We propose an Euler particle transport (EPT) approach for generative learning. The proposed approach is motivated by the problem of finding an optimal transport map from a reference distribution to a target distribution characterized by the Monge-Ampere equation. Interpreting the infinitesimal linearization of the Monge-Ampere equation from the perspective of gradient flows in measure spaces leads to a stochastic McKean-Vlasov equation. We use the forward Euler method to solve this equation. The resulting forward Euler map pushes forward a reference distribution to the target. This map is the composition of a sequence of simple residual maps, which are computationally stable and easy to train. The key task in training is the estimation of the density ratios or differences that determine the residual maps. We estimate the density ratios (differences) based on the Bregman divergence with a gradient penalty using deep density-ratio (difference) fitting. We show that the proposed density-ratio (difference) estimators do not suffer from the “curse of dimensionality” if data is supported on a lower-dimensional manifold. Numerical experiments with multi-mode synthetic datasets and comparisons with the existing methods on real benchmark datasets support our theoretical results and demonstrate the effectiveness of the proposed method.

Key words: Density-ratio estimation; high-dimensional distribution; gradient flow; residual map; sampling; velocity fields

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1 This is an updated version of the manuscript: Gao, Huang, Jiao and Liu (2020). Learning Implicit Generative Models with Theoretical Guarantees. arXiv preprint [arXiv:2002.02862] https://arxiv.org/abs/2002.02862

2 This version: November 27, 2020
1 Introduction

The ability to efficiently sample from complex distributions plays a key role in a variety of prediction and inference tasks in machine learning and statistics (Salakhutdinov, 2015). The long-standing methodology for learning an underlying distribution relies on an explicit statistical data model, which can be difficult to specify in many applications such as image analysis, computer vision and natural language processing. In contrast, implicit generative models do not assume a specific form of the data distribution, but rather learn a nonlinear map to transform a reference distribution to the target distribution. This modeling approach has been shown to achieve impressive performance in many machine learning tasks (Reed et al., 2016; Zhu et al., 2017). Generative adversarial networks (GAN) (Goodfellow et al., 2014), variational auto-encoders (VAE) (Kingma & Welling, 2014) and flow-based methods (Rezende & Mohamed, 2015) are important representatives of implicit generative models.

GANs model the low-dimensional latent structure via deep nonlinear factors. They are trained by sequential differentiable surrogates of two-sample tests, including the density-ratio test (Goodfellow et al., 2014; Nowozin et al., 2016; Mao et al., 2017; Mroueh & Sercu, 2017; Tao et al., 2018) and the density-difference test (Li et al., 2015; Sutherland et al., 2017; Li et al., 2017; Arjovsky et al., 2017; Binkowski et al., 2018), among others. VAE is a probabilistic deep latent factor model trained with variational inference and stochastic approximation. Several authors have proposed improved versions of VAE by enhancing the representation power of the learned latent codes and reducing the blurriness of the generated images in vanilla VAE (Makhzani et al., 2016; Higgins et al., 2017; Tolstikhin et al., 2018; Zhang et al., 2019). Flow-based methods learn a diffeomorphism map between the reference distribution and the target distribution by maximum likelihood using the change of variables formula. Recent work on flow-based methods has been focused on developing training methods and designing neural network architectures to trade off between the efficiency of training and sampling and the representation power of the learned map (Rezende & Mohamed, 2015; Dinh et al., 2015; Papamakarios et al., 2017; Kingma & Dhariwal, 2018; Grathwohl et al., 2019).

We propose an Euler particle transport (EPT) approach for learning a generative model by integrating ideas from optimal transport, numerical ODE, density-ratio estimation and deep neural networks. EPT is motivated by the problem of finding an optimal transport from a reference distribution to the target distribution based on the quadratic Wasserstein distance. Since it is challenging to solve the resulting Monge-Ampère equation that characterizes the optimal transport, we consider the continuity equation derived from the linearization of the Monge-Ampère equation, which is a gradient flows converging to the target distribution. We solve the McKean-Vlasov equation associated with the gradient flow using the forward Euler method. The resulting EPT that pushes forward a reference distribution to the target is a composition of a sequence of simple residual maps, which are computationally stable and easy to train. The residual maps are completely determined by the density ratios between the distributions at the current iterations and the target distribution. We estimate density ratios based on the Bregman divergence with a gradient regularizer using deep density-ratio fitting.

We establish bounds on the approximation errors due to linearization of the Monge-Ampère equation, Euler discretization of the McKean-Vlasov equation, and deep density-ratio estimation. Our result on the error rate for the proposed density-ratio estimators improves the minimax rate of nonparametric estimation via exploring the low-dimensional structure of the data and circumvents the “curse of dimensionality”. Experimental results on multi-mode synthetic data and comparisons with state-of-the-art GANs on benchmark data support our theoretical findings and demonstrate that EPT is computationally more stable and easier to train than GANs.
Using simple ReLU ResNets without batch normalization and spectral normalization, we obtained results that are better than or comparable with those using GANs trained with such tricks.

2 Euler particle transport

Let \( X \in \mathbb{R}^m \) be a random vector with distribution \( \nu \), and let \( Z \) be a random vector with distribution \( \mu \). We assume that \( \mu \) has a known and simple form. Our goal is to construct a transformation \( T \) such that \( T_\# \mu = \nu \), where \( T_\# \mu \) denotes the push-forward distribution of \( \mu \) by \( T \), that is, the distribution of \( T(Z) \). Then we can sample from \( \nu \) by first generating a \( Z \sim \mu \) and calculate \( T(Z) \). In practice, \( \nu \) is unknown and only a random sample \( \{X_i\}_{i=1}^n \) i.i.d. \( \nu \) is available. We must construct \( T \) based on the sample.

There may exist multiple transports \( T \) with \( T_\# \mu = \nu \). The optimal transport is the one that minimizes the quadratic Wasserstein distance between \( \mu \) and \( \nu \) defined by

\[
W_2(\mu, \nu) = \left\{ \inf_{\gamma \in \Gamma(\mu, \nu)} \mathbb{E}(Z, X) \sim \gamma \left[ \|Z - X\|_2^2 \right] \right\}^{1/2},
\]

(2.1)

where \( \Gamma(\mu, \nu) \) denotes the set of couplings of \( (\mu, \nu) \) (Villani, 2008; Ambrosio et al., 2008). Suppose that \( \mu \) and \( \nu \) have densities \( q \) and \( p \) with respect to the Lebesgue measure, respectively. Then the optimal transport map \( T \) such that \( T_\# \mu = \nu \) is characterized by the Monge-Ampère equation (Brenier, 1991; McCann, 1995; Santambrogio, 2015). Specifically, the minimization problem in (2.1) admits a unique solution \( \gamma = (I, T)_\# \mu \) with \( T = \nabla \Psi, \mu \text{-a.e.} \), where \( I \) is the identity map and \( \nabla \Psi \) is the gradient of the potential function \( \Psi : \mathbb{R}^m \to \mathbb{R} \). This function is convex and satisfies the Monge-Ampère equation

\[
\det(\nabla^2 \Psi(z)) = \frac{q(z)}{p(\nabla \Psi(z))}, \ z \in \mathbb{R}^m.
\]

(2.2)

Therefore, to find the optimal transport \( T \), it suffices to solve (2.2) for \( \Psi \). However, it is challenging to solve this degenerate elliptic equation due to its highly nonlinear nature.

Below we first provide an overall description of the proposed EPT method for constructing a transport map that pushes forward a reference \( \mu \) to the target \( \nu \). EPT is motivated by solving a linearized version of the Monge-Ampère equation (2.2). It consists of the following steps: (a) linearizing (2.2) via residual maps, (b) determining the velocity fields governing the stochastic McKean-Vlasov equation resulting from the linearization, (c) calculating the forward Euler particle transport map and, (d) training the EPT map by estimating the velocity fields from data. Since velocity fields are completely determined by density ratios, this step amounts to nonparametric density ratio estimation. We also provide bounds on the errors due to linearization, discretization and estimation. Mathematical details and proofs are given in Section 3 and the appendix.

Linearization via residual map A basic approach to addressing the difficulty due to nonlinearity is linearization. We use a linearization method based on the residual map

\[
T_{t, \Phi} = \nabla \Phi = I + t \nabla \Phi, \ t \geq 0,
\]

(2.3)

where \( \Phi_t : \mathbb{R}^m \to \mathbb{R}^1 \) is a function to be chosen such that the law of \( T_{t, \Phi}(Z) \) is closer to \( \nu \) than that of \( Z \) (Villani, 2008). We then iteratively improve the approximation by repeatedly applying the residual map to the current particles. We give the specific form of \( \Phi \) below, see Theorem 3.1 in Section 3 for details.

This linearization scheme leads to the stochastic process \( X_t : \mathbb{R}^m \to \mathbb{R}^m \) satisfying the McKean-Vlasov equation

\[
\frac{d}{dt} X_t(x) = v_t(X_t(x)), \ t \geq 0, \ \text{with} \ X_0 \sim \mu, \ \mu \text{-a.e.} \ x \in \mathbb{R}^m,
\]

(2.4)
where \( v_t \) is the velocity vector field of \( X_t \). In addition, we have \( v_t = \nabla \Phi_t \). Thus \( v_t \) also determines the residual map \((2.3)\). The detailed derivations are given in Theorems \[3.1\] and \[3.2\] in Section \[3\]. Therefore, the problem of estimating the residual maps \((2.3)\) is equivalent to that of estimating the velocity fields \( v_t \).

The movement of \( X_t \) along \( t \) is completely governed by \( v_t \), given the initial value. We choose a \( v_t \) to decrease the discrepancy between the distribution of \( X_t \), say \( \mu_t \), at time \( t \) and the target \( \nu \) with respect to a properly chosen measure. An equivalent formulation of \((2.4)\) is through the gradient flow \((2.4)\) and the target \( \nu \).

**Determining velocity field** The basic intuition is that we should move in the direction that decreases the differences between \( \mu_t \) and the target \( \nu \). We use an energy functional \( L[\mu_t] \) to measure such differences. An important energy functional \( L[\mu_t] \) is the \( f \)-divergence (Ali & Silvey, 1966).

\[
L[\mu_t] = D_f(\mu_t || \nu) = \int_{\mathbb{R}^m} p(x) f\left( \frac{q_t(x)}{p(x)} \right) \, dx,
\]

where \( q_t \) is the density of \( \mu_t \), \( p \) is the density of \( \nu \) and \( f : \mathbb{R}^+ \to \mathbb{R} \) is assumed to be a twice-differentiable convex function with \( f(1) = 0 \). We choose \( \Phi_t \) such that \( L[\mu_t] \) is minimized. We show in Theorem \[3.1\] in Section \[3\] that \( \Phi_t(x) = -f'(r_t(x)) \) and \( v_t(x) = \nabla \Phi_t(x) \). Therefore,

\[
v_t(x) = -f''(r_t(x)) \nabla r_t(x), \quad \text{where} \quad r_t(x) = \frac{q_t(x)}{p(x)}, \quad x \in \mathbb{R}^m.
\]

For example, if we use the \( \chi^2 \)-divergence with \( f(c) = (c-1)^2/2 \), then \( v_t(x) = \nabla r_t(x) \) is simply the gradient of the density ratio. Other types of velocity fields can be obtained by using different energy functionals such as the Lebesgue norm of the density difference, i.e., \( L[\mu_t] = \int_{\mathbb{R}^m} |q_t(x) - p(x)|^2 \, dx \), see Section \[3\] for details.

