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# MMD-FUSE: LEARNING AND COMBINING KERNELS FOR TWO-SAMPLE TESTING WITHOUT DATA SPLITTING

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## Abstract

We propose novel statistics which maximise the power of a two-sample test based on the Maximum Mean Discrepancy (MMD), by adapting over the set of kernels used in defining it. For finite sets, this reduces to combining (normalised) MMD values under each of these kernels via a weighted soft maximum. Exponential concentration bounds are proved for our proposed statistics under the null and alternative. We further show how these kernels can be chosen in a data-dependent but permutation-independent way, in a well-calibrated test, avoiding data splitting. This technique applies more broadly to general permutation-based MMD testing, and includes the use of deep kernels with features learnt using unsupervised models such as auto-encoders. We highlight the applicability of our MMD-FUSE test on both synthetic low-dimensional and real-world high-dimensional data, and compare its performance in terms of power against current state-of-the-art kernel tests.

## 1. Introduction

The fundamental problem of non-parametric two-sample testing consists in detecting the difference between any two distributions having access only to samples from these. Kernel-based tests relying on the Maximum Mean Discrepancy (MMD; [Gretton et al., 2012a](#))

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as a measure of distance on distributions are well-suited for this framework as they can identify complex non-linear features in the data, and benefit from both strong theoretical guarantees and ease of implementation. This explains their popularity among practitioners and justifies their wide use for real-world applications.

However, the performance of these tests is crucially impacted by the choice of kernel. This is commonly tackled by either: choosing the kernel by some weakly data-dependent heuristic (Gretton et al., 2012a); or splitting off a hold-out set of data for kernel selection, with the other half used for the actual test (Gretton et al., 2012b; Sutherland et al., 2017). This latter method includes training feature extractors such as deep kernels on the first selection half. Both of these methods can incur a significant loss in test power, since heuristics may lead to poor kernel choices, and data splitting reduces the number of data points for the actual test.

Our contribution is to present MMD-based tests which can strongly adapt to the data *without* data splitting. This comes in two parallel parts: firstly we show how the kernel can be chosen in an unsupervised fashion using the entire dataset, and secondly we show how multiple such kernels can be adaptively weighted in a single test statistic, optimising test power.

**Data Splitting.** The data splitting approach selects test parameters on a held-out half of the dataset, and applies the test to the other half. Commonly, this involves optimising a kernel on held-out data in a supervised fashion to distinguish which sample originated from which distribution, either by learning a deep kernel directly (Sutherland et al., 2017; Liu et al., 2020, 2021), or indirectly through the associated witness function (Kübler et al., 2022a,b). Jitkrittum et al. (2016) propose tests which select witness function features (in either spatial or frequency space) on the held-out data, running the analytic representation test of Chwialkowski et al. (2015) on the remaining data.

Our first contribution is to show that it is possible to learn a feature extractor for our test (*e.g.*, a deep kernel) on the *entirety* of the data in an *unsupervised* manner while retaining the desired non-asymptotic test level. Specifically, any method can be used that is ignorant of which distribution generated which samples. We can thus leverage many feature extraction methods, from auto-encoders (Hinton and Salakhutdinov, 2006) to recent powerful developments in self-supervised learning (He et al., 2020; Chen et al., 2020a,b,c; Chen and He, 2021; Grill et al., 2020; Caron et al., 2020; Zbontar et al., 2021; Li et al., 2021). Remarkably, our method applies to *any* permutation-based two-sample test, even non-kernel tests, provided the parameters are chosen in this unsupervised fashion. This includes a very wide array of MMD-based tests, and finally provides a formal justification for the commonly-used median heuristic (Gretton et al., 2012b; Ramdas et al., 2015; Reddi et al., 2015).

