Abstract

The maximum mean discrepancy (MMD) is a recently proposed test statistic for two-sample test. Its quadratic time complexity, however, greatly hampers its availability to large-scale applications. To accelerate the MMD calculation, in this study we propose an efficient method called FastMMD. The core idea of FastMMD is to equivalently transform the MMD with shift-invariant kernels into the amplitude expectation of a linear combination of sinusoid components based on Bochner’s theorem and Fourier transform (Rahimi & Recht, 2007). Taking advantage of sampling of Fourier transform, FastMMD decreases the time complexity for MMD calculation from $O(N^2d)$ to $O(Nd)$, where $N$ and $d$ are the size and dimension of the sample set, respectively. For kernels that are spherically invariant, the computation can be further accelerated to $O(N \log d)$ by using the Fastfood technique (Le et al., 2013). The uniform convergence of our method has also been theoretically proved in both unbiased and biased estimates. We have further provided a geometric explanation for our method, namely ensemble of circular discrepancy, which facilitates us to understand the insight of MMD, and is hopeful to help arouse more extensive metrics for assessing two-sample test. Experimental results substantiate that FastMMD is with similar accuracy as exact MMD, while with faster computation speed and lower variance than the existing MMD approximation methods.

1. Introduction

The two-sample test is one of the most fundamental tests in statistics and has a wide range of applications. It uses samples drawn from two distributions to test whether to accept or reject the null hypothesis that they are the same or different. This task, however, is very difficult and challenging in practice since the underneath distribution information are generally unknown apriori (Bickel, 1969; Friedman & Rafsky, 1979; Hall & Tajvidi, 2002; Biau & Gyofi, 2005). The maximum mean discrepancy (MMD) is the latest test statistic designed for this task by measuring the discrepancy of two distributions by embedding them in a reproducing kernel Hilbert space (Gretton et al., 2012a). The MMD has been attracting much attention in recent two-sample test research due to its solid theoretical fundament (Smola et al., 2008; Sriperumbudur et al., 2010; 2011; Sejdinovic et al., 2013) and successful applications including biological data test (Borgwardt et al., 2006), data integration and attribute matching (Gretton et al., 2009), outlier detection, data classifiability (Sriperumbudur et al., 2009), domain adaption (Gong et al., 2013), etc. By generalizing the MMD to kernel families as the supremum of MMDs on a class of kernels, it has also been effectively used for some basic machine learning problems such as kernel selection (Sriperumbudur et al., 2009).

Albeit its various applications, the exact MMD needs $O(N^2d)$ computational cost, where $N$ and $d$ denote the size and dimension of samples, respectively, to calculate the kernel values between all pairs from the assessed two-sample sets. This quadratic computational complexity greatly hampers its further application to large-scale practical problems. How to speedup the computation of MMD has thus become a hot issue in statistics and machine learning in recent years.

There are mainly two approaches proposed for this problem by approximating MMD on a subsampling set of all sample pairs. The first is MMD-linear, which is the extremely
simplified MMD calculation by only using possibly fastest interactions of sample pairs (Gretton et al., 2012a). While this strategy significantly accelerates the MMD calculation to \(O(Nd)\), it also brings very high variance due to its evident loss of sample pair information. To better leverage the computation cost and calculation accuracy of MMD, B-test is recently proposed (Zaremba et al., 2013). The main idea is to split two-sample sets into corresponding subsets, construct block correspondence between them, and then compute the exact MMD inner each block while omit the inter-block pair information. By changing the block size, it can vary smoothly from MMD-linear with linear complexity to exact MMD with quadratic complexity. In practice, the block size is generally set as a modest value \(\sqrt{N}\) by experience. The complexity is \(O(N^{3/2}d)\), correspondingly.

Actually, as the coming of the big data era, it has become a hot trend to enhancing the efficiency of kernel-based learning methods, such as support vector machines and Gaussian process (Cortes & Vapnik, 1995; Schölkopf & Smola, 2002), throughout machine learning, computer vision, pattern recognition and data mining. Many efforts have been made to speedup the establishment of the kernel information and accelerate the implementation of kernel techniques (Smola & Schölkopf, 2000; Williams & Seeger, 2000; Fine & K.Scheinberg, 2001; Si et al., 2014). Two of the representative developments are Random Kitchen Sinks (Rahimi & Recht, 2007; 2008) and Fastfood (Le et al., 2013), which can significantly speed up the computation for a large range of kernel functions by mapping data into a relatively low-dimensional randomized feature space. These developments inspire us for this MMD-acceleration research topic, which constitutes an important branch along this line of research.

