A Fast and Effective Large-Scale Two-Sample Test Based on Kernels

Hoseung Song and Hao Chen
Department of Statistics, University of California, Davis

Abstract

Kernel two-sample tests have been widely used and the development of efficient methods for high-dimensional large-scale data is gaining more and more attention as we are entering the big data era. However, existing methods, such as the maximum mean discrepancy (MMD) and recently proposed kernel-based tests for large-scale data, are computationally intensive to implement and/or ineffective for some common alternatives for high-dimensional data. In this paper, we propose a new test that exhibits high power for a wide range of alternatives. Moreover, the new test is more robust to high dimensions than existing methods and does not require optimization procedures for the choice of kernel bandwidth and other parameters by data splitting. Numerical studies show that the new approach performs well in both synthetic and real world data.

Keywords: High-dimensional data, Permutation null distribution, General alternatives, Nonparametrics, Block averaging
1 Introduction

1.1 Background

Two-sample hypothesis testing plays a significant role in a variety of scientific applications, such as bioinformatics, social sciences, and image analysis (Fox and Dimmic 2006; Osborne et al. 2013; Kohout and Pevný 2017). As we entering the big data era, high-dimensional and large-scale data is becoming prevalent, particularly in machine learning and deep learning applications, and the attention to the two-sample testing method for large-scale data is also naturally increasing (Sutherland et al. 2016; Grosse et al. 2017; Carlini and Wagner 2017; Gao et al. 2020).

Formally speaking, given two samples $X_1, X_2, \ldots, X_m \overset{iid}{\sim} P$ and $Y_1, Y_2, \ldots, Y_n \overset{iid}{\sim} Q$ where $P$ and $Q$ are distributions in $\mathbb{R}^d$, we consider testing the null hypothesis $H_0: P = Q$ against $H_1: P \neq Q$. Classical approaches focused on univariate data (Kolmogorov 1933; Wald and Wolfowitz 1940; Mann and Whitney 1947). In the multivariate setting, there are many parametric methods (Bai and Saranadasa 1996; Schott 2007; Srivastava and Du 2008; Srivastava and Yanagihara 2010), but they are confined by model assumptions. Nonparametric approaches are more flexible and several tests have been proposed utilizing the rank (Baumgartner et al. 1998; Hettmansperger et al. 1998; Rousson 2002; Oja 2010), interpoint distances (Székely and Rizzo 2013; Biswas and Ghosh 2014), graphs (Friedman and Rafsky 1979; Schilling 1986; Rosenbaum 2005; Chen and Zhang 2013; Chen and Friedman 2017; Chen et al. 2018; Zhang and Chen 2017), ball divergence (Pan et al. 2018), and classifiers (Lopez-Paz and Oquab 2016; Hediger et al. 2019; Liu et al. 2020; Kirchler et al. 2020). In this paper, we focus on kernel two-sample tests, and some of the aforementioned state-of-the-arts tests will be included for comparison in numerical studies.

1.2 A kernel two-sample test

As a nonparametric framework, kernel two-sample tests have been widely used in real data (Liu et al. 2020; Wynne and Duncan 2020). The most well-known kernel two-sample test was proposed by Gretton et al. (2007). Given a kernel $k(\cdot, \cdot)$, the test is based on the
maximum mean discrepancy (MMD), which is the difference between expected features of \( P \) and \( Q \) in a reproducing kernel Hilbert space (RKHS):

\[
\text{MMD}^2(P, Q) = E_{X,X'}[k(X, X')] - 2E_{X,Y}[k(X, Y)] + E_{Y,Y'}[k(Y, Y')],
\]

where \( X \) and \( X' \) are independent random variables drawn from \( P \) and \( Y \) and \( Y' \) are independent random variables drawn from \( Q \).

An unbiased estimate of \( \text{MMD}^2 \) was considered by Gretton et al. (2007):

\[
\text{MMD}^2_u = \frac{1}{m(m-1)} \sum_{i=1}^{m} \sum_{j=1, j \neq i}^{m} k(X_i, X_j) + \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j=1, j \neq i}^{n} k(Y_i, Y_j)
- \frac{2}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} k(X_i, Y_j)
\triangleq \alpha + \beta - 2\gamma.
\]

Here, \( \alpha \) and \( \beta \) represent the average of within-sample kernel values and \( \gamma \) represents the average of between-sample kernel values. When the kernel \( k \) is characteristic, such as the Gaussian kernel or the Laplacian kernel, the MMD behaves as a metric (Sriperumbudur et al., 2010).

Gretton et al. (2007, 2009, 2012a) proposed testing methods based on the asymptotic behaviors of MMD. Gretton et al. (2012b) and Ramdas et al. (2015) studied the choice of the kernel and its bandwidth, and revealed that the performance of the test using Gaussian kernel is independent of the bandwidth as long as the median heuristic, the median of all pairwise distances among observations, is used as the kernel bandwidth.

1.3 Fast kernel two-sample tests and their limitations

Although MMD works well under some settings, it costs \( O(N^2) \) to compute the kernel values for the \( N = m + n \) samples and it is computationally intensive when \( N \) is large. Furthermore, MMD degenerates under the null hypothesis of equal distribution and a few approaches proposed by Gretton et al. (2007, 2009) to approximate the limiting null distribution have some limitations. This low efficiency is problematic since modern scientific applications increasingly deal with large-scale data. To address this, several solutions have
been proposed. Unfortunately, all these approaches have some drawbacks and they are still time-consuming to implement.

1.3.1 MMD-based work

Gretton et al. (2012a) proposed a linear version of MMD, which is a running average over independent pairs of two samples. This approach is computationally more efficient than MMD and its null distribution is also straightforward to compute as a Gaussian distribution. However, there is a trade-off between the computation time and the performance of the test, and it tends to show low test power for finite $N$ due to the increase in the variance of the test statistic.

To balance the test power and the computational cost, Zaremba et al. (2013) considered a block averaging version of MMD that achieves higher test power than the linear version of MMD with a small increase in computation complexity. However, the median heuristic does not work since the median cannot capture the main data variation by perturbations (Gretton et al., 2012b). Hence, one needs to find a suitable kernel bandwidth to guarantee the performance of the test, which increases the time cost.

In addition, both tests only work for the balanced sample design, i.e, the sample sizes of the two samples are the same.