**Adaptive Kernel Selection.** A newer approach originating in Schrab et al. (2021) performs adaptive kernel selection through multiple testing. Aggregating several MMD-based tests with different kernels, each on the whole dataset, results in an overall adaptive test with optimal power guarantees in terms of minimax separation rate over Sobolev balls. Variants of this kernel adaptivity through aggregation have been proposed with linear-time estimators (Schrab et al., 2022b), spectral regularisation (Hagrass et al., 2022), kernel thinning compression (Domingo-Enrich et al., 2023), and in the asymptotic regime (Chatterjee and Bhattacharya, 2023). Another adaptive approach using the entire dataset for both kernel selection and testing is given by Kübler et al. (2020); this leverages the Post Selection Inference framework, but the resulting test suffers from low power in practice.

While our unsupervised feature extraction method is an extremely powerful and general technique, particularly for high-dimensional structured data like images, it is not always

sufficient for data where such feature extraction is difficult. This motivates our second contribution, a method for combining whole-dataset MMD estimates under multiple different kernels into single test statistics, for which we prove exponential concentration. Kernel parameters such as bandwidth can then be chosen in a non-heuristic manner to optimise power, even on data with less structure and varying length scales. Using a single statistic also ensures that a single *test* can be used, instead of the multiple testing approach outlined above, reducing computational expense.

**MMD-FUSE.** By combining these contributions we construct two closely related **MMD-FUSE** tests. Each chooses a set of kernels based on the whole dataset in an unsupervised fashion, and then adaptively weights and *fuses* this (potentially infinite) set of kernels through our new statistics; both parts of this procedure are done using the entire dataset without splitting. On the finite sets of kernels we use in practice the weighting procedure is done in closed form via a weighted soft maximum. We show these new tests to be well-calibrated and give sufficient power conditions which achieve the minimax optimal rate in terms of MMD. In empirical comparisons, our test compares favourably to the state-of-the-art aggregated tests in terms of power and computational cost.

**Outline and Summary of Contributions.** In Section 2 we outline our setting, crucial results underlying our work, and alternative existing approaches. Section 3 covers the construction of permutation tests and discusses how we can choose the parameters for any such test in any unsupervised fashion including with deep kernels and by those methods mentioned above. Section 4 introduces and motivates our two proposed tests. Section 5 discusses sufficient conditions for test power (at a minimax optimal rate in MMD), and the exponential concentration of our statistics. Finally, we show that our test compares favourably with a wide variety of competitors in Section 6 and discuss in Section 7.

## 2. Background

**Two-Sample Testing.** The two sample testing problem is to determine whether two distributions  $p$  and  $q$  are equal or not. In order to test this hypothesis, we are given access to two samples,  $\mathbf{X} := (X_1, \dots, X_n) \stackrel{\text{iid}}{\sim} p$  and  $\mathbf{Y} := (Y_1, \dots, Y_m) \stackrel{\text{iid}}{\sim} q$  as tuples of data points with sizes  $n$  and  $m$ . We write the combined (ordered) sample as  $\mathbf{Z} := (Z_1, \dots, Z_{n+m}) = (\mathbf{X}, \mathbf{Y}) = (X_1, \dots, X_n, Y_1, \dots, Y_m)$ .

We define the null hypothesis  $H_0$  as  $p = q$  and the alternative hypothesis  $H_1$  as  $p \neq q$ , usually with a requirement  $\mathbb{D}(p, q) > \epsilon$  for a distance  $\mathbb{D}$  (such as the MMD) and some  $\epsilon > 0$ . A hypothesis test  $\Delta$  is a  $\{0, 1\}$ -valued function of  $\mathbf{Z}$ , which rejects the null hypothesis if  $\Delta(\mathbf{Z}) = 1$  and fails to reject it otherwise. It will usually be formulated to control the probability of a type I error at some level  $\alpha \in (0, 1)$ , so that  $\mathbb{P}_{p \times p}(\Delta(\mathbf{Z}) = 1) \leq \alpha$ , while simultaneously minimising the probability of a type II error,  $\mathbb{P}_{p \times q}(\Delta(\mathbf{Z}) = 0)$ . In the above we have used the notation  $\mathbb{P}_{p \times p}$  and  $\mathbb{P}_{p \times q}$  to indicate that the sample  $\mathbf{Z}$  is either drawn from the null,  $p = q$ , or the alternative  $p \neq q$ . Similar notation will be used for expectations and variances. When a bound  $\beta \in (0, 1)$  on the probability of a type II error is given (which may depend on the precise formulation of the alternative), we say the test has power  $1 - \beta$ .

