via JKO stepping with ICNNs.

### 3.1 JKO Reformulation via Optimal Push-forwards Maps

Our key idea is to replace the optimization \( 6 \) over probability measures by an optimization over convex functions, an idea inspired by \cite{11}. Thanks to Brenier’s theorem, for any \( \rho \in \mathcal{P}_{2,ac} \) there exists a unique \( \rho^{(k-1)} \)-measurable gradient \( \nabla \psi : \mathbb{R}^D \rightarrow \mathbb{R}^D \) of a convex function \( \psi \) satisfying \( \rho = \nabla \psi \rho^{(k-1)} \). We set \( \rho = \nabla \psi \rho^{(k-1)} \) and rewrite \( 6 \) as an optimization over convex \( \psi \):

\[
\psi^{(k)} \leftarrow \arg \min_{\text{Convex } \psi} \left[ F(\nabla \psi \rho^{(k-1)}) + \frac{1}{2h} \mathcal{W}_2^2(\rho^{(k-1)}, \nabla \psi \rho^{(k-1)}) \right]. 
\]

This formulation avoids the difficulty of computing Wasserstein-2 distances. An additional advantage is that we can sample from \( \psi^{(k)} \). Since \( \rho^{(k)} = [\nabla \psi(0) \circ \cdots \circ \nabla \psi(1)]_{\#} \rho^0 \), one may sample \( x_0 \sim \rho^0 \), and then \( \nabla \psi(0) \circ \cdots \circ \nabla \psi(1)(x_0) \) gives a sample from \( \rho^{(k)} \). Moreover, if functions \( \psi^{(i)} \) are strictly convex, then gradients \( \nabla \psi^{(i)} \) are invertible. In this case, the density \( \frac{d\rho^{(k)}}{dx}(x_k) = [\det \nabla^2 \psi^{(k)}(x_{k-1})]^{-1} \cdots [\det \nabla^2 \psi^{(1)}(x_0)]^{-1} \frac{d\rho^{(0)}}{dx}(x_0) \),

where \( x_i = \nabla \psi^{(i)}(x_{i-1}) \) for \( i = 1, \ldots, k \) and \( \frac{d\rho^{(0)}}{dx} \) is the density of \( \rho^0 \).

### 3.2 Stochastic Optimization for JKO via ICNNs

In general, the solution \( \psi^{(k)} \) of \( 8 \) is intractable since it requires optimization over all convex functions. To tackle this issue, \cite{11} discretizes the space of convex function. The approach also requires discretization of measures \( \rho^{(k)} \) limiting this method to small dimensions.

We propose to parametrize the search space using input convex neural networks (ICNNs) \cite{20} satisfying a universal approximation property among convex functions \cite{20}. ICNNs are parametric models of the form \( \psi_\theta : \mathbb{R}^D \rightarrow \mathbb{R} \) with \( \psi_\theta \) convex w.r.t. the input. ICNNs are constructed from neural network layers, with restrictions on the weights and activation functions to preserve the input-convexity, see \cite{20} §3.1 or \cite{37} §B.2. The parameters are optimized via deep learning optimization techniques such as SGD.

The JKO step then becomes finding the optimal parameters \( \theta^* \) for \( \psi_\theta \):

\[
\theta^* \leftarrow \arg \min_{\theta} \left[ F(\nabla \psi_\theta \rho^{(k-1)}) + \frac{1}{2h} \int_{\mathbb{R}^D} \|x - \nabla \psi_\theta(x)\|_2^2 d\rho^{(k-1)}(x) \right]. 
\]

If the functional \( F \) can be estimated stochastically using random batches from \( \rho^{(k-1)} \), then SGD can be used to optimize \( \theta \). \( F_{\text{PP}} \) given by \( 5 \) is an example of such a functional:

**Theorem 1** (Estimator of \( F_{\text{PP}} \)). Let \( \rho \in \mathcal{P}_{2,ac}(\mathbb{R}^D) \) and \( T : \mathbb{R}^D \rightarrow \mathbb{R}^D \) be a diffeomorphism. For a random batch \( x_1, \ldots, x_N \sim \rho \), the expression \( [\widehat{U}_T(x_1, \ldots, x_N) - \beta^{-1} \Delta \widehat{E}_T(x_1, \ldots, x_N)] \), where

\[
\widehat{U}_T(x_1, \ldots, x_N) \overset{\text{def}}{=} \frac{1}{N} \sum_{n=1}^{N} \Phi(T(x_n)) \text{ and}
\]

\[
\Delta \widehat{E}_T(x_1, \ldots, x_N) \overset{\text{def}}{=} \frac{1}{N} \sum_{n=1}^{N} \log |\det T(x_n)|,
\]

is an estimator of \( F_{\text{PP}}(T_\# \rho) \) up to constant (w.r.t. \( T \)) shift given by \( \beta^{-1} \mathcal{E}(\rho) \).
Proof. \( \hat{U}_T \) is a straightforward unbiased estimator for \( \mathcal{U}(T\rho) \). Let \( p \) and \( p_T \) be the densities of \( \rho \) and \( T\rho \). Since \( T \) is a diffeomorphism, we have \( p_T(y) = p(x) \cdot |\det \nabla T(x)|^{-1} \) where \( x = T^{-1}(y) \). Using the change of variables formula, we write

