Distribution Matching in Deep Generative Models with Kernel Transfer Operators

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Abstract

Generative models which use explicit density modeling (e.g., variational autoencoders, flow-based generative models) involve finding a mapping from a known distribution, e.g. Gaussian, to the unknown input distribution. This often requires searching over a class of non-linear functions (e.g., representable by a deep neural network). While effective in practice, the associated runtime/memory costs can increase rapidly, usually as a function of the performance desired in an application. We propose a substantially cheaper (and simpler) distribution matching strategy based on adapting known results on kernel transfer operators. We show that our formulation enables highly efficient distribution approximation and sampling, and offers surprisingly good empirical performance that compares favorably with powerful baselines, but with significant runtime savings. We show that the algorithm also performs well in small sample size settings (in brain imaging).

1 Introduction

Generative modeling, in its unconditional form, refers to the problem of estimating the data generating distribution: given *i.i.d.* samples $\mathbf{X}$ with an unknown distribution P_X, a generative model seeks to find a parametric distribution that closely resembles P_X. In modern deep generative models, we often approaches this problem by via a *latent variable* – i.e., we assume that there is some variable $Z \in \mathcal{Z}$ associated with the observed data $X \in \mathcal{X}$ that follows a *known* distribution P_Z (also referred to as the *prior* in generative models). Thus, we can learn a mapping $f : Z \to X$ such that the distribution after transformation, denoted by $P_{f(Z)}$, aligns well with the data generating distribution P_X. Therefore, sampling from P_X becomes convenient since P_Z can be efficiently sampled. Frequently, f is parameterized by deep neural networks and optimized with SGD.

Existing generative modeling methods variously optimize the transformation f, most commonly modeling it as a Maximum Likelihood (ML) or distribution matching problem. For instance, given data $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$, a variational autoencoder (VAE) Kingma & Welling (2013) first constructs Z through the approximate posterior $q_{Z|X}$ and maximizes the lower bound of likelihood $p_{f(Z)}(\mathbf{X})$. Generative adversarial networks (GANs) Goodfellow et al. (2014) relies on a simultaneously learned discriminator such that samples of $P_{f(Z)}$ are indistinguishable from $\mathbf{X}$. Results in Arjovsky et al. (2017); Li et al. (2017) suggest that GANs minimize the distributional discrepancies between $P_{f(Z)}$ and P_X. Flow-based generative models optimize $p_{f(Z)}(\mathbf{X})$ explicitly through the *change of variable rule* and efficiently calculating the Jacobian determinant of the inverse mapping f^{-1}.

In all examples above, the architecture or objective notwithstanding, the common goal is to find a suitable function f that reduces the difference between $P_{f(Z)}$ and P_X. Thus, a key component in many deep generative models is to learn a *forward operator* as defined below.

Definition 1.1 (Forward operator)**.** *A forward operator $f^\star \in \mathcal{C} : \mathcal{Z} \to \mathcal{X}$ is defined to be a mapping associated with some latent variable $Z \sim P_Z$ such that $f^\star = \arg\min_{f \in \mathcal{C}} d(P_{f(Z)}, P_X)$ for some function class $\mathcal{C}$ and a distance measure $d(\cdot, \cdot)$.*

Motivation: The specifics of the forward operator may differ from case to case. But its properties and how it is estimated numerically greatly influences the empirical performance

of the model. For instance, mode collapse issues in GANs are well known and interesting solutions continue to emerge Srivastava et al. (2017). To learn the forward operator, VAEs use an approximate posterior $q_{Z|X}$ that may sometimes fail to align with the prior Kingma et al. (2016); Dai & Wipf (2019). Flow-based generative models enable direct access to the posterior likelihood, yet in order to tractably evaluate the Jacobian of the transformation during training, one must either restrict the expressiveness at each layer Dinh et al. (2017); Kingma & Dhariwal (2018) or make use of more involved solutions Chen et al. (2018). Of course, solutions to mitigate these weaknesses Ho et al. (2019) is an active area of research.

The starting point of our work is to evaluate the extent to which we can *radically* simplify the forward operator in deep generative models. Consider some desirable properties of a hypothetical forward operator (in Def. (1.1)): **(a)** Upon convergence, the learned operator $f^\star$ minimizes the distance between P_X and $P_{f(Z)}$ over all possible operators of a certain class. **(b)** The training scheme directly learns the mapping from the prior distribution P_Z, rather than an approximation. **(c)** The forward operator $f^\star$ can be efficiently learned and sample generation is also efficient. It would appear that these criteria violate the "no free lunch rule", and some compromise must be involved. Our goal is to investigate this trade-off: which design choices can make this approach work? Specifically, a well studied result in dynamical systems, namely the Perron-Frobenius operator Lemmens & Nussbaum (2012), suggests an alternative *linear* route to model the forward operator. Here, we show that the forward operator in generative models can be efficiently approximated as the estimation of a *closed-form linear operator* in the reproducing kernel Hilbert space (RKHS).

Contributions. Our results are largely based on results in kernel methods and dynamical systems, but we demonstrate their relevance in generative modeling and complement recent ideas that emphasize interesting links between deep generative models and dynamical systems.. Our contributions are **(a)** We propose a simple framework for transferring a known prior density *linearly* in RKHS to an unknown data density, which is equivalent to learning a nonlinear forward operator in the input space; **(b)** We evaluate this idea in multiple scenarios and show competitive generation performance with pre-trained autoencoders on popular image datasets including MNIST, CIFAR-10, CelebA and FFHQ; **(c)** As a special use case, we demonstrates the advantage of using the proposed framework in generative modeling tasks over other deep generative methods in limited data settings.

2 Preliminaries

We first briefly introduce reproducing kernel Hilbert space (RKHS) and kernel embedding of probability distributions, concepts that we will use frequently.

Definition 2.1 (RKHS Aronszajn (1950))**.** *For a set $\mathcal{X}$, let $\mathcal{H}$ be a set of functions $g : \mathcal{X} \to \mathbf{R}$. Then, $\mathcal{H}$ is a reproducing kernel Hilbert space (RKHS) with a product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ if there exists a function $k : \mathcal{X} \times \mathcal{X} \to \mathbf{R}$ (called a reproducing kernel) such that (i) $\forall x \in \mathcal{X}, g \in \mathcal{H}, g(x) = \langle g, k(x, \cdot) \rangle_{\mathcal{H}}$; (ii) $\mathcal{H} = cl(span(\{k(x, \cdot), x \in \mathcal{X}\}))$, where $cl(\cdot)$ is the set closure.*

The function $\phi(x) = k(x, \cdot) : \mathcal{X} \to \mathcal{H}$ is referred to as the *feature mapping* of the induced RKHS $\mathcal{H}$. A useful identity derived from feature mappings is the *kernel mean embedding*: it defines a mapping from a probablity measure in $\mathcal{X}$ to an element in the RKHS.

Definition 2.2 (Kernel Mean Embedding Smola et al. (2007))**.** *Given a probability measure p on $\mathcal{X}$ with an associated RKHS $\mathcal{H}$ equipped with a reproducing kernel k such that $\sup_{x \in \mathcal{X}} k(x, x) < \infty$, the kernel mean embedding of p in RKHS $\mathcal{H}$, denoted by $\mu_p \in \mathcal{H}$, is defined as $\mu_p = E_p[\phi(x)] = \int k(x, \cdot) p(x) dx$, and the mean embedding operator $\mathcal{E} : L^1(\mathcal{X}) \to \mathcal{H}$ is defined as $\mu_p = \mathcal{E}p$.*

Remark 1. *For characteristic kernels, the operator $\mathcal{E}$ is injective. Thus, two distributions (p, q) in $\mathcal{X}$ are identical iff $\mathcal{E}p = \mathcal{E}q$.*

This property allows using of *Maximum Mean Discrepancy (MMD)* for distribution matching Gretton et al. (2012); Li et al. (2017) and is common, see Muandet et al. (2017); Zhou et al. (2018). For a finite number of samples $\{\mathbf{x}_i\}_{i=1}^n$ drawn from the probabil-

ity measure p, an unbiased empirical estimate of $\mu_{\mathcal{H}}$ is $\hat{\mu}_{\mathcal{H}} = \frac{1}{n}\sum_{i=1}^{n} k(\mathbf{x}_i, \cdot)$ such that $\lim_{n\to\infty} \frac{1}{n}\sum_{i=1}^{n} k(\mathbf{x}_i, \cdot) = \mu_{\mathcal{H}}$.

Next, we review the covariance/cross covariance operators, two widely-used identities in kernel methods Fukumizu et al. (2013); Song et al. (2013) and building blocks of our approach.