1.3.2 Tests based on differences in expectations at spatial or frequency locations

Recently, Chwialkowski et al. (2015) developed two tests with a cost linear in the sample size. They demonstrated that the distance between mean embeddings in RKHS can be evaluated sufficiently at a finite number of randomly chosen test locations. Based on the differences in the analytic representations of distributions, they proposed two linear time two-sample tests, ME test and SCF test. ME test uses the test statistic defined as $n\bar{z}^T S^{-1} \bar{z}$ when $m = n$, where $\bar{z} = \frac{1}{n} \sum_{i=1}^{n} z_i$, $S = \frac{1}{n-1} \sum_{i=1}^{n} (z_i - \bar{z})(z_i - \bar{z})^T$, and $z_i = (k(x_j, v_j) - k(y_j, v_j))_{j=1}^{J} \in \mathcal{R}^J$. The test statistic depends on a set of $J$ test locations $v_j \in \mathcal{R}^d$ for $j = 1, \ldots, J$ and they are arbitrarily chosen. The SCF test uses the test
statistic that has the same form as the ME test statistic with the modified $z_i$ using Fourier transform.

Later, Jitkrittum et al. (2016) extended the approaches in Chwialkowski et al. (2015) and proposed to optimize the test locations and the kernel bandwidth by maximizing a lower bound of the test power. This approach significantly improves the performance of the test with the linear complexity. However, parameters, such as test locations and the kernel bandwidth, should be optimized and these procedures take a lot of time. Specifically, the data has to be split in two sets to learn and this also may lead to a potential loss of power due to a smaller test sample size.

In addition, the test statistics are occasionally not well-defined since $S$ in the test statistics is not invertible and all these approaches only work for the balanced sample design.

### 1.4 Our contribution

In this paper, we develop a fast and effective kernel-based test for high-dimensional large-scale data and provide the asymptotic distribution of the new test statistic, offering easy off-the-shelf tools for large datasets. The main contributions of this paper are summarized below:

- The new approach does not need to resort to the cumbersome procedures, such as optimization procedures for the kernel bandwidth or other parameters by data splitting and grid search, making the new test much faster and more efficient than the existing tests.

- We conduct numerical studies and demonstrate that the new method is more versatile and powerful for a wide range of alternatives in both synthetic and real world data.

- Unlike other fast kernel methods that require the two samples to have the same sample size, the new test statistic can be applied to the unbalanced sample design.

The organization of the paper is as follows. The new test is proposed and discussed in Section 2. Section 3 examines the performance of the new test under various simulation
settings. The new approach is illustrated by real data applications in Section 4. We discuss a few other block approaches along the same line in Section 5 and conclude in Section 6.

2 A new test

The new test statistics build on the block averaging approach with MMD proposed by Zaremba et al. (2013). This block averaging approach was originally proposed in Ho and Shieh (2006). This approach was also utilized in computational chemistry (Kent IV et al., 2007; Grossfield and Zuckerman, 2009).

To achieve a balance between the computational time and the performance of the test, Zaremba et al. (2013) proposed to use the block size $\sqrt{m}$ and this leads to the sub-quadratic time test. However, they proposed the same block sizes for two samples, which is only applicable to the balanced sample design, and this approach also leads to a potential loss of power due to wasted observations (see Section 5). In order for the new test to handle unbalanced sample sizes, we allow the block sizes to be different for the two samples: we split the data into blocks of different sizes for X-sample and Y-sample. Specifically, we define the number of blocks as $b = \left\lceil \sqrt{(m + n)/2} \right\rceil$ and the corresponding block sizes as $[m/b]$ for $X$-sample and $[n/b]$ for $Y$-sample if $b$ is divisible by $m$ and $n$. If $b$ is not divisible by $m$ or $n$, we could let some of the blocks having $[m/b] + 1$ or $[n/b] + 1$ observations so as to make fully use of the observations. Explicitly, let $B_{1,i}$, $B_{2,i}$ be the block size of the $i$th block for $X$-sample and $Y$-sample, respectively, and $r_x = m - b[m/b]$, $r_y = n - b[n/b]$. Then, for $i = 1, \ldots, b$,

$$B_{1,i} = \begin{cases} 
[m/b] & \text{for } i = 1, \ldots, b - r_x, \\
[m/b] + 1 & \text{for } i = b - r_x + 1, \ldots, b,
\end{cases}$$

$$B_{2,i} = \begin{cases} 
[n/b] & \text{for } i = 1, \ldots, b - r_y, \\
[n/b] + 1 & \text{for } i = b - r_y + 1, \ldots, b.
\end{cases}$$

We build upon core statistics proposed in Song and Chen (2020) that can cover more

\[^1[x]\] denotes the largest integer that is no larger than $x$. 

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1[^1]
types of alternatives than MMD. In particular, two statistics are defined as follows:

\[ W_i = \frac{B_{1,i}}{B_i} \alpha_i + \frac{B_{2,i}}{B_i} \beta_i, \]

\[ D_i = B_{1,i}(B_{1,i} - 1)\alpha_i - B_{2,i}(B_{2,i} - 1)\beta_i, \]

for \( i = 1, \ldots, b \) where \( B_i = B_{1,i} + B_{2,i} \). Here, \( \alpha_i \) and \( \beta_i \) are the block version of \( \alpha \) and \( \beta \), respectively, computed in each block. It is expected that \( W_i \) tends to be sensitive to location alternatives and \( D_i \) tends to be sensitive to scale alternatives.

We adopt the permutation distribution as the null distribution, which places \( \frac{1}{(B_i)} \) probability on each of the \( (B_i) \) choices of \( B_{1,i} \) out of the total \( B_i \) observations as the \( X \)-sample for each block and similarly for each block of \( Y \)-sample. The approach in Zaremba et al. (2013) suffers from the choice of a suitable bandwidth in kernels and there is no specific strategy for this. As discussed in Gretton et al. (2012b), the main data variation captured by the median heuristic differs from the lengthscales of the difference between two distributions \( P \) and \( Q \). However, under the permutation null distribution, the median heuristic seems to be a reasonable choice (see Section 3.3 for more discussions).