The main difficulty and challenge of MMD calculation lie in the fact that it needs to compute the kernel values between all sample pairs of two sets. MMD-linear and B-test attain this task by only utilizing a subsampling pair subset from all. Such simplification, however, also decreases the accuracy of MMD calculation due to their neglectness of the entire sample pair information. To this aim, this paper proposes a new efficient MMD calculation strategy, which can implement this task in a more efficient and accurate way. In summary, this paper mainly contains the following four-fold contributions:

1. Through employing Bochner’s theorem and Fastfood technique (Le et al., 2013) for kernels that are spherically invariant, we reduce the MMD computation cost to \(O(N \log d)\), which has lower time complexity than current MMD approximation methods and facilitates MMD’s application in large-scale data. Moreover, our method is easy to be sequentially computed and paralized.

2. The proposed method utilizes the interacted kernel values between all pairs from two sample sets to calculate MMD, which naturally leads to very accurate MMD result. Our experimental results substantiate that our method is with similar accuracy as exact MMD, and with significantly smaller variance than MMD-linear and B-test.

3. We have theoretically proved the uniform convergence of our method in both unbiased and biased cases. Comparatively, both MMD-linear and B-test are only feasible in unbiased cases.

4. We provide a geometrical explanation of our method in calculating MMD with shift-invariant kernels. Under this viewpoint, it is potentially useful for arousing more extensive metrics for two-sample test.

Code is available at https://www.dropbox.com/s/p5vtzqvcdw1swg8/FastMMD.zip.

### 2. Efficient MMD for Shift-Invariant Kernels

Firstly we give a brief review of MMD (Gretton et al., 2012a) and introduce some important properties of shift-invariant kernel (Rahimi & Recht, 2007). Then we propose an efficient MMD approximation method.

Consider a set of samples drawn from two distributions \( S = \{(x_i, \ell_i)\in \mathbb{R}^d \times \{1,2\}\}_{i=1}^N \), where the label \( \ell_i \) indicates the distribution from which \( x_i \) is drawn. The indices of samples with label \( \{1,2\} \) are denoted by \( I_1 = \{i \mid \ell_i = 1\} \) and \( I_2 = \{i \mid \ell_i = 2\} \), respectively.

#### 2.1. Overview of MMD

**Definition 1** Let \( p_1(x), p_2(x) \) be distributions defined on a domain \( \mathbb{R}^d \). Given observations \( \{(x_i, \ell_i)\}_{i=1}^N \), where \( X_1 = \{x_i | \ell_i = 1\} \) and \( X_2 = \{x_i | \ell_i = 2\} \) are i.i.d. drawn from \( p_1(x) \) and \( p_2(x) \), respectively. Denote \( I_1 = \{i | \ell_i = 1\} \) and \( I_2 = \{i | \ell_i = 2\} \). Let \( \mathcal{F} \) be a class of functions \( f: \mathbb{R}^d \rightarrow \mathbb{R} \). Then the maximum mean discrepancy and its empirical estimate are defined as (Definition 2 in Gretton et al. (2012a)):

\[
\text{MMD}[\mathcal{F}, p_1, p_2] = \sup_{f \in \mathcal{F}} (\mathbb{E}_{x \sim p_1} f(x) - \mathbb{E}_{x \sim p_2} f(x)),
\]

\[
\text{MMD}[\mathcal{F}, X_1, X_2] = \sup_{f \in \mathcal{F}} \left( \frac{1}{|I_1|} \sum_{i \in I_1} f(x_i) - \frac{1}{|I_2|} \sum_{i \in I_2} f(x_i) \right).
\]

Usually, \( \mathcal{F} \) is selected to be a unit ball in a universal RKHS \( \mathcal{H} \), defined on the compact metric space \( \mathbb{R}^d \) with associated kernel \( K(\cdot, \cdot) \) and feature mapping \( \phi(\cdot) \). The popular Gaussian and Laplacian kernels are universal (Gretton et al., 2012a). Denote \( \mu(p) = \mathbb{E}_{x \sim p} \phi(x) \) as the expectation of \( \phi(x) \). Then it has been proved that (Lemma 4 in Gretton et al. (2012a)):

\[
\text{MMD}[\mathcal{F}, p_1, p_2] = \|\mu(p_1) - \mu(p_2)\|_{\mathcal{H}}.
\]
Substituting the empirical estimates \( \mu(X_1) := \frac{1}{|I_1|} \sum_{i \in I_1} \phi(x_i) \) and \( \mu(X_2) := \frac{1}{|I_2|} \sum_{i \in I_2} \phi(x_i) \) of the feature space means based on respective samples, an empirical biased estimate of MMD can then be obtained as:

\[
\text{MMD}_b[\mathcal{F}, X_1, X_2] = \left\| \sum_{i=1}^{N} a_i \phi(x_i) \right\|_{\mathcal{F}} = \left( \sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j K(x_i, x_j) \right)^{\frac{1}{2}},
\]

where \( a_i = \frac{1}{|I_1|} \) if \( i \in I_1 \), and \( a_i = \frac{1}{|I_2|} \) if \( i \in I_2 \).

We will investigate how to accelerate its computation to \( O(N \log d) \), especially for shift-invariant kernels.