\[
\mathcal{E}(T\rho) = -\int_{\mathbb{R}^D} p_T(y) \log p_T(y) dy
\]

\[
= -\int_{\mathbb{R}^D} p(x) \cdot |\det \nabla T(x)|^{-1} \log \left[p(x) \cdot |\det \nabla T(x)|^{-1}\right] \cdot |\det \nabla T(x)| dx
\]

\[
= -\int_{\mathbb{R}^D} p(x) \log p(x) dx + \int_{\mathbb{R}^D} p(x) \log |\det \nabla T(x)| dx
\]

\[
= \mathcal{E}(\rho) + \int_{\mathbb{R}^D} p(x) \log |\det \nabla T(x)| dx,
\]

\[
\implies \mathcal{E}_T(\rho) \overset{\text{def}}{=} \mathcal{E}(T\rho) - \mathcal{E}(\rho) = \int_{\mathbb{R}^D} \log |\det \nabla T(x)| d\rho(x)
\]

which explains that \( \mathcal{E}_T \) is an unbiased estimator of \( \Delta \mathcal{E}_T(\rho) \). As the result, \( \hat{U}_T - \beta^{-1} \mathcal{E}_T \) is an estimator for \( \mathcal{F}_\Phi(T\rho) = \mathcal{U}(T\rho) - \beta^{-1} \mathcal{E}(T\rho) \) up to a shift of \( \beta^{-1} \mathcal{E}(\rho) \).

To apply Theorem 1 to our case, we take \( T \leftarrow \nabla \psi_0 \) and \( \rho \leftarrow \rho^{(k-1)} \) to obtain a stochastic estimator for \( \mathcal{F}_\Phi(\nabla \psi_0 \rho^{(k-1)}) \) in (10). Here, \( \beta^{-1} \mathcal{E}(\rho^{(k-1)}) \) is \( \theta \)-independent and constant since \( \rho^{(k-1)} \) is fixed, so the offset of the estimator plays no role in the optimization w.r.t. \( \theta \).

Algorithm 1 details our stochastic JKO method for \( \mathcal{F}_\Phi \). The training is done solely based on random samples from the initial measure \( \rho^0 \): its density is not needed.

**Algorithm 1:** Fokker-Planck JKO via ICNNs

**Input:** Initial measure \( \rho^0 \) accessible by samples;
- JKO discretization step \( h > 0 \), number of JKO steps \( K > 0 \);
- target potential \( \Phi(x) \), diffusion process temperature \( \beta^{-1} \);
- batch size \( N \);

**Output:** Trained ICNN models \( \{\psi^{(k)}\}_{k=1}^K \) representing JKO steps

for \( k = 1, 2, \ldots, K \) do

\[ \psi_0 \leftarrow \text{basic ICNN model} \]

for \( i = 1, 2, \ldots \) do

\[ X \leftarrow \nabla \psi^{(k-1)} \circ \cdots \circ \nabla \psi^{(1)}(Z); \]

\[ W_2 \leftarrow \frac{1}{N} \sum_{x \in X} \| \nabla \psi_{0}(x) - x \|_2^2; \]

\[ \hat{U} \leftarrow \frac{1}{N} \sum_{x \in X} \Phi(\nabla \psi_{0}(x)); \]

\[ \hat{\mathcal{E}} \leftarrow \frac{1}{N} \sum_{x \in X} \log |\det \nabla^2 \psi_{0}(x); \]

\[ \hat{\mathcal{E}} \leftarrow \hat{\mathcal{E}} + \hat{U} - \beta^{-1} \hat{\mathcal{E}}; \]

Perform a gradient step over \( \theta \) by using \( \frac{\partial \hat{\mathcal{E}}}{\partial \theta} \);

\[ \psi^{(k)} \leftarrow \psi_0 \]

This algorithm assumes \( \mathcal{F} \) is the Fokker-Planck diffusion energy functional. However, our method admits straightforward generalization to any \( \mathcal{F} \) that can be stochastically estimated; studying such functionals is a promising avenue for future work.

### 3.3 Computing the Density of the Diffusion Process

Our algorithm provides a computable density for \( \rho^{(k)} \). As discussed in §3.1, it is possible to sample from \( \rho^{(k)} \) while simultaneously computing the density of the samples. However, this approach does not provide a direct way to evaluate \( \frac{d\rho^{(k)}}{dx}(x_k) \) for arbitrary \( x_k \in \mathbb{R}^D \). We resolve this issue below.
If a convex function is strongly convex, then its gradient is bijective on $\mathbb{R}^D$. By the change of variables formula for $x_k \in \mathbb{R}^D$, it holds $\frac{d\rho^{(k)}}{dx}(x_k) = \frac{d\rho^{(k-1)}}{dx}(x_{k-1}) \cdot \left[\det \nabla^2 \psi^{(k)}(x_{k-1})\right]^{-1}$ where $x_k = \nabla \psi^{(k)}(x_{k-1})$. To compute $x_{k-1}$, one needs to solve the convex optimization problem:

$$x_k = \nabla \psi^{(k)}(x_{k-1}) \iff x_{k-1} = \arg \max_{x \in \mathbb{R}^D} \left[\langle x, x_k \rangle - \psi^{(k)}(x)\right].$$

