How many moments does MMD compare?

RUSTEM TAKHANOV∗, School of Sciences and Humanities, Republic of Kazakhstan

We present a new way of study of Mercer kernels, by corresponding to a special kernel $K$ a pseudo-differential operator $p(x, D)$ such that $F \cdot p(x, D)\cdot p(x, D)F^{-1}$ acts on smooth functions in the same way as an integral operator associated with $K$ (where $F$ is the Fourier transform). We show that kernels defined by pseudo-differential operators are able to approximate uniformly any continuous Mercer kernel on a compact set.

The symbol $p(x, y)$ encapsulates a lot of useful information about the structure of the Maximum Mean Discrepancy distance defined by the kernel $K$. We approximate $p(x, y)$ with the sum of the first $r$ terms of the Singular Value Decomposition of $K$, denoted by $p_r(x, y)$. If ordered singular values of the integral operator associated with $p(x, y)$ die down rapidly, the MMD distance defined by the new symbol $p_r$ differs from the initial one only slightly. Moreover, the new MMD distance can be interpreted as an aggregated result of comparing $r$ local moments of two probability distributions.

The latter result holds under the condition that right singular vectors of the integral operator associated with $p$ are uniformly bounded. But even if this is not satisfied we can still hold that the Hilbert-Schmidt distance between $p$ and $p_r$ vanishes. Thus, we report an interesting phenomenon: the MMD distance measures the difference of two probability distributions with respect to a certain number of local moments, $r^*$, and this number $r^*$ depends on the speed with which singular values of $p$ die down.

Additional Key Words and Phrases: kernel methods, maximum mean discrepancy, generative, pseudo-differential operators, moment matching.

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1 INTRODUCTION

Recovering a distribution from a high-dimensional dataset, either in the form of a multivariate probability density function or in the form of a sampling model, is the key task in the plethora of data science applications. The modern approach to that task is based on minimizing a distance function between the so called empirical distribution $\mu_{emp}$, i.e. the probabilistic measure concentrated in data points, and a parameterized model distribution, $\mu_\theta$. Parameters of the model, $\theta$, are the arguments over which the minimization is performed. Many distance functions are used for this purpose, including the Kullback-Leibler divergence, the Wasserstein distance [1], the $f$-divergence [22] and many others. Kernel methods, that are ubiquitous in machine learning, have also been applied to the problem. A key kernel-based distance function in the generative modeling is the Maximum Mean Discrepancy (MMD) metric. The MMD distance is induced by the following inner product between probability measures $\mu$ and $\nu$:

$$\langle \mu, \nu \rangle_K = \int_{\mathbb{R}^n \times \mathbb{R}^n} K(x, y)d\mu(x)d\nu(y)$$

where $K : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ is a Mercer kernel. In other words, MMD is defined by:

$$\text{MMD}_K(\mu, \nu)^2 = \langle \mu, \mu \rangle_K + \langle \nu, \nu \rangle_K - 2\langle \mu, \nu \rangle_K$$

Author’s address: Rustem Takhanov, rustem.takhanov@nu.edu.kz, School of Sciences and Humanities, 53 Kabanbay Batyr Ave, Nur-Sultan city, Republic of Kazakhstan, 010000.
and the corresponding generative modeling task is:

$$\min_\theta \text{MMD}_K(\mu_{\text{emp}}, \mu_\theta)$$

where, usually, $\mu_\theta$ is given in the form of a sampler.

Initial experiments with the MMD based generative modeling, the so called moment matching networks (GMMNs) [10], demonstrated the superiority of more computationally costly generative adversarial networks (GANs) [17]. A weakness of GMMNs in various applications is that MMD is strongly dependent on the underlying kernel $K$. In an attempt to overcome this problem, MMD GANs were introduced [3, 16], with the GAN style architecture that assumes training of the so called critic network. In MMD GANs the kernel that defines MMD depends on parameters. The role of the critic is to tune parameters of the kernel.

In fact, there is a connection between GANs and the MMD based networks that follows from a well-known representation:

$$\text{MMD}_K(\mu, \nu) = \sup_{f \in \mathcal{H}_K} \mathbb{E}_{X \sim \mu} f(X) - \mathbb{E}_{Y \sim \nu} f(Y),$$

where $\mathcal{H}_K$ is RKHS of $K$ [21, 25]. Thus, the task (1) can be represented in the minimax form, and this allows to treat MMD based networks as GANs. Unfortunately, this representation does not give a direct insight into the structure of MMD, because the critic’s space of functions, i.e. a unit ball in $\mathcal{H}_K$, is a nontrivial mathematical object.

Thus, an important general question is: if we change something in $K$ (e.g. the Gaussian kernel’s bandwidth or a degree of a polynomial kernel) how will it affect the structure of the MMD distance? To answer this question we introduce a family of kernels defined by the so called pseudo-differential operators [28]. Pseudo-differential operators are a special kind linear operators between spaces of smooth functions nicely behaving at infinity. Every such operator $L$ is defined by a function $p : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{C}$, which is called a symbol of operator. Their relationship is usually denoted as $L = p(x, D)$. Then we say that a kernel $K$ is defined by $L$ if $\langle Lu, Lv \rangle_{L^2} \propto \langle \hat{u}, \hat{O}_K \hat{v} \rangle_{L^2}$, where $\hat{u}$ denotes the Fourier transform of $u$ and $\hat{O}_K u(x) = \int_{\Omega} K(x, y) u(y) dy$ is an integral operator associated with $K$.

It turns out that many popular Mercer kernels (Gaussian, Poisson, Abel etc) can be given in this way. Moreover, this family of kernels is broad enough to approximate any continuous Mercer kernel $K : \Omega \times \Omega \to \mathbb{R}$ on a compact set $\Omega \subset \mathbb{R}^n$.