The standardized statistics for (2) and (3) are defined as follows:

\[ Z_{W,i} = \frac{W_i - E(W_i)}{\sqrt{\text{Var}(W_i)}}, \]

\[ Z_{D,i} = \frac{D_i - E(D_i)}{\sqrt{\text{Var}(D_i)}}, \]

for \( i = 1, \ldots, b \) where \( E(W_i) \), \( \text{Var}(W_i) \), \( E(D_i) \), and \( \text{Var}(D_i) \) are the expectations and variances of \( W_i \) and \( D_i \), respectively, under the permutation null distribution. Their analytic expressions are provided in Lemma 2.1. Figure 1 illustrates the formulation of the new test statistic.

For pooled observations \( z_1^{(i)}, \ldots, z_{B_i}^{(i)} \) in \( i \)-th block \( (i = 1, \ldots, b) \), \( \alpha_i \) and \( \beta_i \) can be rewritten as

\[ \alpha_i = \frac{1}{B_{1,i}(B_{1,i} - 1)} \sum_{u=1}^{B_i} \sum_{v=1, v \neq u}^{B_i} k(z_u^{(i)}, z_v^{(i)}) I_{g_u^{(i)} = g_v^{(i)} = 0}, \]

\[ \beta_i = \frac{1}{B_{2,i}(B_{2,i} - 1)} \sum_{u=1}^{B_i} \sum_{v=1, v \neq u}^{B_i} k(z_u^{(i)}, z_v^{(i)}) I_{g_u^{(i)} = g_v^{(i)} = 1}, \]
where \( g_u^{(i)} = 0 \) if observation \( z_u^{(i)} \) is from sample \( X \) and \( g_u^{(i)} = 1 \) if observation \( z_u^{(i)} \) is from sample \( Y \) in \( i \)-th block.

**Lemma 2.1.** Let \( k_{uv}^{(i)} = k(z_u^{(i)}, z_v^{(i)}) \) for \( i = 1, \ldots, b \). Under the permutation null, we have

\[
\begin{align*}
E(\alpha_i) &= E(\beta_i) = \frac{1}{B_i(B_i - 1)} R_0^{(i)}, \\
\text{Var}(\alpha_i) &= \frac{1}{B_{1,i}(B_{1,i} - 1)^2} \left( 2R_1^{(i)}p_{1,i} + 4R_2^{(i)}p_{2,i} + R_3^{(i)}p_{3,i} \right) - E(\alpha_i)^2, \\
\text{Var}(\beta_i) &= \frac{1}{B_{2,i}(B_{2,i} - 1)^2} \left( 2R_1^{(i)}q_{1,i} + 4R_2^{(i)}q_{2,i} + R_3^{(i)}q_{3,i} \right) - E(\beta_i)^2, \\
\text{Cov}(\alpha_i, \beta_i) &= \frac{R_3^{(i)}}{B_i(B_i - 1)(B_i - 2)(B_i - 3)} - E(\alpha_i)E(\beta_i),
\end{align*}
\]

where

\[
\begin{align*}
R_0^{(i)} &= \sum_{u=1}^{B_i} \sum_{v=1, v \neq u}^{B_i} k_{uv}^{(i)}, \\
R_1^{(i)} &= \sum_{u=1}^{B_i} \sum_{v=1, v \neq u}^{B_i} (k_{uv}^{(i)})^2, \\
R_2^{(i)} &= \sum_{u=1}^{B_i} \sum_{v=1, v \neq u}^{B_i} \sum_{r=1, r \neq v, r \neq u}^{B_i} k_{uv}^{(i)}k_{ur}^{(i)}, \\
R_3^{(i)} &= \sum_{u=1}^{B_i} \sum_{v=1, v \neq u}^{B_i} \sum_{r=1, r \neq v, r \neq u}^{B_i} \sum_{s=1, s \neq r, s \neq v, s \neq u}^{B_i} k_{uv}^{(i)}k_{ur}^{(i)} k_{rs}^{(i)},
\end{align*}
\]

with

\[
\begin{align*}
p_{1,i} &= \frac{B_{1,i}(B_{1,i} - 1)}{B_i(B_i - 1)}, \\
p_{2,i} &= \frac{B_{1,i}(B_{1,i} - 1)(B_{1,i} - 2)}{B_i(B_i - 1)(B_i - 2)}, \\
p_{3,i} &= \frac{B_{1,i}(B_{1,i} - 1)(B_{1,i} - 2)(B_{1,i} - 3)}{B_i(B_i - 1)(B_i - 2)(B_i - 3)},
\end{align*}
\]
\[ q_{1,i} = \frac{B_{2,i}(B_{2,i} - 1)}{B_i(B_i - 1)}, \quad q_{2,i} = \frac{B_{2,i}(B_{2,i} - 1)(B_{2,i} - 2)}{B_i(B_i - 1)(B_i - 2)}, \quad q_{3,i} = \frac{B_{2,i}(B_{2,i} - 1)(B_{2,i} - 2)(B_{2,i} - 3)}{B_i(B_i - 1)(B_i - 2)(B_i - 3)}. \]

This lemma follows from Song and Chen [2020] straightforwardly.

Given the new test statistics, the next step is to calibrate how large the test statistics need to provide sufficient evidence to reject the null hypothesis. The classical central limit theorem (CLT) usually can be used for the block averaging approaches as in Zaremba et al. [2013]. However, the new test statistics \( Z_{W,i} \)'s are independent variables with respect to \( i \), but not identically distributed under the permutation null distribution. And a similar situation \( Z_{D,i} \)'s. Hence, we use the Lyapunov central limit theorem to handle the dependencies.

We write \( x_b = o(y_b) \) when \( x_b \) is dominated by \( y_b \) asymptotically, i.e., \( \lim_{b \to \infty} \frac{x_b}{y_b} = 0 \).

By the Lyapunov central limit theorem, as \( b \to \infty \),

- \( \sqrt{b} \bar{Z}_W \to N(0, 1) \) when \( \sum_{i=1}^{b} E|Z_{W,i}|^3 = o(b^{1.5}) \),
- \( \sqrt{b} \bar{Z}_D \to N(0, 1) \) when \( \sum_{i=1}^{b} E|Z_{D,i}|^3 = o(b^{1.5}) \).