(11)

If we know the density of $\rho^0$, to compute the density of $\rho^{(k)}$ at $x_k$ we solve $k$ convex problems

$$x_{k-1} = \arg \max_{x \in \mathbb{R}^D} \left[\langle x, x_k \rangle - \psi^{(k)}(x)\right] \quad \ldots \quad x_0 = \arg \max_{x \in \mathbb{R}^D} \left[\langle x, x_1 \rangle - \psi^{(1)}(x)\right]$$

to obtain $x_{k-1}, \ldots, x_0$ and then evaluate the density as

$$\frac{d\rho_k}{dx}(x_k) = \frac{d\rho^0}{dx}(x_0) \cdot \left[\prod_{i=1}^{k} \det \nabla^2 \psi^{(i)}(x_{i-1})\right]^{-1}.$$

Note the steps above provide a general method for tracing back the position of a particle along the flow, and density computation is simply a byproduct.

4 Experiments

In this section, we evaluate our method on toy and real-world applications. Our code is written in PyTorch and is publicly available at

https://github.com/PetrMokrov/Large-Scale-Wasserstein-Gradient-Flows

The experiments are conducted on a GTX 1080Ti. In most cases, we performed several random restarts to obtain mean and variation of the considered metric. As a result, experiments require about 100-150 hours of computation. The details are given in Appendix A.

Neural network architectures. In all experiments, we use the DenseICNN [37] Appendix B.2] architecture for $\psi_\theta$ in Algorithm 1 with SoftPlus activations. The network $\psi_\theta$ is twice differentiable w.r.t. the input $x$ and has bijective gradient $\nabla \psi_\theta : \mathbb{R}^D \to \mathbb{R}^D$ with positive semi-definite Hessian $\nabla^2 \psi_\theta(x) \succeq 0$ at each $x$. We use automatic differentiation to compute $\nabla \psi_\theta$ and $\nabla^2 \psi_\theta$.

Metric. To qualitatively compare measures, we use the symmetric Kullback-Leibler divergence

$$\text{SymKL}(\rho_1, \rho_2) \overset{\text{def}}{=} \text{KL}(\rho_1 \| \rho_2) + \text{KL}(\rho_2 \| \rho_1),$$

(12)

where $\text{KL}(\rho_1 \| \rho_2) \overset{\text{def}}{=} \int_{\mathbb{R}^D} \log \frac{d\rho_1}{d\rho_2} (x) d\rho_1(x)$ is the Kullback-Leibler divergence. For particle-based methods, we obtain an approximation of the distribution by kernel density estimation.

4.1 Convergence to Stationary Solution

Starting from an arbitrary initial measure $\rho^0$, an advection-diffusion process (4) converges to the unique stationary solution $\rho^*$ [56] with density

$$\frac{d\rho^*}{dx}(x) = Z^{-1} \exp(-\beta \Phi(x)),$$

(13)

where $Z = \int_{\mathbb{R}^D} \exp(-\beta \Phi(x)) dx$ is the normalization constant. This property makes it possible to compute the symmetric KL between the distribution to which our method converges and the ground truth, provided $Z$ is known.

We use $\mathcal{N}(0, 16I_D)$ as the initial measure $\rho^0$ and a random Gaussian mixture as the stationary measure $\rho^*$. In our method, we perform $K = 40$ JKO steps with step size $h = 0.1$. We compare with a particle simulation method (with $10^3, 10^4, 10^5$ particles) based on the Euler-Maruyama [EM] approximation [36] [89.2]. We repeat the experiment 5 times and report the averaged results in Figure 1.

In Figure 2 we present qualitative results of our method converging to the ground truth in $D = 13, 32$: the stationary measure in $D = 2, 4, \ldots, 12$
We choose $\rho$ we know for symmetric positive definite $A \in \mathbb{R}^{D \times D}$ and $b \in \mathbb{R}^{D}$. They are among the few examples where we know $\rho_t$ for any $t \in \mathbb{R}^+$ in closed form, when the initial measure $\rho^0$ is Gaussian [67]. This allows us to quantitatively evaluate the computed dynamics of the process, not just the stationary measure. We choose $A, b$ at random and set $p^0$ to be the standard Gaussian measure $\mathcal{N}(0, I_D)$. We approximate the dynamics of the process by our method with JKO step $h = 0.05$ and compute SymKL between the true $\rho_t$ and the approximate one at time $t = 0.5$ and $t = 0.9$. We repeat the experiment 15 times in dimensions $D = 1, 2, \ldots, 12$ and report the performance at in Figure 3. The baselines are [EM] with $10^3, 10^4, 5 \times 10^4$ particles, EM particle simulation endowed with the Proximal Recursion operator [EM PR] with $10^5$ particles [16], and the parametric dual inference method [24] for JKO steps [Dual JKO]. The detailed comparison for times $t = 0.1, 0.2, \ldots, 1$ is given in Appendix C.