### 2.2. Efficient Approximation of MMD

The following classical theorem from harmonic analysis provides the main fundament underlying our approximation method (Genton, 2001).

**Theorem 1 (Bochner)** Every continuous positive definite function is Fourier transform of a positive finite Borel measure. This means that for any shift-invariant kernel \( K(x, y) \), there exists a positive measure \( \mu \) satisfying

\[
K(x, y) = \int_{\mathbb{R}^d} e^{i\omega \cdot (x - y)} \, d\mu(\omega),
\]

where \( \mu(\omega) \) is Fourier transform of kernel \( K(\Delta) \), and its normalization \( p(\omega) = \mu(\omega) / \int d\mu(\omega) \) is a probability measure. Here \( j = \sqrt{-1} \) is the imaginary unit.

We assume that the discussed positive definite kernel is real valued. According to Bochner’s theorem, we have that if a shift-invariant kernel \( K(x, y) \) is positive definite, there exists a proper scaled probability distribution \( p(\omega) \) satisfying

\[
K(x, y) = K(0) \cdot \int_{\mathbb{R}^d} p(\omega) e^{i\omega \cdot (x - y)} \, d\omega.
\]

Since both the probability distribution \( p(\omega) \) and the kernel \( K(\Delta) \) are real, the integrand \( e^{i\omega \cdot (x - y)} \) can be replaced by \( \cos(\omega^T \Delta \cdot x - \omega^T \Delta \cdot y) \) in the above equation. Taking the Gaussian kernel \( K(x, y; \sigma) = e^{-\frac{|x-y|^2}{2\sigma^2}} \) as an example, we can rewrite it as \( K(\Delta; \sigma) = e^{-\frac{\Delta^T \sigma^2 \Delta}{2\sigma^2}} \), where \( \Delta = x - y \).

Its Fourier transform is \( p(\omega; \sigma) = (2\pi)^{-d} e^{-\frac{\omega^2}{2} \sigma^2} \). By proper scaling, \( \omega \) can be viewed as a multivariate Gaussian distribution \( \omega \sim \mathcal{N}(0, \frac{1}{\sigma} I) \), where \( I \) is the \( d \times d \) identity matrix.

**Claim 2** For a shift-invariant kernel \( K(x, y) = \langle \phi(x), \phi(y) \rangle \), suppose \( p(\omega) \) is its corresponding normalized distribution in Bochner’s theorem, then

\[
\frac{1}{|I_1|} \sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j K(x_i, x_j) = K(0) \cdot E_{\omega \sim p(\omega)} \sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j \cos(\omega^T x_i - \omega^T x_j).
\]

Claim 2 can be easily proved by substituting Eqn. (2) into kernel \( K(x_i, x_j) \).

A very interesting thing is that we can fortunately calculate \( \sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j \cos(\omega^T x_i - \omega^T x_j) \) in linear time by applying a classical trigonometric identity. First, the expression can be viewed as a squared amplitude of combined sinusoids. Suppose a linear combination of \( N \) sinusoids is

\[
\frac{1}{|I_1|} \sum_{i=1}^{N} a_i \sin(x - \omega^T x_i) = A \sin(x - \theta),
\]

then its amplitude has a closed form \( A^2 = \sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j \cos(\omega^T x_i - \omega^T x_j) \). Second, the amplitude of sinusoids with the same frequency can be calculated in a sequential way in linear time. By combining the above two observations, we can calculate the expression with linear time complexity. If we set \( a_i \) in Eqn. (3) as that in empirical MMD, it turns out to be the biased estimate of MMD. As a result, Claim 2 finely implies a novel methodology to efficiently approximate MMD.

By the same spirit of Random Fourier features (Rahimi & Recht, 2007), we draw samples from distribution \( p(\omega) \), and then take the average of \( A^2(\omega; X_1, X_2) \) to approximate the empirical estimate of squared MMD. Formally, we sample \( L \) samples \( \{\omega_k\}_{k=1}^{L} \) from the distribution \( p(\omega) \), and then
use them to approximate MMD:
\[
\text{MMD}_b = \left[ \frac{K(0)}{L} \sum_{k=1}^{L} A^2(\omega_k; X_1, X_2) \right]^2, \tag{4}
\]
where \( A(\omega_k; X_1, X_2) \) is the amplitude of linear combination of sinusoids \( \frac{1}{|I_1|} \sum_{i \in I_1} \sin(x - \omega^i x_i) \) and \( \frac{1}{|I_2|} \sum_{i \in I_2} \sin(x - \omega^i x_i) \). We call \( L \) the number of basis functions (Neal, 1994; Le et al., 2013). The efficient calculation for unbiased MMD is similar since we can also rewrite unbiased estimate of MMD as the form in Eqn. (3). The proof is provided in Appendix A. The aforementioned procedure for approximating MMD is described in Algorithm 1.