For the two conditions, they are satisfied if \( E|Z_{W,i}|^3, E|Z_{D,i}|^3 = o(\sqrt{B_i}) \), which are mild conditions as \( Z_{W,i} \)'s and \( Z_{D,i} \)'s are standardized statistics with mean 0 and variance 1. To see how the normal approximations work for finite samples, we check the normal quantile-quantile plots of \( \bar{Z}_W \) and \( \bar{Z}_D \). Figure 2 shows the plots with Gaussian data under different choices of \( m \) and \( n \) when \( d = 100 \). We see that the asymptotic null distributions kick in for relatively small \( m \) and \( n \)’s.

To combine the advantages of the two statistics based on the asymptotic results, we propose to use a Bonferroni test on \( \bar{Z}_W \) and \( \bar{Z}_D \). Let \( p_W \) and \( p_D \) be the approximated \( p \)-values of the test that rejects for large values of \( \sqrt{b} \bar{Z}_W \) or \( \sqrt{b} |\bar{Z}_D| \), respectively, based on their limiting distributions. Then, the proposed test rejects the null if \( 2 \min(p_D, p_W) \) is less than the significance level.

Remark 2.2. Other global testing methods, such as the Simes procedure, might also be considered. Here, \( \bar{Z}_W \) and \( \bar{Z}_D \) are dependent, so it is hard to show the exact level of global testing for the Simes procedure. We observe that \( p_W \) tends to be small under the location alternatives and \( p_D \) tends to be small under the scale alternatives. Thus, the Bonferroni correction does not introduce too much conservativeness.
3 Experiments

In this section, we examine the performance of the new test under diverse settings through simulations. We first focus on the existing fast kernel two-sample tests and compare them for Gaussian data under Python (Section 3.1). In Section 3.2, we compare the new test with other state-of-the-art nonparametric two-sample tests for non-Gaussian data under R. We also briefly check the performance of the new test on different choices of the bandwidth in Section 3.3.

3.1 Simulation I

We compare the new test with the existing fast kernel two-sample tests proposed by Zaremba et al. (2013) and Jitkrittum et al. (2016). We denote the proposed test in Zaremba et al. (2013) by MMD-B and two tests in Jitkrittum et al. (2016) by ME-full and SCF-full, respectively. We also consider the Hotelling’s $T^2$ test as a baseline. We use the Gaussian
kernel for all tests. For ME-full and SCF-full, the bandwidth of Gaussian kernel and test locations are fully optimized on a training sample. For a fair comparison, the bandwidth of Gaussian kernel used in MMD-B is also optimized by a grid search, while the median heuristic is used in the new test. An implementation of the existing methods is available at [https://github.com/wittawatj/interpretable-test](https://github.com/wittawatj/interpretable-test) provided in Jitkrittum et al. (2016).

Here, we follow the simulation setup in Jitkrittum et al. (2016) for the comparison between the test power and sample size \((m = n)/\text{dimension} (d)\). In addition, we check the computational cost of the tests. The number of test locations \(J\) is set to be 5 for ME-full and SCF-full and the significance level is set to be 0.01 for all the experiments.

Table 1: Three toy problems.

| Data | \(P\) | \(Q\) |
|------|------|------|
| GMD  | \(N_d(\mathbf{0}_d, I_d)\) | \(N_d((0.8, 0, \ldots, 0)^T, I_d)\) |
| GVD  | \(N_d(\mathbf{0}_d, I_d)\) | \(N_d(\mathbf{0}_d, \text{diag}(2, 1, \ldots, 1))\) |
| NULL | \(N_d(\mathbf{0}_d, I_d)\) | \(N_d(\mathbf{0}_d, I_d)\) |

3.1.1 Test power vs. sample size \(m\)

We study how the sample size affects test powers and type I error and we consider three settings in Table 1: GMD (location shift), GVD (scale shift), and NULL (no shift). For each sample size, we simulate 500 datasets.

The results are shown in Figure 3 where test powers (GMD and GVD) and type I error (NULL) are plotted against sample sizes. We see that the new test is comparable to the existing tests for the mean difference in distributions. However, the new approach achieves higher power than the existing methods for the variance difference in distributions. The new test also controls the type I error rate well.
3.1.2 Test power vs. dimension $d$

We next study how the dimension of the problem affects the test power and the type I error. Here, we fix the sample size to 10,000 and we simulate 500 datasets for each dimension. The results are presented in Figure 4. We observe that the new test in general dominates in power when two samples differ in both the mean and the variance. This implies that the new test is robust to high dimensions for a wide range of problems, particularly for the scale alternatives. The new test also controls the type I error rate well.
3.1.3 Computational time

In addition, we compare the computational cost of the tests. The one of required properties of the test for large-scale data is the computation time. We check runtimes of the tests for Gaussian data under various $m = n$. All experiments were run by Python on 2.2 GHz Intel Core i7.

Table 2: Average runtimes in seconds from 10 simulations for each sample size $m = n$ when $d = 100$.

| $m = n$ | New  | ME-full | SCF-full | MMD-B |
|---------|------|---------|----------|-------|
| 6000    | 0.179| 10.97   | 31.93    | 2.235 |
| 7000    | 0.194| 12.90   | 34.86    | 2.920 |
| 8000    | 0.205| 13.22   | 40.58    | 3.585 |
| 9000    | 0.249| 15.03   | 49.61    | 3.805 |
| 10000   | 0.267| 20.46   | 54.70    | 4.423 |

Table 2 shows average runtimes for each sample size $m = n$ when $d = 100$. We see that the new approach is the fastest among the existing methods. Although ME-full and SCF-full are linear time tests, they are more computationally expensive than sub-quadratic tests MMD-B and the new test due to the parameter tuning procedures. This crucial drawback makes the existing test computationally inhibitive for large-scale data. This problem would become more severe when the dimension is higher.

3.1.4 Summary

For the existing tests, MMD-B has low power for scale alternatives. The power of SCF-full decreases fast as the dimension increases. The power of ME-full decreases fast as the dimension increases under scale alternatives. The new test is effective for a wide range of testing problems and significantly fast for large-scale data.
3.2 Simulation II

Here, we compare the new test with other state-of-the-art nonparametric two-sample tests: graph-based test (GT) (Chen and Friedman, 2017), ball divergence test (BT) (Pan et al., 2018), and classifier two-sample test (CT) (Lopez-Paz and Oquab, 2016). We consider the multivariate log-normal data: \( \exp(N_d(0_d, \Sigma)) \) vs. \( \exp(N_d(a1_d, \Sigma)) \), where \( \Sigma_{i,j} = 0.4^{|i-j|} \). GT, BT, and CT are publicly available in R packages gTests, Ball, and Ecume, respectively. We simulate 500 datasets and the significance level is set to be 0.01 for all the experiments.