**Maximum Mean Discrepancy.** The Maximum Mean Discrepancy (MMD) is a kernel-based measure of distance between two distributions  $p$  and  $q$ , which is often used for two-sample testing. The MMD quantifies the dissimilarity between these distributions by comparing their mean embeddings in a reproducing kernel Hilbert space (RKHS; Aronszajn, 1950) with kernel  $k(\cdot, \cdot)$ . Formally, if  $\mathcal{H}_k$  is the RKHS associated with kernel function  $k$ ,

the MMD between distributions  $p$  and  $q$  is the integral probability metric defined by:

$$\text{MMD}(p, q; k) := \sup_{f \in \mathcal{H}_k: \|f\|_{\mathcal{H}_k} \leq 1} (\mathbb{E}_{X \sim p}[f(X)] - \mathbb{E}_{Y \sim q}[f(Y)]).$$

The minimum variance unbiased estimate of  $\text{MMD}^2$ , is given by the sum of two U-statistics and a sample average as:<sup>1</sup>

$$\widehat{\text{MMD}}_k^2(\mathbf{Z}) := \frac{1}{n(n-1)} \sum_{(i,i') \in [n]_2} k(X_i, X_{i'}) + \frac{1}{m(m-1)} \sum_{(j,j') \in [m]_2} k(Y_j, Y_{j'}) - \frac{2}{mn} \sum_{i=1}^n \sum_{j=1}^m k(X_i, Y_j),$$

where we introduced the notation  $[n]_2 = \{(i, i') \in [n]^2 : i \neq i'\}$  for the set of all pairs of distinct indices in  $[n] = \{1, \dots, n\}$ . Tests based on the MMD usually reject the null when  $\widehat{\text{MMD}}^2$  exceeds some critical threshold, with the resulting power being greatly affected by the kernel choice. For *characteristic* kernel functions (Sriperumbudur et al., 2011), it can be shown that  $\text{MMD}(p, q; k) = 0$  if and only if  $p = q$ , leading to consistency results. However, on finite sample sizes, convergence rates of MMD estimates typically have strong dependence on the data dimension, so there are settings in which kernels ignoring redundant or unimportant features (*i.e.* non-characteristic kernels) will give higher test power in practice than characteristic kernels (which can over-weight redundant features).

**Permutation Tests.** The tests we discuss in this paper use permutations of the data  $\mathbf{Z}$  to approximate the null distribution. We denote the permutation (or symmetric) group of  $[N]$  by  $\mathfrak{S}_N$  and its elements by  $\sigma \in \mathfrak{S}_N, \sigma : [N] \rightarrow [N]$ . Since  $\sigma \in \mathfrak{S}_{n+m}$  are group elements, we abuse notation slightly to write their action on a sample as  $\sigma \mathbf{Z} = (Z_{\sigma(1)}, \dots, Z_{\sigma(n+m)})$ . We also introduce a quantile operator (analogous to the max and min operators) for a finite set  $\{f(a) \in \mathbb{R} : a \in \mathcal{A}\}$ :

$$\text{quantile}_{q, a \in \mathcal{A}} f(a) := \inf \left\{ r \in \mathbb{R} : \frac{1}{|\mathcal{A}|} \sum_{a \in \mathcal{A}} \mathbf{1}\{f(a) \leq r\} \geq q \right\}. \quad (1)$$