Definition 2.3 (Covariance/Cross-covariance Operator)**.** *Let X, Z be random variables defined on $\mathcal{X} \times \mathcal{Z}$ with joint distribution $P_{X,Z}$ and marginal distributions P_X, P_Z. Let $(l, \phi, \mathcal{H})$ and $(k, \psi, \mathcal{G})$ be two sets of (a) bounded kernel, (b) their corresponding feature map, and (c) their induced RKHS, respectively. The (uncentered) covariance operator $\mathcal{C}_{ZZ} : \mathcal{H} \to \mathcal{H}$ and cross-covariance operator $\mathcal{C}_{XZ} : \mathcal{H} \to \mathcal{G}$ are defined as*

$$\mathcal{C}_{ZZ} \triangleq \mathbb{E}_{z\sim P_Z}[\phi(z) \otimes \phi(z)] \qquad \mathcal{C}_{XZ} \triangleq \mathbb{E}_{(x,z)\sim P_{X,Z}}[\psi(x) \otimes \phi(z)] \tag{1}$$

3 Simplifying estimation of the forward operator

Let us consider the forward operator in generative models as a dynamical system, a view taken by a number of results Chen et al. (2018); Grathwohl et al. (2019); Behrmann et al. (2019). Let us temporarily assume that $\mathcal{Z} = \mathcal{X}$ – this is not true for VAEs and GANs, where the latent variable Z lives in a lower dimensional space relative to the input space (i.e. $|\mathcal{Z}| \ll |\mathcal{X}|$). Nevertheless, since $\mathcal{Z}$ is often modeled as a subspace of $\mathcal{X}$, we can just embed $\mathcal{Z}$ into $\mathcal{X}$ to satisfy the equivalence.

Notations		Meaning
Z	X	Random variable
$\mathcal{Z}$	$\mathcal{X}$	Domain
P_Z	P_X	Distribution
p_Z	p_X	Density function
k	l	Kernel function
$\mathcal{H}$	$\mathcal{G}$	RKHS
$\phi(\cdot)$	$\psi(\cdot)$	Feature mapping
$\mathcal{E}_k$	$\mathcal{E}_l$	Mean embedding operator
μ_Z	μ_X	Kernel mean embedding

Table 1: Notations used in this paper.

Forward operator as a dynamical system:
In Def. 1.1, we define the forward operator as the minimizer of the distance between the data generating distribution p_X and the *post*-transformation prior $p_{f(Z)}$. While the following perspective does not inform our formulation, readers familiar with recent work on hybrid models may easily view the forward operator $f^\star$ as the solution function of a (deterministic) continuous dynamical system, similar to the dynamical-system view of flow-based generative in Neural ODE Chen et al. (2018). Other generative models with explicit layered structure can be viewed as an Euler discretization of the underlying dynamics Behrmann et al. (2019). As an illustration, the dynamics on an element $z(t_0) \in \mathcal{X}$ by applying $f^\star$ is governed by,

$$x = z(t_0) + \int_{t_0}^{t_1} \Delta_t(z(t))dt,$$

We can integrate the RHS and write $g^\star(z(t_0)) = \int_{t_0}^{t_1} \Delta_t(z(t))$. The forward operator $f^\star = (I + g^\star) : \mathcal{X} \to \mathcal{X}$, therefore, controls the discrete evolution of $z(t_0)$ at time t_1 as $x = f^\star(z(t_0))$. So, the marginal density over a subset of the state space $\Lambda \subseteq \mathcal{X}$ can be expressed as

$$\int_\Lambda p_X(x)dx = \int_{z\in f^{\star -1}(\Lambda)} p_Z(z)dz \tag{2}$$

Towards a one-step estimation of forward operator: Both $f^\star$ and $f^{\star -1}$ in (2) will be highly nonlinear in practice. Therefore, learning f requires searching over a large space of nonlinear functions (e.g., functions represented by a given network architecture). Sometimes, evaluations of the RHS integral or its lower bound (i.e., ELBO in VAE and exact likelihood in flow based models) can be expensive. Nevertheless, the dynamical systems literature suggests a simpler, *linear* extension of the transformation of p_Z, namely the *Perron-Frobenius* operator or transfer operator, that conveniently transfers p_Z to p_X.

Definition 3.1 (Perron-Frobenius operator Mayer (1980))**.** *Given a dynamical system $f : \mathcal{X} \to \mathcal{X}$, the Perron-Frobenius (PF) operator $\mathcal{P} : L^1(\mathcal{X}) \to L^1(\mathcal{X})$ is an infinite-dimensional linear operator defined as $\int_\Lambda (\mathcal{P}p_Z)(x)dx = \int_{z\in f^{-1}(\Lambda)} p_Z(z)dz$ for all $\Lambda \subseteq \mathcal{X}$.*

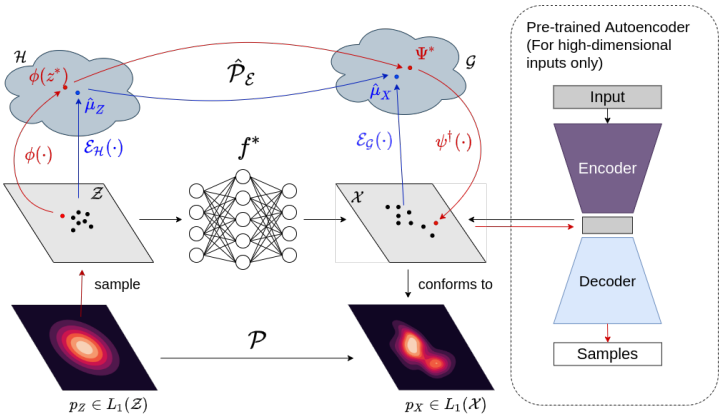


Figure 1: Summary of our proposed framework. Blue arrows demonstrates how densities are empirically embedded and transferred by the kPF operator. Red arrows indicates the steps for new sample generation. The pre-trained autoencoder projects the data onto a *smooth* latent space and is only required when generating high-dimensional data such as images.

With this definition of the PF operator, $\mathcal{P}$, we have

$$p_X = \mathcal{P} p_Z. \tag{3}$$

If $\mathcal{P}$ can be efficiently estimated, we can use it to transfer the tractable probability density p_Z to the target density p_X. However, since $\mathcal{P}$ is an infinite-dimensional operator on $L^1(\mathcal{X})$, it is impractical to instantiate it explicitly and exactly. Nonetheless, common methods for estimating the Perron-Frobenius operator include Ulam's method Ulam (1960) and the extended dynamical mode decomposition (EDMD) Williams et al. (2015a). Both strategies project $\mathcal{P}$ onto a finite number of hand-crafted basis functions – this may suffice in many settings but may fall short in modeling highly complex dynamics.

"Kernel embedded" form of PF operator: A natural extension Klus et al. (2020) is to represent $\mathcal{P}$ by an infinite set of functions, e.g., projecting it onto the bases of an RKHS via the *kernel trick*. There, for a characteristic kernel l, the *kernel mean embedding* uniquely identifies an element $\mu_X = \mathcal{E}_l p_X \in \mathcal{G}$ for $p_X \in L^1(\mathcal{X})$. Thus, to approximate $\mathcal{P}$, we may alternatively solve for the dynamics from p_Z to p_X in their *embedded* form. Using Tab. 1 notations, we have the following linear operator that defines the dynamics between two embedded densities.

Definition 3.2 (Kernel-embedded Perron-Frobenius operator Klus et al. (2020))**.** *Given $p_Z \in L^1(\mathcal{X})$ and $p_X \in L^1(\mathcal{X})$. Denote k as the **input kernel** and l as the **output kernel**. Let $\mu_X = \mathcal{E}_l p_X$ and $\mu_Z = \mathcal{E}_k p_Z$ be their corresponding mean kernel embeddings. The kernel-embedded Perron-Frobenius (kPF) operator, denoted by $\mathcal{P}_\mathcal{E} : \mathcal{H} \to \mathcal{G}$, is defined as*

$$\mathcal{P}_\mathcal{E} = \mathcal{C}_{XZ} \mathcal{C}_{ZZ}^{-1} \tag{4}$$

Proposition 3.1 (Song et al. (2013))**.** *With the above definition, $\mathcal{P}_\mathcal{E}$ satisfies*

$$\mu_X = \mathcal{P}_\mathcal{E} \mu_Z \tag{5}$$

*under the conditions: **(i)** $\mathcal{C}_{ZZ}$ is injective **(ii)** $\mu_t \in range(\mathcal{C}_{ZZ})$ **(iii)** $\mathbb{E}[g(X)|Z = \cdot] \in \mathcal{H}$ for any $g \in G$.*

The last two assumptions can sometimes be difficult to satisfy for certain RKHS (see Theorem 2 of Fukumizu et al. (2013)). In such cases, a relaxed solution can be constructed by replacing $\mathcal{C}_{ZZ}^{-1}$ by a regularized inverse $(\mathcal{C}_{ZZ} + \lambda I)^{-1}$ or a Moore-Penrose inverse $\mathcal{C}_{ZZ}^{\dagger}$.