For kernels that are spherically invariant, the Fastfood technique can be employed to further speedup \( \omega \) sampling in step 2 and \( \omega^i x_i \) calculation in steps 4.5 of Algorithm 1 (Le et al., 2013). This can bring further efficiency gain for MMD calculation from \( O(Nd) \) to \( O(N \log d) \). In the rest of this paper, we call our original algorithm as FastMMD-Fourier and its variant using Fastfood as FastMMD-Fastfood, respectively.

2.3. Computational Complexity

As aforementioned, given a sampling of \( \omega \), the time complexity for calculating \( A(\omega; X_1, X_2) \) is \( O(Nd) \). Since the sampling number \( L \) is preset as a fixed number and are independent on the sample scale, the computational complexity of the entire FastMMD-Fourier is \( O(Nd) \). For FastMMD-Fastfood, the computation speed is further enhanced to \( O(N \log d) \). As compared to the complexities of the previous MMD methods, such as \( O(N^2d) \) for exact MMD (Gretton et al., 2012a), \( O(Nd) \) for MMD-linear (Gretton et al., 2012a), and \( O(N^{3/2}d) \) for B-test (Zaremba et al., 2013), the proposed FastMMD methods evidently get a speed gain. Furthermore, instead of only utilizing a subsampling pair subset from all by the current MMD-calculation-accelerate methods, FastMMD takes into consideration all the interacted information between sample pairs. Our methods are thus expected to be more accurate.

Another interesting thing is that the calculation of \( A(\omega; X_1, X_2) \) can be computed in a sequential way, and thus our method can be naturally implemented in stream computations. Also our method is easy to be parallelized. This further implies the the potential usefulness of the proposed FastMMD methods in real large-scaled applications.

2.4. Approximation Guarantees

In this section, we will prove the approximation ability of the proposed FastMMD methods.

Theorem 3 (Uniform Convergence of FastMMD-Fourier) Let \( \mathcal{M} \) be a compact subset of \( \mathbb{R}^d \) with diameter diam(\( \mathcal{M} \)). Then, for the biased estimate of MMD in Algorithm 1, we have:
\[
\Pr \left[ \sup_{x_1, \ldots, x_N \in \mathcal{M}} \left| \text{MMD}_b^2 - \text{MMD}_b^2 \right| \geq \epsilon \right] 
\leq 2^{12} \left( \frac{\sigma_p \text{diam}(\mathcal{M})}{\epsilon} \right)^2 \exp \left( -\frac{L \epsilon^2}{64(d+2)} \right),
\]
where \( \sigma_p^2 = \mathbb{E}_p[\omega^i \omega^j] \) is the second moment of the Fourier transform of kernel \( K \). This bound also holds for the approximation of unbiased MMD.

Theorem 4 (Uniform Convergence of FastMMD-Fastfood) If we use Fastfood method (Le et al., 2013) to calculate \( \{\omega^i x_i\}^L_{i=1} \) in Algorithm 1, suppose the kernel is Gaussian kernel with bandwidth \( \sigma \) and \( \text{MMD}_b \) is the biased estimate of MMD that arises from a \( d \times d \) block of Fastfood, then we have:
\[
\Pr \left[ \sup_{x_1, \ldots, x_N \in \mathcal{M}} \left| \text{MMD}_b^2 - \text{MMD}_b^2 \right| \geq \epsilon \right] 
\geq \left( \frac{16 \text{diam}(\mathcal{M})}{\sigma} \right)^2 \left( \frac{\log(2/\delta) \log(2d/\delta)}{d} \right) \leq 2\delta.
\]
This bound also holds for the approximation of unbiased MMD.

From Theorems 3 and 4, we can see that the approximation of FastMMD is unbiased. Their proof is provided in the supplementary material.

3. Ensemble of Circular Discrepancy

In the previous section, we proposed an efficient approximation for MMD. In this section, we give a geometric explanation for our methods by using random projection (Blum, 2006) on a circle and circular discrepancy. This explanation is expected to help us more insightfully understand such approximation and inspire more extensive metrics for the two-sample test other than MMD.

3.1. Random Projection on a Unit Circle

If \( \omega \) in Eqn. (2) is fixed, we can see that the positions of points projected on a unit circle sufficiently determine the kernel. In other words, the random variables \( \omega^i x \) and \( \omega^i y \) can be wrapped around the circumference of a unit circle without changing the value of kernel function. We first investigate the circular distribution under fixed \( \omega \) in the following, and later will discuss the cases when \( \omega \) is sampled from a multivariate distribution.