Under the null we note  $\sigma \mathbf{Z} \stackrel{d}{=} \mathbf{Z}$ , while under the alternative, the permuted sample  $\sigma \mathbf{Z}$  for randomised  $\sigma \sim \text{Uniform}(\mathfrak{S}_{n+m})$  can be considered as a sample from the mixture  $\frac{1}{2}(p + q)$ , which simulates the null distribution. We can therefore use permutations to construct an approximate cumulative distribution function (CDF) of our test statistic under the null, and choose an appropriate quantile of this CDF as our test threshold. This quantile must be exceeded under the null with probability less than level  $\alpha$ . Various different results can be used to choose the threshold giving a correct level; in Section 3 we will highlight a very general method for doing this and discuss previously unconsidered implications for using unsupervised feature extraction methods as a part of our tests.

A related approach constructs an MMD Aggregated test (MMDA<sub>agg</sub>; Schrab et al., 2021), which combines multiple MMD-based permutation tests with different kernels, and rejects if *any* of these reject, using distinct quantiles for each kernel. To ensure the overall aggregated test is well-calibrated, these quantiles need to be adjusted, this correction is performed using a *second level* of permutations. This incurs additional computational cost, a pitfall avoided by our fused single statistic.

**Distributions Over Kernels.** In our test statistic, we will consider the case where the kernel  $k \in \mathcal{K}$  is drawn from a distribution  $\rho \in \mathcal{M}_+^1(\mathcal{K})$  (with the latter notation

<sup>1</sup> Kim et al. (2022) notes that  $\widehat{\text{MMD}}_k^2$  can equivalently be written as a two-sample U-statistic with kernel  $h_k(x, x'; y, y') = k(x, x') + k(y, y') - k(x, y') - k(x', y)$ , which is useful for analysis.

denoting a probability measure; *c.f.* Benton et al., 2019 in the Gaussian Process literature). This distribution will be adaptively chosen based on the data subject to a regularisation term based on a “prior”  $\pi \in \mathcal{M}_+^1(\mathcal{K})$  and defined through the Kullback-Liebler divergence:  $\text{KL}(\rho||\pi) := \mathbb{E}_\rho[\log(d\rho/d\pi)]$  for  $\rho \ll \pi$  and  $\text{KL}(\rho||\pi) := \infty$  otherwise. When constructing these statistics the Donsker-Varadhan equality (Donsker and Varadhan, 1975), holding for any measurable  $g : \mathcal{K} \rightarrow \mathbb{R}$ , will be useful:

$$\sup_{\rho \in \mathcal{M}_+^1(\mathcal{A})} \mathbb{E}_\rho[g] - \text{KL}(\rho||\pi) = \log \mathbb{E}_\pi[\exp \circ g]. \quad (2)$$

This can be further related to the notion of soft maxima. If  $\pi$  is a uniform distribution on finite  $\mathcal{K}$  with  $|\mathcal{K}| = r$ , then  $\text{KL}(\rho||\pi) \leq \log(r)$ . Setting  $g = f$  for some  $t > 0$ , Equation (2) relaxes to

$$\max_k f(k) - \frac{\log(r)}{t} \leq \frac{1}{t} \log \left( \frac{1}{r} \sum_k e^{tf(k)} \right) \leq \max_k f(k), \quad (3)$$