For kernels defined by pseudo-differential operators, the MMD distance can be naturally represented as the supremum over a managable unit ball in $L_2(\mathbb{R}^n)$, i.e. not a unit ball in $\mathcal{H}_K$. This allows us to study the structure of a loss function that the critic maximizes during a computation of the MMD distance.

For a pseudo-differential operator $L = p(x, D)$ we observe the following: if the rank of $O_p$, i.e. the dimension of the range of $O_p$, equals $r$, then the MMD distance associated with $L$ can be understood as an aggregated result of a comparison of $r$ “local” moments of two distributions. Motivated by this observation, we study the general situation, i.e. when the rank of $O_p$ is unbounded and $O_p$ needs to be approximated by another operator of finite rank. This setting reminds us of the principal component analysis of an infinite dimensional operator $O_p$.

The approximation error for pseudo-differential operators that we introduced can be naturally measured by two types of norms. The first norm is the operator norm in the space of bounded linear operators from $L_2(\mathbb{R}^n)$ to $L_\infty(\mathbb{R}^n)$, denoted $\| \cdot \|_{L_2, \infty}$. It is natural in a sense that two symbols $p_1, p_2$ with small $\|O_{p_1} - O_{p_2}\|_{L_2, \infty}$ define MMD distances that differ only slightly. We show that the truncated (on $r$th term) Singular Value Decomposition of $O_p$ approximates well $O_p$ in $\| \cdot \|_{L_2, \infty}$-norm if, basically: a) right singular vectors of $O_p$ are uniformly bounded, b) the remaining part $\sum_{i=r+1}^{\infty} \sigma_i$ is small, where $\sigma_1 \geq \sigma_2 \geq \cdots$ are ordered singular values of $O_p$. The second norm that we study is the Hilbert-Schmidt norm. Even when $\|O_{p_1} - O_{p_2}\|_{\text{HS}}$ is small, there is a possibility that corresponding
MMD distances between probability density functions \( u, v \) will differ sharply if \( \|u\|_{L_2}, \|v\|_{L_2} \) blow up. In this case, we only need the remaining part \( \sum_{i=r+1}^{n} \sigma_i^2 \) to be small in order for the truncated SVD to approximate \( O_p \).

Thus, the number \( r^* \) that indicates how many moments we need to compare to approximate the MMD distance, depends on spectral properties of the operator \( O_p \) that defines the kernel \( K \) (through \( p(x, D) \)), rather than on the spectrum of \( O_K \). This situation is different from a set of well-known results in which spectral properties of \( O_K \) are connected with the generalization capability of kernel-based algorithms [2, 6, 13, 15, 18, 20].

Note that pseudo-differential operators have already been used in some data science tasks [4, 7, 23].

## 2 Preliminaries

Throughout this paper we use standard terminology and notation from functional analysis. For details one can address the textbook on the theory of distributions [8]. We assume \( 0 \in \mathbb{N} \). For \( \alpha = (\alpha_1, \cdots, \alpha_n) \in \mathbb{N}^n \), \( |\alpha| \) denotes \( \sum_{i=1}^{n} \alpha_i \), \( D^\alpha \) denotes \( \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}} \), \( x^\alpha \) denotes \( x_1^{\alpha_1} \cdots x_n^{\alpha_n} \). The Schwartz space, denoted by \( S(\mathbb{R}^n) \), is a space of infinitely differentiable functions \( f : \mathbb{R}^n \to \mathbb{C} \) such that \( \forall \alpha, \beta \in \mathbb{N}^n, \sup_{x \in \mathbb{R}^n} |x^\alpha D^\beta f(x)| < \infty \). Its dual space is denoted by \( S'(\mathbb{R}^n) \). The Fourier and inverse Fourier transforms are denoted by \( \mathcal{F}, \mathcal{F}^{-1} : S'(\mathbb{R}^n) \to S' (\mathbb{R}^n) \).

For brevity, we denote \( \mathcal{F} [f] \) by \( \hat{f} \). A set of continuous functions on \( \mathbb{R}^n \) is denoted by \( C(\mathbb{R}^n) \), a set of infinitely differentiable functions on \( \mathbb{R}^n \) is denoted by \( \mathcal{C}^\infty (\mathbb{R}^n) \).

### 2.1 Maximum mean discrepancy (MMD)

Let \( K : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R} \) be a symmetric, positive definite kernel on a set \( \mathbb{R}^n \) and \( \mathcal{H}_K \) be the reproducing kernel Hilbert space that corresponds to \( K \) [11], equipped with the norm \( \|\phi\|_{\mathcal{H}_K} = \sqrt{\langle \phi, \phi \rangle_{\mathcal{H}_K}} \). Thus, for all \( x \in \mathbb{R}^n \), \( K_x = K(x, \cdot) \) is a representation of \( x \) in \( \mathcal{H}_K \). It is a well-known fact that the MMD distance between probability density functions \( p \) and \( q \) on \( \mathbb{R}^n \) can be rewritten in the following way:

\[
\text{MMD}_K (p, q) = \| \mathbb{E}_{X \sim p} [K_x] - \mathbb{E}_{Y \sim q} [K_y] \|_{\mathcal{H}_K}
\]

where we assume that \( \mathbb{E}_{X \sim p} [K_x] = \int_{\mathbb{R}^n} K(x, y)p(y)dy \) is defined and is an element of \( \mathcal{H}_K \).