4.3 Unnormalized Posterior Sampling in Bayesian Logistic Regression

An important task in Bayesian machine learning to which our algorithm can be applied is sampling from an unnormalized posterior distribution. Given the model parameters $x \in \mathbb{R}^D$ with the prior distribution $p_0(x)$ as well as the conditional density $p(S|x) = \prod_{m=1}^M p(s_m|x)$ of the data $S = \{s_1, \ldots, s_M\}$, the posterior distribution is given by

$$p(x|S) = \frac{p(S|x)p_0(x)}{p(S)} \propto p(S|x)p_0(x) = p_0(x) \cdot \prod_{m=1}^M p(s_m|x).$$

Computing the normalization constant $p(S)$ is in general intractable, underscoring the need for estimation methods that sample from $p(S|x)$ given the density only up to a normalizing constant.
In our context, sampling from \( p(x|S) \) can be solved similarly to the task in [4.1]. From (13), it follows that the advection-diffusion process with temperature \( \beta > 0 \) and \( \Phi(x) = -\frac{1}{2} \log \left[ p_0(x) \cdot p(S|x) \right] \), has \( \frac{d\rho}{dx}(x) = p(x|S) \) as the stationary distribution. Thus, we can use our method to approximate the diffusion process and obtain a sampler for \( p(x|S) \) as a result.

The potential energy \( U(x) = \Phi(x) - \log p(x|S) \) can be estimated efficiently by using a trick similar to the ones in stochastic gradient Langevin dynamics [70], which consists in resampling samples in \( S \) uniformly. For evaluation, we consider the Bayesian linear regression setup of [42]. We use the 8 datasets from [47]. The number of features ranges from 2 to 60 and the dataset size from 700 to 7400 data points. We also use the Covertype dataset[4] with 500K data points and 54 features. The prior on regression weights \( w \) is given by \( p_0(w|\alpha) = \mathcal{N}(w|0,\alpha^{-1}) \) with \( p_0(\alpha) = \text{Gamma}(\alpha|1, 0.01) \), so the prior on parameters \( x = [w, \alpha] \) of the model is given by \( p_0(x) = p_0(w|\alpha) \cdot p_0(\alpha) \). We randomly split each dataset into train \( S_{\text{train}} \) and test \( S_{\text{test}} \) ones with ratio 4:1 and apply the inference on the posterior \( p(x|S_{\text{train}}) \). In Table 1 we report accuracy and log-likelihood of the predictive distribution on \( S_{\text{test}} \). As the baseline, we use particle-based Stein Variational Gradient Descent [42]. We use the author’s implementation with the default hyper-parameters.

### 4.4 Nonlinear Filtering

We demonstrate the application of our method to filtering a nonlinear diffusion. In this task, we consider a diffusion process \( X_t \) governed by the Fokker-Planck equation [4]. At times \( t_1 < t_2 < \cdots < t_K \) we obtain noisy observations of the process \( Y_k = X_{t_k} + v_k \), where \( v_k \sim \mathcal{N}(0, \sigma) \). The goal is to compute the predictive distribution \( p_{t_k}(x|Y_{1:k}) \) for \( t \geq t_k \) given observations \( Y_{1:k} \).

For each \( k \) and \( t \geq t_k \), the predictive distribution \( p_{t_k}(x|Y_{1:k}) \) follows the diffusion process on time interval \( [t_k, t] \) with initial distribution \( p_{t_k}(x|Y_{1:k}) \). If \( t_k = t \) then

\[
p_{t_k}(x|Y_{1:k}) \propto p(Y_k|X_{t_k} = x) \cdot p_{t_k}(x|Y_{1:k-1}).
\]

For \( k = 1, \ldots, K \), we sequentially obtain the predictive distribution \( p_{t_k}(x|Y_{1:k}) \) by using the previous predictive distribution \( p_{t_k-1}(x|Y_{1:k-1}) \). First, given access to \( p_{t_k-1}(x|Y_{1:k-1}) \), we approximate the diffusion on interval \( [t_{k-1}, t_k] \) with initial distribution \( p_{t_k-1}(x|Y_{1:k-1}) \) by our Algorithm 1 to get access to \( p_{t_k}(x|Y_{1:k-1}) \). Next, we use (14) to get unnormalized density and Metropolis-Hastings algorithm [57] to sample from \( p_{t_k}(x|Y_{1:k}) \). We give details in Appendix B.

For evaluation, we consider the experimental setup of [24] §6.3. We assume that the 1-dimensional diffusion process \( X_t \) has potential function \( \Phi(x) = \frac{1}{2} \sin(2\pi x) + \frac{1}{2} x^2 \) which makes the process highly nonlinear. We simulate nonlinear filtering on the time interval \( t_{\text{start}} = 0 \) sec., \( t_{\text{fin}} = 5 \) sec. and take the noise observations each 0.5 sec. The noise variance is \( \sigma^2 = 1 \) and \( p(X_0) = \mathcal{N}(X_0|0, 1) \).