which approximates the maximum with error controlled by  $t$ . Our approach in considering these soft maxima is reminiscent of the PAC-Bayesian (McAllester, 1998; Seeger et al., 2001; Maurer, 2004; Catoni, 2007; see Guedj, 2019 or Alquier, 2021 for a survey) approach to capacity control and generalisation. This framework has raised particular attention recently as it has been used to provide the only non-vacuous generalisation bounds for deep neural networks (Dziugaite and Roy, 2017, 2018; Dziugaite et al., 2021; Zhou et al., 2019; Perez-Ortiz et al., 2021; Biggs and Guedj, 2021, 2022a); it has also been fruitfully applied to other varied problems from ensemble methods (Lacasse et al., 2006, 2010; Masegosa et al., 2020; Wu et al., 2021; Zantedeschi et al., 2021; Biggs and Guedj, 2022b; Biggs et al., 2022) to online learning (Haddouche and Guedj, 2022). Our proofs draw on techniques in that literature for U-Statistics (Lever et al., 2013) and martingales (Seldin et al., 2012; Biggs and Guedj, 2023; Haddouche and Guedj, 2023; Chugg et al., 2023). By considering these soft maxima, we gain a major advantage over the standard approaches, as we can obtain concentration and power results for our statistics without incurring Bonferroni-type multiple testing penalties.

**Faster Sub-Optimal Tests.** While the main focus of this paper revolves around the kernel selection problem for optimal, quadratic MMD testing, we also highlight the existence of a rich literature on efficient kernel tests which run in linear (or near-linear) time. These speed improvements are achieved using various tools such as: incomplete U-statistics (Gretton et al., 2012b; Yamada et al., 2019; Lim et al., 2020; Kübler et al., 2020; Schrab et al., 2022b), block U-statistics (Zaremba et al., 2013; Deka and Sutherland, 2022), eigenspectrum approximations (Gretton et al., 2009), Nyström approximations (Cherfaoui et al., 2022), random Fourier features (Zhao and Meng, 2015), analytic representations (Chwialkowski et al., 2015; Jitkrittum et al., 2016), deep linear kernels (Kirchler et al., 2020), kernel thinning (Dwivedi and Mackey, 2021; Domingo-Enrich et al., 2023), *etc.*

The efficiency of these tests usually entail weaker theoretical power guarantees compared to their quadratic-time counterparts, which are minimax optimal<sup>2</sup> (Kim et al., 2022; Li and Yuan, 2019; Fromont et al., 2013; Schrab et al., 2021; Chatterjee and Bhattacharya, 2023). These optimal quadratic tests are either permutation-based non-asymptotic tests (Kim et al., 2022; Schrab et al., 2021) or studentised asymptotic tests (Kim and Ramdas, 2023; Shekhar et al., 2022; Li and Yuan, 2019; Gao and Shao, 2022; Florian et al., 2023). We emphasise that the parameters of any of these permutation-based two-sample tests can

<sup>2</sup>With the exception of the near-linear test of Domingo-Enrich et al. (2023) which achieves the same MMD separation rate as the quadratic test but under stronger assumptions on the data distributions.

be chosen in the unsupervised way we outline in Section 3. We choose to focus in this work on optimal quadratic-time results, but note that our general approach could be extended to sub-optimal faster tests as well.

### 3. Constructing Permutation Tests

In this section we will highlight a very general and easy to use theorem for constructing permutation tests, with implications for the use of unsupervised feature extraction methods as a part of the test. Although this result is not new, we believe that its usefulness has been under-appreciated in the kernel testing community, and that we are the first to point out the way in which it enables such feature extraction and other parameter optimisation in this setting. We begin by stating the result in a fairly general form, so that its use in other close settings such as independence testing (Albert et al., 2022; Rindt et al., 2021) or wild bootstrap-based two-sample tests (Fromont et al., 2012, 2013; Chwialkowski et al., 2014; Schrab et al., 2021) can also be seen.

Let  $\mathcal{G}$  be a group of transformations on  $\mathbf{Z}$ ; in our setting  $\mathcal{G} = \mathfrak{S}_{n+m}$ . Write  $g\mathbf{Z}$  for the action of  $g \in \mathcal{G}$  on  $\mathbf{Z}$ . We will suppose  $\mathbf{Z}$  is invariant under the action of  $\mathcal{G}$  when the sample is drawn from the *null* distribution, *i.e.* if the null is true then  $g\mathbf{Z} \stackrel{d}{=} \mathbf{Z}$  for all  $g \in \mathcal{G}$ . This is clearly the case for  $\mathcal{G} = \mathfrak{S}_{n+m}$  in two-sample testing, since under the null  $\mathbf{Z} = (Z_1, \dots, Z_{m+m}) \stackrel{\text{iid}}{\sim} p$  with  $p = q$ .