3.2.1 Test power vs. sample size \( m/dimension \ d \)

We study how the sample size and the dimension affect test powers and type I error. Here, alternatives in log-normal data yield the changes in both the mean and variance of distributions. The results are shown in Figure 5. We set \( a = 0.03 \), \( a = 0.02 \), and \( a = 0 \) in the left, middle, and right pannel, respectively. We see that the new test exhibit high power for different sample sizes and dimensions, and perform well for asymmetric distributions under moderate to high sample sizes and dimensions. GT and CT perform poorly and they are not sensitive to capturing differences in distributions. Although BT performs well, it is infeasible to use for large-scale data due to computation time (see Section 3.2.2).

![Figure 5: Plots of test power and type I error.](image-url)
3.2.2 Computational time

We compare the computation time of the tests using R on 2.2 GHz Intel Core i7 under various \( m = n \) (Table 3). We see that the new test is the fastest among the existing tests implemented by R. Although BT shows good performance in testing, it takes a long time to run and it is not useful for large-scale data. GT is faster than other existing tests, but R blows up due to the memory issue storing the graph when the sample size is large.

Table 3: Average runtimes in seconds from 10 simulations for each sample size \( m = n \) when \( d = 100 \).

| \( m = n \) | New | GT     | BT   | CT     |
|----------|-----|--------|------|--------|
| 6000     | 0.485 | 80.04  | >2000| 73.20  |
| 7000     | 0.609 | 106.94 | >2000| 116.30 |
| 8000     | 0.748 | -      | >2000| 200.12 |
| 9000     | 0.916 | -      | >2000| 165.23 |
| 10000    | 1.119 | -      | >2000| 238.70 |

3.3 Simulation III

In this section, we briefly check whether the median heuristic is reasonable for the new test through numerical studies. We use Gaussian data \( N_d(0, I_d) \) vs. \( N_d(\mu, \sigma^2 I_d) \) with \( \Delta = \| \mu \|_2 \), and examine the average median heuristic in each setting by 100 trials. The averaged median heuristic is around 10 when \( d = 100 \) and 14 when \( d = 200 \) in our settings. So we choose 8 bandwidths that differ by 2 from each other, starting from the averaged median heuristic -8 to the averaged median heuristic +8 in order to check bandwidths in a wide range. We use 10,000 samples from each distribution and check the performance of the new test for each bandwidth choice under six different settings at 0.05 significance level (Figure 6).

We see that the new test controls the type I error well and there is no significant difference in the performance unless the bandwidth is too small. This result coincides with
our conjecture in that the main data variation captured by the median heuristic reflects the difference between $P$ and $Q$ relatively well under the permutation null distribution. So we use the median heuristic for the proposed test.

4 Real data examples

4.1 Age dataset

We now demonstrate the new test on real data, using the age dataset, namely the IMDb-WIKI database (Rothe et al., 2018) (Figure 7). This dataset is publicly available at [https://data.vision.ee.ethz.ch/cvl/rrothe/imdb-wiki/](https://data.vision.ee.ethz.ch/cvl/rrothe/imdb-wiki/) It consists of 397,949 images of 19,545 celebrities with corresponding age labels, where $d = 4096$. Here, we follow
the preprocessing of Law et al. (2018), and construct two groups according to the celebrity’s age label. For example, let 10-15 represent the images where the celebrity’s age label is between 10 and 15.

One problem for such large-scale datasets is that it is difficult to apply the existing kernel two-sample tests to determine whether the two samples are different or not. For example, the 15-20 age group consists of 16,282 images and the 20-25 age group has 39,957 images. Due to this large number of samples, it is computationally expensive for most existing tests. Table 4 shows the computation time of the tests on 2.2 GHz Intel Core i7. We see that ME-full and SCF-full are too slow to obtain the test results. Although MMD-B is faster than ME-full and SCF-full, the test result would be unreliable due to lower power than ME-full and SCF-full (see Section 3). On the other hand, the new test is still very fast with good performance.

Table 4: Runtimes in seconds for the image dataset.

|                | New | ME-full | SCF-full | MMD-B |
|----------------|-----|---------|----------|-------|
| 15-20 vs 20-25 | 1.641 | >3000   | >3000    | 48.19 |

To illustrate how well the tests distinguish age groups, we conduct the testing procedures on subsets of the whole data so that ME-full and SCF-full are applicable. We randomly select 500 images from each group and repeat 500 times for each experiment. Since this dataset has a lot of noise, we set the significance level to be 0.001.

The power of the tests is shown in Table 5. Since this dataset has pretty strong signals, all tests can tell the difference between two age groups easily. However, the existing tests cannot capture the difference well in some cases. For example, SCF-full has 0 power in comparing the 30-35 and 35-40 age groups. MMD-B has low power in comparing 35-40 vs. 40-45 and 40-45 vs. 45-50. On the other hand, the new test consistently has high power in all these comparisons.
Table 5: Estimated power of the tests for the age dataset using subsets.

| Problem     | New | ME-full | SCF-full | MMD-B |
|-------------|-----|---------|----------|-------|
| 15-20 vs 20-25 | 1.00 | 1.00    | 1.00     | 1.00  |
| 20-25 vs 25-30 | 1.00 | 1.00    | 1.00     | 0.80  |
| 25-30 vs 30-35 | 0.99 | 1.00    | 0.99     | 0.79  |
| 30-35 vs 35-40 | 1.00 | 1.00    | 0.00     | 0.83  |
| 35-40 vs 40-45 | 0.95 | 0.99    | 0.96     | 0.25  |
| 40-45 vs 45-50 | 0.93 | 0.73    | 0.85     | 0.40  |

4.2 Eye movement

In this experiment, we examine how well the new test can distinguish samples of eye movement patterns (Salojärvi et al., 2005). A subject was shown questions and asked to choose a sentence in a list of sentences consisting of the correct answer (C), relevant sentences for the question (R), and irrelevant sentences for the question (I). In each case, 22 features are obtained and these features are commonly used in psychological studies on eye movement. The dataset is publicly available at [https://www.openml.org/d/1044](https://www.openml.org/d/1044).