We predict the conditional density \( p_{\text{test}}(x|Y_{1:9}) \) and compare the prediction with ground truth obtained with numerical integration method by Chang and Cooper [19], who use a fine discrete grid. As the baselines, we use [Dual JKO] [24] as well as the Bayesian Bootstrap filter [BBF] [27], which combines particle simulation with bootstrap resampling at observation times.

We repeat the experiment 15 times. In Figure 4a we report the SymKL between predicted density and true \( p(X_{t_{\text{fin}}}|Y_{1:9}) \). We visually compare the fitted and true conditional distributions in Figure 4b.

### 5 Discussion

**Complexity of training and sampling.** Let \( T \) be the number of operations required to evaluate ICNN \( \psi_{\theta}(x) \), and assume that the evaluation of \( \Phi(x) \) in the potential energy \( U \) takes \( O(1) \) time.

Table 1: Comparison of our method with [SVGD] [42] for Bayesian logistic regression.

| Dataset  | Accuracy | Log-Likelihood |
|----------|----------|----------------|
|          | Ours     | [SVGD]         | Ours     | [SVGD]         |
| covtype  | 0.75     | 0.75           | -0.515   | -0.515         |
| german   | 0.67     | 0.65           | -0.6     | -0.6           |
| diabetes | 0.775    | 0.78           | -0.45    | -0.46          |
| twonorm  | 0.98     | 0.98           | -0.059   | -0.062         |
| ringnorm | 0.74     | 0.74           | -0.5     | -0.5           |
| banana   | 0.55     | 0.54           | -0.69    | -0.69          |
| splice   | 0.845    | 0.85           | -0.36    | -0.355         |
| waveform | 0.78     | 0.765          | -0.485   | -0.465         |
| image    | 0.82     | 0.815          | -0.43    | -0.44          |

Table 2: Comparison of our method with [SVGD] [42] for Bayesian logistic regression.

<https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/binary.html>
Recall that computing the gradient is a small constant factor harder than computing the function itself \[^{41}\]. Thus, evaluation of \(\nabla \psi(x) : \mathbb{R}^D \rightarrow \mathbb{R}^D\) requires \(O(T)\) operations and evaluating the Hessian \(\nabla^2 \psi(x) : \mathbb{R}^D \rightarrow \mathbb{R}^{D \times D}\) takes \(O(DT)\) time.

To compute \(\log \det \nabla^2 \psi(x)\), we need \(O(D^3)\) extra operations. Sampling from \(\rho_{(k-1)} = (\nabla \psi_{(k-1)}) \circ \cdots \circ \nabla \psi_1 \circ \rho_0\) involves pushing \(x_0 \sim \rho_0\) forward by a sequence of ICNNs \(\psi_1\) of length \(k - 1\), requiring \(O((k-1)T)\) operations. The forward pass to evaluate the JKO step objective \(\tilde{L}\) in Algorithm 1 requires \(O(DT + D^3)\) operations, as does the backward pass to compute the gradient \(\frac{\partial \tilde{L}}{\partial \theta}\) w.r.t. \(\theta\).

The memory complexity is more difficult to characterize, since it depends on the autodiff implementation. It does not exceed the time complexity and is linear in the number of JKO steps \(k\).

**Wall-clock times.** All particle-based methods considered in [4] and [Dual JKO] require from several seconds to several minutes per GPU computation time. Our method requires from several minutes to few hours on GPU, the time is explained by the necessity to train a new network at each step.

**Advantages.** Due to using continuous approximation, our method scales well to high dimensions, as we show in [4.1] and [4.2]. After training, we can produce infinitely many samples \(x_k \sim \rho_k\), together with their trajectories \(x_{k-1}, x_{k-2}, \ldots, x_0\) along the gradient flow. Moreover, the densities of samples in the flow \(\frac{d\rho_k}{dx}(x_k), \frac{d\rho_{k-1}}{dx}(x_{k-1}), \ldots, \frac{d\rho_0}{dx}(x_0)\) can be evaluated immediately.

In contrast, particle-based and domain discretization methods do not scale well with the dimension (Figure 3) and provide no density. Interestingly, despite its parametric approximation, [Dual JKO] performs comparably to particle simulation and worse than ours (see additionally [24] Figure 3)).

**Limitations.** To train \(k\) JKO steps, our method requires time proportional to \(k^2\) due to the increased complexity of sampling \(x \sim \rho_k\). This may be disadvantageous for training long diffusions. In addition, for very high dimensions \(D\), exact evaluation of \(\log \det \nabla^2 \psi(x)\) is time-consuming.