Let  $G$  be a vector of elements in  $\mathcal{G}$ ,  $G = (g_1, g_2, \dots, g_{B+1})$ , with  $g_{B+1} = \text{id}$  (the identity permutation). The elements  $g_1, \dots, g_B$  are drawn uniformly from  $\mathcal{G}$  either i.i.d. or without replacement (which includes the possibility of  $G = \mathcal{G}$ ). Recall the quantile operator defined in Equation (1).

**Theorem 1** (Permutation Test; Hemerik and Goeman, 2018, Theorem 2.). *Let  $\tau(\mathbf{Z})$  be a statistic of  $\mathbf{Z}$ . In the setting described above with any  $B \geq 1$ , under the null hypothesis and random draw  $G$ ,*

$$\mathbb{P}_{p \times p, G} \left( \tau(\mathbf{Z}) > \underset{1-\alpha, g \in G}{\text{quantile}} \tau(g\mathbf{Z}) \right) \leq \alpha.$$

In other words, if we compare  $\tau(\mathbf{Z})$  with the empirical quantile of  $\tau(g\mathbf{Z})$  as a test threshold, the type I error rate is no more than  $\alpha$ . The potentially complex task of constructing a permutation test reduces to the trivial task of choosing the statistic  $\tau(\mathbf{Z})$ . This result is also true for *randomised* permutations of any number  $B \geq 1$  *without* approximation, so an exact and computationally efficient test can be straightforwardly constructed this way. We emphasise that this result can also be more conveniently applied than Romano and Wolf (2005, Lemma 1), which requires exchangeability and is commonly used. For example, the proofs of Albert et al. (2022, Proposition 1) and Schrab et al. (2021, Proposition 1) could likely be greatly simplified by direct application of Theorem 1, without the need to explicitly prove exchangeability of the HSIC/MMD test statistic with its permuted variants.

Importantly, Theorem 1 holds for any  $\tau$ . For example, we could use the MMD with a kernel chosen based on the data,  $\tau(\mathbf{Z}) = \widehat{\text{MMD}}_{k=k(\mathbf{Z})}^2(\mathbf{Z})$ ; however, for each permutation  $\sigma$  we would need to re-compute  $\tau(\sigma\mathbf{Z}) = \widehat{\text{MMD}}_{k=k(\sigma\mathbf{Z})}^2(\sigma\mathbf{Z})$ , so the kernel being used would be different for each permutation. This has two major disadvantages: firstly, it might be computationally expensive to re-compute  $k$  for each permutation, especially for a deep kernel<sup>3</sup>. Secondly, the *scale* of the resulting MMD could be dramatically different for each

<sup>3</sup>A possibility envisaged by *e.g.* Liu et al. (2020) and dismissed due to the computational infeasibility.

permutation, so the empirical quantile might not lead to a powerful test. This second problem is related to the problem of combining multiple different MMD values into a single test which our MMD-FUSE statistics are designed to combat (Section 4; *c.f.* also MMDAgg, Schrab et al., 2021).