### 2.2 Pseudo-differential operators

The theory of pseudo-differential operators is a developed branch of mathematics that can be found in many textbooks, e.g. in [28]. The basic definitions is as follows (first given by Hörmander [12] and Kohn-Nirenberg [14]): a class \( \mathcal{S}_0^m \) is defined as a set of functions \( F \in \mathcal{C}^\infty (\mathbb{R}^n \times \mathbb{R}^n) \) such that for any compact \( \Omega \subseteq \mathbb{R}^n \) and any \( \alpha, \beta \in \mathbb{N}^n \) there is \( C_{\Omega, \alpha, \beta} > 0 \) such that

\[
|D_x^\alpha D_y^\beta F(x, y)| \leq C_{\Omega, \alpha, \beta} (1 + |y|)^{m - |\alpha|}
\]

whenever \( x \in \Omega \).

Any \( F \in \mathcal{S}_0^m \) defines a continuous operator \( F(x, D) : \mathcal{S}(\mathbb{R}^n) \to \mathcal{S}(\mathbb{R}^n) \), by the rule

\[
F(x, D)u(x) = \int_{\mathbb{R}^n} F(x, y)\hat{u}(y)e^{ix^Ty}dy.
\]

We call \( F(x, D) \) the pseudo-differential operator (PDO) with symbol \( F \) [28]. For example, \( F(x, y) = \sum_{|\alpha| \leq m} f_\alpha (x)y^\alpha \), then \( F(x, D) \) maps \( u \) to \( \sum_{|\alpha| \leq m} f_\alpha (x)(-i)|\alpha|D^\alpha u(x) \).

If additionally, for any compact \( \Omega \subseteq \mathbb{R}^n \) there is \( C > 0 \) and \( R > 0 \) such that \( |F(x, y)| \geq C(1 + |y|)^m \) whenever \( x \in \Omega \) and \( |y| > R \), then \( F(x, D) \) is called an elliptic operator of order \( m \).

## 3 PDO-based Kernels

Throughout the paper we will study a special type of Mercer kernels defined below.
Definition 3.1. Let \( F(x, D) \) be a PDO and let a function \( K : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R} \) satisfy
\[
\langle F(x, D)[u], F(x, D)[v] \rangle_{L^2} \propto \int_{\mathbb{R}^n \times \mathbb{R}^n} \hat{u}(x)K(x,y)\hat{v}(y)dx\,dy
\]
for \( u, v \in S(\mathbb{R}^n) \). Then, \( K \) is called the PDO-based kernel and is denoted by \( K^F \). In other words, the integral operator \( O_{K^F} \) is proportional to the composition \( \mathcal{F} \circ F(x, D)^{-1} \circ F(x, D) \circ \mathcal{F}^{-1} \).

Example 3.2. Any kernel \( K(x,y) = k(x-y) \) for which \( y = \mathcal{F}^{-1}[k] \) satisfies \( y(x) \geq 0 \) and \( \partial_{\alpha} \sqrt{y(x)} \in C(\mathbb{R}^n) \), is defined by the PDO of the symbol \( p(x,y) = \sqrt{y(x)} \). This case includes the Gaussian kernel, the Laplace kernel, the rational quadratic kernel, the Matérn kernel and many other popular kernels.

3.1 Universality of PDO-based kernels

In this section we show that PDO-based kernels are in a certain sense universal, i.e. a continuous kernel on a compact set can be approximated uniformly with any given accuracy by some PDO-based kernel.

Let \( K \) be a continuous Mercer kernel on \( \mathbb{R}^n \). Thus, its restriction \( K|_\Omega : \Omega \times \Omega \to \mathbb{R} \) on any compact \( \Omega \subseteq \mathbb{R}^n \) is also a continuous Mercer kernel (and also, a Hilbert-Schmidt kernel). The following facts can be found in [26]:

a) RKHS \( \mathcal{H}_{K|_\Omega} \) is a separable space of continuous functions, b) there exists a countable basis of orthonormal functions in \( \mathcal{H}_{K|_\Omega} \), \( e_1, \cdots, e_i, \cdots \), such that \( O_{K|_\Omega} e_i = \lambda_i e_i \), c) the corresponding feature map \( \Phi : \mathbb{R}^n \to \mathcal{H}_{K|_\Omega} \) is continuous, d) finally, Mercer’s theorem gives us that
\[

K(x,y) = \langle \Phi(x), \Phi(y) \rangle_{\mathcal{H}_{K|_\Omega}} = \sum_{i=1}^{\infty} f_i^*(x) f_i(y)
\]
where \( f_i(x) = \langle e_i, \Phi(x) \rangle_{\mathcal{H}_{K|_\Omega}} \) and the convergence is absolute and uniform on \( \Omega \).

Therefore, let us study the kernel
\[
K(x,y) = \sum_{i=1}^{N} e^{-\epsilon^2 \|x-y\|^2} f_i^*(x) f_i(y)
\]
where \( \epsilon > 0, f_i(x) = \sum_{|\alpha| \leq m} c_\alpha^i x^\alpha, i \in [N] \) are polynomials such that \( c_\alpha^i \neq 0 \) if \( |\alpha| = m \). Obviously, finite sums of the form (3) can approximate uniformly continuous kernels on compact sets.

**Proposition 3.3.** The kernel (3) is PDO-based.

**Proof.** The following bilinear forms are proportional:
\[
\langle \hat{u}, O_K \hat{v} \rangle = \sum_{i=1}^{N} \langle f_i \hat{u}, O_{e^{-\epsilon^2 \|x-y\|^2}} f_i \hat{v} \rangle \propto \sum_{i=1}^{N} \langle f_i(D)u, e^{-\|x\|^2/4\epsilon^2} f_i(D)v \rangle = \langle u, Lu \rangle
\]
where \( L = \sum_{i=1}^{N} f_i(D)^\top e^{-\|x\|^2/4\epsilon^2} f_i(D) \).