The following proposition shows commutativity between the (kernel-embedded) PF operator and the mean embedding operator, showing its equivalence to $\mathcal{P}$ when l is characteristic.

Proposition 3.2 (Klus et al. (2020))**.** *With the above notations, $\mathcal{E}_l \circ \mathcal{P} = \mathcal{P}_\mathcal{E} \circ \mathcal{E}_k$.*

Transferring embedded densities with the kPF operator: The kPF operator is a powerful tool that allows transferring embedded densities in RKHS. The main steps are:

(1) Use mean embedded operator $\mathcal{E}_l$ on p_Z. Let us denote it by μ_Z.
(2) Transfer μ_Z using kPF operator $\mathcal{P}_\mathcal{E}$ to get mean embedded p_X, given by μ_X.

Of course, in practice with finite data, $\{\mathbf{x}_i\}_{i\in[n]} \sim P_X$ and $\{\mathbf{z}_i\}_{i\in[n]} \sim P_X$, $\mathcal{P}_\mathcal{E}$ must be estimated empirically (See Klus et al. (2020) for an error analysis).

$$\hat{\mathcal{P}}_\mathcal{E} = \hat{\mathcal{C}}_{XZ}(\hat{\mathcal{C}}_{ZZ})^{-1} \approx \Psi(\Phi^T\Phi + \lambda n I)^{-1}\Phi^T \approx \Psi(\Phi^T\Phi)^\dagger\Phi^T$$

where $\Phi = [k(\mathbf{z}_1, \cdot), \cdots, k(\mathbf{z}_n, \cdot)]$, $\Psi = [l(\mathbf{x}_1, \cdot), \cdots, l(\mathbf{x}_n, \cdot)]$ are simply the corresponding feature matrices for samples of P_X and P_Z, and λ is a small penalty term.

Learning kPF for unconditional generative modeling: Some generative modeling methods such as VAEs and flow-based formulations explicitly model the latent variable Z as conditionally dependent on the data variable X. This allows deriving/optimizing the likelihood $p_{f(Z)}(X)$. This is desirable but may not be critical in all applications. To learn a kPF, however, X and Z can be independent RVs. While it may not be immediately obvious why we could assume this independence, we can observe the following property for the empirical kPF operator, assuming that the empirical covariance operator $\hat{\mathcal{C}}_{ZZ}$ is non-singular:

$$\hat{\mathcal{P}}_\mathcal{E}\hat{\mu}_Z = \hat{\mathcal{C}}_{XZ}\hat{\mathcal{C}}_{ZZ}^{-1}\hat{\mu}_Z = \underbrace{\Psi\Phi^\top}_{\hat{\mathcal{C}}_{XZ}}(\underbrace{\Phi\Phi^\top}_{\hat{\mathcal{C}}_{ZZ}})^{-1}\Phi 1_n = \Psi(\Phi^\top\Phi)^{-1}\Phi^\top\Phi 1_n = \Psi 1_n = \hat{\mu}_X \tag{6}$$

Suppose that $\{\mathbf{x}_i\}_{i\in[n]}$ and $\{\mathbf{z}_j\}_{i\in[n]}$ are independently sampled from the marginals P_X and P_Z. It is easy to verify that that (6) holds for any pairing $\{(\mathbf{x}_i, \mathbf{z}_j)\}_{(i,j)\in[n]\times[n]}$. Learning the kPF operator is similar in spirit to other implicit density models such as GAN, where the search criteria is based on sample discrepancy rather than explicit likelihoods.

Mapping Z to $\mathcal{G}$: Now, since $\mathcal{P}_\mathcal{E}$ is a *deterministic* linear operator, we can easily set up a scheme to map samples of Z to elements of $\mathcal{G}$ where the expectation of the mapped samples equals μ_X

Define $\phi(z) = k(z, \cdot)$ and $\psi(x) = l(x, \cdot)$ as feature maps of kernels k and l. We can rewrite μ_X as

$$\mu_X = \mathcal{P}_\mathcal{E}\mathcal{E}_k p_Z = \mathcal{P}_\mathcal{E} E_Z[\phi(Z)] = E_Z[\mathcal{P}_\mathcal{E}(\phi(Z))] = E_Z[\psi\left(\psi^{-1}\left(\mathcal{P}_\mathcal{E}\phi\left(Z\right)\right)\right)] \tag{7}$$

Here ψ^{-1} is the inverse or the *preimage map* of ψ. Such an inverse, in general, may not exist Kwok & Tsang (2004); Honeine & Richard (2011). We will discuss a procedure to approximate ψ^{-1} in §4.1. In what follows, we will temporarily assume that an exact preimage map exists and is tractable to compute.

Define $\Psi^* = \hat{\mathcal{P}}_\mathcal{E}\phi(Z)$ as the *transferred sample* in $\mathcal{G}$ using the empirical embedded PF operator $\hat{\mathcal{P}}_\mathcal{E}$. Then the following result shows that asymptotically the transferred samples converge in distribution to the target distribution.

Proposition 3.3. *As $n \to \infty$, $\psi^{-1}(\Psi^*) \xrightarrow{\mathcal{D}} P_X$. In other words, the preimage of the transferred sample approximately conforms to P_X under the previous assumptions when n is large.*

Proof. $\mathbb{E}[\psi(\psi^{-1}(\Psi^*))] = \mathbb{E}[\Psi^*] = \mathbb{E}[\hat{\mathcal{P}}_\mathcal{E}\phi(Z)] = \hat{\mathcal{P}}_\mathcal{E}\mu_Z \overset{\text{asymp.}}{=} \mu_X$ □

4 Sample generation using the Kernel transfer operator

At this point, the transferred sample Ψ^*, obtained by the kPF operator, remains an element of RKHS $\mathcal{G}$. To translate the samples back to the input space, we must find the preimage x^* such that $\psi(x^*) = \Psi^*$.

4.1 Solving for an approximate preimage

Solving the preimage in kernel-based methods is known to be ill-posed Mika et al. (1999) because the mapping $\psi(\cdot)$ is not necessarily surjective, i.e., a unique preimage $\mathbf{x}^* = \psi^{-1}(\Psi^*), \Psi^* \in \mathcal{H}$ may not exist. Often, an approximate preimage $\psi^\dagger(\mathbf{X}, \Psi^*) \approx \psi^{-1}(\Psi^*)$ is constructed instead based on relational properties among the training data in the RKHS. We consider two options in our framework **(1)** MDS-basd method Kwok & Tsang (2004); Honeine & Richard (2011),

$$\psi^\dagger_{\text{MDS}}(\mathbf{X}, \Psi^*) = \tfrac{1}{2}(\mathbf{X}'\mathbf{X}'^\top)^{-1}\mathbf{X}'(\text{diag}(\mathbf{X}'^\top\mathbf{X}') - \mathbf{d}^\top), \text{where } \forall i \in [\gamma], \mathbf{d}_i = \|l(\mathbf{x}'_i, \cdot) - \Psi^*\|_{\mathcal{G}} \tag{8}$$

which optimally preserves the distances in RKHS to the preimages in the input space, and **(2)** weighted Fréchet mean Friedman et al. (2001), which in Euclidean space takes the form

$$\psi^\dagger_{\text{wFM}}(\mathbf{X}, \Psi^*) = \psi^\dagger_{\text{wFM}}(\mathbf{X}'; \mathbf{s}) = \mathbf{X}'\mathbf{s}/\|\mathbf{s}\|_1, \text{where } \forall i \in [\gamma], \mathbf{s}_i = \langle l(\mathbf{x}'_i, \cdot), \Psi^* \rangle \tag{9}$$

The weighted Fréchet mean preimage uses the inner product weights $\langle \Psi^*, \psi(\mathbf{x}_i) \rangle$ as measures of similarities to interpolate training samples. Similar to Kwok & Tsang (2004), we only consider a neighborhood $\mathbf{X}'$ of γ training samples based on pairwise distance or similarity in RKHS. On the toy data (as in Fig. 2), weighted Fréchet mean produces fewer samples that deviate from the true distribution and is easier to compute. Based on this observation, we use the weighted Fréchet mean as the preimage module for all experiments that requires samples, while acknowledging that other preimage methods can also be substituted in.