Since this dataset consists of around 3000 samples (I: 3,804, R: 4,262, C:2,870) with low dimension, we focus more on the performance of the tests. We first conduct two-sample testing for the whole data to determine whether each group is different or not. Since only the new test can be applied to the unbalanced sample design, we draw the number of samples in the group with the smaller sample from the other group in each comparison. The results are shown in Table 6. We see that the new test and MMD-B reject all cases at 0.001 significance level. However, SCF-Full is not significant for the two comparisons, I vs. R and I vs. C, and also not significant for R vs. C at 0.001 significance level. ME-full is not significant for the comparison I vs. R.

We investigate the test statistics in more detail for this comparison. Table 7 shows $p$-values of the new test statistics. We see that most $p$-values are almost zero, but $p$-value of $\bar{Z}_D$ for the case I vs. R is very large (0.460). This implies that the mean difference is
Table 6: \( p \)-values for the eye movement dataset.

| Problem | New  | ME-full | SCF-full | MMD-B |
|---------|------|---------|----------|-------|
| I vs. R | 0.000| 0.197   | 0.516    | 0.000 |
| I vs. C | 0.000| 0.000   | 0.800    | 0.000 |
| R vs. C | 0.000| 0.000   | 0.013    | 0.000 |

mainly significant for the case I vs. R, while both the mean and the variance differences are significant for the other two cases. When the mean mainly differs (I vs. R), the new test captures this signal, while ME-full and SCF-full cannot capture this signal. MMD-B also captures this signal since MMD is very sensitive to the mean change (seearguement in Song and Chen (2020)). Indeed, Salojärvi et al. (2005) carried out linear discriminant analysis with the visualization to obtain a classification result and revealed that relevant and irrelevant sentences are relatively harder to separate than the other two cases.

Table 7: \( p \)-values of the new test statistics.

| p-values | \( \bar{Z}_W \) | \( \bar{Z}_D \) |
|----------|-----------------|-----------------|
| I vs. R  | 0.000           | 0.460           |
| I vs. C  | 0.000           | 0.000           |
| R vs. C  | 0.000           | 0.000           |

For the two cases that most tests are significant (I vs. C and R vs. C), we also examine the performance of the tests using the subsets of the whole data. For each sample size, we generate 1,000 randomly selected subsets of the whole data and the significance level is set to be 0.001 for all tests. The results are shown in Table 8. We see that SCF-full has no power and MMD-B shows lower power than the new test in all cases. ME-full exhibits higher power than SCF-full and MMD-B, but it is in general outperformed by the new test.
Table 8: Estimated power of the tests for the eye movement dataset using subsets.

|       | I vs. C |       |
|-------|---------|-------|
| $m = n$ | New | ME-full | SCF-full | MMD-B |
| 100   | 0.826 | 0.561 | 0.003 | 0.374 |
| 200   | 0.998 | 0.865 | 0.002 | 0.850 |
| 300   | 1.000 | 0.943 | 0.002 | 0.985 |
| 400   | 1.000 | 0.993 | 0.000 | 1.000 |

|       | R vs. C |       |
|-------|---------|-------|
| $m = n$ | New | ME-full | SCF-full | MMD-B |
| 100   | 0.670 | 0.538 | 0.002 | 0.236 |
| 200   | 0.969 | 0.701 | 0.000 | 0.685 |
| 300   | 0.999 | 0.987 | 0.000 | 0.941 |
| 400   | 1.000 | 1.000 | 0.002 | 0.988 |

5 Discussion

In this section, we briefly discuss some other blocking approaches along the same line as $b$, $B_1$, and $B_2$.

- **Approach 1 (A1):** $B_1 = \left[ \frac{m}{\sqrt{m}} \right]$, $B_2 = \left[ \frac{n}{\sqrt{n}} \right]$, $b = \min(\left[ \frac{m}{B_1} \right], \left[ \frac{n}{B_2} \right])$.

- **Approach 2 (A2):** $B_1 = \left[ \frac{m}{b} \right]$, $B_2 = \left[ \frac{n}{b} \right]$, $b = \sqrt{\min(m,n)}$.

- **Approach 3 (A3):** $B_1 = \left[ \frac{m}{b} \right]$, $B_2 = \left[ \frac{n}{b} \right]$, $b = \sqrt{\max(m,n)}$.

Note that, under the balanced design, all approaches are equivalent to the block approach in [Zaremba et al. (2013)].

To compare these three approaches to the new test, we check the performance of tests under the simulation setting used in Section 3.2. Here, the ratio of the two sample sizes $m$ and $n$ is fixed at 4:1 and 6:1.
Table 9: Estimated power of the tests. $m = 4n$.

| $d = 100$ | Sample sizes change ($a = 0.03$) | Sample sizes change ($a = 0.04$) |
|-----------|---------------------------------|---------------------------------|
| Approach  | A1     | A2     | A3     | New    | A1     | A2     | A3     | New    |
| $n = 500$  | 0.146  | 0.194  | **0.208** | **0.208** | 0.346  | 0.432  | **0.460** | 0.440  |
| $n = 800$  | 0.264  | **0.374** | 0.360  | 0.360  | 0.494  | 0.634  | 0.620  | **0.646** |
| $n = 1100$ | 0.410  | **0.532** | 0.502  | 0.514  | 0.710  | 0.792  | 0.796  | **0.806** |
| $n = 1400$ | 0.530  | 0.648  | 0.622  | **0.656** | 0.836  | **0.916** | 0.906  | **0.916** |
| $n = 1700$ | 0.640  | 0.764  | 0.758  | **0.768** | 0.902  | 0.950  | 0.944  | **0.958** |

| $n = 2000$ | Dimensions change ($a = 0.01$) | Dimensions change ($a = 0.02$) |
|-----------|---------------------------------|---------------------------------|
| Approach  | A1     | A2     | A3     | New    | A1     | A2     | A3     | New    |
| $d = 100$  | 0.166  | 0.218  | 0.218  | **0.224** | 0.282  | 0.370  | **0.378** | 0.364  |
| $d = 200$  | 0.288  | 0.356  | 0.352  | **0.368** | 0.530  | 0.628  | **0.638** | 0.636  |
| $d = 300$  | 0.332  | **0.464** | 0.456  | 0.444  | 0.692  | **0.804** | **0.804** | **0.804** |
| $d = 400$  | 0.438  | **0.574** | 0.548  | 0.564  | 0.790  | **0.892** | 0.880  | **0.892** |
| $d = 500$  | 0.574  | 0.688  | 0.678  | **0.700** | 0.880  | **0.942** | 0.940  | **0.942** |