**The forward Euler method** Numerically, we need to discretize the McKean-Vlasov equation \((2.4)\). Let \( s > 0 \) be a small step size. We use the forward Euler method defined iteratively by:

\[
\begin{align*}
T_{k} &= I + sv_k, \\
X_{k+1} &= T_{k}(X_k), \\
\mu_{k+1} &= (T_{k})_# \mu_k,
\end{align*}
\]

where \( X_0 \sim \mu, \mu_0 = \mu, v_k \) is the velocity field at the \( k \)th step, \( k = 0, 1, ..., K \) for some large \( K \). The particle process \( \{X_k\}_{k \geq 0} \) is a discretized version of the continuous process \( \{X_t\}_{t \geq 0} \) in \((2.4)\). The final transport map is the composition of a sequence of simple residual maps \( T_0, T_1, ..., T_K \), i.e., \( \hat{T} = T_K \circ T_{K-1} \circ \cdots \circ T_0 \). This updating scheme is based on the forward Euler method for solving equation \((2.4)\). This is the reason we refer to the proposed method as Euler particle transport (EPT).

**Training EPT** When the target \( \nu \) is unknown and only a random sample is available, it is natural to learn \( \nu \) by first estimating the discrete velocity fields \( v_k \) at the sample level and then plugging the estimator of \( v_k \) in \((2.6)\). For example, if we use the \( f \)-divergence as the energy functional, estimating \( v_k(x) = -f''(r_k(x)) \nabla r_k(x) \) boils down to estimating the density ratios \( r_k(x) = q_k(x)/p(x) \) dynamically at each iteration \( k \). Nonparametric density-ratio estimation using Bregman divergences and gradient regularizer are discussed in Section \[4\] below. Let \( \hat{v}_k \) be the estimated velocity fields at the \( k \)th iteration. The \( k \)th estimated residual map is \( \hat{T}_k = I + s\hat{v}_k \). Finally, the trained map is

\[
\hat{T} = \hat{T}_K \circ \hat{T}_{K-1} \circ \cdots \circ \hat{T}_0.
\]
We are now ready to describe EPT in details. Specifically, we describe the gradient flows associated with EPT when training the EPT map, we use the deep neural networks to estimate the density ratios (density differences) with samples. In Theorem 4.1, we provide an estimation error bound that improves the minimax rate of deep nonparametric estimation via exploring the low-dimensional structure of data and circumvents the “curse of dimensionality.” Thus this result is of independent interest in nonparametric estimation using deep neural networks.

3 Gradient flows associated with EPT

For convenience, we first describe the notation used in the remaining sections. Let \( \mathcal{P}_2(\mathbb{R}^m) \) denote the space of Borel probability measures on \( \mathbb{R}^m \) with finite second moments, and let \( \mathcal{P}_2^0(\mathbb{R}^m) \) denote the subset of \( \mathcal{P}_2(\mathbb{R}^m) \) in which measures are absolutely continuous with respect to the Lebesgue measure (all distributions are assumed to satisfy this assumption hereinafter). \( \text{Tan}_\mu \mathcal{P}_2(\mathbb{R}^m) \) denotes the tangent space to \( \mathcal{P}_2(\mathbb{R}^m) \) at \( \mu \). Let \( \mathcal{AC}_{loc}^\mu(\mathbb{R}^+, \mathcal{P}_2(\mathbb{R}^m)) = \{ \mu_t : I \to \mathcal{P}_2(\mathbb{R}^m) \text{ is absolutely continuous, } [\mu_t] \in L^2(I), I \subset \mathbb{R}^+ \} \). \( \text{Lip}_{loc}(\mathbb{R}^m) \) denotes the set of functions that are Lipschitz continuous on any compact set of \( \mathbb{R}^m \). For any \( \ell \in [1, \infty) \), we use \( L^\ell(\mu, \mathbb{R}^m) \) (\( L^\ell_{loc}(\mu, \mathbb{R}^m) \)) to denote the \( L^\ell \) space of \( \mu \)-measurable functions on \( \mathbb{R}^m \) (on any compact set of \( \mathbb{R}^m \)). With \( 1, \det \) and \( tr \), we refer to the identity map, the determinant and the trace. We use \( \nabla, \nabla^2 \) and \( \Delta \) to denote the gradient or Jacobian operator, the Hessian operator and the Laplace operator, respectively.

We are now ready to describe EPT in details. Specifically, we describe the gradient flows associated with EPT and the corresponding Mckean-Vlasov equation. Let \( X \sim q \), and let

\[
\tilde{X} = T_{t, \Phi}(X) = X + t \nabla \Phi(X), \quad t \geq 0.
\]

Here we let \( \Phi \) be independent of \( t \) for the moment. Denote the distribution of \( \tilde{X} \) by \( \tilde{q} \). With a small \( t \), the map \( T_{t, \Phi} \) is invertible according to the implicit function theorem. By the change of variables formula, we have

\[
\det(\nabla^2 \Psi)(x) = |\det(\nabla T_{t, \Phi})(x)| = \frac{q(x)}{\tilde{q}(\tilde{x})},
\]

where

\[
\tilde{x} = T_{t, \Phi}(x).
\]
Using the fact that the derivative
\[
\frac{d}{dt}\bigg|_{t=0} \det(A + tB) = \det(A) \text{tr} (A^{-1}B) \forall A, B \in \mathbb{R}^{m \times m},
\]
provided that $A$ is invertible, and applying the first order Taylor expansion to (3.1), we have
\[
\log q(\bar{x}) - \log q(x) = - t \Delta \Phi(x) + o(t).
\] (3.3)

Let $t \to 0$ in (3.2) and (3.3), we obtain a random process $\{x_t\}$ and its law $q_t$ satisfying
\[
\frac{dx_t}{dt} = \nabla \Phi(x_t), \quad \text{with} \quad x_0 \sim q,
\] (3.4)
\[
\frac{d\ln q_t(x_t)}{dt} = - \Delta \Phi(x_t), \quad \text{with} \quad q_0 = q.
\] (3.5)

Equations (3.4) and (3.5) resulting from linearization of the Monge-Ampère equation (2.2) can be interpreted as gradient flows in measure spaces (Ambrosio et al., 2008). Thanks to this connection, we can resort to solving a continuity equation characterized by a McKean-Vlasov equation, an ODE system that is easier to work with.

For $\mu \in \mathcal{P}_2^m(\mathbb{R}^m)$ with density $q$, let
\[
\mathcal{L}[\mu] = \int_{\mathbb{R}^m} F(q(x))dx : \mathcal{P}_2^m(\mathbb{R}^m) \to \mathbb{R}^+ \cup \{0\}
\]
be an energy functional satisfying $\nu \in \arg\min \mathcal{L}[\cdot]$, where $F(\cdot) : \mathbb{R}^+ \to \mathbb{R}^1$ is a twice-differentiable convex function. Among the widely used metrics on $\mathcal{P}_2^m(\mathbb{R}^m)$ in implicit generative learning, the following two are important examples of $\mathcal{L}[\cdot]$:

1. $f$-divergence given in (2.5) (Ali & Silvey, 1966);
2. Lebesgue norm of density difference:
\[
\|\mu - \nu\|^2_{L^2(\mathbb{R}^m)} = \int_{\mathbb{R}^m} |q(x) - p(x)|^2 dx.
\] (3.7)

**Definition.** We call $\{\mu_t\}_{t \in \mathbb{R}^+} \subset AC_{loc}(\mathbb{R}^+, \mathcal{P}_2(\mathbb{R}^m))$ a gradient flow of the functional $\mathcal{L}[\cdot]$, if $\{\mu_t\}_{t \in \mathbb{R}^+} \subset \mathcal{P}_2^m(\mathbb{R}^m)$ a.e., $t \in \mathbb{R}^+$ and the velocity vector field $v_t \in \text{Tan}_{\mu_t}\mathcal{P}_2(\mathbb{R}^m)$ satisfies $v_t = -\partial \mathcal{L}[\mu_t]$ a.e. $t \in \mathbb{R}^+$, where $\partial \mathcal{L}[\cdot]$ is the subdifferential of $\mathcal{L}[\cdot]$.

The gradient flow $\{\mu_t\}_{t \in \mathbb{R}^+}$ of $\mathcal{L}[\cdot]$ enjoys the following nice properties.

**Proposition 3.1.**

(i) The following continuity equation holds in the sense of distributions.
\[
\frac{\partial}{\partial t} \mu_t = -\nabla \cdot (\mu_t v_t) \quad \text{in} \quad \mathbb{R}^+ \times \mathbb{R}^m \quad \text{with} \quad \mu_0 = \mu, t \geq 0.
\] (3.8)

(ii) Energy decay along the gradient flow: $\frac{d}{dt} \mathcal{L}[\mu_t] = -\|v_t\|^2_{L^2(\mu_t, \mathbb{R}^m)}$ a.e. $t \in \mathbb{R}^+$. In addition,
\[
W_2(\mu_t, \nu) = \mathcal{O}(\exp^{-\lambda t}),
\] (3.9)

if $\mathcal{L}[\mu]$ is $\lambda$-geodetically convex with $\lambda > 0$.

$^3$A metric $d$ on $\mathcal{P}_2^m(\mathbb{R}^m)$ is said to be $\lambda$-geodetically convex if there exists a constant $\lambda > 0$ such that for every $\mu_1, \mu_2 \in \mathcal{P}_2^m(\mathbb{R}^m)$, there exists a constant speed geodesic $\gamma : [0, 1] \to \mathcal{P}_2^m(\mathbb{R}^m)$ such that $\gamma_0 = \mu_1, \gamma_1 = \mu_2$ and
\[
\mathcal{L}(\gamma_s) \leq (1 - s)\mathcal{L}(\mu_1) + s\mathcal{L}(\mu_2) - \frac{\lambda}{2}s(1 - s)d(\mu_1, \mu_2), \ \forall s \in [0, 1],
\]
where $d$ is a metric defined on $\mathcal{P}_2^m(\mathbb{R}^m)$ such as the quadratic Wasserstein distance.
(iii) Conversely, if \( \{ \mu_t \} \), is the solution of continuity equation (3.8) in (i) with \( v_t(x) \) specified by (3.10) in (ii), then \( \{ \mu_t \} \) is a gradient flow of \( L[\cdot] \).

