Relative Error RKHS Embeddings for Gaussian Kernels

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Abstract

We show how to obliviously embed into the reproducing kernel Hilbert space associated with Gaussian kernels, so that distance in this space (the kernel distance) only has $(1 + \varepsilon)$-relative error. This only holds in comparing any point sets at a kernel distance at least $\alpha$; this parameter only shows up as a poly-logarithmic factor of the dimension of an intermediate embedding, but not in the final embedding. The main insight is to effectively modify the well-traveled random Fourier features to be slightly biased and have higher variance, but so they can be defined as a convolution over the function space. This result provides the first guaranteed algorithmic results for LSH of kernel distance on point sets and low-dimensional shapes and distributions, and for relative error bounds on the kernel two-sample test.
1 Introduction

Kernel methods are a pillar of machine learning and general data analysis. These approaches consider classic problems such as PCA, linear regression, linear classification, k-means clustering which at their heart fit a linear subspace to a complex data set. Each of these methods can be solved by only inspecting the data via a dot product \( \langle x, t \rangle \). Kernel methods, and specifically the “kernel trick,” simply replaces these Euclidean dot products with a non-linear inner product operation. Two most common inner products are the polynomial kernel \( K_p(x, t) = (\langle x, t \rangle + 1)^p \) and the RBF kernel \( K(x, p) = \exp(-\|x - t\|^2) \) (e.g., the Gaussian kernel).

The “magic” of the kernel method works mainly because of the existence of a reproducing kernel Hilbert space (RKHS) \( \mathcal{H}_K \) associated with any positive definite (pd) kernel \( K \). It is a function space, so for any data point \( x \in \mathbb{R}^d \), there is a mapping \( \phi : \mathbb{R}^d \rightarrow \mathcal{H}_K \) so \( \phi(x) = K(x, \cdot) \). Since \( \phi(x) \) is a function with domain \( \mathbb{R}^d \), and each coordinate of \( \phi(x) \) is associated with another point \( t \in \mathbb{R}^d \), there are an infinite number of coordinates, and \( \mathcal{H}_K \) can be infinite dimensional. However, since \( \langle \phi(x), \phi(t) \rangle_{\mathcal{H}_K} = K(x, t) \), this embedding does not ever need to be computed, we can simply evaluate \( K(x, t) \). And life was good.

However, at the dawn of the age of big data, it became necessary to try to explicitly, but approximately, compute this map \( \phi \). Kernel methods typically start by computing the \( n \times n \) gram matrix \( G \) where \( G_{i,j} = K(p_i, p_j) \) for a data sets \( P \) of size \( n \). As \( n \) became huge, this became untenable. In a hallmark paper, Rahimi and Recht [27] devised random Fourier features (RFFs) for RBF pd kernels (with max value 1, e.g., Gaussians) that compute a random map \( \tilde{\phi} : \mathbb{R}^d \rightarrow \mathbb{R}^D \) so \( \langle \tilde{\phi}(p), \tilde{\phi}(t) \rangle \) is an unbiased estimate of \( K(p, t) \), and with probability at least \( 1 - \delta \) has error \( |K(p, t) - \langle \tilde{\phi}(p), \tilde{\phi}(t) \rangle| \leq \varepsilon \). For just one pair of points they require \( \tilde{D} = O((1/\varepsilon^2) \log(1/\delta)) \), or for all comparisons among \( n \) points \( \tilde{D}_n = ((1/\varepsilon^2) \log(n/\delta)) \), or for any points in a region \( \Lambda \) of volume \( \text{vol}(\Lambda) \leq V \), then \( \tilde{D}_V = ((1/\varepsilon^2) \log(V/\delta)) \).

For polynomial kernels, there is an explicit exact embedding by “linearizing” the polynomial, so such techniques are not necessary. However, approximate embeddings with improved dimensionality are possible [9]: these preserve relative error on the inner product.

Relative-error-preserving RKHS embeddings for RBF kernels have eluded the community. Indeed recently, Avron et al. [8] shows a lower bound which almost implies that RFFs cannot achieve relative error for inner products. It shows a \( \lambda \)-regularized problem requires \( \Omega(n/\lambda) \) dimensional RFFs to achieve some relative error, however, requires \( \lambda \geq 10/n > 0 \); so it stops just short of showing a lower bound for the unregularized version. Instead, to obtain relative-error results in big data sets, researchers have relied on other approaches such as sampling [32], devising modified RFFs which still have dependence on regularization terms (which are probably \( \sqrt{n} \)) for kernel regression [8], or building data structures for kernel density estimate queries [12].

The kernel distance. To address these difficulties, we turn our attention from the inner product \( \langle \phi(x), \phi(t) \rangle_{\mathcal{H}_K} = K(x, t) \) in the RKHS to the natural distance it implies, the kernel distance [20] [22] (alternatively known as the current distance [19] or maximum mean discrepancy [20] [28])

\[
\text{D}_K(x, t) = \|\phi(x) - \phi(t)\|_{\mathcal{H}_K} = \sqrt{\langle \phi(x), \phi(x) \rangle_{\mathcal{H}_K} + \langle \phi(x), \phi(t) \rangle_{\mathcal{H}_K} - 2 \langle \phi(x), \phi(t) \rangle_{\mathcal{H}_K}}.
\]

Under a slightly restricted class of kernels (a subset of pd kernels), called characteristic kernels [29], this distance is a metric. These include the Gaussian kernels which we focus on hereafter. This distance looks and largely acts like Euclidean distance; indeed, restricted to any finite-dimensional subspace, it is equivalent to Euclidean distance.

So a natural question to ask is if this distance is preserved within relative error via some approximate lifting. Clearly RFFs guarantee additive \( \varepsilon \)-error. However, if we relate this problem to the Johnson-
Lindenstrauss Lemma \cite{Lindenstrauss}, this describes a family of random projections from a high-dimensional space to a $D'$-dimensional space which preserve $(1 + \varepsilon)$-relative error on Euclidean distance, again with $D' = O((1/\varepsilon^2) \log(n/\delta))$ for any \( \binom{n}{2} \) pairs of distances, but only guarantees additive error on inner products.

Moreover, it is possible to apply the JL Lemma to create such an approximate embedding. First for any set of $n$ points, we can create $n \times n$ Gram matrix $G$, and orthogonalize it to obtain a $n$-dimensional orthogonal basis. The Euclidean distance in this basis is exactly the kernel distance between points \cite{Chen et al.} \cite{Charikar and Siminelakis}. Then we can apply JL to obtain such an approximate embedding. However, this embedding is not oblivious to the data (necessary for many big data applications like streaming) and still requires $\Omega(n^2)$ time just to create the Gram matrix, not to mention the time for orthogonalization.

Another recent approach \cite{Chen et al.} attempted to analyze RFFs for this task, and shows that these approximate embeddings do guarantee relative error on the kernel distance, but only between pairs of points $x, t \in \mathbb{R}^d$ (e.g., so $\|\phi(x) - \phi(t)\|_{\mathcal{H}_K(x,t)} \in (1 \pm \varepsilon)$), and as we describe many downstream analysis tasks require the distance preserved between point sets.

**Data Set Embeddings.** A powerful aspect of RKHS embeddings is how they represent point sets $P \subset \mathbb{R}^d$, or in general any probability distribution $\mu_P$ with domain $\mathbb{R}^d$. If we treat $P$ as a discrete probability distribution with uniform $1/|P|$ weight on each point, then we can represent this in $\mathcal{H}_K$ as $\Phi(P) = \frac{1}{|P|} \sum_{x \in P} \phi(x)$, known as the kernel mean \cite{Rahimi and Recht}. Indeed, for any query point $t$, the inner product $\langle \Phi(P), \phi(t)\rangle_{\mathcal{H}_K} = \frac{1}{|P|} \sum_{x \in P} K(x,t)$ precisely the kernel density estimate at $t$. Moreover, to run kernel $k$-means we are computing objects which lie in the convex combination of the points $\{\phi(x_1), \phi(x_2), \ldots\} \subset \mathcal{H}_K$. Hence the Chen et al. \cite{Chen et al.} result does not guarantee anything about these analysis.