Since \( \langle u, Lu \rangle \geq 0 \), then \( L \) is a positive semidefinite self-adjoint operator. Additionally, \( L \) is an elliptic operator of order \( 2m \), because there is
\[
p(x,y) = \sum_{\alpha,\beta: |\alpha| \leq 2m, |\beta| \leq 2m} c_{\alpha,\beta} x^\alpha e^{-\|x\|^2/4\epsilon^2} y^\beta \in S_{2m}^{2m}
\]
such that $L = p(x, D)$. The ellipticity property is satisfied because the principal part of $p(x, y)$ is

$$\sum_{i=1}^{N} \sum_{\alpha = |\alpha| = m} |c_\alpha|^2 e^{-|\alpha|^2/4x^2} y^{2\alpha}.$$

According to Seeley (see [24]) the square root for such an operator is also elliptic self-adjoint pseudo-differential operator of order $m$. In other words, there exists a function $F(x, y) \in S_{1,0}^m$ such that $F(x, D)F(x, D) = p(x, D)$. It is easy to see that $\langle F(x, D)[u], F(x, D)[v]\rangle_{L^2} \propto \int_{\mathbb{R}^n \times \mathbb{R}^n} \hat{u}(x)K(x, y)\hat{v}(y)dx dy$. Therefore, $K$ is defined by $F$, i.e. $K = K^F$. □

4 GAN-STYLE INTERPRETATION OF MMD

For a probability density function $u \in S(\mathbb{R}^n)$, $\chi_u$ denotes its characteristic function, i.e. $\chi_u(x) = \mathbb{E}_{\xi \sim u} e^{i\xi^T x} = \mathcal{F}^{-1}[u](x)$. For $F \in S_{1,0}^m$, $F(D, x)$ denotes $\mathcal{F} \circ F(x, D)^{\dagger} \circ \mathcal{F}^{-1}$, a continuous operator from $S(\mathbb{R}^n)$ to $S(\mathbb{R}^n)$.

**Proposition 4.1.** Let $u, v \in S(\mathbb{R}^n)$ be two probability density functions and $F(x, D)$ be a PDO. Then, the MMD distance defined by $K^F$ satisfies:

$$\text{MMD}_{K^F}(u, v) \propto \sup_{||f||_{L_2(\mathbb{R}^n)} \leq 1} \mathbb{E}_{X \sim u} F(D, x)f(X) - \mathbb{E}_{Y \sim v} F(D, x)f(Y) \quad (5)$$

**Proof.** The MMD distance defined by $K^F$ can be expressed:

$$\text{MMD}_{K^F}(u, v) \propto ||F(x, D)[\chi_u] - F(x, D)[\chi_v]||_{L_2} = \sup_{f \in S(\mathbb{R}^n) : ||f||_{L_2(\mathbb{R}^n)} \leq 1} \langle F(x, D)^{\dagger} f, \chi_u - \chi_v \rangle_{L_2} \propto \sup_{f \in S(\mathbb{R}^n) : ||f||_{L_2(\mathbb{R}^n)} \leq 1} \langle F(x, D)^{\dagger} f, u - v \rangle_{L_2}$$

$$= \sup_{f \in S(\mathbb{R}^n) : ||f||_{L_2(\mathbb{R}^n)} \leq 1} \langle F(D, x)^{\dagger} f, u - v \rangle_{L_2} \quad (6)$$

From the latter proposition the following is straightforward.

**Proposition 4.2.** Let $F = F_1 + F_2$, then

$$\text{MMD}_{K^F}(u, v) \leq \text{MMD}_{K^{F_1}}(u, v) + \text{MMD}_{K^{F_2}}(u, v)$$

The last representation of MMD distance allows to put the MMD minimization into the minimax framework. Let us now consider a pseudo-differential operator with a symbol $F$ such that the range of $O_F$ is finite-dimensional.
4.1 A finite sum case

In applications, a finite sum case is important:

\[ F(x, y) = \sum_{i=1}^{l} f_i(x)g_i(y) \]

(7)

where \( \hat{f}_i \in L_1(\mathbb{R}^n) \). The latter implies that \( f_i \) is bounded.

**Proposition 4.3.** If \( F \) satisfies (7), then it can be represented as \( F(x, y) = \sum_{i=1}^{L} h_i(x)t_i(y) \) where \( L \leq 4l, \hat{h}_i \) is a pdf, i.e. \( \hat{h}_i(x) \geq 0, \int_{\mathbb{R}^n} \hat{h}_i(x)dx = 1 \).

**Proof.** By substituting each term \( f_i(x)g_i(y) = (f_i(x)+f_i(-x)+\frac{f_i(x)+f_i(-x)}{2})g_i(y) \) with two terms \( \frac{f_i(x)+f_i(-x)}{2}g_i(y) \) we can turn a sum with \( l \) terms into a sum with \( 2l \) terms in such a way that in all resulting terms \( h_i(x)t_i(y) \), \( \hat{h}_i(x) \) is a real valued function. This operation costs us the doubling of the number of terms.

Let us now consider the term \( f_i(x)g_i(y) \) such that \( \hat{f}_i(x) \) is a real valued function.

Suppose \( F[\hat{f}_i] = f'_i \) and both inverse images \( (f'_i)^{-1}[\mathbb{R}_+] \) and \( (f'_i)^{-1}[\mathbb{R}_-] \) have nonzero Lebesgue measure. Note that \( f'_i \in L_1(\mathbb{R}^n) \), therefore \( f'_i(x) = \alpha p'_i(x) - \beta p'_i(x) \), where \( p'_i(x) = \max\{0, f'_i(x)\}/\alpha, p'_i(-x) = -\min\{0, f'_i(x)\}/\beta \) and \( \alpha = ||\max\{0, f'_i(x)\}||_{L_1}, \beta = ||\min\{0, f'_i(x)\}||_{L_1} \). Thus, we can substitute \( f_i(x)g_i(y) \) with \( \hat{f}_i(x)\hat{g}_i(y) \) where \( f'_i = \mathcal{F}^{-1}[p'_i], g'_i(y) = \alpha g_i(y), f''_i = \mathcal{F}^{-1}[\hat{f}_i] \text{ and } \hat{g}_i(y) = -\beta g_i(y) \).