**Remark 3.1.** In part (ii) of Proposition 3.1, for general \( f \)-divergences, we assume the functional \( L \) to be \( \lambda \)-geodesically convex for the convergence of \( \mu_t \) to the target \( \nu \) in the quadratic Wasserstein distance. However, for the KL divergence, the convergence can be guaranteed if \( \nu \) satisfies the log-Sobolev inequality (Otto & Villani, 2000). In addition, the distributions that are strongly log-concave outside a bounded region, but not necessarily log-concave inside the region satisfy the log-Sobolev inequality, see, for example, Holley & Stroock (1987). Here the functional \( L \) can even be nonconvex, an example includes the densities with double-well potential.

**Remark 3.2.** Equation (8.48) in Proposition 8.4.6 of and Ambrosio et al. (2008) shows the connection (locally) of the velocity \( v_t \) of the gradient flow \( \mu_t \) and the optimal transport along \( \mu_t \), i.e., \( T^h_{\mu_t} \) be the optimal transport from \( \mu_t \) to \( \mu_{t+h} \) for a small \( h > 0 \), then \( T^h_{\mu_t} = I + hv_t + o(h) \) in \( L^p \). So locally, \( I + hv_t \) approximates the optimal transport map from \( \mu_t \) to \( \mu_{t+h} \) on \( [t, t+h] \). However, the global approximation property of the proposed method is not clear. This is a challenging problem that requires further study and is beyond the scope of this paper.

Theorem 3.1. (i) Representation of the velocity fields: if the density \( q_t \) of \( \mu_t \) is differentiable, then
\[
    v_t(x) = -\nabla F'(q_t(x)) \quad \mu_t \text{-a.e. } x \in \mathbb{R}^m.  \tag{3.10}
\]

(ii) If we let \( \Phi \) be time-dependent in (3.4)–(3.5), i.e., \( \Phi \), then the linearized Monge-Ampère equations (3.4)–(3.5) are the same as the continuity equation (3.8) by taking \( \Phi_t(x) = -F'(q_t(x)) \).

Theorem 3.1 and (3.9) in Proposition 3.1 imply that \( \{ \mu_t \} \), the solution of the continuity equation (3.8) with \( v_t(x) = -\nabla F'(q_t(x)) \), converges rapidly to the target distribution \( \nu \). Furthermore, the continuity equation has the following representation under mild regularity conditions on the velocity fields.

**Theorem 3.2.** Assume \( \|v_t\|_{L^1(\mu_t, \mathbb{R}^m)} \in L^1_{\text{loc}}(\mathbb{R}^+ \times \mathbb{R}^m) \) and \( v_t(\cdot) \in L^1_{\text{loc}}(\mathbb{R}^m) \) with upper bound \( B_t \) and Lipschitz constant \( L_t \) such that \( (B_t + L_t) \in L^1_{\text{loc}}(\mathbb{R}^+) \). Then the solution of the continuity equation (3.8) can be represented as \( \mu_t = (X_t)_{t\geq t} \), where \( X_t(x) : \mathbb{R}^+ \times \mathbb{R}^m \rightarrow \mathbb{R}^m \) satisfies the McKean-Vlasov equation (2.4).

As shown in Lemma 3.1 below, the velocity fields associated with the \( f \)-divergence (2.5) and the Lebesgue norm (3.7) are determined by density ratio and density difference, respectively.

**Lemma 3.1.** The velocity fields \( v_t \) satisfy
\[
    v_t(x) = \begin{cases} 
        -f''(r_t(x)) \nabla r_t(x), & \mathcal{L}[\mu] = D_f(\mu \parallel \nu), \text{ where } r_t(x) = \frac{q_t(x)}{p(x)}, \\
        -2 \nabla d_t(x), & \mathcal{L}[\mu] = \|\mu - \nu\|_{L^2(\mathbb{R}^m)}, \text{ where } d_t(x) = q_t(x) - p(x).
    \end{cases}
\]

Several methods have been developed to estimate density ratio and density difference in the literature. Examples include probabilistic classification approaches, moment matching and direct density-ratio (difference) fitting, see Sugiyama et al. (2012a,b); Kanamori & Sugiyama (2014); Mohamed & Lakshminarayanan (2016) and the references therein.

**Proposition 3.2.** For any finite \( T > 0 \), suppose that the velocity fields \( v_t \) are Lipschitz continuous with respect to \( (x, \mu_t) \) for \( t \in [0, T] \), that is, there exists a finite constant \( L_v > 0 \) such that
\[
    \|v_t(x) - v_t(\tilde{x})\| \leq L_v \|x - \tilde{x}\| + W_2(\mu_t, \mu_t), t, \tilde{t} \in [0, T] \text{ and } x, \tilde{x} \in \mathbb{R}^m.  \tag{3.11}
\]
Then the bound \((2.11)\) on the discretization error holds:
\[
\sup_{t \in [0,T]} W_2(\mu_t, \mu_t^*) = O(s).
\]

**Remark 3.3.** If we take \(f(x) = (x - 1)^2/2\) in Lemma 3.1 then the velocity fields \(v_t(x) = \nabla r_t(x)\), where \(r_t(x) = q_t(x)/p(x)\). In the proof of Theorem 3.1 part (ii), it is shown that \(q_t\) satisfies \(\partial_t q_t/\partial t = -\nabla \cdot (q_t \nabla \Phi_t)\). Thus for this simple \(f\)-divergence function, the verification of the Lipschitz condition \((3.11)\) amounts to verifying that \(\nabla r_t(x)\) is Lipschitz in the sense of \((3.11)\).

### 4 Deep Density-Ratio Fitting

The evaluation of velocity fields depends on the dynamic estimation of a discrepancy between the push-forward distribution \(q_t\) and the target distribution \(p\). Density-ratio and density-difference fitting with the Bregman score provides a unified framework for such discrepancy estimation without estimating each density separately (Gneiting & Raftery [2007], Dawid [2007], Sugiyama et al. [2012], Kanamori & Sugiyama [2014]).

Let \(r(x) = q(x)/p(x)\) be the density ratio between a given density \(q(x)\) and the target \(p(x)\). Let \(g : \mathbb{R} \to \mathbb{R}\) be a differentiable and strictly convex function. The separable Bregman score with the base probability \(p\) for measuring the discrepancy between \(r\) and a measurable function \(R : \mathbb{R}^m \to \mathbb{R}^1\) is
\[
\mathcal{B}(r, R) = \mathbb{E}_{X \sim p}[g'(R(X))R(X) - g(R(X))] - \mathbb{E}_{X \sim q}[g'(R(X))].
\]

Here we focus on the widely used least-squares density-ratio (LSDR) fitting with \(g(x) = (x - 1)^2\) as a working example, i.e.,
\[
\mathcal{B}_{LSDR}(r, R) = \mathbb{E}_{X \sim p}[R(X)^2] - 2\mathbb{E}_{X \sim q}[R(X)] + 1. \tag{4.1}
\]

For other choice of \(g\), such as \(g(x) = x \log x - (x + 1) \log(x + 1)\) corresponding to estimating \(r\) via the logistic regression (LR), and the scenario of density difference fitting will be presented in Section 4.

#### 4.1 Gradient Regularizer

The distributions of real data may have a low-dimensional structure with their support concentrated on a low-dimensional manifold, which may cause the \(f\)-divergence to be ill-posed due to non-overlapping supports. To exploit such underlying low-dimensional structures and avoid ill-posedness, we derive a simple weighted gradient regularizer \(\frac{\lambda}{2} \mathbb{E}_p[\|\nabla R\|^2]\), motivated by recent works on smoothing via noise injection (Sønderby et al. [2017], Arjovsky & Bottou [2017]). This serves as a regularizer for deep density-ratio fitting. For example, with \(g(c) = (c - 1)^2\), the resulting gradient regularizer is
\[
\mathbb{E}_p[\|\nabla R\|^2], \tag{4.2}
\]
which recovers the well-known squared Sobolev semi-norm in nonparametric statistics. Gradient regularization stabilizes and improves the long time performance of EPT. The detailed derivation is presented in Section 4.

#### 4.2 LSDR Estimation with Gradient Regularizer

Let \(\{X_i\}_{i=1}^n\) and \(\{Y_i\}_{i=1}^n\) be two collections of i.i.d data from densities \(p(x)\) and \(q(x)\), respectively. Let \(\mathcal{H} = \mathcal{H}_{D,W,S,B}\) be the set of ReLU neural networks \(R_\phi\) with parameter \(\phi\), depth \(D\), width \(W\), size \(S\), and
\|R_\phi\|_\infty \leq B. We combine the least squares loss \([4.1]\) with the gradient regularizer \([4.2]\) as our objective function. The resulting gradient regularized LSDR estimator of \(r = p/q\) is given by

\[
\hat{R}_\phi \in \arg\min_{R_\phi \in \mathbb{R}^n} \frac{1}{n} \sum_{i=1}^{n} [R_\phi(X_i)^2 - 2R_\phi(Y_i)] + \alpha \frac{1}{n} \| \nabla R_\phi(X_i) \|_2^2,
\]

where \(\alpha \geq 0\) is a regularization parameter.

### 4.3 Estimation Error Bound

We first show that the density ratio \(r\) is identifiable through the objective function by proving that, at the population level, we can recover the density ratio \(\hat{r}\) via minimizing

\[
\mathcal{B}^\alpha_{\text{LSDR}}(R) = \mathcal{B}_{\text{LSDR}}(r, R) + \alpha \mathbb{E}_p[|\|\nabla R\|_2^2|] + C,
\]

where \(\mathcal{B}_{\text{LSDR}}\) is defined in \([4.1]\) and \(C = \mathbb{E}_{X \sim q}[r^2(X)] - 1\).

**Lemma 4.1.** For any \(\alpha \geq 0\), we have \(r = \arg\min_R \mathcal{B}^\alpha_{\text{LSDR}}(R)\). In addition, \(\mathcal{B}^\alpha_{\text{LSDR}}(R) \geq 0\) for any \(R\) with \(\mathbb{E}_{X \sim p}R^2(X) < \infty\), and \(\mathcal{B}^\alpha_{\text{LSDR}}(R) = 0\) iff \(R(x) = r(x) = 1\) \((q, p)\)-a.e. \(x \in \mathbb{R}^m\).

This identifiability result shows that the target density ratio is the unique minimizer of the population version of the empirical criterion in \((4.3)\). This provides a basis for establishing the convergence result of deep nonparametric density-ratio estimation.

Next we bound the nonparametric estimation error \(\|\hat{R}_\phi - r\|_{L^2(\nu)}\) under the assumptions that the support of \(\nu\) is concentrated on a compact low-dimensional manifold and \(r\) is Lipschitz continuous. Let \(\mathcal{M} \subseteq [-c, c]^m\) be a Riemannian manifold \([\text{Lee, 2010}]\) with dimension \(m\), condition number \(1/\tau\), volume \(V\), geodesic covering regularity \(R\), and \(m \ll M = O(m \ln(m) (\mathcal{V}/\tau)) \ll m\). Denote \(\mathcal{M}_\epsilon = \{x \in [-c, c]^m : \inf \{|x - y|_2 : y \in \mathcal{M}\} \leq \epsilon\}, \epsilon \in (0, 1)\).