The kernel distance has a natural extension to these point set representations as

$$D_K(P, Q) = \|\Phi(P) - \Phi(Q)\|_{\mathcal{H}_K} = \sqrt{\kappa(P, P) + \kappa(Q, Q) - 2\kappa(P, Q)},$$

where $\kappa(P, Q) = \frac{1}{|P||Q|} \sum_{x \in P} \sum_{y \in Q} K(p, q)$. Several concrete applications work directly on this kernel distance between point sets. The kernel two-sample test \cite{Chen et al.} \cite{Rahimi and Recht} is a non-parametric way to perform hypothesis tests between two distributions; simply, the null hypothesis of the distributions being the same is rejected if the kernel distance is sufficiently large. Also, devising a Locality Sensitive Hash (LSH) between point sets (or geometrically-aware LSH for probability distributions) has lacked a great general solution. While there are recent solutions for polygons \cite{recent solutions for polygons}, more general distances between geometric distributions, like Earth-Mover distance require $\Omega(\log s)$ distortion when defined on a domain with at least $s$ discrete points \cite{recent solutions for polygons}. While the kernel two-sample test is useful under additive error \cite{Chen et al.} (but would of course rather have relative error), an LSH requires relative error to properly provide $(1 + \varepsilon)$-approximate nearest neighbor results. Hence, we aim to show relative-error embeddings for the kernel distance to address these issues.

If we assume that $D_K^2(P, Q) > \alpha$, then standard RFFs can provide a relative error guarantee using $\hat{D} = O\left(\frac{1}{\sqrt{\alpha}} \log \frac{1}{\varepsilon}\right)$. However, such a large factor in $\alpha$ is undesirable.

**Comparison to relevant recent work.** We note that recent related works on kernel approximation do not provide such guarantees, although they provide some conditional relative error on the Gaussian kernel inner products.

Chiarikar and Siminelakis \cite{Chen et al.} describe a data structure of size $n \hat{D}$ and query time $\hat{D}$, which answers KDE$_P(t)$ queries within $(1 + \varepsilon)$-relative error as long as KDE$_P(t) > \alpha$; it requires $\hat{D} = O\left(\frac{1}{\sqrt{\alpha}} \log \frac{1}{\varepsilon} \log 23 / n \log \log n\right)$. However, this cannot argue much about how large $D_K(P, Q)$ has to be for this to achieve relative error on the kernel distance since it could be $D_K(P, Q)$ is small but $\kappa(P, t)$ and $\kappa(P, P)$ are both large. Moreover, its
guarantees only work for a single point set $P$ with point queries $t$, not for two or more points sets $P,Q$, as we argue, most downstream data analysis requires.

Alternatively Avron et al. [8] modify the sampling probability for $v'$ in RFFs to be from a domain which it modeled after the statistical leverage in the kernel space. It is uniform over a region $[-\tilde{\gamma}, \tilde{\gamma}]^d$, with $\tilde{\gamma} = 10\sqrt{\log(n/\lambda)}$ (somewhat similar to a region $[-\gamma, \gamma]^d$ we will define), but then decays smoothly as it extends beyond the area. This approximates a $\lambda$-regularized kernel regression problem, creating a $D$-dimensional embedding; that is for an $n \times n$ gram matrix $G$, and a regularization parameter $\lambda$ it creates a $n \times D$ matrix $Z$ so that

$$(1 - \varepsilon)(G + \tilde{\lambda}I_n) \preceq ZZ^* + \tilde{\lambda}I_n \preceq (1 + \varepsilon)(G + \lambda I_n).$$

It sets $D = O(\frac{1}{\varepsilon^2} (V \log^{d/2}(n/\lambda) + \log^{2d}(n/\lambda)) \log(s_{\lambda}^2(K)/\delta))$, where $V$ is a bound on the volume of an area which contains all of the data points, and $s_{\lambda}(K) = \text{Tr}((G + \tilde{\lambda}I)^{-1}G)$, and can roughly be thought of as the number of eigenvalues of $G$ larger than $\lambda$. Typically uses cases set $\tilde{\lambda}$ so $s_{\lambda} \approx \sqrt{n}$ [11]. This effectively provides relative error for inner products along directions which are aligned with a lot of data, but not for directions which are not (they are dominated by the $\tilde{\lambda}$ component). It is not clear how to translate these bounds to argue about $D_K$.

**Our Results.** We show the first data-oblivious $(1 + \varepsilon)$-relative error RKHS embedding for the Gaussian kernel distance, between point sets (beyond the trivial $O(\frac{1}{\varepsilon^2})$-dimension RFF). The guarantee hold for pairs of point sets $P,Q$ satisfying $D_K^2(P,Q) \geq \alpha$ for some $\alpha > 0$. The dimensionality of this embedding only depends poly-logarithmically on $1/\alpha$; for at most $1 - \delta$ probability of failure, its dimension is $D = O(\frac{1}{\varepsilon^2} \log \frac{1}{\varepsilon} \cdot V \log \frac{d}{\varepsilon n})$ where $P,Q \subset \Lambda$, and $V$ upper bounds the volume of an $\log^d \frac{1}{\alpha}$ expansion of $\Lambda$. These bounds can be specified to $D_n = O\left(n^2 \left(\log \frac{1}{\alpha}\right)^d \left(\log \frac{1}{\varepsilon n}\right)^d \frac{1}{\varepsilon} \log \frac{1}{\varepsilon}\right)$ when $|P \cup Q| \leq n$ and to $D_L = O\left(L + \sqrt{\log \frac{1}{\varepsilon}}\right)^{2d} \left(\log \frac{1}{\varepsilon}\right)^d \frac{1}{\varepsilon} \log \frac{1}{\varepsilon}$ when $P \cup Q$ must lie in the region $[-L, L]^d$.

Furthermore, this embedding can be composed with a Johnson-Lindenstrauss-type embedding [21] [2] [3] [11] [22] to create an overall oblivious embedding of dimension roughly $O(\frac{1}{\varepsilon^2} \log \frac{1}{\varepsilon})$, that is with no dependence on $\alpha$ or $V$ (or $n$ or $L$), and roughly the same guarantees.

This immediately implies the first linear time, $(1 + \varepsilon)$-relative error results for the kernel two-sample test [20] and for an LSH for kernel distance between two point sets (after composing with Euclidean LSH), and a $(1 + \varepsilon)$-approximate nearest neighbor data structure for $D_K$. That means we can describe an oblivious map to a Euclidean vector space that preserves $(1 + \varepsilon)$-relative error between point sets and geometrically-defined probability distributions.

### 2 Definition of our Hash Family

Our hash family $\mathcal{H}_{n,\varepsilon}$ includes hash functions that lift points $x \in \mathbb{R}^d$ to some space $\mathbb{R}^D$. We will show that these sufficiently well captures the Euclidean nature of the kernel distance $D_K$ for the Gaussian kernel $K(x,t) = \exp(-\|x - t\|^2)$.