If \( f'_i(x) \geq 0 \text{ a.s.} \), then we can substitute \( f_i(x)g_i(y) \) with \( \hat{f}_i(x)\hat{g}_i(y) \) where \( \hat{f}_i(x) = \frac{f_i(x)}{f''_i} \text{ and } \hat{g}_i(y) = ||f''_i||_{L_1}g_i(y) \). Analogously the case \( f_i(x) \leq 0 \) is treated.

Thus, any such term can be substituted with 2 terms of the form \( h_i(x)t_i(y) \) where \( \hat{h}_i \) is a pdf. Both operations cost at most the doubling of the number of terms. If we apply them sequentially, then we obtain at most 4l terms.

Due to proposition 4.3, let us additionally assume in (7) that \( \hat{f}_i = p_i \) and \( p_i(x) \geq 0, \int_{\mathbb{R}^n} p_i(x)dx = 1 \). Then, we obtain:

\[ f(x) \xrightarrow{F_i \in L_1(\mathbb{R}^n)} \sum_{i=1}^{l} g'_i f_i \mathcal{F} \left[ f'_i \mathcal{F}^{-1}[f] \right] \propto \sum_{i=1}^{l} g'_i(x)(q_i \ast f)(x) \]

where \( q_i(x) = p_i(-x) = \hat{f}_i^* \). Thus, if \( u \) is a smooth probability density function, then:

\[ \mathbb{E}_{x-u} F(D, x)f(x) \propto \mathbb{E}_{x-u} \sum_{i=1}^{l} g'_i(x)(q_i \ast f)(x) = \]

\[ \sum_{i=1}^{l} \int_{\mathbb{R}^n \times \mathbb{R}^n} u(x)g'_i(x)q_i(y)f(x-y)dxdy = \]

\[ \sum_{i=1}^{l} \mathbb{E}_{x-u, y-q_i} g'_i(x)f(x-y) \]
Now, using (6) we finally obtain a characterization of MMD as supremum:

$$\text{MMD}_{K^F}(u, v) \propto \sup_{f: ||f||_{L^2(U^n)} \leq 1} \sum_{i=1}^{l} \mathbb{E}_{x \sim u, y \sim q_i} f'(x - y) - \mathbb{E}_{x \sim v, y \sim q_i} f'(x - y)$$

(8)

Note that if \(l = 1\) and \(q_1(x) = 1\), \(\text{MMD}_{K^F}(u, v)\) is proportional to:

$$\sup_{f: ||f||_{L^2(U^n)} \leq 1} \mathbb{E}_{x \sim u, \epsilon \sim p_1} [f(x + \epsilon)] - \mathbb{E}_{x \sim v, \epsilon \sim p_1} [f(x + \epsilon)]$$

where \(q_1(x) = p_1(-x)\). In this case we have \(K(x, y) = \tilde{f}_2^1(x - y)\) (the translation invariant kernel case [9]). This case captures the Gaussian kernel, the Poisson, kernel, the Abel kernel, and many other kernels.

From the last expression the GAN-style interpretation of generative networks based on MMD distance directly follows. In the minimax task (1), which is equivalent to \(\min_{\theta} \sup_{f: ||f||_{L^2(U^n)} \leq 1} \mathbb{E}_{x \sim \mu_0, \epsilon \sim p_1} f(x + \epsilon) - \mathbb{E}_{x \sim \mu_{emp}, \epsilon \sim p_1} f(x + \epsilon)\), the generator always adds noise, distributed according to \(p_1(x)\), to vectors generated from empirical and model distributions. The critic optimizes over functions from unit ball in \(L_2(\mathbb{R}^n)\) and tries to increase the \(f's\) value in regions for which probabilities of \(\mu_{emp}\) and \(\mu_0\) differ.

Note that the GAN-style interpretation of (8) is also straightforward. Let us introduce:

$$m_i(t, u) = \mathbb{E}_{x \sim u, \epsilon \sim p_1} [g_i^*(x) | x + \epsilon = t]$$

(9)

for \(q_i(x) = p_i(-x)\) and \(i \in [l]\). The expression (9) is the expectation of the feature \(g_i^*(x)\) when \(x\) is sampled according to distribution \(u\), under condition that the sum of \(x\) and the noise vector \(\epsilon\) equals \(t\). In other words, \(m_i(t, u)\) is a \(g_i^*\)-moment of \(u\) in the neighbourhood of \(t\).

Thus,

$$\text{MMD}_{K^F}(u, v) \propto \sup_{f: ||f||_{L^2(U^n)} \leq 1} \sum_{i=1}^{l} \mathbb{E}_{x \sim u, \epsilon \sim p_1} [f(x + \epsilon)] \left( m_i(x + \epsilon, u) - m_i(x + \epsilon, v) \right)$$

From the latter formula we can make the following conclusions:

- The critic tries to increase \(f\) in regions for which "local" expectations of \(g_i^*(x)\) for empirical and model distributions, i.e. \(m_i(x + \epsilon, u) - m_i(x + \epsilon, v)\), differ sharply. Thus, the MMD distance measures the difference between distributions of the feature vector \(G(x) = [g_i^*(x)]_{i=1}^l\) for \(x \sim u\) and \(x \sim v\) around each point \(t\).
- Different features affect the critic’s objective simultaneously. That is why it is important to generate noise for different features, \(g_i^*\) and \(g_j^*\), according to different distributions, \(p_i\) and \(p_j\). Otherwise, if \(p_i = p_j\), then the MMD distance will compare the distributions of a single feature, \(g_i^* + g_j^*\). For example, suppose \(p_i\) is a pdf of the Gaussian noise with the bandwidth \(\sigma_i\). In the design of MMD’s kernel, the bandwidth \(\sigma_i\) rather than being the same for all features, better be adapted to the feature \(g_i^*\). E.g. for the kurtosis of a distribution (4th moment), it is natural to have a larger bandwidth than for the expected value.