**Theorem 4.1.** Assume \(\text{supp}(r) = \mathcal{M}\) and \(r(x)\) satisfies \(|r(x)| \leq B\) for a finite constant \(B > 0\) and is Lipschitz continuous with Lipschitz constant \(L\). Suppose the topological parameter of \(\mathcal{H}_{D, W, S, B}\) in \((4.3)\) with \(\alpha = 0\) satisfies \(D = O(\log n), W = O(n^{\frac{M}{2(2+M)}} / \log n), S = O(n^{\frac{M-2}{2}} / \log^4 n),\) and \(B = 2B\). Then,

\[
\mathbb{E}_{(X, Y) \sim \nu} \|\hat{R}_\phi - r\|_{L^2(\nu)}^2 \leq C(B^2 + cLmM)n^{-2/(2+M)},
\]

where \(C\) is a universal constant.

The error bound established in Theorem 4.1 for the nonparametric deep density-ratio fitting is new. This result is of independent interest for nonparametric estimation with deep neural networks. The above derived rate \(O(n^{-\frac{2}{2+M}})\) is faster than the optimal rate of convergence for nonparametric estimation of a Lipschitz target in \(\mathbb{R}^m\), where the optimal rate is \(O(n^{-\frac{1}{M+2}})\) \([\text{Stone, 1982}]\) \([\text{Schmidt-Hieber, 2020}]\) as long as the intrinsic dimension \(M\) of the data is much smaller than the ambient dimension \(m\). Therefore, the proposed density-ratio estimators circumvent the “curse of dimensionality” if data is supported on a lower-dimensional manifold. Low-dimensional structure of complex data is a common phenomenon in image analysis, computer vision and natural language processing.

### 5 Implementation

We now described how to implement EPT and train the optimal transport \(T\) with an i.i.d. sample \(\{X_i\}_{i=1}^n \subset \mathbb{R}^m\) from an unknown target distribution \(\nu\). The EPT map is trained via the forward Euler iteration \((2.6)-(2.8)\)
with a small step size \( s > 0 \). The resulting map is a composition of a sequence of residual maps, i.e., \( T_K \circ T_{K-1} \circ \ldots \circ T_0 \) for a large \( K \). As implied by Theorem 4.1 in Section 4, each \( T_k, k = 0, \ldots, K \) can be estimated with high accuracy by \( \tilde{T}_k = I + s\tilde{v}_k \), where \( \tilde{v}_k(x) = -f''(\tilde{R}_\phi(x))\nabla \tilde{R}_\phi(x) \). Here \( \tilde{R}_\phi \) is the density-ratio estimator defined in (4.3) below based on \( \{Y_i\}_{i=1}^n \) and the data \( \{X_i\}_{i=1}^n \sim p \). Therefore, according to the EPT map (2.9), the particles

\[
\tilde{T}(\tilde{Y}_i) = T_K \circ T_{K-1} \circ \ldots \circ T_0(\tilde{Y}_i), \quad i = 1, \ldots, n
\]
solve \( \min_{\phi} \mathcal{D}(\tilde{R}_{\phi}, R_{\phi}) \) for a large \( K \).

In many applications, high-dimensional complex data such as images, texts and natural languages, tend to have low-dimensional latent features. To learn generative models with latent low-dimensional structures, it is beneficial to have the option of first sampling particles \( \{Z_i\}_{i=1}^n \) from a low-dimensional reference distribution \( \tilde{\mu} \in \mathcal{P}(\mathbb{R}^\ell) \) with \( \ell \ll d \). Then we apply \( \tilde{T} \) to particles \( \tilde{Y}_i = G_{\theta}(Z_i), i = 1, \ldots, n \), where we introduce another deep neural network \( G_{\theta} : \mathbb{R}^\ell \rightarrow \mathbb{R}^m \) with parameter \( \theta \). We can estimate \( G_{\theta} \) via fitting the pairs \( \{(Z_i, \tilde{Y}_i)\}_{i=1}^n \). We describe the EPT algorithm below.

- **Outer loop for modeling low dimensional latent structure (optional)**
  - Sample \( \{Z_i\}_{i=1}^n \subset \mathbb{R}^\ell \) from a low-dimensional reference distribution \( \tilde{\mu} \) and let \( \tilde{Y}_i = G_{\theta}(Z_i), i = 1, 2, \ldots, n \).
  - **Inner loop for finding the push-forward map**
    - If there are no outer loops, sample \( \tilde{Y}_i \sim \mu, i = 1, \ldots, n \).
    - Get \( \tilde{v}(x) = -f''(\tilde{R}_\phi(x))\nabla \tilde{R}_\phi(x) \) via solving (4.3) below with \( Y_i = \tilde{Y}_i \). Set \( \tilde{T} = I + s\tilde{v} \) with a small step size \( s \).
    - Update the particles \( \tilde{Y}_i = \tilde{T}(\tilde{Y}_i), i = 1, \ldots, n \).
  - **End inner loop**
  - If there are outer loops, update the parameter \( \theta \) of \( G_{\theta}(\cdot) \) via solving \( \min_{\theta} \sum_i^n \|G_{\theta}(Z_i) - \tilde{Y}_i\|^2/n \).
  - **End outer loop**

6 RELATED WORK

We discuss connections between EPT and the existing related works. The existing generative models, such as VAEs, GANs and flow-based methods, parameterize a transform map with a neural network, say \( G \), that solves

\[
\min_{G} \mathcal{D}(G_{#}\mu, \nu), \quad (6.1)
\]

where \( \mathcal{D}(\cdot, \cdot) \) is an integral probability discrepancy. The original GAN (Goodfellow et al. 2014), \( f \)-GAN (Nowozin et al. 2016) and WGAN (Arjovsky et al. 2017) solve the dual form of (6.1) by parameterizing the dual variable using another neural network with \( \mathcal{D} \) as the JS-divergence, the \( f \)-divergence and the 1-Wasserstein distance, respectively. Based on the fact that the 1-Wasserstein distance can be evaluated from samples via linear programming (Sriperumbudur et al. 2012), Liu et al. (2018) and Genevay et al. (2018) proposed training the primal form of WGAN via a two-stage method that solves the linear program. SWGAN (Deshpande et al. 2018) and MMDGAN (Li et al. 2017; Binkowski et al. 2018) use the sliced quadratic Wasserstein distance and the maximum mean discrepancy (MMD) as \( \mathcal{D} \), respectively.
Vanilla VAE (Kingma & Welling, 2014) approximately solves the primal form of (6.1) with the KL-divergence loss under the framework of variational inference. Several authors have proposed methods that use optimal transport losses, such as various forms of Wasserstein distances between the distribution of learned latent codes and the prior distribution as the regularizer in VAE to improve performance. These methods include WAE (Tolstikhin et al., 2018), Sliced WAE (Kolouri et al., 2019) and Sinkhorn AE (Patrini et al., 2019).

Discrete time flow-based methods minimize (6.1) with the KL divergence loss (Rezende & Mohamed, 2015; Dinh et al., 2015; 2017; Kingma et al., 2016; Papamakarios et al., 2017; Kingma & Dhariwal, 2018). Grathwohl et al. (2019) proposed an ODE flow approach for fast training in such methods using the adjoint equation (Chen et al., 2018b). By introducing the optimal transport tools into maximum likelihood training, Chen et al. (2018a) and Zhang et al. (2018) considered continuous time flow. Chen et al. (2018a) proposed a gradient flow in measure spaces in the framework of variational inference and then discretized it with the implicit movement minimizing scheme (De Giorgi, 1993; Jordan et al., 1998). Zhang et al. (2018) considered gradient flows in measure spaces with time invariant velocity fields. CFGGAN (Johnson & Zhang, 2018) derived from the perspective of optimization in the functional space is a special form of EPT with $L_2$ taken as the KL divergence. SW flow (Liutkus et al., 2019) and MMD flow (Arbel et al., 2019) are gradient flows in measure spaces. MMD flow can be recovered from EPT by first choosing $L_2$ as the Lebesgue norm and then projecting the corresponding velocity vector fields onto reproducing kernel Hilbert spaces, please see Appendix B.3 for a proof. However, neither SW flow nor MMD flow can model hidden low-dimensional structure with the particle sampling procedure.

SVGD in (Liu, 2017) and the proposed EPT are both particle methods based on gradient flow in measure spaces. However, the SVGD samples from an un-normalized density, while EPT focuses on generative leaning, i.e., learning the distribution from samples. At the population level, projecting the velocity fields of EPT with KL divergence onto reproducing kernel Hilbert Spaces will recover the velocity fields of SVGD. The proof is given in Appendix B.3. Score-based methods in (Song & Ermon, 2019; 2020; Ho et al., 2020) are also particle methods based on unadjusted Langevin flow and deep score estimators. At the population level, the velocity fields of these score-based methods are random since they have a Brownian motion term, while the velocity fields of EPT are deterministic. At the sample level, these score-based methods need to learn a vector-valued deep score function. While in EPT we only need to estimate the density ratios which are scalar functions.

7 Experiments

The implementation details on numerical settings, network structures, SGD optimizers and hyper-parameters are given in the appendix. All experiments are performed using NVIDIA Tesla K80 GPUs. The PyTorch code of EPT is available at [https://github.com/anonymous/EPT](https://github.com/anonymous/EPT).

7.1 2D Simulated Data

We use EPT to learn 2D distributions adapted from (Grathwohl et al., 2019) with multiple modes and density ridges. The first row in Figure 1 shows kernel density estimation (KDE) plots of 50k samples from target distributions including (from left to right) 8Gaussians, pinwheel, moons, checkerboard, 2spirals, and circles. The second and third rows show the KDE plots of the learned samples via EPT with f-divergence and the surface plots of estimated density ratios after 20k iterations. The fourth and fifth rows show the KDE plots of the learned sample via EPT with Lebesgue norm of the density difference. Clearly, the generated samples via
EPT are nearly indistinguishable from those of the target samples and the estimated density-ratio/ difference functions are approximately equal to 1/0, indicating the learnt distribution matches the target well.

Next, we demonstrate the effectiveness of using the gradient penalty \(^{4.2}\) by visualizing the transport maps learned in the generative learning tasks with the learning targets \(5\text{quares}\) and \(large\text{Agaussians}\) from \(4\text{quares}\) and \(small\text{Agaussians}\), respectively. We use 200 particles connected with grey lines to manifest the learned transport maps. As shown in Figure 2(a), the central squares of \(5\text{quares}\) were learned better with the gradient penalty, which is consistent with the result on the estimated density-ratio in Figure 2(b). For \(large\text{Agaussians}\), the learned transport map exhibited some optimality under quadratic Wasserstein distance due to the obvious correspondence between the samples in Figure 2(a), and the gradient penalty also improves the density-ratio estimation as expected.