**Our Proposal.** In two-sample testing we propose to use a statistic  $\tau_\theta$  parameterised by some  $\theta$ , where  $\theta$  is fixed for all permutations, but depends on the data in an *unsupervised* or *permutation-invariant* way. Specifically, we allow such a parameter to depend on  $\langle \mathbf{Z} \rangle := \{Z_1, \dots, Z_{n+m}\}$ , the *unordered* combined sample. Since our tests will not depend on the internal ordering of  $\mathbf{X}$  and  $\mathbf{Y}$  (which are assumed i.i.d. under both hypotheses), the only additional information contained in  $\mathbf{Z}$  over  $\langle \mathbf{Z} \rangle$  is the *label* assigning  $Z_i$  to its initial sample. This is justified since  $\langle \mathbf{Z} \rangle = \langle \sigma \mathbf{Z} \rangle$  for all  $\sigma \in \mathfrak{S}_{n+m}$ , so setting  $\tau(\mathbf{Z}) = \tau_\theta(\langle \mathbf{Z} \rangle)(\mathbf{Z})$  gives a fixed  $\theta$  and statistic for all permutations to use in Theorem 1. The information in  $\langle \mathbf{Z} \rangle$  can be used to fine-tune test parameters for any test fitting this setup. This solves both the computation and scaling issues mentioned above.

The above also provides a first formal justification for the use of the median heuristic in Gretton et al. (2012a), since it is a permutation-invariant function of the data. However, a far richer set of possibilities are available even when restricting ourselves to these permutation-free functions of  $\mathbf{Z}$ . For example, we can use any unsupervised or self-supervised learning method to learn representations for use as the input to an MMD-based test statistic, while paying no cost in terms of calibration and needing to train such methods only once. Given the wide variety of methods dedicated to feature extraction and dimensionality reduction, this opens up a huge range of possibilities for the design of new and principled two-sample tests. Pointing out this powerful and widely-applicable possibility represents one of our most practical contributions.

## 4. MMD-FUSE: Fusing U-Statistics by Exponentiation

We use two different test statistics based on  $\widehat{\text{MMD}}^2$  with normalised and un-normalised variants. Both use a ‘‘prior’’  $\pi(\langle \mathbf{Z} \rangle)$ , which is either fixed independently of the data, or is a function of the data which is invariant under permutation (as discussed in Section 3). This prior is (a function mapping to) a distribution on a space of kernels  $\mathcal{K}$ . Our statistics also use a regularisation parameter  $\lambda > 0$ , the choice of which will drive the power results discussed in Section 5.

**Definition 1** (MMD-FUSE-N). *We define the normalised test statistic*

$$\widehat{\text{FUSE}}_N(\mathbf{Z}) := \frac{1}{\lambda} \log \left( \mathbb{E}_{k \sim \pi(\langle \mathbf{Z} \rangle)} \left[ \exp \left( \lambda \frac{\widehat{\text{MMD}}^2(\mathbf{X}, \mathbf{Y}; k)}{\sqrt{\widehat{N}_k(\mathbf{Z})}} \right) \right] \right)$$

where  $\widehat{N}_k(\mathbf{Z}) := \frac{1}{n(n-1)} \sum_{(i,j) \in [n+m]_2} k(Z_i, Z_j)^2$  is permutation invariant.

Although this statistic appears complex, we note that in the case where  $\pi$  has finite support, its calculation reduces to a log-sum-exp of MMD estimates normalised by  $\widehat{N}_k$ . This is even clearer when  $\pi$  is also uniform on its support, then Equation (3) shows that our statistic reduces to a soft maximum. The parameter  $\lambda$  can be seen as a ‘‘temperature’’ parameter controlling the smoothness of this soft maximum. We discuss this point further in Section 4.2.



Our test (for sampled set  $S$  of permutations as described above) is given in terms of  $\widehat{\text{FUSE}}_N$  as

$$\Delta_{\text{FUSE}_N}(\mathbf{Z}) := \mathbf{1} \left\{ \widehat{\text{FUSE}}_N(\mathbf{Z}) > \underset{1-\alpha, \sigma \in S}{\text{quantile}} \widehat{\text{FUSE}}_N(\sigma \mathbf{Z}) \right\}. \quad (4)$$

It compares the test statistic  $\widehat{\text{FUSE}}_N$  with its quantiles under permutation, and rejects if the overall value exceeds a quantile controlled by  $\alpha$ . We note that since  $\widehat{N}_k(\mathbf{Z})$  is permutation invariant, it only needs to be calculated once per kernel (and not separately for each permutation).