Algorithm 1 Sample Generation from kPF

Input: Training data $\mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$, Optional autoencoder (E, D), input/output kernels (k, l), neighborhood size γ
Training
  $\mathbf{X} = (E(\mathbf{x}_1), \ldots, E(\mathbf{x}_n))$ if E is provided
  Sample $\{\mathbf{z}_i\}_{i\in[n]} \sim P_Z$ independently
  Construct $L, K \in R^{n\times n}$ s.t.
    $L_{ij} = l(\mathbf{x}_i, \mathbf{x}_j), K_{ij} = k(\mathbf{z}_i, \mathbf{z}_j)$
  $K_{\text{inv}} = (K + \lambda n I)^{-1}$ or $K^\dagger$
Inference
  Generate new prior sample $\mathbf{z}^* \sim P_Z$
  $\mathbf{s} = L \cdot K_{\text{inv}}[k(\mathbf{z}_1, \mathbf{z}^*) \ldots k(\mathbf{z}_n, \mathbf{z}^*)]^\top$
  $ind = \text{argsort}(\mathbf{s})[-\gamma :]$
  $\mathbf{x}^* = \psi^\dagger_{\text{wFM}}(\mathbf{X}[ind]\,; \mathbf{s}[ind])$.
Output $D(\mathbf{x}^*)$ if D is provided else $\mathbf{x}^*$

With all the ingredients in hand, we now present an algorithm for sample generation using the kPF operator in Alg. 1. The idea is simple yet powerful: at training time, we construct the empirical kPF operator $\hat{\mathcal{P}}_{\mathcal{E}}$ using the training data $\{\mathbf{x}_i\}_{i\in[s]}$ and samples of the known prior $\{\mathbf{z}_i\}_{1\in[n]}$. At test time, we will transfer new points sampled from P_Z to feature maps in $\mathcal{H}$, and construct their preimages as the generated output samples.

4.2 Image generation

Image generation is a common application for generative models Goodfellow et al. (2014); Dinh et al. (2017). While our framework is not specific to images, constructing sample preimages in a high dimensional space with limited training samples can be challenging, since the space of images is usually not dense in a reasonably sized neighborhood. However, empirically images often lie near a low dimensional manifold in the ambient space Seung & Lee (2000), and one may utilize an autoencoder (AE) (E, D) to embed the images onto a latent space that represents coordinates on a learned manifold. If the learned manifold lies close to the true manifold, we can learn densities on the manifold directly Dai & Wipf (2019).

Therefore, for image generation tasks, the training data is first projected onto the latent space of a pretrained AE. Then, the operator will be constructed using the projected latent representations, and samples will be mapped back to image space with the decoder of AE. Our setup can be viewed analogously to other generative methods based on so called "*ex-post*" density estimation of latent variables Ghosh et al. (2020). We also restrict the AE latent space to a hypersphere $\mathbf{S}^{n-1}$ to ensure that **(a)** $k(\cdot,\cdot)$ and $l(\cdot,\cdot)$ are bounded and **(b)** the space is geodesically convex and complete, which is required by the preimage computation. To compute the weighted Fréchet mean on a hypersphere, we adopt the recursive algorithm in Chakraborty & Vemuri (2015) (see appendix D for details).

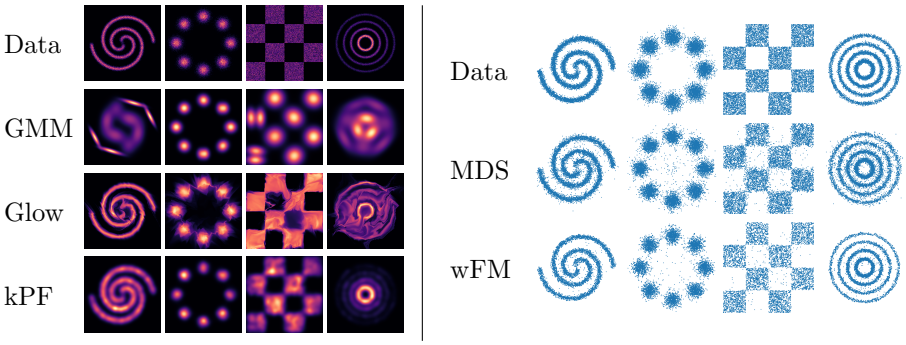


Figure 2: *Left figure:* Density estimation on 2D toy data. **Top to bottom: (1)** Training data samples, and learned densities of **(2)** GMM **(3)** Glow **(4)** Proposed kPF operator. More details in appendix. *Right figure:* Sample generation results. **Top:** Data samples **Middle:** MDS-based preimage samples **Bottom:** Weighted Fréchet mean samples.

5 Experimental Results

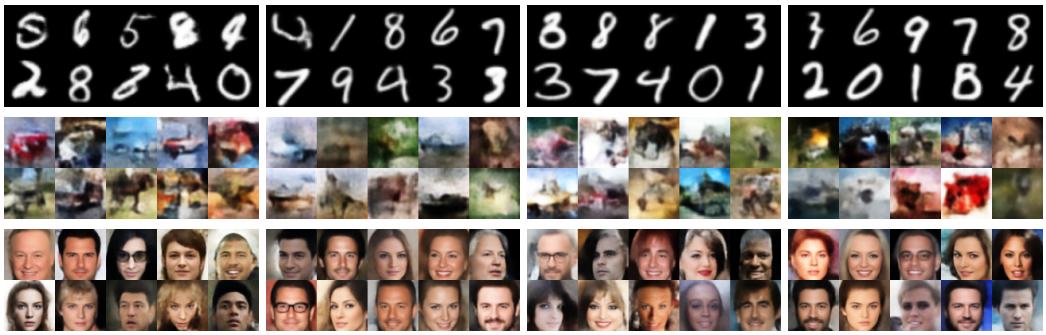
Goals. In our experiments, we seek to answer three questions: **(a)** With sufficient data, can our method generate new data with comparable performance with other state-of-the-art generative models? **(b)** If only limited data samples were given, can our method still estimate the density with reasonable accuracy? **(c)** What are the runtime benefits, if any?

Datasets/setup. To answer the first question, we evaluate our method on standard vision datasets, including MNIST, CIFAR10, and CelebA, where the number of data samples is much larger than the latent dimension. We compare our results with other VAE variants (Two-stage VAE Dai & Wipf (2019), WAE Arjovsky et al. (2017), CV-VAE Ghosh et al. (2020)) and flow-based generative models (Glow Kingma & Dhariwal (2018), CAGlow Liu et al. (2019)) The second question is due to the broad use of kernel methods in small sample size settings. For this more challenging case, we randomly choose 100 training samples ($< 1\%$ of the full dataset) from CelebA and evaluate the quality of generation compared to other density approximation schemes. We also use a dataset of T1 Magnetic Resonance (MR) images from the Alzheimer's Disease Neuromaging Initiative (ADNI) study.

Distribution matching with many data samples. We evaluate the quality by calculating the Fréchet Inception Distance (FID) Heusel et al. (2017) with 10K generated images from each model. Here, we use a pretained regularized autoencoder Ghosh et al. (2020) with a latent space restricted to the hypersphere (denoted by SRAE) to encourage *smooth* latent representations. All implemented models share the same encoder/decoder structure used in Ghosh et al. (2020). The subscript indicates different types of density estimators learned on the latent variables, including Glow Kingma & Dhariwal (2018), Gaussian mixture model (GMM), and two proposed kPF operators with Gaussian kernel as the input kernel (RBF-kPF) and with NTK as the input kernel (NTK-kPF). The use of NTK is motivated by promising results at the interface of kernel methods and neural networks Jacot et al. (2018); Arora et al. (2020). Implementation details are included in the appendix. We also provide a code implementation along with the submission.

Comparative results are shown in Table 2. We see that for images with structured feature spaces, e.g., MNIST and CelebA, our method matches or outperforms other non-adversarial generative models, which provides evidence in support of the premise that the forward

Figure 3: Representative samples from learned kPF on pre-trained NVAE latent space



Two-stage VAE | $\text{SRAE}_{\text{Glow}}$ | SRAE_{GMM} | $\text{SRAE}_{\text{NTK-kPF}}$

Figure 4: Comparison of different sampling techniques using AE trained on CelebA 64x64. Left to right: samples of (1) Two-Stage VAE (Dai & Wipf, 2019) (2) $\text{SRAE}_{\text{Glow}}$ (Kingma & Dhariwal, 2018) (3) SRAE_{GMM} (4) SRAE $_{\text{NTK-kPF}}$ using 10k latent points.

operator can be simplified. Further, we present qualitative results on all datasets (in Fig. 4), where we compare our kPF operator based model with other density estimation techniques on the latent space. Observe that our model generates comparable visual results as $\text{SRAE}_{\text{Glow}}$.