![Figure 1: KDE plots of the target samples (the first row). The second and third rows show the KDE plots of the learned samples via EPT with \(f\)-divergence and the surface plots of estimated density ratios after 20k iterations. The fourth and fifth rows show the KDE plots of the learned sample via EPT with Lebesgue norm of the density difference after 20k iterations.](image)

### 7.2 Benchmark Image Data

We show the performance of applying EPT to benchmark data MNIST (LeCun et al., 1998), CIFAR10 (Krizhevsky & Hinton, 2009) and CelebA (Liu et al., 2015) using ReLU ResNets without batch normalization and spectral normalization. The particle evolutions on MNIST and CIFAR10 without using outer loop are shown in Figure 3. Clearly, EPT can transport samples from a multivariate normal distribution into a target distribution.

We further compare EPT using the outer loop with the generative models including WGAN, SNGAN and MMDGAN. We considered different \(f\)-divergences, including Pearson’s \(\chi^2\), KL, JS and logD (Gao et al.)
Figure 2: Learned transport maps and estimated density-ratio in learning 5squares from 4squares, and learning large4gaussians from small4gaussians.

Figure 3: Particle evolution of EPT on MNIST and CIFAR10.

Table 1 shows FID (Heusel et al., 2017) evaluated with five bootstrap sampling of EPT with four divergences on CIFAR10. We can see that EPT using ReLU ResNets without batch normalization and spectral normalization attains (usually better) comparable FID scores with the state-of-the-art generative models. Comparisons of the real samples and learned samples on MNIST, CIFAR10 and CelebA are shown in Figure 4, where high-fidelity learned samples are comparable to real samples visually.

7.3 Numerical Convergence

Finally, we illustrate the convergence property of the learning dynamics of EPT on synthetic datasets pinwheel, checkerboard and 2spirals. As shown in Figure 5 on the three test datasets, the dynamics of both the estimated LSDR fitting losses in (4.3) with $\alpha = 0$ and the estimated value of the gradient norms $E_{X \sim q_k} [\| \nabla R_\phi(X) \|_2]$ demonstrate the estimated LSDR loss converges to the theoretical value $-1$.  

Table 1: Mean (standard deviation) of FID scores on CIFAR10. The FID score of NSCN is reported in Song & Ermon (2019) and results in the right table are adapted from Arbel et al. (2018).

| Models       | CIFAR10 (50k) | Models       | CIFAR10 (50k) |
|--------------|---------------|--------------|---------------|
| EPT-LSDR-χ²  | 24.9 (0.1)    | WGAN-GP      | 31.1 (0.2)    |
| EPT-LR-KL    | 25.9 (0.1)    | MMDGAN-GP-L2 | 31.4 (0.3)    |
| EPT-LR-JS    | 25.3 (0.1)    | SN-GAN       | 26.7 (0.2)    |
| EPT-LR-logD  | 24.6 (0.1)    | SN-SMMDGAN   | 25.0 (0.3)    |
| NCSN         | 25.3          |              |               |

Figure 4: Visual comparisons between real images (left 3 panels) and generated images (right 3 panels) by EPT-LSDR-χ² on MNIST, CIFAR10 and CelebA.

8 Conclusion and future work

EPT is a new approach for generative learning via training a transport map that pushes forward a reference to the target. This approach uses the forward Euler method for solving the McKean-Vlasov equation, which results from linearizing the Monge-Ampère equation that characterizes the optimal transport map. The EPT map is a composition of a sequence of simple residual maps. The key task in training is the estimation of density ratios that completely determine the residual maps. We estimate density ratios based on the Bregman divergence with gradient penalty using deep density-ratio fitting. We establish bounds on the approximation errors due to linearization, discretization, and density-ratio estimation. Our results provide strong theoretical guarantees for the proposed method and ensure that the EPT map converges fast to the target. We also show that the proposed density-ratio (difference) estimators do not suffer from the “curse of dimensionality” if data is supported on a lower-dimensional manifold. This is an interesting result in itself since density-ratio estimation is an important basic problem in machine learning and statistics. Because EPT is easy to train, computationally stable, and enjoys strong theoretical guarantees, we expect it to be a useful addition to the methods for generating learning.
There are two important ingredients in EPT: the velocity field and density-ratio estimation. With a suitable choice of the velocity and a density-ratio estimation procedure, EPT can recover several existing generative models such as MMD flow and SVGD. Thus our theoretical results also provide insights into the properties of these methods. Simulation results on multi-mode synthetic datasets and comparisons with the existing methods on real benchmark datasets using simple ReLU ResNets without batch normalization and spectral normalization support our theoretical analysis and demonstrate the effectiveness.

Some aspects and results in this paper are of independent interest. For example, density-ratio estimation is an important problem and of general interest in machine learning and statistics. The estimation error bound established in Theorem 4.1 for the nonparametric deep density-ratio fitting procedure are new. This provides an important example showing that deep nonparametric estimation can circumvent the curse of dimensionality via exploring the data structure. It is of interest to use the techniques developed here to investigate the generalization errors in setting of deep nonparametric regressions and classifications.

The proposed EPT method is motivated by the Monge–Ampère equation that characterizes the optimal transport map. However, while EPT pushes forward a reference distribution to the target, it is not an estimate of the optimal transport map itself. How to consistently estimate the Monge–Ampère optimal map remains a challenging and open problem.
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Algorithm 1: EPTv1: Euler particle transport

| Input: | $K \in \mathbb{N}^+, s > 0, \alpha > 0$ // maximum loop count, step size, regularization coefficient |
|--------|---------------------------------------------------|
| $X_i \sim \nu, \tilde{Y}_i^0 \sim \mu, i = 1, 2, \ldots, n$ // real samples, initial particles |
| $k \leftarrow 0$ |
| while $k < K$ do |
| $\hat{R}_k^i \in \arg \min R_\phi \frac{1}{n} \sum_{i=1}^{n} [R_\phi(X_i)^2 + \alpha \|\nabla R_\phi(X_i)\|_2^2 - 2R_\phi(\tilde{Y}_i^k)]$ via SGD // determine the density ratio |
| $\hat{v}^k(x) = -f''(\hat{R}_k^i(x))\nabla \hat{R}_k^i(x)$ // approximate the velocity field |
| $\tilde{T}_k = 1 + s\hat{v}^k$ // define the forward Euler map |
| $\tilde{Y}_i^{k+1} = \tilde{T}_k(\tilde{Y}_i^k), i = 1, 2, \ldots, n$ // update particles |
| $k \leftarrow k + 1$ |
| end |

Output: $\tilde{Y}_i^k \sim \tilde{\mu}_k, i = 1, 2, \ldots, n$ // transported particles

APPENDIX

In the appendix, we provide the implementation details on numerical settings, network structures, SGD optimizers, and hyper-parameters in the paper. We show the numerical convergence of EPT with simulated datasets and compare the learning and inference of EPT with other generative models. We give detailed theoretical background and proofs of the results mentioned in the paper. We also provide proofs MMD flow and SVGD can be derived from EPT by choosing appropriate $f$-divergences.

A A P P E N D I X : N U M E R I C A L E X P E R I M E N T S

A.1 Algorithm details

We provide the details of two versions of the EPT algorithm, EPTv1 in Algorithm 1 and EPTv2 in Algorithm 2 below. In Algorithm 1 we describe the algorithm without outer loops. In Algorithm 2 we describe the algorithm with a latent structure and outer loops.

A.2 Implementation details, network structures, hyper-parameters

We provide the details of two versions of the EPT algorithm, EPTv1 in Algorithm 1 and EPTv2 in Algorithm 2 below. In Algorithm 1 we describe the algorithm without outer loops. In Algorithm 2 we describe the algorithm with a latent structure and outer loops.

A.2.1 2D Examples

Experiments on 2D examples in our work were performed with deep LSDR fitting and the Pearson $\chi^2$ divergence. We use the EPTv1 (Algorithm 1) without outer loops. In inner loops, only a multilayer perceptron (MLP) was utilized for dynamic estimation of the density ratio between the model distribution $q_k$ and the target distribution $p$. The network structure and hyper-parameters in EPT and deep LSDR fitting were shared in all 2D experiments. We adopt EPT to push particles from a predrawn pool consisting of 50k i.i.d. Gaussian
Algorithm 2: EPTv2: Euler particle transport with latent structure

**Input**: $I_L, O_L \in \mathbb{N}^s, s > 0, \alpha > 0$  // maximum inner loop count, maximum outer loop count, step size, regularization coefficient

$X_i \sim \nu, i = 1, 2, \cdots, n$  // real samples

$\hat{G}_0^\theta \leftarrow G_0^{\text{init}}$  // initialize the transport map

$j \leftarrow 0$  /* outer loop */

while $j < O_L$ do

$Z_j^i \sim \mu, i = 1, 2, \cdots, n$  // latent particles

$\tilde{Y}_0^i = \hat{G}_j^\theta (Z_j^i), i = 1, 2, \cdots, n$  // intermediate particles

$k \leftarrow 0$  /* inner loop */

while $k < I_L$ do

$k \leftarrow k + 1$  // define the forward Euler map

$k \leftarrow k + 1$  // update particles

end

$\hat{G}_j^{O_L} \theta \leftarrow \arg \min_{G_\theta} \frac{1}{n} \sum_{i=1}^{n} \| G_\theta (Z_j^i) - \tilde{Y}_i^{IL} \|^2$ via SGD  // fit the transport map

end

**Output**: $\hat{G}_j^{O_L} \theta : \mathbb{R}^d \rightarrow \mathbb{R}^d$  // transport map with latent structure

particles to evolve in 20k steps. We used RMSProp with the learning rate 0.0005 and the batch size 1k as the SGD optimizer. The details are given in Table A1 and Table A2. We note that $s$ is the step size, $n$ is the number of particles, $\alpha$ is the penalty coefficient, and $T$ is the mini-batch gradient descent times of deep LSDR fitting or deep logistic regression in each inner loop hereinafter.

**Table A1**: MLP for deep LSDR fitting.

| Layer | Details      | Output size |
|-------|--------------|-------------|
| 1     | Linear, ReLU | 64          |
| 2     | Linear, ReLU | 64          |
| 3     | Linear, ReLU | 64          |
| 4     | Linear       | 1           |
Table A2: Hyper-parameters in EPT on 2D examples.

| Parameter | s    | n   | α   | T   |
|-----------|------|-----|-----|-----|
| Value     | 0.005| 50k | 0 or 0.5 | 5   |

A.2.2 Real image data

Datasets. We evaluated EPT on three benchmark datasets including two small datasets MNIST, CIFAR10 and one large dataset CelebA from GAN literature. MNIST contains a training set of 60k examples and a test set of 10k examples as $28 \times 28$ bilevel images which were resized to $32 \times 32$ resolution. There are a training set of 50k examples and a test set of 10k examples as $32 \times 32$ color images in CIFAR10. We randomly divided the 200k celebrity images in CelebA into two sets for training and test according to the ratio 9:1. We also pre-processed CelebA images by first taking a $160 \times 160$ central crop and then resizing to the $64 \times 64$ resolution. Only the training sets are used to train our models.