The results are shown in Table 9 and 10. When $m = 4n$, we see that A2 and the new test perform well when the sample size is small. On the other hand, the new test dominates in power when the sample size is large. When the dimension is low, A3 and the new test are doing better than other approaches, while A2 and the new test exhibit high power when the dimension is high. When $m = 6n$, A2 exhibits high power when the sample size is large, while the new approach in general show good performance when the dimension is high. Therefore, we still recommend the proposed block approach in general scenarios.
Table 10: Estimated power of the tests. $m = 6n$.

| Approach | $d = 100$ | Sample sizes change ($a = 0.03$) | Sample sizes change ($a = 0.04$) |
|----------|-----------|----------------------------------|----------------------------------|
|          |           | A1 | A2 | A3 | New | A1 | A2 | A3 | New |
| $n = 400$|            |    |    |    |     |    |    |    |     |
|          |           | 0.122 | 0.188 | 0.165 | **0.198** | 0.271 | **0.384** | 0.362 | 0.367 |
| $n = 600$|            | 0.220 | **0.303** | 0.299 | 0.295 | 0.428 | 0.547 | 0.527 | **0.548** |
| $n = 800$|            | 0.295 | 0.392 | **0.402** | 0.398 | 0.549 | **0.697** | 0.671 | 0.667 |
| $n = 1000$|           | 0.400 | **0.507** | 0.504 | 0.487 | 0.670 | **0.796** | 0.766 | 0.754 |
| $n = 1200$|           | 0.483 | **0.610** | 0.588 | 0.600 | 0.775 | **0.880** | 0.869 | 0.872 |

| Approach | $d = 100$ | Dimensions change ($a = 0.01$) | Dimensions change ($a = 0.02$) |
|----------|-----------|----------------------------------|----------------------------------|
|          |           | A1 | A2 | A3 | New | A1 | A2 | A3 | New |
| $d = 100$|            |    |    |    |     |    |    |    |     |
|          |           | 0.146 | 0.186 | **0.212** | 0.196 | 0.210 | 0.282 | 0.276 | **0.296** |
| $d = 200$|            | 0.258 | 0.354 | 0.362 | **0.364** | 0.402 | **0.540** | 0.518 | **0.540** |
| $d = 300$|            | 0.388 | 0.488 | **0.522** | 0.516 | 0.514 | 0.642 | 0.644 | **0.648** |
| $d = 400$|            | 0.458 | 0.548 | 0.558 | **0.576** | 0.628 | 0.724 | 0.742 | **0.778** |
| $d = 500$|            | 0.574 | 0.692 | 0.698 | **0.706** | 0.738 | 0.834 | **0.846** | 0.844 |

6 Conclusion

In this paper, we proposed a new kernel two-sample test for large-scale data. The new test combines the strengths of two statistics and it enables the proposed test to detect the differences in distributions effectively. The asymptotic distributions of the test statistics facilitate its application to large datasets. The new approach is robust to high dimensions, applicable to the unbalanced sample design, and it does not need parameter tuning procedures by data splitting, making the new test computationally efficient. We experimentally demonstrated that the new test exhibits high power for a wide range of problems.
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References

Bai, Z. and Saranadasa, H. (1996), “Effect of high dimension: by an example of a two sample problem,” *Statistica Sinica*, 311–329.

Baumgartner, W., Weiß, P., and Schindler, H. (1998), “A nonparametric test for the general two-sample problem,” *Biometrics*, 1129–1135.

Biswas, M. and Ghosh, A. K. (2014), “A nonparametric two-sample test applicable to high dimensional data,” *Journal of Multivariate Analysis*, 123, 160–171.

Carlini, N. and Wagner, D. (2017), “Adversarial examples are not easily detected: bypassing ten detection methods,” in *Proceedings of the 10th ACM workshop on artificial intelligence and security*.

Chen, H., Chen, X., and Su, Y. (2018), “A weighted edge-count two-sample test for multivariate and object data,” *Journal of the American Statistical Association*, 113, 1146–1155.

Chen, H. and Friedman, J. H. (2017), “A new graph-based two-sample test for multivariate and object data,” *Journal of the American statistical association*, 112, 397–409.

Chen, H. and Zhang, N. R. (2013), “Graph-based tests for two-sample comparisons of categorical data,” *Statistica Sinica*, 1479–1503.

Chwialkowski, K. P., Ramdas, A., Sejdinovic, D., and Gretton, A. (2015), “Fast two-sample testing with analytic representations of probability measures,” in *Advances in Neural Information Processing Systems*.

Fox, R. J. and Dimmic, M. W. (2006), “A two-sample Bayesian t-test for microarray data,” *BMC bioinformatics*, 7, 1–11.
Friedman, J. H. and Rafsky, L. C. (1979), “Multivariate generalizations of the Wald-Wolfowitz and Smirnov two-sample tests,” *The Annals of Statistics*, 697–717.

Gao, R., Liu, F., Zhang, J., Han, B., Liu, T., Niu, G., and Sugiyama, M. (2020), “Maximum mean discrepancy is aware of adversarial attacks,” *arXiv preprint arXiv:2010.11415*.

Gretton, A., Borgwardt, K. M., Rasch, M., Schölkopf, B., and Smola, A. J. (2007), “A kernel method for the two-sample-problem,” in *Advances in neural information processing systems*.

Gretton, A., Fukumizu, K., Harchaoui, Z., and Sriperumbudur, B. K. (2009), “A fast, consistent kernel two-sample test,” in *Advances in neural information processing systems*.

Gretton, A. et al. (2012a), “A kernel two-sample test,” *Journal of Machine Learning Research*, 13, 723–773.

— (2012b), “Optimal kernel choice for large-scale two-sample tests,” in *Advances in neural information processing systems*.

Grosse, K., Manoharan, P., Papernot, N., Backes, M., and McDaniel, P. (2017), “On the (statistical) detection of adversarial examples,” *arXiv preprint arXiv:1702.06280*.