Since kPF learns the distribution on a pre-trained AE latent space for image generation, using a more powerful AE can offer improvements in generation quality. In Fig. 3, we present representative images by learning our kPF on NVAE Vahdat & Kautz (2020) latent space, pre-trained on the FFHQ dataset. NVAE builds a hierarchical prior and achieves state-of-the-art generation quality among VAEs. We see that kPF can indeed generate high-quality and diverse samples with the help of NVAE encoder/decoder. In fact, any AE/VAE may be substituted in, assuming that the latent space is *smooth*.

Summary: When a sufficient number of samples are available, our algorithm performs as well as the alternatives, which is attractive given the efficient training. In Fig. 5, we present training time comparison until convergence for all latent space models (excluding the time to pre-train AE) and show that our method is much faster than other deep generative methods.

Distribution matching with limited data samples. Next, we present our evaluations when only a limited number of samples are available. Here, each of the density estimators was trained on latent representations of the same set of 100 randomly sampled CelebA images, and 10K images were generated to evaluate FID (see Table 3). Our method outperforms Glow and VAE, while offering competitive performance with GMM. Surprisingly, GMM remains a strong baseline for both tasks, which agrees with results in Ghosh et al. (2020).

	MNIST	CIFAR	CelebA
Glow‡	25.8	-	103.7
CAGlow‡	26.3	-	104.9
Vanilla VAE	**13.7**	111.0	52.1
CV-VAE†	33.8	94.8	48.9
WAE†	20.4	117.4	53.7
Two-stage VAE	18.3	110.3	44.7
$\text{SRAE}_{\text{Glow}}$	23.7	110.7	59.8
SRAE_{GMM}	16.7	79.2	42.0
$\text{SRAE}_{\text{RBF-kPF}}$ (*ours*)	21.7	77.9	41.9
$\text{SRAE}_{\text{NTK-kPF}}$ (*ours*)	21.5	**77.5**	**41.0**

Table 2: Comparative FID values. SRAE indicates an autoencoder with hyperspherical latent space and spectral regularization following Ghosh et al. (2020). Results reported from ‡: Liu et al. (2019). †: Ghosh et al. (2020).

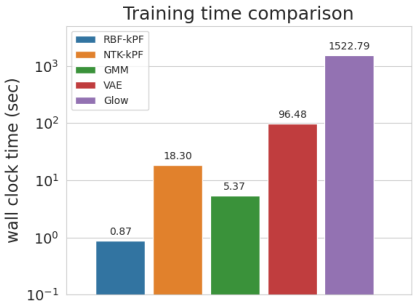


Figure 5: Comparison of additional training time for density estimation on latent space. All models were fitted on the latent representations of CelebA images encoded by an SRAE.

However, note that GMM is restricted by its parametric form and is less flexible than our method (as shown in Fig 2)

VAE	Glow	GMM	RBF-kPF	NTK-kPF
59.3	77.0	39.6	40.6	40.9

Table 3: FID values for few samples setting density approximation on CelebA.

Learning from few samples is common in biomedical applications where acquisition is costly. We present results on generating high-resolution ($160 \times 196 \times 160$) brain images: 183 samples from group AD (diagnosed as Alzheimer's disease) and 291 samples from group CN (control normals). For $n = 474 \ll d = 5017600$, it is often difficult to model the data distribution due to the high variance of the data or the memory-inefficiency of the operations. Using properties of our kernel operator, we can generate high-quality samples that are in-distribution. We present comparative results with VAEs. The generated samples in Fig. 6 clearly show that our method generates sharper images. To check if the results are also scientifically meaningful, we test consistency between group difference testing (i.e., cases versus controls differential tests on each voxel) on the real images (groups were AD and CN) and the same test was performed on the generated samples (AD and CN groups), using a FWER corrected two-sample t-test Ashburner & Friston (2000) consistent with standard practice. The results (see Fig 6) show that while there is a deterioration in regions identified to be affected by disease (different across groups), many statistically-significant regions from tests on the original images are preserved in voxel-wise tests on the generated images.

Summary: We achieve improvements in the small sample size setting compared to other generative methods. This is useful in many data-poor settings. For larger datasets, our method still compares competitively with alternatives, but with a smaller resource footprint.

6 Limitations

Our proposed simplifications can be variously useful, but deriving the density of the posterior given a mean embedding or providing an exact preimage for the generated sample in RKHS is unresolved at this time. While density estimation from kPF has been partially addressed in Schuster et al. (2020b), finding the pre-image is often ill-posed. The weighted Fréchet mean preimage only provides an approximate solution and evaluated empirically. Finally, like other kernel-based methods, the memory/compute cost can be a bottleneck on very large datasets where kernel approximation methods (Rahimi & Recht, 2009) may have to be applied.

7 Conclusions

We show that using recent developments in regularized autoencoders, a linear kernel transfer operator can potentially be an efficient substitute for the forward operator in some generative models. Our proposal, despite its simplicity, shows comparable empirical results to other state-of-the-art generative models, while enjoying much better computational efficiency. Results on brain images also show promise for applications to high-resolution 3D imaging data generation, which is being pursued actively in the community.

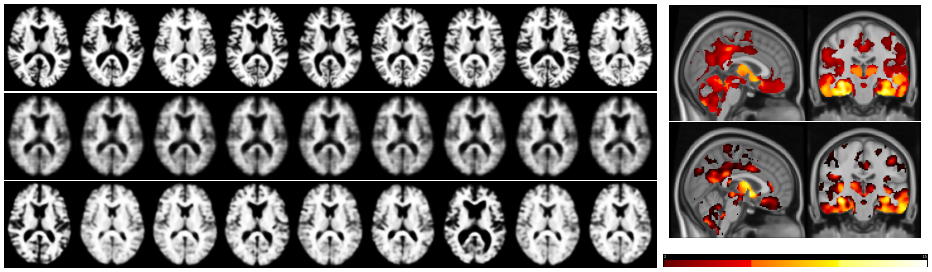


Figure 6: **Left.** *Top: data*, generated samples of *Middle: VAE , Bottom: kPF with SRAE*. **Right.** Statistically significant regions *Top: voxel-wise tests on real data, Bottom: voxel-wise tests on generated samples* are shown in negative log p-value thresholded at $\alpha = 0.01$.

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A Choice of Kernel is relevant yet flexible

In some cases, one would focus on identifying (finite) eigenfuntions and modes of the underlying operator Williams et al. (2015b); Brunton et al. (2016). But rather than finding certain modes that best characterize the dynamics, we care most about minimizing the error of the transferred density and therefore whether the span of functions is rich/expressive enough. In particular, condition (iii) in Proposition 3.2 requires an input RKHS spanned by sufficiently rich bases (Fukumizu et al., 2013). For this reason, the choice of kernel here cannot be completely ignored since it determines the family of functions contained in the induced RKHS.

To explore the appropriate kernel setup for our application, we empirically evaluate the effect of using several different kernels via a simple experiment on MNIST. We first train an autoencoder to embed MNIST digits on to a hypersphere S^2, then generate samples from kPF by the procedure described by Alg. 1 using the respective kernel function as the input kernel k. Subplot (b) and (c) in Fig. 7 show the generated samples using Radial Basis Function (RBF) kernel and arc-cosine kernel, respectively. Observe that the choice of kernel has an influence on the sample population, and a kernel function with superior empirical behavior is desirable.

Motivated by this observation, we evaluated the Neural Tangent Kernel (NTK) Jacot et al. (2018), a well-studied neural kernel in recent works. We use it for a few reasons, **(a)** NTK, in theory, corresponds to a trained infinitely-wide neural network, which spans a rich set of functions that satisfies the assumption. **(b)** For well-conditioned inputs (i.e., no duplicates) on hypersphere, the positive-definiteness of NTK is proved in Jacot et al. (2018). Therefore, invertibility of the Gram matrix $K_{ZZ} = \Phi^T \Phi$ is *almost guaranteed* if the prior distribution p_Z is restricted on a hypersphere **(c)** NTK can be non-asymptotically approximated Arora et al. (2019). **(d)** Unlike other parametric kernels such as RBF kernels, NTK is less sensitive to hyperparameters, as long as the number of units used is large enough Arora et al. (2019). Subplot (d) of Fig. 7 shows that kPF learned with NTK as input kernel is able to generate samples that are more consistent with the data distribution. However, we should note that NTK is merely a convenient choice of kernel that requires less tuning, and is not otherwise central to our work. In fact, as shown in our experiment in Tab. 2, a well-tuned RBF kernel may also achieve a similar performance. Indeed, in practice, any suitable choice of kernel may be conveniently adopted into the proposed framework without major modifications.