We assume throughout that the ambient dimension $d$ is constant. And the error parameter $\varepsilon$ is assumed to be less than $1/2$. Also, our hash family will only present guarantees on the kernel distance $D_K$ between two point sets $P,Q$ if they are sufficiently different. Specifically we only argue about $P,Q$ such that $D_K^2(P,Q) > \alpha$ for some $\alpha > 0$. If $P = Q$, then our hash functions will map them to the same representative object.
A hash function \( h_v \in \mathcal{H}_{\alpha, \varepsilon} \) is defined by two vectors \( v \in \mathbb{R}^d \). These defining vectors \( v \in \mathbb{R}^d \) are chosen \( v \sim \text{Unif}([-\gamma, \gamma]^d) \) where \( \gamma = \sqrt{\frac{4}{\ln(\frac{16d}{\sqrt{\pi} \varepsilon \alpha})}} \). Now the hash function applied to a point \( x \in \mathbb{R}^d \) generates two coordinates as

\[
h_v(x) = (2\gamma)^{d/2} \left( \frac{1}{4\pi} \right)^{d/4} \exp(-\|v\|^2/8) \begin{bmatrix} \cos(\langle v, x \rangle) \\ \sin(\langle v, x \rangle) \end{bmatrix}.
\]

**Remark:** Recall that the random Fourier features (RFFs) approach of Rahimi and Recht [27] (the cos-sin variant [31]) defines the hash family \( \mathcal{H} \) as follows. It first choose a Gaussian random variable \( v' \sim \mathcal{N}(0, 2) \) (i.e. with pdf \( \left(\frac{1}{4\pi}\right)^{d/2} \exp\left(-\frac{\|v'\|^2}{4}\right) \)) and then the hash is defined

\[
h_{v'}(x) = \begin{bmatrix} \cos(\langle v', x \rangle) \\ \sin(\langle v', x \rangle) \end{bmatrix}.
\]

This means that probability density of \( v' \) times the inner product of its value at \( x \) and \( y \) (something like the expected value) is now

\[
\left(\frac{1}{4\pi}\right)^{d/2} \exp\left(-\frac{\|v'\|^2}{4}\right) \cdot \cos(\langle v', x - y \rangle)
= \left\langle \left(\frac{1}{4\pi}\right)^{d/4} \exp\left(-\frac{\|v'\|^2}{8}\right) \begin{bmatrix} \cos(\langle v', x \rangle) \\ \sin(\langle v', x \rangle) \end{bmatrix}, \left(\frac{1}{4\pi}\right)^{d/4} \exp\left(-\frac{\|v'\|^2}{8}\right) \begin{bmatrix} \cos(\langle v', y \rangle) \\ \sin(\langle v', y \rangle) \end{bmatrix} \right\rangle
\]

which looks quite reminiscent of what the same is for our hash function. Our choice of hash functions initially seem suboptimal in two ways. In explicitly samples from only \([-\gamma, \gamma]^d\), instead of implicitly from all of \( \mathbb{R}^d \), this indeed create a small bias in the hash functions; we quantify and bound it in Section 3.3. Also, because this we sampled over \([-\gamma, \gamma]^d\) and then weight by \( \exp(-\|v\|^2/8) \), as opposed to directly sampling explicitly from \( \exp(-\|v\|^2/8) \), our hash function has an increased variance. In effect, RFFs are close to an importance-sampling variant of our hash, and the extra \( \gamma^{d/2} \) variance term shows up in the number of hash functions \( D \) required obtain \( (1 + \varepsilon) \) error.

However, these two important differences, the extra \( \exp(-\|v\|^2/8) \) factor, and choosing a random variable over \( \text{Unif}([-\gamma, \gamma]^d) \) instead of \( \mathcal{N}(0, 2) \), turn out to be essential in our analysis.

As we are going to show in Lemma 5 for \( h_v(x) = (2\gamma)^{d/2} \begin{bmatrix} \eta_{\cos}(x) \\ \eta_{\sin}(x) \end{bmatrix} \) that

\[
\eta_{\cos}(x) = \left(\frac{\pi}{2}\right)^{d/2} \exp(-\|v\|^2/8) \cos(\langle v, x \rangle) = \int_{t \in \mathbb{R}^d} \exp(-2\|x - t\|^2) \cos(\langle v, t \rangle) dt.
\]

This means if we don’t have the extra \( \exp(-\|v\|^2/8) \) factor, the above integral form (on the RHS) has an extra \( \exp(||v||^2/8) \) (note that it is positive index). Our integral form is critical as we will use Schwarz’s Inequality in Lemma 7. This extra \( \exp(||v||^2/8) \) makes the random variable unbounded which causes our approach to fail. That is why we need the factor \( \exp(-\|v\|^2/8) \) on the LHS above, and in our hash function.

However, this exponential factor \( \exp(-\|v\|^2/8) \) is exactly the factor that compensates the pdf of \( \mathcal{N}(0, 2) \). Namely, the expectation is no longer close to \( \exp(||x - y||^2) \) if we sample \( v \sim \mathcal{N}(0, 2) \) or similar (even if we tune the coefficient). Fortunately, this density function has exponentially decaying tail, so we can sample from a uniform distribution on the region around the center of Gaussian function, and as long as the region
is large enough, the truncated error is small. The factor $(2\gamma)^d$ which increases the variance, and hence the dimension $D$ derived, is then required to cancel the pdf of our uniform distribution. Indeed, as mentioned, the recently proposed modified RFFs of Avron et al. \[8\] uses similar sampling regime.

3 Analysis of New Kernel Hash Family

In this section we show that although our hash function is biased, and perhaps high variance, it can provide relative error for the kernel distance. To do so, we first observe specifically how \( \mathcal{D}_K^2 \) acts like a squared-Euclidean distance over an infinite dimensional function space. Second we calculate that inner products for the hash family is nearly unbiased, and bound the amount of bias. Third, we show these hash functions can be viewed as convolutions over the function space vectors, which critically allows us to invoke Shwarz's lemma to decompose the estimator and bound the error. We are then ready for to put together our hash functions into lifting map \( F \) to \( D \)-dimensions, and bound their error. We present two bounds for the size of \( D \) based on with the point sets \( P, Q \) being of finite size \( n \) or within a bounded region \([-L, L]^d\).

3.1 Preliminary Observations

Before we really begin, we will prove a few basic facts that will be useful throughout our calculations.

(F1) For vectors \( x, y, t \in \mathbb{R}^d \) then \( \|x - t\|^2 + \|y - t\|^2 = \|x - y\|^2 + 2 \|t - \frac{x + y}{2}\|^2 \).

(F2) For any \( s > 0 \) and vector \( x \in \mathbb{R}^d \), then \( \int_{t \in \mathbb{R}^d} \exp(-\|t - x\|^2/s)dt = (s\pi)^{d/2} \).

(F3) For any \( a \in \mathbb{R} \) and \( b > 0 \), then \( \int_{t \in \mathbb{R}} \exp(-t^2/b) \cos(at)dt = \sqrt{b\pi} \exp(-ba^2/4) \).

(F4) For any \( a > 0 \) then \( \int_{x > a} \exp(-ax)dx = \frac{a}{2} \exp(-a^2) \).

We now make observations of how to integrate out some variables.

In particular, combining facts (F1) and (F2) with \( \exp(a) \exp(b) = \exp(a + b) \), for any \( c > 0 \), we can immediately see

\[
\int_{t \in \mathbb{R}^d} \exp(-c\|x - t\|^2) \exp(-c\|y - t\|^2)dt = \exp(-\frac{\|x - y\|^2}{2c}) \int_{t \in \mathbb{R}^d} \exp(-2c\|t - \frac{x + y}{2}\|^2)dt
\]

\[
= \exp(\frac{\|x - y\|^2}{2b})(\pi/2c)^{d/2}. \tag{1}
\]

Second we can consider the following integral over \( t \in \mathbb{R}^d \). For any \( r \in \mathbb{R}^d \), denote \( S_r = \{ t \in \mathbb{R}^d \mid t = ar \text{ for some } a \in \mathbb{R} \} \) and \( S_{\perp} = \{ t \in \mathbb{R}^d \mid \langle r, t \rangle = 0 \} \). \( S_r \) is one dimensional subspace and \( S_{\perp} \) is \( (d - 1) \) dimensional subspace. Also, we can also decompose \( t = t_r + t_{\perp} \) where \( t_r \in S_r \) and \( t_{\perp} \in S_{\perp} \). Now after the decomposition we can apply (F3) on \( t_r \) and (F2) on \( t_{\perp} \).

\[
\int_{t \in \mathbb{R}^d} \exp(-\|t\|^2/b) \cos(\langle t, r \rangle)dt = \left( \int_{t \in S_r} \exp(-\|t_r\|^2/b) \cos(\|t_r\|\|r\|)dt_r \right) \left( \int_{t \in S_{\perp}} \exp(-\|t_{\perp}\|^2/b)dt_{\perp} \right)
\]

\[
= \left( \sqrt{b\pi} \exp(-b\|r\|^2/4) \right) \left( (b\pi)^{(d-1)/2} \right)
\]

\[
= (b\pi)^{d/2} \exp(-b\|r\|^2/4). \tag{2}
\]
3.2 Expressing $D^2_K(P, Q)$ as an Infinite-Dimensional Euclidean Function

We focus entirely on the Gaussian kernel $K: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ defined for any $x, y \in \mathbb{R}^d$, $K(x, y) = \exp(-\|x - y\|^2)$.