Let us denote \(\text{Feat}_F = \{\lambda_1, g_1 + \ldots + \lambda_l | \lambda_i \in \mathbb{C}\}\), i.e. the span of those functions. Thus, it becomes clear that \(\text{Feat}_F\) serves as a space of features whose distribution we compare. The dimension of \(\text{Feat}_F\) can be naturally called a dimension of the kernel \(K^F\). It is easy to see that this dimension equals \(\dim \mathcal{R}[O_F]\).
5 A NATURAL NORM ON PDOS DEFINING KERNELS

For an operator $O : S(\mathbb{R}^n) \to S(\mathbb{R}^n)$ let us define

$$||O||_{2,\infty} = \sup_{f \in S(\mathbb{R}^n) : ||f||_{L_1(\mathbb{R}^n)} \leq 1} ||Of||_{L_\infty(\mathbb{R}^n)}.$$ 

For any function $F : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ such that $A = \sup_x \int_{\mathbb{R}^n} |F(x,y)|^2 dy < \infty$, we have $||O_F||_{2,\infty} = \sqrt{A}$. In other words, the norm $|| \cdot ||_{2,\infty}$ can be easily calculated for integral operators. The following two proposition show that the calculation of $||F(x, D)||_{2,\infty}$ is also simple.

**Proposition 5.1.** If $F \in S^m_{1,0}, ||O_F||_{2,\infty} < \infty$, then diagonal elements of Schwartz kernels of $F(x, D)F(x, D)^\dagger$ and $O_FO_F^\dagger$ are the same, i.e. there are smooth functions $M, N$ such that $F(x, D)F(x, D)^\dagger = O_M, O_FO_F^\dagger = O_N$ and $M(\xi, \xi) \propto N(\xi, \xi)$.

**Proof.** The Schwartz kernel of $F(x, D)$ is $K_1(\xi', x) = \int e^{i\xi'^T y} F(\xi', y)e^{-i\xi x} dy'$. Therefore, the Schwartz kernel of $F(x, D)^\dagger$ is $K_2(\xi, x) = K_1(\xi, x)^* = \int e^{i\xi' y} F(\xi, y)^* e^{-i\xi x} dy$. Thus,

$$\langle u, F(x, D)(F(x, D)^\dagger u) \rangle \propto \int u(\xi')^* e^{i\xi'^T y} F(\xi', y)^* e^{-i\xi' y} e^{i\xi x} y F(\xi, y)^* e^{-i\xi x} y dy' d\xi'$$

Thus, the Schwartz kernel of $F(x, D)F(x, D)^\dagger$ is

$$M(\xi', \xi) = \int e^{i\xi'^T y} F(\xi', y)^* e^{-i\xi' y} e^{i\xi x} y F(\xi, y)^* e^{-i\xi x} y dydy'$$

The diagonal element equals:

$$M(\xi, \xi) = \int e^{i\xi'^T y} F(\xi, y)^* e^{-i\xi' y} e^{i\xi x} y F(\xi, y)^* e^{-i\xi x} y dydy' = \int e^{-i(\xi - \xi')^T (y - y')} F(\xi, y)^* F(\xi, y) dydy'$$

after we set $G_b(a) = F(b, -a), F_b(a) = F(b, a)^*$

$$\int e^{-i(\xi - \xi')^T \lambda} G_\xi(\lambda) F_\xi(y) dy d\lambda dx = \int e^{-i(\xi - \xi')^T \lambda} \{G_\xi * F_\xi\}(\lambda) d\lambda dx \propto$$

$$\int \mathcal{T} [\{G_\xi * F_\xi\}](\xi - x) dx = \int \widehat{G_\xi}(\xi - x) \widehat{F_\xi}(\xi - x) dx = (\widehat{G_\xi}, \widehat{F_\xi})_{L_2} = (G_\xi(-x)^*, F_\xi(x))_{L_2} = \int F(\xi, x)(\xi, x)^* dx$$

The latter equals the diagonal element of $O_FO_F^\dagger$. \hfill \square
Proposition 5.2. If $F \in S_{1,0}^m$, then

$$
||F(x, D)||_{2, \infty} \propto ||O_F||_{2, \infty} = \sup_x \int_{\mathbb{R}^n} |F(x, y)|^2 dy
$$

(10)

Proof. The norm of the integral operator $O_F$ can be expressed as:

$$
||O_F||_{2, \infty} = \sup_x \sup_{u: ||u||_{L^2(\mathbb{R}^n)} \leq 1} \int_{\mathbb{R}^n} F(x, y)u(y)dy = \sup_x \sup_{||F(x, \cdot)||_{L^2}} \sqrt{\int_{\mathbb{R}^n} |F(x, y)|^2 dy} = \sup_x \int_{\mathbb{R}^n} F(x, y)^*F(x, y)dy = \sqrt{\sup_x N_F(x, x)}
$$

where $N_F$ is the Schwartz kernel of $O_F^\dagger$. Let $O_F^\dagger = F(x, D)$. Due to proposition 5.1, diagonal elements of $O_F^\dagger O_F$ and $O_F^\dagger O_F^\dagger$ are the same, i.e $N_F(x, x) = N_F(x, x)$. Therefore, supremum of those diagonal elements, $\sup_x N_F(x, x)$ and $\sup_x N_F^\dagger(x, x)$, are also the same. Thus, $||F(x, D)||_{2, \infty} = ||O_F^\dagger||_{2, \infty} = ||O_F||_{2, \infty}$. □

Proposition 5.3. If $F_1 \in S_{1,0}^m$ and $F_2 \in S_{1,0}^m$, then

$$
|MMD_{K_F^1}(u, v) - MMD_{K_F^2}(u, v)| \leq c ||F_1(D, x) - F_2(D, x)||_{L^2}
$$

(11)

where $c$ is some constant.