Evaluation metrics. Fréchet Inception Distance (FID) (Heusel et al., 2017) computes the Wasserstein distance $W_2$ with summary statistics (mean $\mu$ and variance $\Sigma$) of real samples $x$ and generated samples $g$ in the feature space of the Inception-v3 model (Szegedy et al., 2016), i.e., $FID = \|\mu_x - \mu_g\|^2 + \text{Tr}(\Sigma_x + \Sigma_g - 2(\Sigma_x \Sigma_g)^{\frac{1}{2}})$. Here, FID is reported with the TensorFlow implementation and lower FID is better.

Network architectures and hyper-parameter settings. We employed the ResNet architectures used by Gao et al. (2019) in our EPT algorithm. Especially, the batch normalization (Ioffe & Szegedy, 2015) and the spectral normalization (Miyato et al., 2018) of networks were omitted for EPT-LSDR-$\chi^2$. To train neural networks, we set SGD optimizers as RMSProp with the learning rate 0.0001 and the batch size 100. Inputs $\{Z_i\}_{i=1}^n$ in EPTv2 (Algorithm 2) were vectors generated from a 128-dimensional standard normal distribution on all three datasets. Hyper-parameters are listed in Table A3 where $IL$ expresses the number of inner loops in each outer loop. Even without outer loops, EPTv1 (Algorithm 1) can generate images on MNIST and CIFAR10 as well by making use of a large set of particles. Table A4 shows the hyper-parameters.

Table A3: Hyper-parameters in EPT with outer loops on real image datasets.

| Parameter | $\ell$ | s    | n   | α   | T   | IL  |
|-----------|--------|------|-----|-----|-----|-----|
| Value     | 128    | 0.5  | 1k  | 0   | 1   | 20  |

Table A4: Hyper-parameters in EPT without outer loops on real image datasets.

| Parameter | s    | n   | α   | T   |
|-----------|------|-----|-----|-----|
| Value     | 0.5  | 4k  | 0   | 5   |

A.3 Learning and Inference

The learning process of EPT performs particle evolution via solving the McKean-Vlasov equation using forward Euler iterations. The iterations rely on the estimation of the density ratios (difference) between the
pushforward distributions and the target distribution. To make the inference of EPTv1 more amendable, we propose EPTv2 based on EPTv1. EPTv2 takes advantage of a neural network to fit the pushforward map. The inference of EPTv2 is fast since the pushforward map is parameterized as a neural network and only forward propagation is involved. These aspects distinguish EPTv2 from score-based generative models Song & Ermon (2019; 2020) which simulate Langevin dynamics to generate samples.

**B Appendix: Proofs**

**B.1 Proof for Section 3**

**Proof of Proposition 3.1.** (i) The continuity equation (3.8) follows from the definition of the gradient flow directly, see, page 281 in (Ambrosio et al., 2008). (ii) The first equality follows from the chain rule and integration by part, see, Theorem 24.2 of Villani (2008). The second one on linear convergence follows from Theorem 24.7 of Villani (2008), where the assumption on $\lambda$ in equation (24.6) is equivalent to the $\lambda$-geodetically convex assumption here. (iii) Similar to (i) see, page 281 in Ambrosio et al. (2008). □

**Proof of Theorem 3.1.** (i) Recall $L[\mu]$ is a functional on $P^2_\mathbb{R}^m$. By the classical results in calculus of variation (Gelfand & Fomin, 2000),

$$\frac{\partial L}{\partial q}(\mathbf{x}) = \frac{d}{dt} L[q + t \xi] |_{t=0} = F'(q(\mathbf{x})), $$

where $\frac{\partial L}{\partial q}$ denotes the first order of variation of $L[\cdot]$ at $q$, and $q, \xi$ are the densities of $\mu$ and an arbitrary $\xi \in P^2_\mathbb{R}^m$, respectively. Let

$$F(z) = zF'(z) - F(z) : \mathbb{R}^1 \to \mathbb{R}^1.$$ 

Some algebra shows,

$$\nabla F'(q(\mathbf{x})) = q(\mathbf{x})\nabla F'(q(\mathbf{x})).$$

Then, it follows from Theorem 10.4.6 in (Ambrosio et al., 2008) that

$$\nabla F'(q(\mathbf{x})) = \partial^\circ L(\mu),$$

where, $\partial^\circ L(\mu)$ denotes the one in $\partial L(\mu)$ with minimum length. The above display and the definition of gradient flow implies the representation of the velocity fields $\mathbf{v}_t$.

(ii) The time dependent form of (3.4)–(3.5) reads

$$\frac{d}{dt} \mathbf{x}_t = \nabla \Phi_t(\mathbf{x}_t), \quad \text{with} \quad \mathbf{x}_0 \sim q,$$

$$\frac{d}{dt} \ln q_t(\mathbf{x}_t) = -\Delta \Phi_t(\mathbf{x}_t), \quad \text{with} \quad q_0 = q.$$

By chain rule and substituting the first equation into the second one, we have

$$\frac{1}{q_t}(\frac{d q_t}{dt} + q_t \frac{d \mathbf{x}_t}{dt}) = \frac{1}{q_t}(\frac{d q_t}{dt} + \nabla q_t \nabla \Phi_t(\mathbf{x}_t)) = -\Delta \Phi_t(\mathbf{x}_t),$$

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which implies,
\[
\frac{dq_t}{dt} = -q_t \Delta \Phi_t(x_t) - \nabla q_t \nabla \Phi_t(x_t) = -\nabla \cdot (q_t \nabla \Phi_t).
\]
By (3.10), the above display coincides with the continuity equation (3.8) with \(v_t = \nabla \Phi_t = -\nabla F' (q_t(x))\).
\[\square\]

**Proof of Theorem 3.2.** The Lipschitz assumption of \(v_t\) implies the existence and uniqueness of the McKean-Vlasov equation (2.4) according to the classical results in ODE (Arnold, 2012). By the uniqueness of the solution of (2.4) in a weak sense, see Proposition 8.1.7 in Ambrosio et al. (2008), it is sufficient to show that \(\mu_t = (X_t)_{\#} \mu\) satisfies the continuity equation (3.8) in a weak sense. This can be done by the standard test function and smoothing approximation arguments, see, Theorem 4.4 in Santambrogio (2015) for details. \[\square\]

**Proof of Lemma 3.1.** By definition,
\[
F(q_t(x)) = \begin{cases} 
 p(x) \frac{f(p(x))}{p(x)} \lambda \mu = \mathbb{D}_f(\mu \| \nu), \\
(q_t(x) - p(x))^2, \quad \mathcal{L}[\mu] = ||\mu - \nu||^2_{L^2(\mathbb{R}^m)}.
\end{cases}
\]
Direct calculation shows
\[
F'(q_t(x)) = \begin{cases} 
 f'(\frac{q_t(x)}{p(x)}) \lambda \nu = \mathbb{D}_f(\mu \| \nu), \\
2(q_t(x) - p(x)), \quad \mathcal{L}[\mu] = ||\mu - \nu||^2_{L^2(\mathbb{R}^m)}.
\end{cases}
\]
Then, the desired result follows from the above display and (3.10). \[\square\]

**Proof of Proposition 3.2.** Without loss of generality let \(K = \frac{T}{s} > 1\) be an integer. Recall \(\{\mu^t_s \mid t \in [ks, (k + 1)s]\}\) is the piecewise constant interpolation between \(\mu_k\) and \(\mu_{k+1}\) defined as
\[
\mu^t_s = (T^{k,s}_t)_{\#} \mu_k,
\]
where,
\[
T^{k,s}_t = 1 + (t - ks)v_k,
\]
\(\mu_k\) is defined in (16)-(18) with \(v_k = v_{ks}\), i.e., the continuous velocity in (3.10) at time \(ks, k = 0, ..., K - 1\), \(\mu_0 = \mu\). Under assumption (B.1) we can first show in a way similar to the proof of Lemma 10 in Arbel et al. (2019) that
\[
\mathcal{W}_2(\mu_{ks}, \mu_k) = \mathcal{O}(s). \tag{B-1}
\]
Let \(\Gamma\) be the optimal coupling between \(\mu_k\) and \(\mu_{ks}\), and \((X, Y) \sim \Gamma\). Let \(X_t = T^{k,s}_t(X)\) and \(Y_t\) be the solution of (2.4) with \(X_0 = Y\) and \(t \in [ks, (k + 1)s]\). Then
\[
X_t \sim \mu^t_s, \quad Y_t \sim \mu_t
\]
and
\[
Y_t = Y + \int_{ks}^t v_t(Y_{\hat{t}})d\hat{t}.
\]
It follows that
\[
\mathcal{W}^2_2(\mu_t, \mu_{ks}) \leq \mathbb{E}[\|Y_t - Y\|^2_2] \tag{B-2}
\]
\[\leq \mathbb{E}[\int_{ks}^t \|v_t(Y_{\hat{t}})\|^2_2 d\hat{t}]
\]
\[\leq \mathbb{E}[\int_{ks}^t \|v_t(Y_t)\|^2 d\hat{t}] \leq \mathcal{O}(s^2).
\]
where, the first inequality follows from the definition of $\mathcal{W}_2$, and the last equality follows from the the uniform bounded assumption of $v_t$. Similarly,

$$\mathcal{W}_2^2(\mu_k, \mu_k^*) \leq \mathbb{E}[\|X - X_t\|_2^2] = \mathbb{E}[\|(t - ks)v_k(X)\|_2^2] \leq \mathcal{O}(s^2).$$

Then,

$$\mathcal{W}_2(\mu_t, \mu_k^*) \leq \mathcal{W}_2(\mu_t, \mu_k) + \mathcal{W}_2(\mu_k, \mu_k^*) \leq \mathcal{O}(s),$$

where the first inequality follows from the triangle inequality, see for example Lemma 5.3 in Santambrogio (2015), and the second one follows from (B-1)-(B-3).

### B.2 Derivation and Proofs of the Results in Section 4

#### B.2.1 Bregman Score for Density Ratio/Difference

The separable Bregman score with the base probability measure $p$ to measure the discrepancy between a measurable function $R : \mathbb{R}^m \rightarrow \mathbb{R}^1$ and the density ratio $r$ is

$$\mathcal{B}_{\text{ratio}}(r, R) = \mathbb{E}_{X \sim p}\left[g'(R(X))(R(X) - r(X)) - g(R(X))\right]$$

$$= \mathbb{E}_{X \sim p}\left[g'(R(X))R(X) - g(R(X))\right] - \mathbb{E}_{X \sim q}\left[g'(R(X))\right].$$

It can be verified that $\mathcal{B}_{\text{ratio}}(r, R) \geq \mathcal{B}_{\text{ratio}}(r, r)$, where the equality holds iff $R = r$.