We will also mainly analyze the squared kernel distance, using the following formulation

$$D^2_K(P, Q) = \kappa(P, P) - 2\kappa(P, Q) + \kappa(Q, Q) = \sum_{x \in P \cup Q} \sum_{y \in P \cup Q} \beta_x \beta_y \exp(-\|x - y\|^2)$$

where $\beta_x$ is $\frac{1}{|P|}$ if $x \in P$ and $-\frac{1}{|Q|}$ if $x \in Q$. This observation that we can write it as weighted (double) sum over $\exp(\|x - y\|^2)$ terms is critical for our analysis. In particular, we can now express $D^2_K(P, Q)$ as squared $L_2$-norm of a function.

**Lemma 1.** Given two point sets $P, Q \subset \mathbb{R}^d$, $D^2_K(P, Q) = \int_{t \in \mathbb{R}^d} (f(t))^2 dt$ where

$$f(t) = \sum_{x \in P \cup Q} \beta_x \left(\frac{4}{\pi}\right)^{d/4} \exp(-2\|x - t\|^2).$$

**Proof.** After expanding

$$\int_{t \in \mathbb{R}^d} (f(t))^2 dt = \sum_{x \in P \cup Q} \sum_{y \in P \cup Q} \beta_x \beta_y \left(\frac{4}{\pi}\right)^{d/2} \int_{t \in \mathbb{R}^d} \exp(-2\|x - t\|^2) \exp(-2\|y - t\|^2) dt$$

we just need to invoke Observation (1) below from Section 3.1 to see

$$\left(\frac{4}{\pi}\right)^{d/2} \int_{t \in \mathbb{R}^d} \exp(-2\|x - t\|^2) \exp(-2\|y - t\|^2) dt = \exp(-\|x - y\|^2).$$

Intuitively, comparing to Euclidean distance, the above lemma describes how squared kernel distance is squared Euclidean distance of a vector with infinitely many coordinates. Each $t$ of $f$ represents one coordinate. Like JL Lemma, the high level hope is to find a random function $g$ that the convolution of $f$ and $g$ is like a random projection of $f$ on $g$. Also, $L_2$-norm of $f$ is bounded which means that most of its coordinate are negligible. We just need to identify the region of these significant coordinates.

3.3 Showing Hash Functions are Nearly Unbiased

The biggest deviation in our approach from previous approaches is that we do not require that our hash functions are completely unbiased in their estimate. But we show they are nearly unbiased; in particular for points $x, y \in \mathbb{R}^d$, they are off by at most an additive term $\mathcal{E}_{x,y}$, which we can bound.

**Lemma 2.** For any $x, y \in \mathbb{R}^d$

$$\mathbb{E}_{h_x \sim \mathcal{H}_\alpha, \gamma} [\langle h_x(x), h_v(y) \rangle] = \exp(-\|x - y\|^2) + \mathcal{E}_{x,y}$$

where the error term is defined

$$\mathcal{E}_{x,y} = -\left(\frac{1}{4\pi}\right)^{d/2} \int_{\mathbb{R}^d \setminus [-\gamma, \gamma]^d} \exp(-\|v\|^2/4) \cos(\langle v, x - y \rangle) dv$$
Proof. We start by expanding
\[
\langle h_v(x), h_v(y) \rangle = (2\gamma)^d \left( \frac{1}{4\pi} \right)^{d/2} \exp(-\|v\|^2/4) \cos(\langle v, x - y \rangle),
\]
with the last term following by expanding the dot-product and applying the identity \( \cos a \cos b + \sin a \sin b = \cos(a - b) \) with \( a = \langle v, x \rangle \) and \( b = \langle v, y \rangle \).

Then the expected value can be written by integrating over the possible values of \( v \) as
\[
\mathbb{E}_{h_v \sim \mathcal{H}_{\alpha, \varepsilon}} [\langle h_v(x), h_v(y) \rangle] = \int_{v \in [-\gamma, \gamma]^d} \left( \frac{1}{2\pi} \right)^d \left( \frac{1}{4\pi} \right)^{d/2} \exp(-\|v\|^2/4) \cos(\langle v, x - y \rangle) dv
\]
\[
= \left( \frac{1}{4\pi} \right)^{d/2} \int_{v \in [-\gamma, \gamma]^d} \exp(-\|v\|^2/4) \cos(\langle v, x - y \rangle) dv
\]
\[
= \left( \frac{1}{4\pi} \right)^{d/2} \int_{v \in \mathbb{R}^d} \exp(-\|v\|^2/4) \cos(\langle v, x - y \rangle) dv + \mathcal{E}_{x,y}
\]
\[
= \exp(-\|x - y\|^2) + \mathcal{E}_{x,y}
\]
The last line is from Observation 2 from Section 3.1 by taking \( b = 4 \) and \( r = x - y \).

Recall that \( f \) is linear combination of Gaussian functions. By directly applying this fact, we have the following corollary. Lemma 13 calculates \( |\mathcal{E}| \leq \varepsilon \alpha \) when \( D_K^2(P, Q) > \alpha \).

**Corollary 3.** Given two point sets \( P, Q \in \mathbb{R}^d \),
\[
\mathbb{E}_{h_v \sim \mathcal{H}_{\alpha, \varepsilon}} \left[ \left\| \sum_{x \in P \cup Q} \beta_x h_{u,v}(x) \right\|^2 \right] = D_K^2(P, Q) + \mathcal{E}
\]
where \( \mathcal{E} = \sum_{x \in P \cup Q} \sum_{y \in P \cup Q} \beta_x \beta_y \mathcal{E}_{x,y} \). Recall that \( \beta_x \) is \( \frac{1}{|P|} \) if \( x \in P \) and \( -\frac{1}{|Q|} \) if \( x \in Q \).

Now, we can conclude that the expectation of squared norm of our hash function is an \((1+\varepsilon)\)-approximation of \( D_K^2(P, Q) \). Indeed, we did not need to make this random variable to be unbiased.

**Corollary 4.** Still assuming \( D_K^2(P, Q) \geq \alpha \), for any choice for \( \varepsilon > 0 \),
\[
(1 - \varepsilon)D_K^2(P, Q) \leq \mathbb{E}_{h_v \sim \mathcal{H}_{\alpha, \varepsilon}} \left[ \left\| \sum_{x \in P \cup Q} \beta_x h_{u,v}(x) \right\|^2 \right] \leq (1 + \varepsilon)D_K^2(P, Q)
\]

### 3.4 Showing Convolution Properties

As mentioned before, the following lemma is to prove that \( h_v \) is actually the convolution of a Gaussian function and random function \( \cos(\langle v, \cdot \rangle), \sin(\langle v, \cdot \rangle) \). Namely, \( \cos(\langle v, \cdot \rangle) \) and \( \sin(\langle v, \cdot \rangle) \) are the random function we are actually generating. This convolution property is basically Fourier Transformation. For completeness, we still prove it in our context.
Lemma 5. For any $v, x \in \mathbb{R}^d$, we have

$$h_v(x) = (2\gamma)^{d/2} \left( \frac{1}{\pi} \right)^{3d/4} \left[ \int_{t \in \mathbb{R}^d} \exp(-2\|x - t\|^2) \cos(\langle v, t \rangle) \, dt \right]$$

Proof. Recall that

$$h_v(x) = (2\gamma)^{d/2} \left( \frac{1}{4\pi} \right)^{d/4} \exp(-\|v\|^2/8) \cos(\langle v, x \rangle)$$