**Future work.** To reduce the computational complexity of sampling from \(\rho_k\), at step \(k\) one may regress an invertible network \(H : \mathbb{R}^D \rightarrow \mathbb{R}^D [9, 31]\) to satisfy \(H(x_0) \approx \nabla \psi_k(x_k) \circ \cdots \circ \nabla \psi_1(x_0)\) and use \(H_\ast \rho_0 \rightarrow \rho_k\) to simplify sampling. An alternative is to use variational inference [12, 54, 71] to approximate \(\rho_k\). To mitigate the computational complexity of computing \(\log \det \nabla \psi(x)\), fast approximation can be used [66, 28]. More broadly, developing ICNNs with easily-computable exact Hessians is a critical avenue for further research as ICNNs continue to gain attention in machine learning [44, 37, 38, 30, 23, 5].

**Potential impact.** Diffusion processes appear in numerous scientific and industrial applications, including machine learning, finances, physics, and population dynamics. Our method will improve models in these areas, providing better scalability. Performance, however, might depend on the expressiveness of the ICNNs, pointing to theoretical convergence analysis as a key topic for future study to reinforce confidence in our model.
In summary, we develop an efficient method to model diffusion processes arising in many practical tasks. We apply our method to common Bayesian tasks such as unnormalized posterior sampling (§4.3) and nonlinear filtering (§4.4). Below we mention several other potential applications:

• **Population dynamics.** In this task, one needs to recover the potential energy $\Phi(x)$ included in the Fokker-Planck free energy functional $F_{FP}$ based on samples from the diffusion obtained at timesteps $t_1, \ldots, t_n$, see [29]. This setting can be found in computational biology, see §6.3 of [29]. A recent paper [14] utilizes ICNN-powered JKO to model population dynamics.

• **Reinforcement learning.** Wasserstein gradient flows provide a theoretically-grounded way to optimize an agent policy in reinforcement learning, see [55, 72]. The idea of the method is to maximize the expected total reward (see (10) in [72]) using the gradient flow associated with the Fokker-Planck functional (see (12) in [72]). The authors of the original paper proposed discrete particle approximation method to solve the underlying JKO scheme. Substituting their approach with our ICNN-based JKO can potentially improve the results.

• **Refining Generative Adversarial Networks.** In the GAN setting, given trained generator $G$ and discriminator $D$, one can improve the samples from $G$ by $D$ via considering a gradient flow w.r.t. entropy-regularized $f$-divergence between real and generated data distribution (see [7], in particular, formula (4) for reference). Using KL-divergence makes the gradient flow consistent with our method: the functional $F$ defining the flow has only entropic and potential energy terms. The usage of our method instead of particle simulation may improve the generator model.

• **Molecular Discovery.** In [3], in parallel to our work the JKO-ICNN scheme is proposed. The authors consider the molecular discovery as an application. The task is to increase the drug-likeness of a given distribution $\rho$ of molecules while staying close to the original distribution $\rho_0$. The task reduces to optimizing the functional $F(\rho) = E_{x \sim \rho} \Phi(x) + D(\rho, \rho_0)$ for a certain potential $\Phi$ (in the notation of [3]) and a discrepancy $D$. The authors applied the JKO-ICNN method to minimize $F$ on MOSES [53] molecular dataset and obtained promising results.

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A Experimental Details

General details. We use DenseICNN architecture [37] Appendix B.2 for $\psi_y$ with 2 hidden layers and vary the width of the model depending on the task. We use Adam optimizer with learning rate decreasing with the number of JKO steps. We initialize the ICNN models either via pretraining to satisfy $\nabla \psi_y(x) \approx x$ or by using parameters $\theta$ obtained from the previous JKO step.

For Dual JKO, we used the implementation provided by the authors with default hyper-parameters. For [EM PR] we implemented the Proximal Recursion operator following the pseudocode of [16] and used the default hyper-parameters but we increased the number of particles for fair comparison with the vanilla [EM] algorithm. Note we limited the number of particles to $N = 10^4$ because of the high computational complexity of the method. For [SVGD], we used the official implementation available at https://github.com/dilinwang820/Stein-Variational-Gradient-Descent.

In particle-based simulations [EM], [BBF] and [EM PR] we used the particle propagation timestep $dt = 10^{-3}$.

We estimate the SymKL [12] using Monte Carlo (MC) on $10^4$ samples. In our method, MC estimate is straightforward since the method permits both sampling and computing the density. In particle-based methods, we use kernel density estimator to approximate the density utilizing scipy implementation of gaussian_kde with bandwidth chosen by Scott’s rule. In [Dual JKO], we employ importance sampling procedure and normalization constant estimation as detailed in [24].

We set $\beta$ to be equal to 1 throughout our experiments.

A.1 Converging to Stationary Distribution

As the stationary measure $\rho^*$ we consider random Gaussian mixture
\[ \frac{1}{N} \sum_{m=1}^{M} N(\mu_m, I_D), \] where $\mu_1, \ldots, \mu_M \sim \text{Uniform}([-\frac{1}{2}, \frac{1}{2}]^D)$.

We set the width $w$ of used ICNNs $\psi_y$ depending on dimension $D$. The parameters are summarized in Table 3.