Proof. Using (6) we can express:

$$
MMD_{K_F^1}(u, v) - MMD_{K_F^2}(u, v) = \sup_{f_1 \in S(\mathbb{R}^n): ||f_1||_{L^2(\mathbb{R}^n)} \leq 1} \langle F_1(D, x)f_1, u - v \rangle_{L^2} - \sup_{f_2 \in S(\mathbb{R}^n): ||f_2||_{L^2(\mathbb{R}^n)} \leq 1} \langle F_2(D, x)f_2, u - v \rangle_{L^2} \leq \sup_{f \in S(\mathbb{R}^n): ||f||_{L^2(\mathbb{R}^n)} \leq 1} \langle (F_1(D, x) - F_2(D, x))f, u - v \rangle_{L^2} \leq \sup_{f \in S(\mathbb{R}^n): ||f||_{L^2(\mathbb{R}^n)} \leq 1} ||F_1(D, x) - F_2(D, x)||_{L^2} ||u - v||_{L^1}
$$

using Holder inequality

$$
\leq 2||F_1(D, x) - F_2(D, x)||_{L^2} ||u - v||_{L^1}
$$

because $||u - v||_{L^1} \leq 2$ and $||F_1(D, x) - F_2(D, x)||_{L^\infty} \leq ||F_1(D, x) - F_2(D, x)||_{L^2}$. Analogously, we bound $MMD_{K_F^1}(u, v) - MMD_{K_F^2}(u, v)$ and this completes the proof. □

A natural norm on the PDO $F(x, D)$ defining the MMD distance $K_F$, is $||F(D, x)||_{L^2}$. A partial justification of this statement is the proposition (5.3) and the following proposition.
Proposition 5.4. Let $F \in S_{1,0}^m$, $f_i \in L_2(\mathbb{R}^n)$, $g_i \in L_{\infty}(\mathbb{R}^n)$ for $i = 1, \infty$, and $\sum_{i=1}^N f_i(x)g_i(y) \xrightarrow{N \to \infty} F$ wrt $|| \cdot ||_{2,\infty}$ norm. Then,

$$||F(D,x)||_{2,\infty} \leq C \sum_{i=1}^N ||f_i||_{L_2}||g_i||_{L_{\infty}}.$$

Proof. Let $F_N(x,y) = \sum_{i=1}^N f_i(x)g_i(x)$, $F_N(x,D)$ is a continuous operator from $L_2(\mathbb{R}^n)$ to $L_2(\mathbb{R}^n)$ defined by $F_N(x,D)f(x) = \int_{\mathbb{R}^n} F_N(x,y)\hat{f}(y)dy$, and $F_N(x,D)$ is $\mathcal{F} \circ F_N(x,D) \circ \mathcal{F}^{-1}$.

For any $f : ||f||_{L_2(\mathbb{R}^n)} \leq 1$ we have

$$||F_N(D,x)f||_{L_\infty} \leq \sum_{i=1}^N ||g_i||_{L_{\infty}}||\mathcal{F}[f_i^*f^{-1}[f]]||_{L_{\infty}} \leq \sum_{i=1}^N ||g_i||_{L_{\infty}}||\mathcal{F}[f_i^*f^{-1}[f]]||_{L_{\infty}}.$$

Since,

$$|\mathcal{F}[f_i^*f^{-1}[f]](\xi)| \leq \int f_i^*(x)f^{-1}[f](x)e^{-i\xi^T x}dx \leq \int \mathcal{F}[f_i^*f^{-1}[f]](\xi)dx \leq \sqrt{\int |f_i^*(x)|^2dx \int |f^{-1}[f](x)|^2dx} \leq C||f_i||_{L_2}||f||_{L_2}.$$ 

we obtain the bound $||F_N(D,x)||_{2,\infty} \leq C \sum_{i=1}^N ||f_i||_{L_2}||g_i||_{L_{\infty}}$. Finally, using $F_N \xrightarrow{N \to \infty} F$ we obtain the needed inequality. \hfill $\Box$

6 INTRINSIC DIMENSIONALITY OF PDO-BASED KERNELS

In Section 4.1 we learned that if $G \in S_{1,0}^m$ satisfies $\mathcal{R}[O_G^1] = r$, then MMD$_{K^G}$ reflects the similarity of two distributions with respect to $r$ local moments. Therefore, it is a natural idea to approximate arbitrary PDO-based kernel by some $K^G$ where $\mathcal{R}[O_G^1] = r$.

Let $K$ be a Mercer kernel such that

$$\text{Sym}(K) = \{ F \in S_{1,0}^m | m \in \mathbb{N}, K^F = K \}$$

is nonempty. Let us introduce

$$d_K(r) = \inf_{(F,G) \in \Pi(K,r)} ||F(D,x) - G(D,x)||_{2,\infty} \quad (12)$$

where

$$\Pi(K,r) = \{ (F,G) | F \in \text{Sym}(K), G \in S_{1,0}^m, \dim \mathcal{R}[O_G^1] = r \}.$$ 

The function $d_K(r)$ plays the same role as the retained variance in the Principal Component Analysis. We will study the behaviour of $d_K(r)$ as $r \to \infty$. 