Given a fixed \( \omega \), we wrap two classes of samples on a unit circle separately. The probability density functions (PDFs) of the wrapped two random variables \( X_1(\omega) \) and \( X_2(\omega) \)
can be mathematically expressed as:

\[ p_1(x; \omega) = \frac{1}{|I_1|} \sum_{i \in I_1} \delta(x - \text{mod}(\omega' x_i, 2\pi)), \quad (5) \]

\[ p_2(x; \omega) = \frac{1}{|I_2|} \sum_{i \in I_2} \delta(x - \text{mod}(\omega' x_i, 2\pi)), \quad (6) \]

where \( \text{mod}(\cdot, \cdot) \) is the modular arithmetic, and \( \delta(\cdot) \) is the Dirac delta function. Distributions \( p_1(x; \omega) \) and \( p_2(x; \omega) \) are zero when \( x \in (-\infty, 0) \cup [2\pi, +\infty) \). Such distributions are called circular distributions or polar distributions (Fisher, 1993).

### 3.2. Circular Discrepancy

We now define a metric for measuring the discrepancy between \( X_1(\omega) \) and \( X_2(\omega) \). Later we will show that this definition is closely related to MMD.

**Definition 2** Given two independent circular distributions \( X_1 \sim P_1 \) and \( X_2 \sim P_2 \), we define the circular discrepancy as:

\[ \eta(X_1, X_2) = \sup_{Q} (\mathbb{E}_{Q} p_1(Y - X_1) - \mathbb{E}_{Q} p_2(Y - X_2)), \quad (7) \]

where \( Y \sim Q \) is also a circular distribution.

In this definition, we choose sine function as the measure for assessing the distance between two circular distributions.

**Claim 5** The circular discrepancy as defined in (7) is equal to:

\[ \eta(X_1, X_2) = \sup_{y \in [0, 2\pi]} \int_{0}^{2\pi} (p_1(x) - p_2(x)) \sin(y - x) \, dx. \quad (8) \]

If \( p_1(x) \) and \( p_2(x) \) are probability mass functions (linear combination of Dirac delta functions), let \( p_1(x) - p_2(x) = \sum_{i=1}^{N} a_i \delta(x - x_i) \), and then the circular discrepancy is equal to

\[ \eta(X_1, X_2) = \left[ \sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j \cos(x_i - x_j) \right]^\frac{1}{2}. \quad (9) \]

The proof is provided in Appendix B. We can see that the circular discrepancy has a close connection with MMD, see Claim 2. In fact, if \( p_1(x) \) and \( p_2(x) \) are probability mass functions, the object function \( \int(p_1(x) - p_2(x)) \sin(y - x) \, dx \) in Eqn. (8) is a linear combination of sinusoids with the same frequency. The maximum of this problem is the amplitude of the combined sinusoid, and this is consistent with MMD.

From Eqn. (8) in Claim 5, it can be seen that the optimal distribution of random variable \( Q \) in problems (7) is a Dirac delta function. For the integral in Eqn. (8), if we change \( y \) to \( \text{mod}(y + \pi, 2\pi) \), the value of this expression will change its sign. Based on this observation, it is clear that there are two distributions of \( Q \) that can maximize and minimize the object function, respectively. The difference of their non-zero positions is \( \pi \). These two distributions construct a “optimal decision diameter” for the projected samples on a unit circle.

We then give a geometric explanation for problem (7). Note that the sine function is a distance measure with sign for two points on a circle (suppose positive angles are counterclockwise), so the definition of circular discrepancy aims to find a diameter that possibly largely separates the projected samples of two different classes. An example is shown in Fig. 1, where the orientation of the diameter corresponds to the non-zero elements of distribution \( Q \). We can see that this diameter maximizes the mean margin of two sample classes.

### 3.3. Ensemble of Circular Discrepancy

We have discussed the circular discrepancy for a given random projection \( \omega \) on a unit circle. For shift-invariant kernels, \( \omega \) is not a fixed value, but randomly sampled from a distribution, see Eqn. (2). We use sampling method for ensemble of circular discrepancy under different random projections. This ensemble turns out to be an efficient approximation of empirical estimate of MMD, so Algorithm 1 can be explained as ensemble of circular discrepancy.

**Definition 3** Suppose \( p(\omega) \) is the normalized distribution in Eqn. (2) for kernel \( K \); \( X_1 \) and \( X_2 \) are two circular distributions depending on \( \omega \) according to Eqn. (5)(6). The ensemble of circular discrepancy for \( X_1 \) and \( X_2 \) with shift-
invariant kernel $K$ is defined as:
\[
\eta(X_1(\omega), X_2(\omega); p(\omega)) = \left[ \mathbb{E}_{\omega \sim p(\omega)} \eta^2(X_1(\omega), X_2(\omega)) \right]^{1/2}.
\] (10)

Claim 6  For a shift-invariant kernel $K(x, y) = \langle \phi(x), \phi(y) \rangle$, $K(0) = 1$; denote $\mathcal{H}$ as the associated Hilbert space with kernel $K$; $p(\omega)$ as the normalized distribution in Eqn. (2); $X_1$ and $X_2$ as two circular distributions depending on $\omega$ defined by Eqn. (5)(6). Then the ensemble of circular discrepancy is
\[
\eta(X_1(\omega), X_2(\omega); p(\omega)) = \frac{1}{|I_1|} \sum_{i \in I_1} \phi(x_i) - \frac{1}{|I_2|} \sum_{i \in I_2} \phi(x_i) \right\|_{\mathcal{H}}.
\] (11)