Each JKO step uses 1000 gradient descent iterations of Algorithm 1. For dimensions $D = 2, 4, \ldots, 12$ the first 20 JKO transitions are optimized with $lr = 5 \cdot 10^{-3}$ and the remaining steps use $lr = 2 \cdot 10^{-3}$. For qualitative experiments in $D = 13, 32$ we perform 50 and 70 JKO steps with step size $h = 0.1$. The learning rate setup in these cases is similar to quantitative experiment setting but has additional stage with $lr = 5 \cdot 10^{-4}$ on the final JKO steps. The batch size is $N = 512$.

| $D$ | $M$ | $l$ | $w$ |
|-----|-----|-----|-----|
| 2   | 5   | 10  | 256 |
| 4   | 6   | 10  | 384 |
| 6   | 7   | 10  | 512 |
| 8   | 8   | 10  | 512 |
| 10  | 9   | 10  | 512 |
| 12  | 10  | 10  | 1024 |
| 13  | 10  | 10  | 512 |
| 32  | 10  | 6   | 1024 |

Table 3: Hyper-parameters in the convergence exp.

A.2 Modeling Ornstein-Uhlenbeck Processes

Matrices $A \in \mathbb{R}^{D \times D}$ are randomly generated using sklearn.datasets.make_spd_matrix. Vectors $b \in \mathbb{R}^D$ are sampled from standard Gaussian measure. All ICNNs $\psi_y$ have $w = 64$ and we train each of them for 500 iterations per JKO step with $lr = 5 \cdot 10^{-3}$ and batch size $N = 1024$.

A.3 Unnormalized Posterior Sampling

To remove positiveness constraint on $\alpha$ we consider $[w, \log(\alpha)]$ as the regression model parameters instead of $[w, \alpha]$. To learn the posterior distribution $p(x|S_{\text{train}})$ we use JKO step size $h = 0.1$. Let iter denote the number of gradient steps over $\theta$ per each JKO step. The used hyper-parameters for each dataset are summarized in Table 4.

| Dataset | $w$ | $lr$ | iter | batch | $K$ |
|---------|-----|------|------|-------|-----|
| cowtype | 512 | $2 \cdot 10^{-5}$ | $10^4$ | 1024 | 6   |
| german  | 512 | $2 \cdot 10^{-4}$ | 5000 | 512   | 5   |
| diabetes| 128 | $5 \cdot 10^{-5}$ | 6000 | 1024  | 16  |
| twonorm | 512 | $5 \cdot 10^{-5}$ | 5000 | 1024  | 7   |
| ringnorm| 512 | $5 \cdot 10^{-5}$ | 5000 | 1024  | 2   |
| banana  | 128 | $2 \cdot 10^{-4}$ | 5000 | 1024  | 5   |
| splice  | 512 | $2 \cdot 10^{-3}$ | 2000 | 512   | 5   |
| waveform| 512 | $5 \cdot 10^{-5}$ | 5000 | 512   | 2   |
| image   | 512 | $5 \cdot 10^{-5}$ | 5000 | 512   | 5   |

Table 4: Hyper-parameters we use in Bayesian logistic regression experiment.
on \( p(x|S_{\text{true}}) \), we use straightforward MC estimate on \( 2^{12} \) random parameter samples.

**B Nonlinear Filtering Details**

For \( k = 1, 2, \ldots \) we progressively obtain access to samples (and their un-normalized density) from predictive distribution \( p_{t_k, X}(x|Y_{1:k}) \) for step \( k \) given \( k \) observations \( Y_1, \ldots, Y_k \). First, at each step \( k \), we access \( p_{t_k, X}(x|Y_{1:k}) \) through \( p_{t_{k-1}, X}(x|Y_{1:k-1}) \). To do this, we use our Algorithm 2 below. The algorithm builds a chain where we substitute (14) sequentially for \( p \).

Let \( \mu \) for \( x \).

Select \( \mu \) for \( x \).

\[ \text{Algorithm 2: Metropolis-Hastings algorithm} \]

**Input**: Unnormalized density \( \pi(\cdot) \); family of proposal distributions \( q_x(\cdot) \) \( x \in \mathbb{R}^D \)

**Output**: Sequence \( x(1), x(2), x(3), \ldots \) of samples from \( \pi \)

Select \( x^{(0)} \in \mathbb{R}^D \)

for \( j = 1, 2, \ldots \) do

\[
\begin{align*}
\text{Sample } y & \sim q_{x(j-1)}; \\
\text{Compute } \alpha(x^{(j-1)}, y) &= \min \left( 1, \frac{\pi(y) q_x(x^{(j-1)})}{\pi(x^{(j-1)}) q_{x^{(j-1)}}(y)} \right) \\
\text{With probability } \alpha(x^{(j-1)}, y) \text{ set } x^{(j)} \leftarrow y; \text{ otherwise set } x^{(j)} \leftarrow x^{(j-1)}
\end{align*}
\]