B Density Estimation with kPF Operator

The displayed transferred density with the kPF operator on toy data in Fig. 1 of the main text is *approximated* using the empirical kernel conditional density operator (CDO) Schuster et al. (2020a), since there is currently no known methods that can exactly reconstruct density from the transferred mean embeddings. The marginalized transferred density $p_{\mathcal{P}_\mathcal{E}}$ has the following form

$$p_{\mathcal{P}_\mathcal{E}} = C_\rho^{-1} \mathcal{P}_\mathcal{E} \mu_Z = C_\rho^{-1} C_{XZ} C_{ZZ}^{-1} \mu_Z, \tag{10}$$

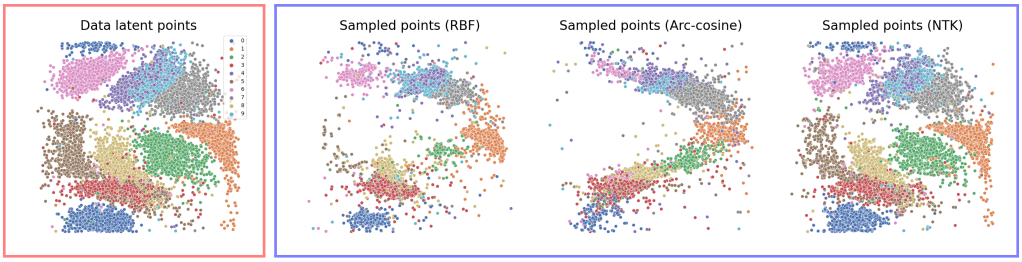

Figure 7: 10k samples from MNIST dataset (*left to right*) (a) projected on $\mathbf{S}^2$ shown in (θ, ϕ) using auto-encoder, and 10K generated samples from kPF with input kernel of type (b) RBF (c) arccos (d) NTK. Color of sampled points represents the class of their nearest training set neighbor in the output RKHS.

where $C_\rho = E_{y\sim\rho}[l(y,\cdot)\otimes l(y,\cdot)]$ is the covariance operator of a independent reference density ρ in $\mathcal{G}$. The above density function is also an element of RKHS $\mathcal{G}$, and therefore we can evaluate the density at x^* by using the reproducing property $p_{\mathcal{P}_\mathcal{E}}(x^*) = \langle p_{\mathcal{P}_\mathcal{E}}, l(x^*,\cdot)\rangle$. The results in Schuster et al. (2020a) show that the empirical estimate of $p_{\mathcal{P}_\mathcal{E}}$ may be constructed from m samples of the reference density $\{y_i\}_{i\in[m]}$ and n training samples $\{x_i\}_{i\in[n]}$ and $\{z_i\}_{i\in[n]}$ as

$$\hat{p}_{\mathcal{P}_\mathcal{E}} = (\hat{C}_\rho + \alpha' I)^{-1}\hat{C}_{XZ}(\hat{C}_{ZZ} + \alpha I)^{-1}\hat{\mu}_Z = \sum_{i=1}^{m}\beta_i l(y_i,\cdot) \tag{11}$$

where

$$\beta = m^{-2}(L_Y + \alpha' I)^{-2}L_{YX}(K_Z + \alpha I)^{-1}\Phi^\top\hat{\mu}_Z \tag{12}$$

and

$$L_Y = [l(y_i,y_j)]_{ij} \in \mathbb{R}^{m\times m}, L_{YX} = [l(y_i,x_j)]_{ij} \in \mathbb{R}^{m\times n}, K_Z = [k(z_i,z_j)]_{ij} \in \mathbb{R}^{n\times n} \tag{13}$$

In Fig. 8, we use a uniform density in the square $(\pm 4, \pm 4)$ as the reference density ρ and constructed $\hat{p}_{\mathcal{P}_\mathcal{E}}$ using $m = 10000$ samples $\{y_i\}_{i\in[m]}$ from ρ. Due to the form of the empirical kernel CDO, where the estimated density function $\hat{p}_{\mathcal{P}_\mathcal{E}}$ is a linear combination of $\{l(y_i,\cdot)\}_{i\in[m]}$ (as in Eq. 11), the approximation can be inaccurate if reference samples are relatively sparse and the densities are 'sharp'. In those cases, to obtain a better density estimate, we may either increase the number of reference samples used to construct the empirical CDO (which can be computationally difficult due to the need to compute $(L_Y + \alpha' I)^{-2}$), or, with some prior knowledge to the true distribution, choose a reference density which is localized around the ground truth density.

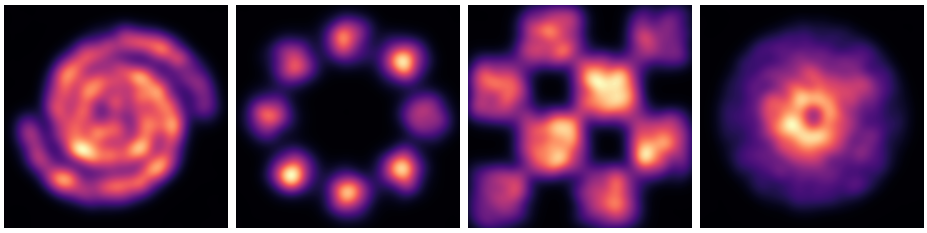

Figure 8: Inaccurate density estimation result from kernel CDO using 10k samples from uniform reference density ρ

Therefore, to show a more faithful density estimate of the transferred distribution for visualization purpose, we use a composite of the uniform density and the true density with weight $4:1$ as the reference density ρ in Fig. 2. In this case, approximately 20% of the reference samples concentrates around the high-density areas of the true density, which helps to form a better basis for $\hat{p}_{\mathcal{P}_\mathcal{E}}$. Note that the choice of ρ does not affect the transferred density embedding $\hat{\mathcal{P}}_\mathcal{E}\hat{\mu}_Z$ since it is independent of p_X and p_Z. After this modification, the reconstructed density more accurately reflects the true density compared to GMM and GLOW, indicating the transferred distribution by kPF in RKHS matches better to the ground truth distribution. This is also reflected in the generated samples in Fig. 9, where samples generated by the kPF operator are clearly more aligned with the ground truth distribution.

C Effect of γ on Sample Quality

In the sampling stage, our proposed method finds the approximate preimage of the transferred kernel embeddings by taking the weighted Fréchet mean of the top γ neighbors among the training samples. The choice of γ therefore influences the quality of generation.

From Figure 10, we can observe that, in general, FID worsens as γ increases. This observation aligns with our intuition of preserving only the local similarities represented by the kernel, and similar ideas have been previously used in the literature Hastie et al. (2001); Kwok &

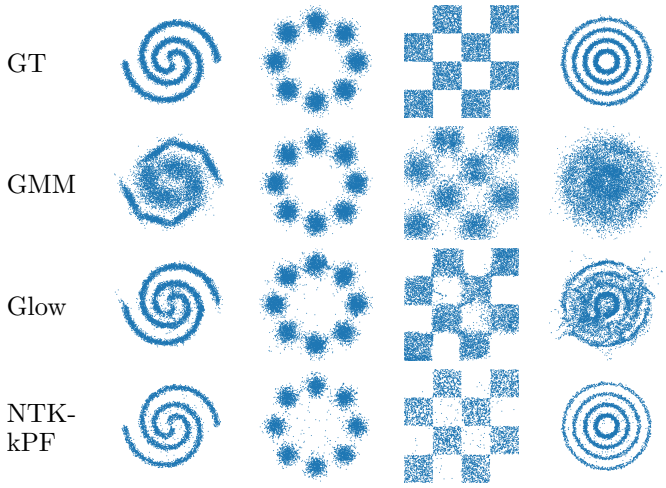

Figure 9: Sample comparisons of the distribution matching methods

Tsang (2004). However, significantly decreasing γ leads to the undesirable result where the generator merely generates the training samples (in the extreme case where $\gamma = 1$, generated samples will just be reconstructions of training samples). Therefore, in our experiments, we choose $\gamma = 5$ to achieve a balance between generation quality and the distance to training samples.