Proposition 6.1. Let $K$ be a Mercer kernel, $F \in \text{Sym}(K)$ be a Hilbert-Schmidt kernel, $\sigma_1 \geq \sigma_2 \geq \cdots$ be singular values of the operator $O_F$ such that $\sum_{i=1}^{\infty} \sigma_i$ converges. Also, let

$$C_F = \sup_{u \neq 0, O_F u = \lambda u} \frac{||u||_\infty}{||u||_2} < \infty.$$ 

Then,

$$d_K(r) \leq C_F \sum_{i=r+1}^{\infty} \sigma_i.$$

Note that requiring $C_F < \infty$ means that the right singular vectors of $O_F$ (or, eigenvectors of $O_F^2$) are uniformly bounded. This condition is popular in various statements concerning Mercer kernels, though it is believed that it is hard to check. Discussions of that issue can be found in [19, 27, 29].

Proof. Using Singular Value Decomposition we obtain:

$$\sum_{i=1}^{N} \sigma_i f_i(x) g_i(y)^* \overset{N \to \infty}{\to} F(x, y) \text{ in } L_2(\mathbb{R}^n \times \mathbb{R}^n)$$

where $\{f_i\}_{i=1}^{\infty} \subseteq L_2(\mathbb{R}^n)$ and $\{g_i\}_{i=1}^{\infty} \subseteq L_2(\mathbb{R}^n)$ are systems of orthonormal vectors in $L_2(\mathbb{R}^n)$ and $g_i$ is an eigenvector of $O_F^2$.

Since $C_F < \infty$, we can write

$$||g_i||_{L_\infty} \leq C_F$$

As in the proof of proposition 5.4, let us denote $F_r(x, y) = \sum_{i=r+1}^{N} \sigma_i f_i(x) g_i(y)^*$ and bound

$$\left| \left| \sum_{i=r+1}^{r+N} \sigma_i f_i(D) g_i(x)^* \right| \right|_{L_1} \leq \sum_{i=r+1}^{r+N} ||\sigma_i g_i||_{L_\infty} ||f_i||_{L_2} \leq \sum_{i=r+1}^{r+N} \sigma_i C_F$$

Therefore, $F_r(D, x)$ is a Cauchy sequence in the Banach space of bounded operators $\mathcal{B}(L_2(\mathbb{R}^n), L_\infty(\mathbb{R}^n))$ with the operator norm. Thus, $F_r(D, x) \overset{r \to \infty}{\to} F(D, x)$ with respect to the norm $|| \cdot ||_{L_1}$.

Moreover, the norm of the remaining part is bounded:

$$||F(x, D) - F_r(x, D)||_{L_\infty} \leq C_F \sum_{i=r+1}^{\infty} \sigma_i$$

By construction $\text{dim} \mathcal{R}[O_F^2] = r$, i.e. $(F, F_r) \in \Pi(K, r)$. Therefore,

$$d_K(r) \leq ||F(x, D) - F_r(x, D)||_{L_\infty} \leq C_F \sum_{i=r+1}^{\infty} \sigma_i$$

$\square$

Sometimes $C_F = \infty$ or $\sum_{i=1}^{\infty} \sigma_i$ diverges, which makes the last proposition useless. Still some guarantees can be given, though we have to change the norm in the definition of $d_K(r)$ to the Hilbert-Schmidt norm:

$$d_K^H(r) = \inf_{(F, G) \in \Pi(K, r)} ||F(D, x) - G(D, x)||_{HS}$$

To obtain a bound on $d_K^H(r)$ we need a simple observation.
Proposition 6.2. Let \( F \in S^m_{\alpha}, \) then
\[
\|O_F\|_{\text{HS}} = \|F(x, D)\|_{\text{HS}}.
\]

Proof. This fact follow directly from proposition 5.1. Since \( O_F O_F^\dagger \) has the same diagonal as \( F(x, D)F(x, D)^\dagger \), we conclude that \( \text{Tr} (O_F O_F^\dagger) = \text{Tr} (F(x, D)F(x, D)^\dagger) \). Therefore, \( \|O_F\|_{\text{HS}} = \|F(x, D)\|_{\text{HS}} \). \( \square \)

Proposition 6.3. Let \( K \) be a Mercer kernel, \( F \in \text{Sym}(K) \) be a Hilbert-Schmidt kernel, \( \sigma_1 \geq \sigma_2 \geq \cdots \) be singular values of the operator \( O_F \). Then,
\[
d_K^0 (r) \leq \sqrt{\sum_{i=r+1}^{\infty} \sigma_i^2}.
\]

Proof. Again, \( \dim \mathcal{R}[O_F^\dagger] = r \), i.e. \( (F, F_i) \in \Pi(K, r) \). Therefore, using proposition 6.2 we obtain:
\[
d_K^0 (r) \leq \|F(D, x) - F_r(D, x)\|_{\text{HS}} = \sqrt{\sum_{i=r+1}^{\infty} \sigma_i^2}.
\]

Unfortunately, many interesting kernels cannot be defined by Hilbert-Schmidt kernel \( F \), but those cases can be partially captured by the following simple generalization whose proof is straightforward.

Proposition 6.4. Let \( F \) be a kernel such that \( \dim \mathcal{R}[O_F^\dagger] = d \) and \( \delta F \) be a Hilbert-Schmidt kernel such that \( K = K^{F + \delta F} \) and \( \sigma_1 \geq \sigma_2 \geq \cdots \) are singular values of the operator \( O_{\delta F} \). Then, for any \( n \geq d \) we have
\[
d_K (n) \leq c \sqrt{\sum_{i=n-d+1}^{\infty} \sigma_i^2}
\]
where \( c \) is a constant.

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