To sample from \( p_{t_k, X}(x|Y_{1:k}) \) we use Algorithm 2 with \( \pi \) equal to unnormalized density (16). We note that computing \( \pi(x_k) \) for \( x_k \in \mathbb{R}^D \) is not easy since it requires computing pre-images \( x_{k-1}, \ldots, x_0 \) by inverting \( B_k, B_{k-1}, \ldots, B_1 \). As the consequence, this makes computation of acceptance probability \( \alpha(\cdot, \cdot) \) hard. To resolve this issue, we choose special \( x \)-independent proposals

\[ q = q_x \overset{\text{def}}{=} (B_k \circ B_{k-1} \circ \cdots \circ B_1) \mu_{p_0, X}. \] (17)

In this case, all \( \det \) terms in \( \alpha(x, y) \) vanish simplifying the computation (we write \( x = x_k, y = y_k \)):
\[
p_{0,X}(y_0) \prod_{i=1}^{k} p_{t_i,Y}(Y_i|X_{t_i} = y_i) \prod_{i=1}^{k} \det \nabla B_i(x_{i-1}) \cdot p_{0,X}(x_0) \prod_{i=1}^{k} \det \nabla B_i(y_{i-1}) = \\
p_{0,X}(x_0) \prod_{i=1}^{k} p_{t_i,Y}(Y_i|X_{t_i} = x_i) \prod_{i=1}^{k} \det \nabla B_i(y_{i-1}) \cdot p_{0,X}(y_0) \prod_{i=1}^{k} \det \nabla B_i(x_{i-1}) \prod_{i=1}^{k} p_{t_i,Y}(Y_i|X_{t_i} = y_i) \prod_{i=1}^{k} p_{t_i,Y}(Y_i|X_{t_i} = x_i)
\]

To compute (18) one needs to know preimages \(x_{k-1}, \ldots, x_0\) and \(y_{k-1}, \ldots, y_0\) of points \(y = y_k\) and \(x = x_k\) respectively. They can be straightforwardly computed when sampling from \(q\) happens \([17]\).

**Experimental details.** To obtain the noise observations \(Y_k = X_{t_k} + v_k\) from the process, we simulate a particle \(X_0\) randomly sampled from the initial measure \(\mathcal{N}(0, 1)\) by using Euler-Maruyama method to obtain the trajectory \(X_t\). At observation times \(t_1 = 0.5, \ldots, t_9 = 4.5\) we add random noise \(v_k \sim \mathcal{N}(0, 1)\) to obtain observations \(Y_1, \ldots, Y_9\).

We utilize Chang and Cooper \([19]\) numerical integration method to compute true \(p(X_{t_m}|Y_{1:9})\). We construct regular fine grid on the segment \([-5, 5]\) with 2000 points and numerically solve the SDE with timestep \(dt = 10^{-3}\). At observation times \(t_k, k \in 1, \ldots, 9\) we multiply the obtained probability density function \(p_{t_k,X}(x|Y_{1:k-1})\) by the density of the normal distribution \(p(Y_k|X_{t_k} = x)\) estimated at the grid which results in unnormalized \(p_{t_k,X}(x|Y_{1:k})\). After normalization on the grid, \(p_{t_k,X}(x|Y_{1:k})\) can be used in the new diffusion round on time interval \([t_k, t_{k+1}]\). At final time \(t_{\text{fin}}\) we estimate SymKL between the true distribution and ones obtained via other competitive methods by numerically integrating (12) on the grid.

We implement [BBF] following the original article \([27]\). Particle propagation performed via Euler-Maruyama method with timestep \(dt = 10^{-3}\). The final distribution \(p(X_{t_m}|Y_{1:9})\) is estimated using kernel density estimator as described in Appendix A.

For [Dual JKO] we use the code provided by the authors with the default hyper-parameters.

In our method, we use JKO step size \(h = 0.1\) and model it by ICNN with width \(w = 256\). Each JKO step takes 700 optimization iterations with \(lr = 5 \cdot 10^{-3}\) and batch size \(N = 1024\). At observation times \(t_k, k \in 1, 2, \ldots, 9\) we use the Metropolis-Hastings algorithm\([2] with acceptance probability \(\alpha\) calculated by \([15]\). Starting from the randomly sampled \(x^{(1)}\) we skip the first 1000 values of the Markov Chain generated by the algorithm which allows the series to converge to the distribution of interest \(p_{t_k,X}(x|Y_{1:k})\). We take each second element from the chain in order to decorrelate the samples. To simultaneously sample the batch of size \(N\), we run \(N\) chains in parallel. To compute SymKL, we normalize the resulting distribution \(p(X_{t_m}|Y_{1:9})\) on the Chang-Cooper support grid.

**C Additional Experiments**

In Figure 5 we compare the true distribution \(p_t\) with the predicted distribution via the competitive methods when modelling Ornstein-Uhlenbeck processes (34.2). The comparison is given for time \(t = 0.1, 0.2, \ldots, 1.0\).
Figure 5: SymKL values between the computed measures and the true measure at $t = 0.1, 0.2, \ldots, 1$ in dimensions $D = 1, 2, \ldots, 12$. Best viewed in color.