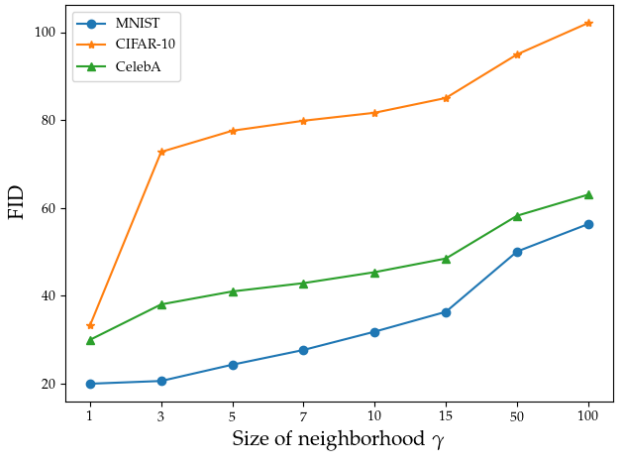

Figure 10: FID *versus* γ on computer vision datasets

D Weighted Fréchet Mean on Hypersphere

While the weighted Fréchet Mean in Euclidean space can be computed in closed-form as a weighted arithmetic mean (as in Eq. 9), on hypersphere there is no known closed-form solution. Thus, we adopt the iterative algorithm in Chakraborty & Vemuri (2015) for an approximate solution given data points $\mathbf{X} = \{\mathbf{x}_1 \dots \mathbf{x}_\gamma\}$ and weight vector $\mathbf{s}$:

$$M_1 = \mathbf{x}_1$$
$$M_{i+1} := \cos(\|\mathbf{s}_{i+1}\mathbf{v}\|)M_i + \sin(\|\mathbf{s}_{i+1}\mathbf{v}\|)\frac{\mathbf{v}}{\|\mathbf{v}\|}$$

where, $\mathbf{v} = \frac{\theta}{\sin(\theta)}\left(X_{i+1} - M_i\cos(\theta)\right), \theta = \arccos(M_i^t X_{i+1})$. This algorithm iterates through the data points once, yielding a complexity of only $O(\gamma d)$, where d is the dimension of $\mathcal{X}$.

Under the prescribed iteration, M_n converges asymptotically to the true Fréchet mean for finite data points. We refer the readers to Chakraborty & Vemuri (2015) for further details.

E Fast approximation of Moore-Penrose inverse

When computing the inverted kernel matrix K_{inv} in Algo. 1, conventional approaches typically performs SVD or Cholesky decomposition. Both procedures are hard to parallelize, and therefore maybe slow when K is large. Alternatively, we can utilize an iterative procedure proposed in Razavi et al. (2014) to approximate the Moore-Penrose inverse.

$$Z_1 = K/(\|K\|_1 \|K\|_\infty) \tag{14}$$

$$Z_{i+1} := Z_i(13I - KZ_i(15I - KZ_i(7I - KZ_i))) \tag{15}$$

where

$$\|K\|_1 = \max_j \sum_{i=0}^{n} K_{ij}, \|K\|_\infty = \max_i \sum_{j=0}^{n} K_{ij} \tag{16}$$

Since this iterative procedure mostly involves matrix multiplications, it can be efficiently parallelized and implemented on GPU. The same procedure has also seen success in approximating large self-attention matrices in language modeling Xiong et al. (2021). For the NVAE experiment, we run this iteration for 10 steps and use $K_{\text{inv}} = Z_{10}$.

F Experimental Details

In this section, we provide the detailed specifications for all of our experiments. We have also provided our code in the supplemental material.

F.1 Density Estimation on Toy Densities

We generated 10000 samples from each of the toy densities to learn the kPF operator. The input kernel k is a ReLU-activated NTK corresponding to a fully-connected network with depth $L = 4$ and width $w = 10000$ at each layer, and the output kernel l is a Gaussian kernel. Unless specified otherwise, we always uses a Gaussian kernel as the output kernel for the remainder of this appendix. The bandwidth of the output kernel was adjusted separately for density estimation and sampling for the purpose of demonstration. For comparison, we also fit/estimate a 10-component GMM and a Glow model with 50 coupling layers, where each of them were trained until convergence.

F.2 Image Generation with Computer Vision Datasets

To generate results in Tab. 2 and Tab. 3, we first trained an autoencoder for each dataset following the model setup in Ghosh et al. (2020), which uses a modified Wasserstein autoencoder Tolstikhin et al. (2018) architecture with batch normalization. Additionally, we applied spectral normalization on both the encoder and the decoder, following Ghosh et al. (2020), to obtain a regularized autoencoder. The latent representations were projected onto a hypersphere before decoding to image space. We trained the models on two NVIDIA GTX 1080TI GPUs. A detailed model specification is provided below in Table 4.

We used an NTK with $L = 8$ and $w = 10000$ as the input kernel k (i.e. the embedding kernel of p_Z) for NTK-kPF, and a Gaussian kernel with bandwidth $\sigma = \sqrt{2|\mathcal{Z}|}/8$ for RBF-kPF. The bandwidth for the output Gaussian kernel is selected based on cross-validation of a degree 3 polynomial kernel MMD between the sampled and the ground-truth latent points. Further, to mitigate the deterioration of performance of kernel methods in a high-dimensional setting due to the curse of dimensionality Evangelista et al. (2006), in practice, we model $\mathcal{Z}$ as a space with fewer dimensions than the input space $\mathcal{X}$. As a rule of the thumb, we choose $\mathcal{Z}$ such that $|\mathcal{Z}| = |\mathcal{X}|/4$.

To generate images from kPF learned on NVAE latent space, we used the pre-trained checkpoints provided in Vahdat & Kautz (2020) to obtain the latent embeddings for 2000 FFHQ images. We then construct the kPF from the concatenated latent space of the lowest resolution (8×8). During sampling, prior samples at those resolutions are replace by the kPF samples, while for other resolutions samples remain generated from inferred Gaussian distributions. The batchnorm statistics were readjusted for 500 iterations following Vahdat & Kautz (2020). We use rbf kernels as input and output kernels, with bandwidths σ_k, σ_l chosen by the *median heuristic* (~ 100 for input and ~ 70 for output in our experiments).

	MNIST	CIFAR-10	CelebA
Encoder	$\text{Conv}^{4\times4}_{128}$ $\text{Conv}^{4\times4}_{256}$ $\text{Conv}^{4\times4}_{512}$ $\text{Conv}^{4\times4}_{1024}$	$\text{Conv}^{4\times4}_{128}$ $\text{Conv}^{4\times4}_{256}$ $\text{Conv}^{4\times4}_{512}$ $\text{Conv}^{4\times4}_{1024}$	$\text{Conv}^{5\times5}_{128}$ $\text{Conv}^{5\times5}_{256}$ $\text{Conv}^{5\times5}_{512}$ $\text{Conv}^{5\times5}_{1024}$
Decoder	$\text{ConvT}^{4\times4}_{512}$ $\text{ConvT}^{4\times4}_{256}$ $\text{ConvT}^{4\times4}_{1}$	$\text{ConvT}^{4\times4}_{512}$ $\text{ConvT}^{4\times4}_{256}$ $\text{ConvT}^{4\times4}_{3}$	$\text{ConvT}^{5\times5}_{512}$ $\text{ConvT}^{5\times5}_{256}$ $\text{ConvT}^{5\times5}_{128}$ $\text{ConvT}^{5\times5}_{3}$

Table 4: Model architecture for computer vision experiments. Subscript denotes the number of output channels and superscript denotes the window size of the convolution kernel. Batch normalization and activation is applied between each pair of convolution layers

Encoder	5x5 conv, stride 4
	$\text{ResBlock}_{64} \times 2$
	$\text{ResBlock}_{64} \times 2$
	$\text{ResBlock}_{128} \times 2$
	$\text{ResBlock}_{256} \times 2$
Decoder	$\text{ResBlock}_{256} \times 2$
	$\text{ResBlock}_{128} \times 2$
	$\text{ResBlock}_{64} \times 2$
	$\text{ResBlock}_{64} \times 2$
	5x5 conv, stride 4

Table 5: Model architecture for experiments for image generation on brain imaging dataset. Subscript denotes the number of output channels. Upsampling and downsampling are performed using strided convolutions.

F.3 Image Generation for Brain Images

For the high-resolution brain imaging dataset, we used a custom version of ResNet He et al. (2016) with 3D convolutions. The detailed architecture is shown in Fig. 5. Due to the large size of the data, we trained the model on 4 NVIDIA Tesla V100 GPUs.

Mandatory ADNI statement regarding data use. Data used in preparation of this article were obtained from the Alzheimer's Disease Neuroimaging Initiative (ADNI) database (adni.loni.usc.edu). As such, the investigators within the ADNI contributed to the design and implementation of ADNI and/or provided data but did not participate in analysis or writing of this report. A complete listing of ADNI investigators can be found in the ADNI Acknowledgement List.