So to complete the proof, we need to prove

$$\int_{t \in \mathbb{R}^d} \exp(-2\|x - t\|^2) \cos(\langle v, t \rangle) \, dt = \left( \frac{\pi}{2} \right)^{d/2} \exp(-\|v\|^2/8) \cos(\langle v, x \rangle)$$

and

$$\int_{t \in \mathbb{R}^d} \exp(-2\|x - t\|^2) \sin(\langle v, t \rangle) \, dt = \left( \frac{\pi}{2} \right)^{d/2} \exp(-\|v\|^2/8) \sin(\langle v, x \rangle)$$

We can again use sum of angle formula $\cos(a + b) = \cos(a) \cos(b) - \sin(a) \sin(b)$, specifically as

$$\cos(\langle v, t \rangle) = \cos(\langle v, t - x \rangle) \cos(\langle v, x \rangle) - \sin(\langle v, t - x \rangle) \sin(\langle v, x \rangle).$$

Now since $\exp(-2\|y\|^2) \sin(\langle v, y \rangle)$ is an odd function which means its integral over the entire $\mathbb{R}^d$ is 0. Combining these two facts together with $y = t - x$, we can zero out the $(\sin a \sin b)$ term so

$$\int_{t \in \mathbb{R}^d} \exp(-2\|t - x\|^2) \cos(\langle v, t \rangle) \, dt$$

$$= \int_{t \in \mathbb{R}^d} \exp(-2\|t - x\|^2) \cos(\langle v, t - x \rangle) \cos(\langle v, x \rangle) \, dt$$

$$= \cos(\langle v, x \rangle) \left( \frac{\pi}{2} \right)^{d/2} \exp(-\|v\|^2/8)$$

by Obs (2) with $b = \frac{1}{2}$

Similarly, we have

$$\int_{t \in \mathbb{R}^d} \exp(-2\|x - t\|^2) \sin(\langle v, t \rangle) \, dt = \left( \frac{\pi}{2} \right)^{d/2} \exp(-\|v\|^2/8) \sin(\langle v, x \rangle).$$

Corollary 6. Given two point sets $P, Q \in \mathbb{R}^d$,

$$\left\| \sum_{x \in P \cup Q} \beta_x h_v(x) \right\|^2 = \left( \frac{2}{\pi} \right)^d \left( \int_{t \in \mathbb{R}^d} f(t) \cos(\langle v, t \rangle) \, dt \right)^2 + \left( \int_{t \in \mathbb{R}^d} f(t) \sin(\langle v, t \rangle) \, dt \right)^2$$

Recall that $f(t) = \sum_{x \in P \cup Q} \beta_x \left( \frac{4}{\pi} \right)^{d/4} \exp(-2\|x - t\|^2)$.
Proof. By Lemma 5, we have

\[ \sum_{x \in P \cup Q} \beta_x h_v(x) = \sum_{x \in P \cup Q} \beta_x (2\gamma)^{d/2} \left( 1 \over \pi \right)^{3d/4} \left[ \int_{t \in \mathbb{R}^d} \exp(-2 \|x - t\|^2) \cos(\langle v, t \rangle) dt \right] \]

\[ = (2\gamma)^{d/2} \left( 1 \over 4\pi^2 \right)^{d/4} \left[ \int_{t \in \mathbb{R}^d} \left( \sum_{x \in P \cup Q} \beta_x \left( \frac{1}{\alpha} \right)^{d/4} \exp(-2 \|x - t\|^2) \right) \cos(\langle v, t \rangle) dt \right] \]

\[ = (2\gamma)^{d/2} \left( 1 \over 4\pi^2 \right)^{d/4} \left[ \int_{t \in \mathbb{R}^d} f(t) \cos(\langle v, t \rangle) dt \right] \]

3.5 The Final Bound

In order to apply Chernoff bound, the following lemma is to bound the random variable by its expectation up to a large factor.

**Lemma 7.** Given two point sets $P, Q \in \mathbb{R}^d$ and a region $\Lambda \subset \mathbb{R}^d$,

\[ \left\| \sum_{x \in P \cup Q} \beta_x h_v(x) \right\|^2 \leq 4 \left( \gamma \over \pi \right)^d (\text{vol}(\Lambda) \mathcal{D}_R^2(P, Q) + \mathcal{E}_\Lambda) \]

Here, $\text{vol}(\Lambda) = \int_{t \in \Lambda} 1 dt$ and $\mathcal{E}_\Lambda = \left( \int_{t \in \mathbb{R}^d \setminus \Lambda} |f(t)| dt \right)^2$.

**Proof.** From Corollary 5, recall that

\[ \left\| \sum_{x \in P \cup Q} \beta_x h_v(x) \right\|^2 = \left( \gamma \over \pi \right)^d \left( \left( \int_{t \in \mathbb{R}^d} f(t) \cos(\langle v, t \rangle) dt \right)^2 + \left( \int_{t \in \mathbb{R}^d} f(t) \sin(\langle v, t \rangle) dt \right)^2 \right) \]

We first analyze the term $\left( \int_{t \in \mathbb{R}^d} f(t) \cos(\langle v, t \rangle) dt \right)^2$. Note that, by $(a + b)^2 \leq 2a^2 + 2b^2$ for any $a, b \in \mathbb{R}^d$,

\[ \left( \int_{t \in \mathbb{R}^d} f(t) \cos(\langle v, t \rangle) dt \right)^2 \leq 2 \left( \int_{t \in \mathbb{R}^d} f(t) \cos(\langle v, t \rangle) dt \right)^2 + 2 \left( \int_{t \in \mathbb{R}^d \setminus \Lambda} f(t) \cos(\langle v, t \rangle) dt \right)^2 \]

For the first term $\left( \int_{t \in \Lambda} f(t) \cos(\langle v, t \rangle) dt \right)^2$, by Schwarz’s Inequality,

\[ \left( \int_{t \in \Lambda} f(t) \cos(\langle v, t \rangle) dt \right)^2 \leq \left( \int_{t \in \Lambda} f(t)^2 dt \right) \left( \int_{t \in \Lambda} \cos(\langle v, t \rangle)^2 dt \right) \]

\[ \leq \left( \int_{t \in \mathbb{R}^d} f(t)^2 dt \right) \left( \int_{t \in \Lambda} 1 dt \right) \]

\[ = \text{vol}(\Lambda) \cdot \mathcal{D}_R^2(P, Q) \]

For the second term $\left( \int_{t \in \mathbb{R}^d \setminus \Lambda} f(t) \cos(\langle v, t \rangle) dt \right)^2$,

\[ \left( \int_{t \in \mathbb{R}^d \setminus \Lambda} f(t) \cos(\langle v, t \rangle) dt \right)^2 \leq \left( \int_{t \in \mathbb{R}^d \setminus \Lambda} |f(t)| dt \right)^2 = \mathcal{E}_\Lambda. \]
Putting these together we have
\[
\left( \int_{t \in \mathbb{R}^d} f(t) \cos((v, t)) dt \right)^2 \leq 2 \text{vol}(\Lambda) d^2_K(P, Q) + 2 \mathcal{E}_\Lambda.
\]
Similarly, we also have \( \left( \int_{t \in \mathbb{R}^d} f(t) \sin((v, t)) dt \right)^2 \leq 2 \text{vol}(\Lambda) d^2_K(P, Q) + 2 \mathcal{E}_\Lambda. \) Now, we can conclude
\[
\left\| \sum_{x \in P \cup Q} \beta_x h_v(x) \right\|^2 \leq 4 \left( \frac{\gamma}{\pi} \right)^d \left( \text{vol}(\Lambda) d^2_K(P, Q) + \mathcal{E}_\Lambda \right).
\]

**Corollary 8.** If \( \mathcal{E}_\Lambda \leq d^2_K(P, Q) \), then for constant \( C = 16(1/\pi)^d \),
\[
\left\| \sum_{x \in P \cup Q} \beta_x h_v(x) \right\|^2 \leq 4 \left( \frac{\gamma}{\pi} \right)^d \left( \text{vol}(\Lambda) d^2_K(P, Q) + \mathcal{E}_\Lambda \right).
\]