For deep density-difference fitting, a neural network $D : \mathbb{R}^m \rightarrow \mathbb{R}^1$ is utilized to estimate the density-difference $d(x) = q(x) - p(x)$ between a given density $q$ and the target $p$. The separable Bregman score with the base probability measure $w$ to measure the discrepancy between $D$ and $d$ can be derived similarly,

$$\mathcal{B}_{\text{diff}}(d, D) = \mathbb{E}_{X \sim p}\left[w(X)g'(D(X))] - \mathbb{E}_{X \sim q}[w(X)g'(D(X))\right] + \mathbb{E}_{X \sim w}[g'(D(X))D(X) - g(D(X))].$$

Here, we focus on the widely used least-squares density-ratio (LSDR) fitting with $g(c) = (c - 1)^2$ as a working example for estimating the density ratio $r$. The LSDR loss function is

$$\mathcal{B}_{\text{LSDR}}(r, R) = \mathbb{E}_{X \sim p}[R(X)^2] - 2\mathbb{E}_{X \sim q}[R(X)] + 1.$$ 

#### B.2.2 Gradient Penalty

We consider a noise convolution form of $\mathcal{B}_{\text{ratio}}(r, R)$ with Gaussian noise $\epsilon \sim \mathcal{N}(0, \alpha I)$,

$$\mathcal{B}_{\text{ratio}}^\alpha(r, R) = \mathbb{E}_{X \sim p}\mathbb{E}_{\epsilon}[g'(R(X + \epsilon))R(X + \epsilon) - g(R(X + \epsilon))] - \mathbb{E}_{X \sim q}\mathbb{E}_{\epsilon}[g'(R(X + \epsilon))].$$

Taylor expansion applied to $R$ gives

$$\mathbb{E}_\epsilon[R(x + \epsilon)] = R(x) + \frac{\alpha}{2} \Delta R(x) + \mathcal{O}(\alpha^2).$$

Using equations (13)-(17) in Roth et al. (2017), we get

$$\mathcal{B}_{\text{ratio}}^\alpha(r, R) \approx \mathcal{B}_{\text{ratio}}(r, R) + \frac{\alpha}{2} \mathbb{E}_{\epsilon}[g''(R)\|\nabla R\|_2^2],$$

i.e., $\frac{1}{2} \mathbb{E}_{\epsilon}[g''(R)\|\nabla R\|_2^2]$ serves as a regularizer for deep density-ratio fitting when $g$ is twice differentiable.
B.2.3 Proofs in Section 4

Below we prove Lemma 4.1 and Theorem 4.1 in Section 4.

Proof Lemma 4.1. By definition, it is easy to check
\[
\mathcal{B}^0_{\text{LSDR}}(R) = \mathcal{B}_{\text{ratio}}(r, R) - \mathcal{B}_{\text{ratio}}(r, r),
\]
where \(\mathcal{B}_{\text{ratio}}(r, R)\) is the Bregman score with the base probability measure \(p\) between \(R\) and \(r\). Then \(r \in \arg \min_{\text{measureable } R} \mathcal{B}^0_{\text{LSDR}}(R)\) follow from the fact \(\mathcal{B}_{\text{ratio}}(r, R) \geq \mathcal{B}_{\text{ratio}}(r, r)\) and the equality holds iff \(R = r\). Since
\[
\mathcal{B}^0(r) = \mathcal{B}^0_{\text{LSDR}}(R) + \alpha \mathbb{E}_p[\|\nabla R\|^2_2] \geq 0,
\]
Then,
\[
\mathcal{B}^0(r) = 0
\]
iff
\[
\mathcal{B}^0_{\text{LSDR}}(R) = 0 \text{ and } \mathbb{E}_p[\|\nabla R\|^2_2] = 0,
\]
which is further equivalent to
\[
R = r \text{ is constant } (q, p)-\text{a.e.},
\]
and the constant = 1 since \(r\) is a density ratio. \(\square\)

Proof of Theorem 4.1. We use \(\mathcal{B}(r)\) to denote \(\mathcal{B}^0_{\text{LSDR}} - C\) for simplicity, i.e.,
\[
\mathcal{B}(r) = \mathbb{E}_{X \sim p}[|R(X)|^2] - 2\mathbb{E}_{X \sim q}|R(X)|.
\tag{B-4}
\]
Rewrite \((20)\) with \(\alpha = 0\) as
\[
\hat{R}_\phi \in \arg \min_{R_\phi \in \mathcal{H}_{D,W,S,B}} \mathcal{B}(R_\phi) = \sum_{i=1}^n \frac{1}{n} (R_\phi(X_i)^2 - 2R_\phi(Y_i)).
\tag{B-5}
\]
By Lemma 4.1 and Fermat’s rule \([\text{Clarke}1990]\), we know \(0 \in \partial \mathcal{B}(r)\). Then, \(\forall R\) direct calculation yields,
\[
\|R - r\|_{L^2(\nu)}^2 = \mathcal{B}(R) - \mathcal{B}(r) - (\partial \mathcal{B}(r), R - r) = \mathcal{B}(R) - \mathcal{B}(r).
\tag{B-6}
\]
And \(\forall \hat{R}_\phi \in \mathcal{H}_{D,W,S,B}\) we have,
\[
\|\hat{R}_\phi - r\|_{L^2(\nu)}^2 = \mathcal{B}(\hat{R}_\phi) - \mathcal{B}(r) \leq \mathcal{B}(\hat{R}_\phi) - \mathcal{B}(r) + \mathcal{B}(\hat{R}_\phi) - \mathcal{B}(\hat{R}_\phi) \leq 2 \sup_{R \in \mathcal{H}_{D,W,S,B}} |\mathcal{B}(R) - \mathcal{B}(\hat{R}(R))| + \|\hat{R}_\phi - r\|_{L^2(\nu)}^2,
\tag{B-7}
\]
where the inequality uses the definition of \(\hat{R}_\phi, R_\phi\) and \((B-6)\). We prove the theorem by upper bounding the expected value of the right hand side term in \((B-7)\). To this end, we need the following auxiliary results \((B-8)-(B-10)\).
\[
\mathbb{E}_{\{Z_i\}_i}[\sup_R |\mathcal{B}(R) - \mathcal{B}(\hat{R}(R))|] \leq 4C_1 (2B + 1) \mathcal{G}(H),
\tag{B-8}
\]
where
\[
\mathcal{G}(H) = \mathbb{E}_{\{Z_i, \epsilon_i\}_i} \left[ \sup_{R \in \mathcal{H}_{D,W,S,B}} \left| \frac{1}{n} \sum_{i=1}^n \epsilon_i R(Z_i) \right| \right].
\]

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is the Gaussian complexity of $\mathcal{H}_{D,W,S,B}$ (Bartlett & Mendelson 2002).

**Proof of (B-8).** Let $g(c) = c^2 - c$, $z = (x,y) \in \mathbb{R}^m \times \mathbb{R}^m$,

$$\tilde{R}(z) = (g \circ R)(z) = R^2(x) - R(y).$$

Denote $Z = (X,Y)$, $Z_i = (X_i,Y_i)$, $i = 1,\ldots,n$ with $X_i$ i.i.d. $\sim p$, $Y_i$ i.i.d. $\sim q$. Let $\tilde{Z}_i$ be an i.i.d. copy of $Z_i$, and $\sigma_i(\epsilon_i)$ be i.i.d. Rademacher random (standard normal) variables that are independent of $Z_i$ and $\tilde{Z}_i$. Then,

$$\mathcal{B}(R) = \mathbb{E}_Z[\tilde{R}(Z)] = \frac{1}{n} \mathbb{E}_{\tilde{Z}_i}[\tilde{R}(\tilde{Z}_i)],$$

and

$$\hat{\mathcal{B}}(R) = \frac{1}{n} \sum_{i=1}^n \tilde{R}(Z_i).$$

Denote

$$\mathfrak{R}(\mathcal{H}) = \frac{1}{n} \mathbb{E}_{\{Z_i,\sigma_i\}} \left[ \mathbb{E}_{\{Z_i,\tilde{Z}_i\}} \sup_{R \in \mathcal{H}_{D,W,S,B}} \left| \sum_{i=1}^n \sigma_i R(Z_i) \right| \right]$$

as the Rademacher complexity of $\mathcal{H}_{D,W,S,B}$ (Bartlett & Mendelson 2002). Then,

$$\mathbb{E}_{\{Z_i\}} \left[ \sup_{R} \left| \mathcal{B}(R) - \hat{\mathcal{B}}(R) \right| \right] = \frac{1}{n} \mathbb{E}_{\{Z_i\}} \left[ \sup_{R} \left| \sum_{i=1}^n (\mathbb{E}_{\tilde{Z}_i}[\tilde{R}(\tilde{Z}_i)] - \tilde{R}(Z_i)) \right| \right]$$

$$\leq \frac{1}{n} \mathbb{E}_{\{Z_i,\tilde{Z}_i\}} \left[ \mathbb{E}_{\{Z_i,\tilde{Z}_i\}} \sup_{R} \left| \tilde{R}(\tilde{Z}_i) - \tilde{R}(Z_i) \right| \right]$$

$$= \frac{1}{n} \mathbb{E}_{\{Z_i,\tilde{Z}_i,\sigma_i\}} \left[ \mathbb{E}_{\{Z_i,\tilde{Z}_i,\sigma_i\}} \sup_{R} \left| \sum_{i=1}^n \sigma_i (\tilde{R}(\tilde{Z}_i) - \tilde{R}(Z_i)) \right| \right]$$

$$\leq \frac{1}{n} \mathbb{E}_{\{Z_i,\sigma_i\}} \left[ \sup_{R} \left| \sum_{i=1}^n \sigma_i \tilde{R}(Z_i) \right| \right] + \frac{1}{n} \mathbb{E}_{\{\tilde{Z}_i,\sigma_i\}} \left[ \sup_{R} \left| \sum_{i=1}^n \sigma_i \tilde{R}(\tilde{Z}_i) \right| \right]$$

$$= 2\mathfrak{R}(g \circ \mathcal{H})$$

$$\leq 4(2B + 1)\mathfrak{R}(\mathcal{H})$$

$$\leq 4C_1(2B + 1)\mathfrak{B}(\mathcal{H}),$$

where, the first inequality follows from the Jensen’s inequality, and the second equality holds since the distribution of $\sigma_i(R(\tilde{Z}_i) - \tilde{R}(Z_i))$ and $\tilde{R}(\tilde{Z}_i) - \tilde{R}(Z_i)$ are the same, and the last equality holds since the distribution of the two terms are the same, and last two inequality follows from the Lipschitz contraction property where the Lipschitz constant of $g$ on $\mathcal{H}_{D,W,S,B}$ is bounded by $2B + 1$ and the relationship between the Gaussian complexity and the Rademacher complexity, see for Theorem 12 and Lemma 4 in Bartlett & Mendelson (2002), respectively.