Grossfield, A. and Zuckerman, D. M. (2009), “Quantifying uncertainty and sampling quality in biomolecular simulations,” *Annual reports in computational chemistry*, 5, 23–48.

Hediger, S., Michel, L., and Näf, J. (2019), “On the use of random forest for two-sample testing,” *arXiv preprint arXiv:1903.06287*.

Hettmansperger, T. P., Möttönen, J., and Oja, H. (1998), “Affine invariant multivariate rank tests for several samples,” *Statistica Sinica*, 785–800.

Ho, H.-c. and Shieh, G. S. (2006), “Two-stage U-statistics for Hypothesis Testing,” *Scandinavian journal of statistics*, 33, 861–873.
Jitkrittum, W., Szabó, Z., Chwialkowski, K. P., and Gretton, A. (2016), “Interpretable distribution features with maximum testing power,” *Advances in Neural Information Processing Systems*, 29, 181–189.

Kent IV, D. R., Muller, R. P., Anderson, A. G., Goddard III, W. A., and Feldmann, M. T. (2007), “Efficient algorithm for “on-the-fly” error analysis of local or distributed serially correlated data,” *Journal of computational chemistry*, 28, 2309–2316.

Kirchler, M., Khorasani, S., Kloft, M., and Lippert, C. (2020), “Two-sample testing using deep learning,” in *International Conference on Artificial Intelligence and Statistics*, PMLR.

Kohout, J. and Pevný, T. (2017), “Network traffic fingerprinting based on approximated kernel two-sample test,” *IEEE Transactions on Information Forensics and Security*, 13, 788–801.

Kolmogorov, A. (1933), “Sulla determinazione empirica di una legge di distribuzione,” .

Law, H. C. L., Sutherland, D., Sejdinovic, D., and Flaxman, S. (2018), “Bayesian approaches to distribution regression,” in *International Conference on Artificial Intelligence and Statistics*.

Liu, F., Xu, W., Lu, J., Zhang, G., Gretton, A., and Sutherland, D. J. (2020), “Learning deep kernels for non-parametric two-sample tests,” in *International Conference on Machine Learning*, PMLR.

Lopez-Paz, D. and Oquab, M. (2016), “Revisiting classifier two-sample tests,” *arXiv preprint arXiv:1610.06545*.

Mann, H. B. and Whitney, D. R. (1947), “On a test of whether one of two random variables is stochastically larger than the other,” *The annals of mathematical statistics*, 50–60.

Oja, H. (2010), *Multivariate nonparametric methods with R: an approach based on spatial signs and ranks*, Springer Science & Business Media.
Osborne, D., Patrangenaru, V., Ellingson, L., Groisser, D., and Schwartzman, A. (2013), “Nonparametric two-sample tests on homogeneous Riemannian manifolds, Cholesky decompositions and diffusion tensor image analysis,” *Journal of Multivariate Analysis*, 119, 163–175.

Pan, W., Tian, Y., Wang, X., and Zhang, H. (2018), “Ball divergence: nonparametric two sample test,” *Annals of statistics*, 46, 1109.

Ramdas, A., Reddi, S. J., Poczos, B., Singh, A., and Wasserman, L. (2015), “Adaptivity and computation-statistics tradeoffs for kernel and distance based high dimensional two sample testing,” *arXiv preprint arXiv:1508.00655*.

Rosenbaum, P. R. (2005), “An exact distribution-free test comparing two multivariate distributions based on adjacency,” *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 67, 515–530.

Rothe, R., Timofte, R., and Van Gool, L. (2018), “Deep expectation of real and apparent age from a single image without facial landmarks,” *International Journal of Computer Vision*, 126, 144–157.

Rousson, V. (2002), “On distribution-free tests for the multivariate two-sample location-scale model,” *Journal of multivariate analysis*, 80, 43–57.

Salojärvi, J., Puolamäki, K., Simola, J., Kovanen, L., Kojo, I., and Kaski, S. (2005), “Inferring relevance from eye movements: Feature extraction,” in *Workshop at NIPS 2005, in Whistler, BC, Canada, on December 10, 2005*.

Schilling, M. F. (1986), “Multivariate two-sample tests based on nearest neighbors,” *Journal of the American Statistical Association*, 81, 799–806.

Schott, J. R. (2007), “A test for the equality of covariance matrices when the dimension is large relative to the sample sizes,” *Computational Statistics & Data Analysis*, 51, 6535–6542.
Song, H. and Chen, H. (2020), “Generalized Kernel Two-Sample Tests,” *arXiv preprint arXiv:2011.06127*.

Sriperumbudur, B. K., Gretton, A., Fukumizu, K., Schölkopf, B., and Lanckriet, G. R. (2010), “Hilbert space embeddings and metrics on probability measures,” *Journal of Machine Learning Research*, 11, 1517–1561.

Srivastava, M. S. and Du, M. (2008), “A test for the mean vector with fewer observations than the dimension,” *Journal of Multivariate Analysis*, 99, 386–402.

Srivastava, M. S. and Yanagihara, H. (2010), “Testing the equality of several covariance matrices with fewer observations than the dimension,” *Journal of Multivariate Analysis*, 101, 1319–1329.

Sutherland, D. J., Tung, H.-Y., Strathmann, H., De, S., Ramdas, A., Smola, A., and Gretton, A. (2016), “Generative models and model criticism via optimized maximum mean discrepancy,” *arXiv preprint arXiv:1611.04488*.

Székely, G. J. and Rizzo, M. L. (2013), “Energy statistics: A class of statistics based on distances,” *Journal of statistical planning and inference*, 143, 1249–1272.

Wald, A. and Wolfowitz, J. (1940), “On a test wether two samples are from the same distribution,” *Ann. Math. Stat.*, 11, 147–162.

Wynne, G. and Duncan, A. B. (2020), “A kernel two-sample test for functional data,” *arXiv preprint arXiv:2008.11095*.

Zaremba, W., Gretton, A., and Blaschko, M. (2013), “B-test: A non-parametric, low variance kernel two-sample test,” in *Advances in neural information processing systems*.

Zhang, J. and Chen, H. (2017), “Graph-Based Two-Sample Tests for Discrete Data,” *arXiv preprint arXiv:1711.04349*.