**Proof.** By Lemma 7 we immediately have
\[
\left\| \sum_{x \in P \cup Q} \beta_x h_v(x) \right\|^2 \leq 4 \left( \frac{\gamma}{\pi} \right)^d \left( \text{vol}(\Lambda) d^2_K(P, Q) + \mathcal{E}_\Lambda \right)
\]
\[
\leq 4 \left( \frac{\gamma}{\pi} \right)^d \left( \text{vol}(\Lambda) + 1 \right) d^2_K(P, Q)
\]
\[
\leq 8(1/\pi)^d \cdot \gamma^d \text{vol}(\Lambda) \cdot d^2_K(P, Q).
\]
Also, by Corollary 8 and assuming \( \varepsilon < 1/2 \),
\[
\left\| \sum_{x \in P \cup Q} \beta_x h_v(x) \right\|^2 \leq C \cdot \gamma^d \text{vol}(\Lambda) \cdot E_{h_v \sim \mathcal{K}_{\alpha, \varepsilon}} \left[ \left\| \sum_{x \in P \cup Q} \beta_x h_v(x) \right\|^2 \right].
\]

We now present our near-final result for abstract region \( \Lambda \); we specify for a few special cases shortly.

**Theorem 9.** Fix \( \varepsilon, \delta, \alpha, V > 0 \). There is a mapping \( F : S \to \mathbb{R}^D \) with \( D = O \left( (\log \frac{1}{\varepsilon \alpha})^d V^2 \frac{1}{\varepsilon^2} \log \frac{1}{\delta} \right) \) where \( S \) is the set of subset of \( \mathbb{R}^d \), such that, for any \( P, Q \in \Lambda \) that

- there exist a region \( \Lambda \in \mathbb{R}^d \) that \( \mathcal{E}_\Lambda \leq d^2_K(P, Q) \) and \( \text{vol}(\Lambda) \leq V \)
- if \( P \neq Q \) then \( D^2_K(P, Q) > \alpha \)

then the following guarantee is held with probability at least \( 1 - \delta \)
\[
(1 - \varepsilon) D_K(P, Q) \leq \| F(P) - F(Q) \| \leq (1 + \varepsilon) D_K(P, Q).
\]
Proof. Draw $D$ random vectors $v_1, v_2, \ldots, v_D$ from $[-\gamma, \gamma]^d$ uniformly. Recall $\gamma = \Theta(\sqrt{\log \frac{1}{\epsilon \delta}})$. Define the mapping $F$ as the follows.

$$F(P) = \frac{1}{\sqrt{D}} \sum_{x \in P} \frac{1}{|P|} \left[ \begin{array}{c} h_{v_1}(x) \\ \vdots \\ h_{v_D}(x) \end{array} \right]$$

for any $P \in \mathbb{R}^d$.

Recall that one version of Chernoff bound is the following. Given $m$ i.i.d. random variables $X_1, X_2, \ldots, X_m$ such that, for all $i, a \leq X_i \leq b$ for some $a, b \in \mathbb{R}$. Let $X = \frac{1}{m} \sum_{i=1}^m X_i$ and $E(X) = \mu > 0$. Then, for any $\epsilon > 0$, $|X - \mu| \leq \epsilon \mu$ with probability at least $1 - 2 \exp\left(\frac{-m \epsilon^2 \mu^2}{2b^2}\right)$.

In our setting, each random variable

$$X_i = \left( \sum_{x \in P} \frac{1}{|P|} h_{v_i}(x) - \sum_{y \in Q} \frac{1}{|Q|} h_{v_i}(y) \right) = \left( \sum_{x \in P \cup Q} \beta_x h_{v_i}(x) \right)^2.$$

By Lemma 8 we can set $a = 0$ and $b = C \cdot \gamma d \cdot V \cdot \mu$. Finally, $m$ represents $D$, setting the probability of failure at $\delta$ and solving for $D = m$ in $\delta \leq 2 \exp\left(-\frac{D \beta_x^2 \mu^2}{C \cdot \gamma d \cdot V \cdot \mu}\right)$ reveals that we can set $D = C \frac{1}{\epsilon \delta} (\gamma d V^2) \ln \frac{2}{\delta}$, and this ensures that

$$(1 - \epsilon) \mu \leq \frac{1}{D} \sum_{i=1}^D \left( \sum_{x \in P \cup Q} \beta_x h_{v_i}(x) \right)^2 \leq (1 + \epsilon) \mu.$$

Now by Corollary 11 we have $\mu \in (1 \pm \epsilon) D_2(\mathbb{P} \cup \mathbb{Q}, \mathbb{P})$, so this implies that

$$(1 - \epsilon)^2 D_2(\mathbb{P} \cup \mathbb{Q}) \leq \|F(\mathbb{P}) - F(\mathbb{Q})\|^2 \leq (1 + \epsilon)^2 D_2(\mathbb{P} \cup \mathbb{Q}).$$

and hence as desired

$$(1 - \epsilon) D(\mathbb{P} \cup \mathbb{Q}) \leq \|F(\mathbb{P}) - F(\mathbb{Q})\| \leq (1 + \epsilon) D(\mathbb{P} \cup \mathbb{Q}).$$

\subsection{Defining Safe Regions $\Lambda$}

We introduce a value $\gamma' = \sqrt{\frac{1}{4} \ln\left(\frac{8d^2 \epsilon^d}{\pi \alpha}\right)} > 1$. For a point $x = (x_1, x_2, \ldots, x_d) \in \mathbb{R}^d$ let

$$\Gamma_x = [x_1 - \gamma', x_1 + \gamma'] \times [x_2 - \gamma', x_2 + \gamma'] \times \ldots \times [x_d - \gamma', x_d + \gamma].$$

The next lemma is essentially to defining safe regions.

\textbf{Lemma 10.} If for all points $x \in \mathbb{P} \cup \mathbb{Q}$ we have $\Gamma_x \subset \Lambda$ then $\mathcal{E}_\Lambda \leq \alpha$.

\textbf{Proof.} Recall that $\mathcal{E}_\Lambda = \left( \int_{t \in \mathbb{R}^d \setminus \Lambda} |f(t)| \, dt \right)^2$ and $|f(t)| = \sum_{x \in \mathbb{P} \cup \mathbb{Q}} |\beta_x| \left(\frac{1}{\pi}\right)^{d/4} \exp(-2 \|x - t\|^2)$. Denote
\[ U_i = \{ t \in \mathbb{R}^d \mid |t_i| > \gamma' \}. \] For any \( x = (x_1, x_2, \ldots, x_d) \in P \cup Q, \)

\[
\int_{t \in \mathbb{R}^d \setminus \Lambda} \exp(-2 \|x - t\|^2)dt \\
\leq \int_{t \in \mathbb{R}^d \setminus \bigcup_{i=1}^d [x_i - \gamma', x_i + \gamma']} \exp(-2 \|x - t\|^2)dt \\
\leq \sum_{i=1}^d \int_{t \in U_i} \exp(-2 \|t\|^2)dt \\
= \sum_{i=1}^d \left( \int_{|t_i| > \gamma'} \exp(-2t_i^2) dt \right) \left( \frac{\pi}{2} \right)^{(d-1)/2} \text{ by (F2)} \\
= 2d \left( \frac{\pi}{2} \right)^{(d-1)/2} \left( \int_{t > \gamma'} \exp(-2t^2) dt \right) \\
\leq 2d \left( \frac{\pi}{2} \right)^{(d-1)/2} \left( \int_{t > \gamma'} \exp(-2\gamma'^2) dt \right) \text{ by } t > \gamma' \\
= 2d \left( \frac{\pi}{2} \right)^{(d-1)/2} \frac{1}{2\gamma'} \exp(-2\gamma'^2) \text{ by (F4)} \\
\leq d \left( \frac{\pi}{2} \right)^{(d-1)/2} \exp(-2\gamma'^2) \text{ by } \gamma' > 1
\]