Proof. By substituting Eqn. (9) into Eqn. (10) and utilizing Bochner’s theorem, we can obtain

\[
(\text{Left hand})^2 = \sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j \mathbb{E}_{\omega \sim p(\omega)} \cos(\omega'(x_i - x_j))
= \sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j K(x_i, x_j) = (\text{Right hand})^2.
\]

where $a_i = \frac{1}{|I_1|}$ if $i \in I_1$, and $a_i = \frac{1}{|I_2|}$ if $i \in I_2$. □

Fig. 2 demonstrates the relationship between MMD, circular discrepancy and our approximation. The blue and red contours are two distributions, and $p(\omega)$ is the distribution determined by Fourier transform of the kernel. We i.i.d. generate samples $\omega$ from distribution $p(\omega)$. For each generated $p(\omega)$, we project samples on a unit circle and calculate the circular discrepancy. The ensemble of discrepancy then corresponds to the MMD. We can see that the circular discrepancy constructs classifiers implicitly.

![Flowchart of circular discrepancy ensemble.](image)

It is interesting that if we use other similarity measurements such as Mallows Distance (earth movers distance) (Werman et al., 1986; Levina & Bickel, 2001), other than the sine function utilized in Definition 2, more extensive metrics for two-sample test can be naturally obtained. Furthermore, it should be noted that in Definition 3, we use $L_2$-norm average for ensemble. If we use other norms, we can also generalize more measures other than MMD for this task. All these extensions are hopeful directions for our future investigation.

4. Experimental Results

4.1. Approximation Quality

We begin by investigating how well our methods can approximate the exact MMD as the sampling number $L$ increases. Following previous work on kernel hypothesis testing (Gretton et al., 2012b; Zaremba et al., 2013), our synthetic distribution is designed as $5 \times 5$ grids of 2D Gaussian blobs. We specify two distributions, $P$ and $Q$. For distribution $P$ each Gaussian has identity covariance matrix, while for distribution $Q$ the covariance is non-spherical with a ratio $\epsilon$ of large to small covariance eigenvalues. Samples drawn from $P$ and $Q$ are presented in Fig. 3. The ratio $\epsilon$ is set as 4, and the sample number for each distribution is set as 1000.

![Synthetic data. (a) Distribution P; (b) Distribution Q.](image)

We used a Gaussian kernel with $\sigma = 1$, which approximately matches the scale of the variance of each Gaussian in mixture $P$. The MMD approximation results are shown in Fig. 4. We use the relative difference between exact (biased and unbiased) MMD and the approximation to quantify the error. The absolute difference also exhibits similar behavior and is thus not shown due to space limit. The results are presented as averages from 1000 trials. As can be seen, as $L$ increases, both FastMMD-Fourier and FastMMD-Fastfood converge quickly to exact MMD in both biased and unbiased cases. Their performance are indistinguishable. It can be easily observed that for both methods, the good approximation can be obtained even from a modest number of basis.

4.2. Accuracy Test

In some situations, MMD with a kernel family is preferred (Sriperumbudur et al., 2009). Here we present an exper-
Figure 4. MMD approximation errors of FastMMD with respect to number of basis function $L$. (a) biased MMD; (b) unbiased MMD.

The experiment that illuminates the superiority of our FastMMD methods on accuracy of MMD calculation. The synthesis data are generated as follows. All samples are constrained into a two-dimensional rectangle: $-5 \leq x_1, x_2 \leq 5$. The points, which are located within a circular ring in between by $x_1^2 + x_2^2 = 1$ and $x_1^2 + x_2^2 = 16$ are labeled as $+1$, while other points are labeled as $-1$. We generate 200 samples for each distribution randomly as the test set. Then we use these samples to calculate MMD for a kernel family. Here the kernel family includes multivariate isotropic Gaussians with bandwidth varying between 0.1 and 100, with a multiplicative step-size of $10^{1/5}$.

We compare our method with exact MMD, MMD-linear (Gretton et al., 2012a), and B-test (Zaremba et al., 2013). Note that the latter two methods are only valid for unbiased MMD. In our methods, the number of basis function $L$ is set as 1024. The block size in B-test is set to the default choice, i.e., the square of sample size $\sqrt{N}$. For our method, we repeat 1000 times and use the curves and error bars to represent means and standard deviations of MMD, respectively. Since both MMD-linear and B-test depend on the permutation of data samples, we make 1000 permutations of the samples. From Fig. 5, it can be seen that the means of all these methods are consistent with the true values. Also it can be seen that our FastMMD-Fourier and FastMMD-Fastfood have similar accuracy, and their deviations are much smaller than those of MMD-linear and B-test.