$$\mathfrak{B}(\mathcal{H}) \leq C_2 B \sqrt{\frac{n}{D \mathcal{S} \log \mathcal{S}}} \log \frac{n}{D \mathcal{S} \log \mathcal{S}} \exp(- \log^2 \frac{n}{D \mathcal{S} \log \mathcal{S}}).$$

(B-9)
Proof of (B-9). Since $\mathcal{H}$ is negation closed,

$$\mathcal{G}(\mathcal{H}) = \mathbb{E}(Z_1\epsilon_1 i_{\mathbb{R}}^{\mathcal{H}}\sup_{R \in \mathcal{H}_{D,W,B}} \frac{1}{n} \sum_{i=1}^{n} \epsilon_i R(Z_i))$$

$$= \mathbb{E}_{Z_1}[\mathbb{E}_{\epsilon_1}\sup_{R \in \mathcal{H}_{D,W,B}} \frac{1}{n} \sum_{i=1}^{n} \epsilon_i R(Z_i)]_{\{Z_i\}_{i=1}}.$$ 

Conditioning on $\{Z_i\}_{i=1}^{n}, \forall R, \tilde{R} \in \mathcal{H}_{D,W,B}$ it easy to check

$$\forall \epsilon_i, \frac{1}{n} \sum_{i=1}^{n} \epsilon_i (R(Z_i) - \tilde{R}(Z_i)) = \frac{d_H^2(R, \tilde{R})}{\sqrt{n}},$$

where, $d_H^2(R, \tilde{R}) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (R(Z_i) - \tilde{R}(Z_i))^2$. Observing the diameter of $\mathcal{H}_{D,W,B}$ under $d_H^2$ is at most $\mathcal{B}$, we have

$$\mathcal{G}(\mathcal{H}) \leq C_3 \frac{1}{\sqrt{n}} \mathbb{E}_{\{Z_i\}_{i=1}} \left[ \int_{0}^{\mathcal{B}} \sqrt{\log \mathcal{N}(\mathcal{H}, d_H^2, \delta)} d\delta \right]$$

$$\leq C_3 \frac{1}{\sqrt{n}} \mathbb{E}_{\{Z_i\}_{i=1}} \left[ \int_{0}^{\mathcal{B}} \sqrt{\log \mathcal{N}(\mathcal{H}, d_H^2, \delta)} d\delta \right]$$

$$\leq C_3 \frac{1}{\sqrt{n}} \left[ \mathcal{B} \sqrt{\log \mathcal{V}C_{\mathcal{H}} \log \frac{6 \mathcal{B} \mathcal{N}}{\delta \mathcal{V}C_{\mathcal{H}}}} \right]$$

$$\leq C_4 \mathcal{B} \left( \frac{n}{\mathcal{V}C_{\mathcal{H}}} \right)^{1/2} \log(\frac{n}{\mathcal{V}C_{\mathcal{H}}}) \exp\left(-\log^2\left(\frac{n}{\mathcal{V}C_{\mathcal{H}}}\right)\right)$$

$$\leq C_2 \mathcal{B} \sqrt{\frac{n}{\mathcal{D} \mathcal{S} \log \mathcal{S}}} \log(\frac{n}{\mathcal{D} \mathcal{S} \log \mathcal{S}}) \exp\left(-\log^2\left(\frac{n}{\mathcal{D} \mathcal{S} \log \mathcal{S}}\right)\right)$$

where, the first inequality follows from the chaining Theorem 8.1.3 in Vershynin (2018), and the second inequality holds due to $d_H^2 \leq d_H^2$, and in the third inequality we used the relationship between the matric entropy and the VC-dimension of the ReLU networks $\mathcal{H}_{D,W,B}$ (Anthony & Bartlett (2009)), i.e.,

$$\log \mathcal{N}(\mathcal{H}, d_H^2, \delta) \leq \mathcal{V}C_{\mathcal{H}} \log \frac{6 \mathcal{B} \mathcal{N}}{\delta \mathcal{V}C_{\mathcal{H}}},$$

and the fourth inequality follows by some calculation, and the last inequality holds due to the upper bound of VC-dimension for the ReLU network $\mathcal{H}_{D,W,B}$ satisfying

$$\mathcal{V}C_{\mathcal{H}} \leq C_5 \mathcal{D} \mathcal{S} \log \mathcal{S},$$

see Bartlett et al. (2019).

For any two integer $M, N$, there exists a $\tilde{R}_6 \in \mathcal{H}_{D,W,B}$ with width $W = \max\{8MN^{1/4} + 4M, 12N + 14\}$ and depth $D = 9M + 12$, and $B = 2B$, such that

$$\|r - \tilde{R}_6\|^2_{L_2(\nu)} \leq C_6 \mathcal{L} \mathcal{M} \mathcal{N} (NM)^{-4/4} \mathcal{M}.$$

(B-10)

Proof of (B-10). We use Lemma 4.1, Theorem 4.3, 4.4 and following the proof of Theorem 1.3 in Shen et al. (2019). Let $A$ be the random orthoprojector in Theorem 4.4, then it is to check $A(\mathcal{M}) \subset A([-c, c]^n) \subset [-c\sqrt{m}, c\sqrt{m}]^4$. Let $r$ be an extension of the restriction of $r$ on $\mathcal{M}$, which is defined similarly as $\hat{g}$ on page 30 in Shen et al. (2019). Since we assume the target $r$ is Lipschitz continuous with the bound $B$ and the
Lipschitz constant $L$, let $\epsilon$ small enough, then by Theorem 4.3, there exist a ReLU network $\tilde{R}_\phi \in \mathcal{H}_{D,W,S,B}$ with width

$$ W = \max\{8MN^{1/M} + 4M, 12N + 14\}, $$

and depth

$$ D = 9M + 12, $$

and $B = 2B$, such that

$$ \|\tilde{r} - \tilde{R}_\phi\|_{L^\infty(\mathbb{R},\mathcal{N})} \leq 80cL\sqrt{mM/(NM)}^{-2/m}, $$

and

$$ \|\tilde{R}_\phi\|_{L^\infty(\mathbb{R}^d)} \leq B + 3Lc\sqrt{mM}, $$

where, $\mathcal{N}$ is a $\nu$-negligible set with $\nu(\mathcal{N})$ can be arbitrary small. Define $\tilde{R}_\phi = \tilde{R}_\phi \circ A$. Then, following the proof after equation (4.8) in Theorem 1.3 of Shen et al. (2019), we get our (B-10) and

$$ \|\tilde{R}_\phi\|_{L^\infty(\mathbb{R},\mathcal{N})} \leq 2B, \|\tilde{R}_\phi\|_{L^\infty(\mathcal{N})} \leq 2B + 3Lc\sqrt{mM}. $$

Let $DS \log S < n$, combing the results (B-7) - (B-10), we have

$$ \mathbb{E}_{(X,Y)} \left[ \|\tilde{R}_\phi - r\|_{L^2(\nu)}^2 \right] \leq 8C_1(2B + 1)\Theta(H) + C_6cLM(NM)^{-4/M} $$

$$ \leq 8C_1(2B + 1)C_2B \sqrt{\frac{DS \log S}{n}} \log \frac{n}{DS \log S} $$

$$ + C_6cLM(NM)^{-4/M} $$

$$ \leq C(B^2 + cLMn)^{2/(2+M)}, $$

where, last inequality holds since we choose $M = \log n$, $N = n^{M/2+M} / \log n$, $S = n^{M+2} / \log^4 n$, i.e., $D = 9 \log n + 12$, $W = 12n^{M/2+M} / \log n + 14$. \hfill \square

B.3 The relationship between EPT and MMD flow

Here we show that MMD flow can be considered a special case of EPT.

**Proof.** Let $\mathcal{H}$ be a reproducing kernel Hilbert space with characteristic kernel $K(x, z)$. Recall in MMD flow,

$$ L[\mu] = \frac{1}{2} \|\mu - \nu\|_{\text{mmd}}^2, $$

and

$$ \frac{\partial L[\mu]}{\partial \mu}(x) = \int K(x, z) d\mu(z) - \int K(x, z) d\nu(z), $$

and the vector fields

$$ v^\text{mmd}_t = -\nabla \frac{\partial L[\mu]}{\partial \mu_t} $$

$$ = \int \nabla_x K(x, z) d\nu(z) - \int \nabla_x K(x, z) d\mu_t(z) $$

$$ = \int \nabla_x K(x, z) p_t(z) dz - \int \nabla_x K(x, z) q_t(z) dz $$

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By Lemma 3.1, the vector fields corresponding the Lebesgue norm $\frac{1}{2} \| \mu - \nu \|^2_{L^2(\mathbb{R}^m)} = \frac{1}{2} \int_{\mathbb{R}^m} |q(x) - p(x)|^2dx$ are defined as 

$$v_t = \nabla p(x) - \nabla q_t(x).$$

Next, we will show the vector fields $v_t^\text{mmd}$ is exactly by projecting the vector fields $v_t$ on to the reproducing kernel Hilbert space $\mathcal{H}^m = \mathcal{H}^\otimes m$. By the definition of reproducing kernel we have, 

$$p(x) = \langle p(\cdot), K(x, \cdot) \rangle_{\mathcal{H}} = \int K(x, z)p(z)dz,$$

and 

$$q_t(x) = \langle q_t(\cdot), K(x, \cdot) \rangle_{\mathcal{H}} = \int K(x, z)q_t(z)dz.$$

Hence, 

$$v_t(x) = \nabla p(x) - \nabla q_t(x)$$

$$= \int \nabla_x K(x, z)(p(z) - q_t(z))dz$$

$$= v_t^\text{mmd}(x).$$

This completes the proof. □

B.4 Proof of the relation between EPT and SVGD

Here we show that SVGD can be derived from EPT.

**Proof.** Let $f(u) = u \log u$ in (2.5). With this $f$ the velocity fields $v_t = -f''(r_t) \nabla r_t = -\frac{\nabla r_t(x)}{r_t(x)}$ Let $g$ in a Stein class associated with $q_t$. 

$$\langle v_t, g \rangle_{\mathcal{H}(q_t)} = -\int g(x)^T \nabla r_t(x) q_t(x)dx$$

$$= -\int g(x)^T \nabla \log r_t(x) q_t(x)dx$$

$$= -E_{X \sim q_t(x)}[g(x)^T \nabla \log q_t(X) + g(x)^T \nabla \log p(X)]$$

$$+ E_{X \sim q_t(x)}[g(x)^T \nabla \log p(X) + \nabla \cdot g(x)]$$

$$= -E_{X \sim q_t(x)}[T_p \cdot g] + E_{X \sim q_t(x)}[T_p \cdot g]$$

$$= E_{X \sim q_t(x)}[T_p \cdot g],$$

where the last equality is obtained by restricting $g$ in a Stein class associated with $q_t$, i.e., $E_{X \sim q_t(x)}[T_p \cdot g] = 0$. This is the velocity fields of SVGD [Liu 2017]. □