That means, recall that \( \gamma' = \sqrt{\frac{1}{4} \ln \left( \frac{8d\pi^d/4}{\epsilon} \right)} \),

\[
\left( \int_{t \in \mathbb{R}^d \setminus \Lambda} |f(t)| dt \right)^2 \leq \left( \sum_{x \in P \cup Q} |\beta_x| \left( \frac{4}{\pi} \right)^{d/4} \left( \frac{\pi}{2} \right)^{(d-1)/2} \exp(-2\gamma'^2) \right)^2 \\
\leq \left( \frac{2\sqrt{\pi}}{\sqrt{\pi}} d\pi^{d/4} \exp(-2\gamma'^2) \right)^2 \\
= \alpha \\
\]

**Bounded Size Case.** Suppose \( P \) and \( Q \) are any point sets with total cardinality less than \( n \). Define the region \( \Lambda \) to be \( \bigcup_{x \in P \cup Q} \prod_{i=1}^d [x_i - \gamma', x_i + \gamma'] \). It is easy to see that \( \text{vol}(\Lambda) \leq n(2\gamma')^d \), and satisfies the conditions of Lemma 10. Thus we can directly invoke Theorem 9 to obtain.

**Theorem 11.** Given \( \epsilon, \delta, \alpha > 0 \) and positive integer \( n \), there is a mapping \( F : S \to \mathbb{R}^{D_n} \) with \( D_n = O \left( n^2 \left( \log \frac{1}{\alpha} \right)^d \left( \log \frac{1}{\epsilon \alpha} \right)^d \frac{1}{\epsilon} \log \frac{1}{\delta} \right) \) where \( S \) is the set of subset of \( \mathbb{R}^d \) such that, for any \( P, Q \in \mathbb{R}^d \) satisfying the following conditions

- \( |P \cup Q| \leq n \)
- if \( P \neq Q \) then \( D_K(P, Q) > \alpha \),

the following guarantee is held with probability at least \( 1 - \delta \)

\[
(1 - \epsilon)D_K(P, Q) \leq \|F(P) - F(Q)\| \leq (1 + \epsilon)D_K(P, Q)
\]
This bound may seem vacuous because the dimensionality is greater than $n^2$ required for the Mercer, exact embedding. However, this bound still has two advantages. First, it does not require to orthogonalization, which to do exactly takes $O(n^3)$ time, and approximate variants introduce their own inaccuracies. Second, it is data oblivious. The definition of this mapping $F$ does not need to know the precise location of the data points, only the maximum size $n$ which may ever occur. So for instance, consider a streaming scenario, where the data points for $P, Q$ are coming in online. If we allocate some $D$ dimensions for the feature space, then as more data points arise, the accuracy gracefully declines. The $\alpha$ lower bound on distance, influences the $\gamma$ value in the hash family definition, while the $n$ upper bound on point set size only affects the volume bound, and hence the error in each estimate. So as long as $D^2(P, Q) \geq \alpha$, then we maintain that $\|F(P) - F(Q)\| \in (1 \pm \varepsilon_n)D(P, Q)$ where $\varepsilon_n$ increases (roughly linearly) with $n$.

**Bounded Region Case.** Now, suppose we do not have a bound on the size of the point sets $P$ and $Q$, and infact they may represent continuous distributions with bounded support. In this case we only need to define some bounded region which contains them. Here we consider a region $[-L, L]^d$ for some $L > 0$, and enforce that $P, Q \subset [-L, L]^d$ (or are probability measures with bounded support in $[-L, L]^d$). Then to satisfy the conditions of Lemma 10 we define $\Lambda = [-L - \gamma', L + \gamma']^d$. So now $\text{vol}(\Lambda) = (2L + 2\gamma')^d$ and $\mathcal{E}_\Lambda \leq \alpha$. By invoking Theorem 9 we obtain the following.

**Theorem 12.** Given $\varepsilon, \delta, \alpha, L > 0$, there is a mapping $F : \mathcal{S} \rightarrow \mathbb{R}^{D_L}$ with $D_L = O\left(\left(L + \sqrt{\log \frac{1}{\alpha}}\right)^{2d} (\log \frac{1}{\eta})^d \frac{1}{\varepsilon \delta} \log \frac{1}{\varepsilon \delta}\right)$ where $\mathcal{S}$ is the set of subset of $\mathbb{R}^d$ such that, for any $P, Q \in \mathbb{R}^d$ satisfying the following conditions

- $P, Q \subset [-L, L]^d$
- if $P \neq Q$ then $D^2(P, Q) > \alpha$,

the following guarantee is held with probability at least $1 - \delta$

$$(1 - \varepsilon)D(P, Q) \leq \|F(P) - F(Q)\| \leq (1 + \varepsilon)D(P, Q)$$

4 Extensions and Data Analysis Implications

There are many data analysis applications where improved bounds almost immediately follow from this new embedding. Before we begin, we start by improving the dimensionality of the embedding with a simple post-processing. We can applying a Johnson-Lindenstrauss-type embedding [21, 2, 3, 1] to the $D$-dimensional space to obtain $\rho$-dimensional vectors that, with probability at least $(1 - \delta)$ preserve $\text{poly}(m)$ pairwise distances using $\rho = O\left(\frac{1}{\varepsilon^2} \log \frac{\delta}{m}\right)$. For applications in kernel two-sample hypothesis testing and nearest neighbor searching $m$ directly depends on how many queries we make, for instances the bounded number needed for $k$-means clustering [15], now applied to kernel $k$-means. In general this takes time $O(nD\rho)$ to project all $n$ vectors of dimension $D$ to ones of dimension $\rho$, although when $\rho = O(d^{1/2 - \eta})$ for some $\eta > 0$, then the runtime can be improved to $O(nD \log \rho)$ [2, 8].

These results are useful for reducing the storage space of data representations. However, they in general do not lead to faster algorithms since often the cost is already dominated by $O(nD)$ time to generate the $D$-dimensional vectors, and the $O(nD\rho)$ or $O(nD \log \rho)$ time to reduce the dimension would only increase that runtime. Hence, because these properties follow fairly directly from previous results, we do not explicitly restate the bounds.
Kernel Two-Sample Test. The Kernel two-sample test \cite{20} is a “non-parametric” hypothesis test between two probability distributions represented by finite samples \( P \) and \( Q \); let \( n = |P \cup Q| \). Then this test simply calculates \( D_K(P, Q) \), and if the value is large enough it rejects the null hypothesis that \( P \) and \( Q \) represent the same distribution. Since its introduction a few years ago it has seen many applications and relations; see the recent 140 page survey \cite{25}. Zhao and Deng \cite{35} proposed to speed this test up for large sets using RFFs which improves runtime and in some cases even statistical power. While several improvements are suggested \cite{34} including using FastFood \cite{23}, these all only provide additive \( \varepsilon \)-error.

If the distributions are known to inhabit a bounded region \([-L, L]^d\), then we can invoke Theorem \ref{thm:gap} to obtain two vectors of size \( D_L = O \left( (L + \sqrt{\log \frac{1}{\alpha}})^d \left( \log \frac{1}{\varepsilon \alpha} \right)^d \frac{1}{\varepsilon \alpha} \log \frac{1}{\delta} \right) \) in \( O(nD) \) time, and compute a kernel means \( \Phi(P) \) and \( \Phi(Q) \) for each, and then compare their distances in \( O(D) \) time. Hence the entire estimate takes \( O(nD) \) time. As long as \( D_K(P, Q) > \alpha \), this guarantees the estimate of \( D_K(P, Q) \) is within \( \varepsilon \) of the correct value.

One way to determine if this value should estimate \( P \) and \( Q \) as distinct, is to run permutation tests. That is for some large number (e.g., \( m = 1000 \)) of trials, select two sets \( P_j, Q_j \) iid from \( P \cup Q \), of size \( |P| \) and \( |Q| \) respectively. For each generated pair we calculate (or estimate using Theorem \ref{thm:gap}) the value of \( D_K(P_j, Q_j) \), and then use the 95th-percentile of these values as a threshold. Note since each \( P_j, Q_j \) is drawn from the same domain \([-L, L]^d\) as \( P, Q \), then the guarantees on the accuracy of the featurized estimate carries over directly.