For some applications, we need to find the kernel that has the maximal MMD. Since our methods have lower variance, they incline to find the correct $\sigma$ with higher probability than MMD-linear and B-test.

4.3. Efficiency Test

In order to evaluate the efficiency of our methods, we generate samples uniformly from $[0, 0.95]^d$ and $[0.95, 1]^d$. The efficiency of different methods is shown in Fig. 6. In Fig. 6(a), the number of samples is varied from $10^3$ to $10^9$, and the data dimension $d$ is set as 16. In Fig. 6(b), the number of samples is set as $10^4$, and the dimension $d$ is varied from 8 to 1024.

Figure 5. MMD approximation for kernel family with different bandwidth $\sigma$. (a) biased MMD; (b) unbiased MMD; (c) standard deviations of approximated unbiased MMD in (b).

Figure 6. Efficiency comparison of different methods. Our methods have better scalability than the exact solution. (a) Fix $d = 16$ and $L = 128$, change number of samples $N$; (b) Fix $N = 10^4$ and $L = 8192$, change $d$. Note the axises are log-scale.

All competing methods are implemented in Matlab except that we use Spiral\(^1\) to perform the Fast Walsh-Hadamard transform. The comparison methods include exact MMD, MMD-linear and B-test\(^2\). We run all the codes on a PC with AMD Athlon X2 250 (800 MHz) CPU and 4 GB RAM memory.

From Fig. 6, we can see that when $N$ or $d$ varies from small to large, our methods gradually become more efficient than exact MMD and B-test. When $d = 16$ and $N = 10^3$, FastMMD-Fourier and FastMMD-Fastfood are 2000/5x and 4000/10x faster than exact MMD/B-test, respectively. As for MMD-linear, since it is the extreme simplified subsampling version of MMD calculation, it always

\(^1\)http://www.spiral.net/
\(^2\)https://github.com/wozaremba/btest
runs very fast. However, as the sample size or dimension increases, the computation times of our methods still depict a more slowly increase trend than that of MMD-linear. This empirically confirms the efficiency of the proposed Fast MMD methods.

4.4. Type II Error

Given MMD, several strategies can be employed to calculate the test threshold (Gretton et al., 2009; 2012a). The bootstrap strategy (Arcones & Giné, 1992) is utilized in our experiments since it can be easily integrated into our Fast-MMD method. Also the bootstrap is preferred for large-scale datasets since it costs $O(N^3 d)$, faster than most other methods for this task such as Person, with cost $O(N^3 d)$ (Gretton et al., 2012a).

The data used for this experiment is generated from Gaussian blob distributions as described in Section 4.1. The sample size is set as 1000 for two distributions. The bandwidth is selected by maximizing MMD. The selected bandwidth is $\sigma = 1$, and it approximately matches the scale of variance of each Gaussian blob in distribution $P$. We find that all of biased/unbiased FastMMD methods have similar good performance, and we thus only demonstrate the result of MMD-Fourier for biased MMD.

The level $\alpha$ for Type I error is set as 0.05. The Type II error is shown in Fig. 7. From Fig. 7(a), we can see that the Type II error drops quickly when increasing number of basis. It demonstrates empirically that increasing number of basis can decrease the Type II error. In Fig. 7(b), FastMMD have the same performance as exact MMD in this case.

$$\text{Figure 7. Type II error when using FastMMD-Fourier for biased MMD. (a) Fix } \epsilon = 4, \text{ change } L; \text{ (b) Fix } L = 1024; \text{ the ratio of variance eigenvalues is varied from 1.1 to 3.0. Average on 1000 trials.}$$

5. Conclusions

In this paper, we propose a method, called FastMMD, for efficiently calculating the maximum mean discrepancy (MMD) for shift-invariant kernels. Taking advantage of Fourier transform of shift-invariant kernels, we get a linear time complexity method. We prove the theoretical convergence of the proposed method in both unbiased and biased cases, and further present a geometric explanation for it. This explanation on one side delivers new insight for intrinsic MMD mechanism, and on the other side is hopeful to inspire more extensive new metrics for two-sample test, which will be investigated in our future research. Future work also includes finding the significance threshold using more efficient and effective strategies other than bootstrap.

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Appendix

A. Relationship between biased and unbiased estimate of MMD: The unbiased estimate of MMD is (See Lemma 6 in Gretton et al. (2012a))

$$\text{MMD}_{\epsilon}^{2}(\mathcal{F}, X_1, X_2) = \frac{1}{m(m-1)} \sum_{i \in I_1} \sum_{j \in I_1, j \neq i} K(x_i, x_j) + \frac{1}{n(n-1)} \sum_{i \in I_2} \sum_{j \in I_2, j \neq i} K(x_i, x_j) - \frac{2}{mn} \sum_{i \in I_1} \sum_{j \in I_2} K(x_i, x_j),$$

where $m = |I_1|, n = |I_2|$.