The T1 MR brain dataset we utilize consists of images from 184 subjects diagnosed with Alzheimers's disease and 292 healthy controls/ normal subjects. Images were first coregistered to a MNI template and segmented to preserve only the white matter and grey matter. Then, all images were resliced and resized to $160 \times 196 \times 160$ and rescaled to the range of $[-1, 1]$. Voxel-based morphometry (VBM) was used to obtain the p-value map of data and generated images.

G More Samples

In this section we present additional uncurated set of samples on MNIST, CIFAR-10, CelebA based on pre-trained SRAE and FFHQ based on NVAE. From the figures, it can be seen that kPF produces consistent and diverse samples, often better in quality than the alternatives.

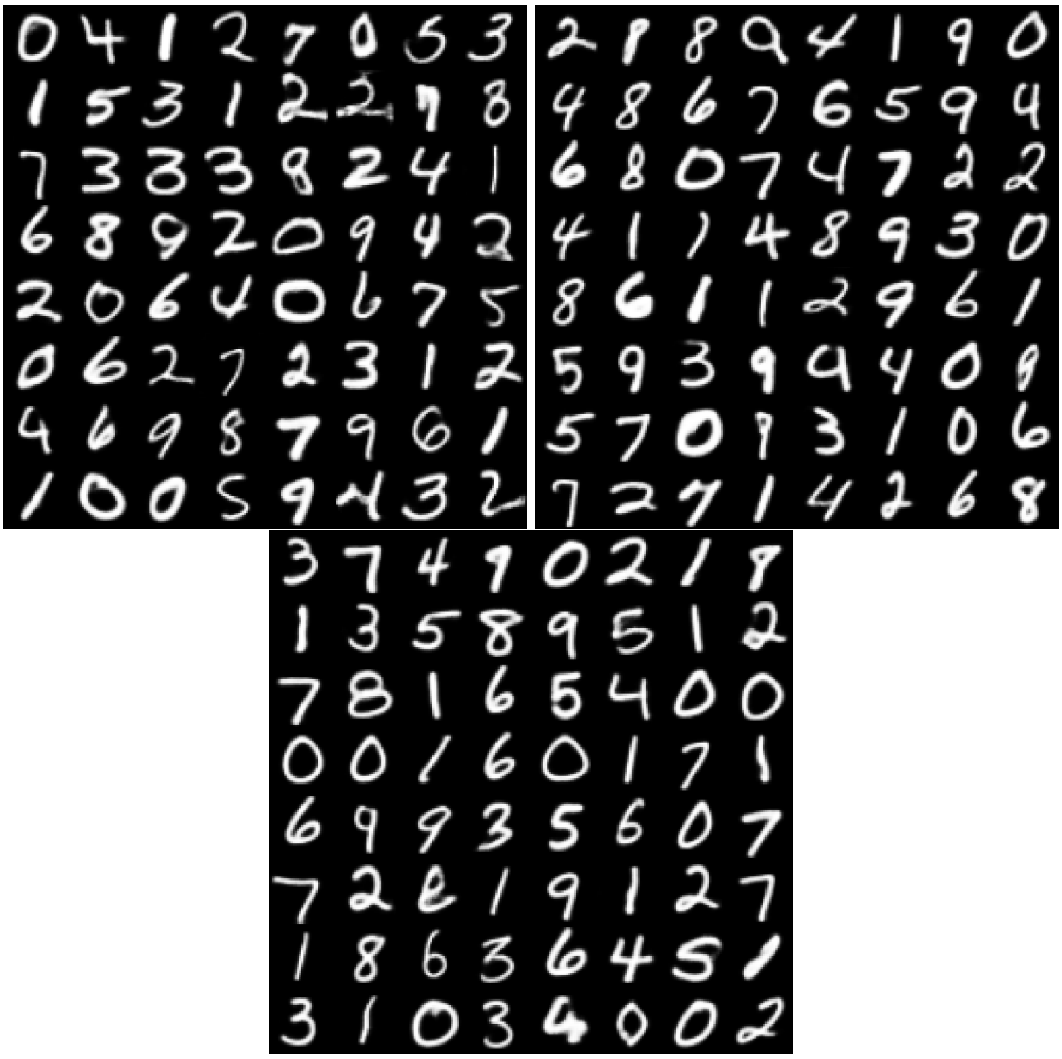

Figure 11: MNIST results from SRAE_{GMM} (top left), SRAE_{Glow} (top right) and our $\text{SRAE}_{\text{NTK-kPF}}$.

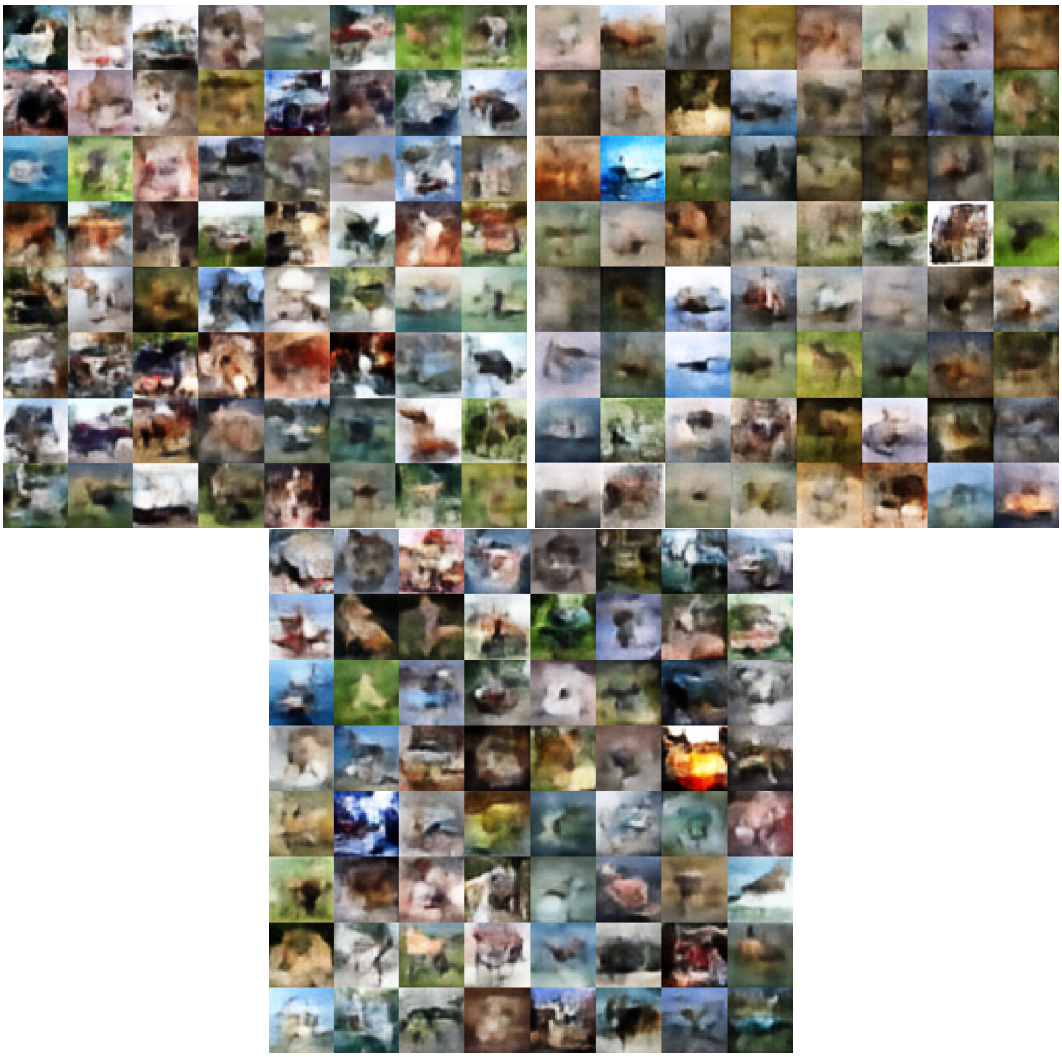

Figure 12: CIFAR results from SRAE_{GMM} (top left), SRAE_{Glow} (top right) and our $\text{SRAE}_{\text{NTK-kPF}}$.

Figure 13: CelebA results from SRAE_{GMM} (top left), SRAE_{Glow} (top right) and our $\text{SRAE}_{\text{NTK-kPF}}$ (bottom).

Figure 14: Additional samples from kPF+NVAE pre-trained on FFHQ