LSH for point sets, geometric distributions. The new results also allow us to immediately design LSH and nearest neighbor students for the kernel distance by relying on standard Euclidean LSH \cite{5}. Build a search engine for low-dimensional shapes \cite{18} has long been a goal in computational geometry and geometric modeling. A difficulty arises in that many of the best-known shape distance measures require an alignment (e.g., Frechet \cite{17} \cite{4} or earth movers \cite{10}) which creates many challenges in designing LSH-type procedures. Some methods have been designed, but with limitations, e.g., on point set size for earth mover distance \cite{6} or number of segments in curves for discrete Frechet \cite{16}. The kernel distance provides an alternative distance to shapes, low-dimensional distributions, or curves \cite{22}.

Now after embedding to \( D_n \) dimensions for a bounded number of points (via Theorem \ref{thm:embedding}) or to \( D_L \) dimensions for objects from a bounded \([-L, L]^d\) domain (via Theorem \ref{thm:gap}), standard Euclidean LSH can be applied \cite{5}. Given a family of point sets \( \mathcal{F} = \{P_1, P_2, \ldots, P_m\} \), an \( \varepsilon \)-approximate nearest neighbor of a query point set \( Q \) is a point set \( \hat{P} \in \mathcal{F} \) so that \( D_K(P_j, Q) \leq (1 + \varepsilon) \min_{P \in \mathcal{F}} D_K(P_j, Q) \). For \( \varepsilon \leq 1/2 \), we can embed each \( P_j \) to \( F(P_j) \in \mathbb{R}^D \), and then invoke the key result from Andoni and Indyk \cite{6} for a \( c' \)-approximate nearest neighbor, so \( (1 + c')(1 + \varepsilon) \leq (1 + (1 + \varepsilon)c' + \varepsilon) \). Overall, retrieve a \( c \)-approximate nearest neighbor (with \( c = (1 + \varepsilon)c' + \varepsilon \)) to a query \( Q \) with \( O(mn^{1/c^2+o(1)}) \) query time after using \( O(mn^{1+1/c^2+o(1)} + mnD) \) preprocessing.

5 Conclusion

We have designed a new \((1 + \varepsilon)\)-relative error feature map to an approximate RKHS for the kernel distance on Gaussian kernels. It only holds when \( D_K(P, Q) > \alpha \), but the dimension only depends polylogarithmically on \( 1/\alpha \). By focusing on the kernel distance instead of the inner product, we are able to obtain stronger and we believe simpler bounds between lifted points and point sets. The modification from the classic RFFs unintuitively adds a bias and variance, but this allows a new form of analysis which can achieve relative
error. We have shown a few immediate implications of these new feature maps, but we are hopefully it will span several more, through a focus on the kernel distance, not the inner products.

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A Proofs of Basic Facts

Here are some deferred proofs of the useful facts.

(F1) For vectors $x, y, t \in \mathbb{R}^d$ then $\|x - t\|^2 + \|y - t\|^2 = \|x - y\|^2 + 2\|t - \frac{x+y}{2}\|$.  

Proof.  
\[
\|x - t\|^2 + \|y - t\|^2 = \|x\|^2 - 2\langle x, t \rangle + \|t\|^2 + \|y\|^2 - 2\langle y, t \rangle + \|t\|^2 \\
= 2\left(\|t\|^2 - 2\left\langle t, \frac{x+y}{2} \right\rangle + \left\| \frac{x+y}{2} \right\|^2 - \left\| \frac{x+y}{2} \right\|^2 \right) + \|x\|^2 + \|y\|^2 \\
= 2\left\| t - \frac{x+y}{2} \right\|^2 - \left( \frac{\|x\|^2}{2} + \frac{\|y\|^2}{2} - 2\frac{\langle x, y \rangle}{2} \right) + \|x\|^2 + \|y\|^2 \\
= 2\left\| t - \frac{x+y}{2} \right\|^2 + \left( \frac{\|x\|^2}{2} + \frac{\|y\|^2}{2} + \frac{2\langle x, y \rangle}{2} \right) \\
= 2\left\| t - \frac{x+y}{2} \right\|^2 + \frac{\|x-y\|^2}{2}
\]

(F4) For any $a > 0$ then $\int_{x>a} \exp(-ax)dx = \frac{1}{a} \exp(-a^2)$.

Proof. Define a variable $y = -ax$ so $x = y/(-a)$. We will change the integration to over $y$, noting that
when \( x = a \), then \( y = -ax = -a^2 \) and when \( x = \infty \) then \( y = -\infty \). Now
\[
\int_{x>a} \exp(-ax) \, dx = \int_{x=a}^{\infty} \exp(-ax) \, dx
\]
\[
= \int_{y=-ax}^{\infty} \frac{1}{y}\exp(y) \, dy
\]
\[
= \frac{1}{a} \{ \exp(-\infty) - \exp(-a^2) \}
\]
\[
= \frac{1}{a} \exp(-a^2)
\]

\[\square\]

### B Some Deferred Calculations on Bounding Error

The following lemma is to bound the error term \( \mathcal{E} \) is small. From the definition of the error term, it is easy to see that it is true so long as \( \gamma \) is large enough.

**Lemma 13.** Given two point sets \( P, Q \in \mathbb{R}^d \) and any \( 0 < \varepsilon < 1/2 \), \( |\mathcal{E}| \leq \varepsilon \alpha \). Recall that \( D_K(P, Q) > \alpha \) if \( P \neq Q \).

**Proof.** We give a bound on \( |\mathcal{E}_{x,y}| \). Recall that \( \gamma = \sqrt{4 \ln(\frac{16d}{\varepsilon \alpha})} > 1 \). Denote \( V_i = \{ v \in \mathbb{R}^d \mid |v_i| > \gamma \} \).

\[
|\mathcal{E}_{x,y}| = \left( \frac{1}{4\pi} \right)^{d/2} \left| \int_{v \in \mathbb{R}^d \setminus [-\gamma, \gamma]^d} \exp(-\|v\|^2/4) \cos(\langle v, x-y \rangle) \, dv \right|
\]
\[
\leq \left( \frac{1}{4\pi} \right)^{d/2} \int_{v \in \mathbb{R}^d \setminus [-\gamma, \gamma]^d} \exp(-\|v\|^2/4) \, dv
\]
\[
\leq \left( \frac{1}{4\pi} \right)^{d/2} \sum_{i=1}^{d} \int_{v \in V_i} \exp(-\|v\|^2/4) \, dv \quad \text{note that } \bigcup_{i=1}^{d} V_i = \mathbb{R}^d \setminus [-\gamma, \gamma]^d
\]
\[
= \left( \frac{1}{4\pi} \right)^{d/2} \sum_{i=1}^{d} \left( \int_{|v| > \gamma} \exp(-v_i^2/4) \, dv_i \right) \left( \sqrt{4\pi} \right)^{d-1}
\]
\[
= \left( \frac{1}{4\pi} \right)^{1/2} \left( 2d \right) \left( \int_{v > \gamma} \exp(-v^2/4) \, dv \right)
\]
\[
\leq \left( \frac{1}{4\pi} \right)^{1/2} \left( 2d \right) \left( \frac{4}{\gamma} \exp(-\gamma^2/4) \right) \quad \text{by (F4)}
\]
\[
\leq \left( \frac{4d}{\sqrt{\pi}} \right) \exp(-\gamma^2/4) \quad \text{by } \gamma > 1
\]
\[
= \frac{1}{4} \varepsilon \alpha
\]
That means

\[ |\mathcal{E}| \leq \sum_{x \in P \cup Q} \sum_{y \in P \cup Q} |\beta_x| |\beta_y| |\mathcal{E}_{x,y}| \leq 4 \cdot \frac{1}{4} \varepsilon \alpha \leq \varepsilon \alpha. \]