Denote $S_1 = \frac{1}{m^2} \sum_{i \in I_1} \sum_{j \in I_1} K(x_i, x_j)$, $S_2 = \frac{1}{n^2} \sum_{i \in I_2} \sum_{j \in I_2} K(x_i, x_j)$. If the kernel $K$ is shift-invariant, let $k_0 = K(0, 0) = K(x_i, x_i)$ for any $x_i$, and then we have

$$\text{MMD}_{\epsilon}^{2} = (\text{MMD}_{\epsilon}^{2} - S_1 - S_2) + \frac{m}{m-1} (S_1 - k_0/m) + \frac{n}{n-1} (S_2 - k_0/n) = \text{MMD}_{\epsilon}^{2} + \frac{1}{m-1} S_1 + \frac{1}{n-1} S_2 - \frac{m + n - 2}{(m-1)(n-1)} k_0.$$

Denote $\mu_1 = \frac{1}{m} \sum_{i \in I_1} \phi(x_i)$ and $\mu_2 = \frac{1}{n} \sum_{i \in I_2} \phi(x_i)$. The biased and unbiased estimate of MMD can be reformulated as:

$$\text{MMD}_{\epsilon}^{2} = \|\mu_1 - \mu_2\|_{\mathcal{F}}^2,$$

$$\text{MMD}_{\epsilon}^{2} = \|\mu_1 - \mu_2\|_{\mathcal{G}}^2 + \frac{1}{m-1} \|\mu_1\|_{2\mathcal{C}}^2 + \frac{1}{n-1} \|\mu_2\|_{2\mathcal{C}}^2 - \frac{m + n - 2}{(m-1)(n-1)} k_0.$$

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In this paper, we propose a method, called FastMMD, for efficiently calculating the maximum mean discrepancy (MMD) for shift-invariant kernels. Taking advantage of Fourier transform of shift-invariant kernels, we get a linear time complexity method. We prove the theoretical convergence of the proposed method in both unbiased and biased cases, and further present a geometric explanation for it. This explanation on one side delivers new insight for intrinsic MMD mechanism, and on the other side is hopeful to inspire more extensive new metrics for two-sample test, which will be investigated in our future research. Future work also includes finding the significance threshold using more efficient and effective strategies other than bootstrap.

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where $m = |I_1|, n = |I_2|$.

Denote $S_1 = \frac{1}{m^2} \sum_{i \in I_1} \sum_{j \in I_1} K(x_i, x_j)$, $S_2 = \frac{1}{n^2} \sum_{i \in I_2} \sum_{j \in I_2} K(x_i, x_j)$. If the kernel $K$ is shift-invariant, let $k_0 = K(0, 0) = K(x_i, x_i)$ for any $x_i$, and then we have

$$\text{MMD}_{\epsilon}^{2} = (\text{MMD}_{\epsilon}^{2} - S_1 - S_2) + \frac{m}{m-1} (S_1 - k_0/m) + \frac{n}{n-1} (S_2 - k_0/n) = \text{MMD}_{\epsilon}^{2} + \frac{1}{m-1} S_1 + \frac{1}{n-1} S_2 - \frac{m + n - 2}{(m-1)(n-1)} k_0.$$
We then have
\[
\mathbb{E}_{Q,P_1} \sin(Y - X_1) - \mathbb{E}_{Q,P_2} \sin(Y - X_2) = \int \int q(y)p_1(x) \sin(y - x) \, dx \, dy - \int \int q(y)p_2(x) \sin(y - x) \, dx \, dy
\]
\[
= \int q(y) \left[ \sum_{i=1}^{N} a_i \sin(x_i - y) \right] \, dy.
\]
Since \(q(y) \geq 0\) and \(\int q(y) \, dy = 1\), the maximum of the previous expression with respect to all possible \(q(y)\) is
\[
\sup_y \int (p_1(x) - p_2(x)) \sin(y - x) \, dx.
\]
If \(p_1(x) - p_2(x) = \sum_{i=1}^{N} a_i \delta(x - x_i)\), then
\[
\int (p_1(x) - p_2(x)) \sin(y - x) \, dx = \sum_{i=1}^{N} a_i \sin(y - x_i) = A \sin(y - \theta).
\]
The second equation holds because the sum of sinusoids with the same frequency is also a sinusoid with that frequency. According to the trigonometric identity, it holds that
\[
A = \sqrt{\sum_{i=1}^{N} \sum_{j=1}^{N} a_i a_j \cos(x_i - x_j)},
\]
\[
\theta = \text{atan2} \left( \sum_{i=1}^{N} a_i \sin x_i, \sum_{i=1}^{N} a_i \cos x_i \right),
\]
where \text{atan2} is the four-quadrant arctangent function. The supremum of this problem is \(A\) when \(y = \theta\).

References