#### 4.1. Un-Normalised Variant

We further introduce a second FUSE statistic in which the normaliser term  $\widehat{N}_k$  is neglected. The FUSE-1 test  $\Delta_{\text{FUSE}_1}$  is defined in an analogous way to  $\Delta_{\text{FUSE}_N}$  in Equation (4).

**Definition 2** (MMD-FUSE-1). *We define the un-normalised test statistic*

$$\widehat{\text{FUSE}}_1(\mathbf{Z}) := \frac{1}{\lambda} \log \left( \mathbb{E}_{k \sim \pi(\langle \mathbf{Z} \rangle)} \left[ \exp \left( \lambda \widehat{\text{MMD}}^2(\mathbf{X}, \mathbf{Y}; k) \right) \right] \right).$$

Although this test has worse performance in practice, the variant statistic is interesting in its own right because of various theoretical properties as we discuss below. Firstly, we introduce the *mean* kernel  $K_\rho(x, y) = \mathbb{E}_{k \sim \rho} k(x, y)$  under a ‘‘posterior’’  $\rho \in \mathcal{M}_+^1(\mathcal{K})$ , which is indeed a reproducing kernel in its own right. In the finite case, this is simply a weighted sum of ‘‘base’’ kernels.

Note that the linearity of  $\widehat{\text{MMD}}^2$  and  $\text{MMD}^2$  in the kernel implies that  $\mathbb{E}_{k \sim \rho} \text{MMD}^2(p, q; k) = \text{MMD}^2(p, q; K_\rho)$ , and similarly for  $\widehat{\text{MMD}}^2$ . Combining this linearity with the dual formulation of  $\widehat{\text{FUSE}}_1$  via Equation (2) gives

$$\widehat{\text{FUSE}}_1(\mathbf{Z}) = \sup_{\rho \in \mathcal{M}_+^1(\mathcal{K})} \widehat{\text{MMD}}^2(\mathbf{X}, \mathbf{Y}; K_\rho) - \frac{\text{KL}(\rho, \pi)}{\lambda}.$$

This re-states our statistic in terms of ‘‘posterior’’  $\rho$ , and makes the interpretation of our statistic as a KL-regularised kernel-learning method clear. In the finite case our test simply optimises the weightings of the different kernels in a constrained way. We note that for certain *infinite* kernel sets and choices of prior it is possible to express the mean kernel in closed form. This happens because, *e.g.* the expectation of a Gaussian kernel with respect to a Gamma prior over the bandwidth is simply a (closed form) rational quadratic kernel. We discuss this point further in Appendix B.

Terms very similar to the above, with  $\text{MMD}^2(p, q; K_\rho)$  and  $\text{KL}(\rho, \pi)$  will appear in our power results (Section 5), which are stated in terms of posteriors  $\rho$ .

#### 4.2. Aside: Why Not Set $\lambda \rightarrow \infty$ ?

Theorem 1 shows that setting  $\lambda \rightarrow \infty$  will not prevent us from controlling the level of our test by  $\alpha$ . This is equivalent to considering the maximum, *c.f.* Equations (2) and (3), over a set of MMD-based statistics; note though that for each permutation we would take this maximum separately. Cárcamo et al. (2022) show that for certain kernel choices the supremum of the MMD values with respect to the bandwidth is a valid integral probability metric (Müller, 1997).

There are however a few problems with this approach: firstly, if the class over which we are maximising is sufficiently rich (for example a complex neural network), then the maximum may be able to effectively memorise the entire sample for each possible permutation, saturating the statistic for every permutation and limiting test power. Secondly, any convergence results would need to hold simultaneously for every  $k$  in  $\mathcal{K}$ , and so power results would suffer. If  $|\mathcal{K}|$  is finite then we would effectively incur a sub-optimal Bonferroni correction; while for infinite classes, results would need to involve capacity control quantities like Rademacher complexity. Our approach here, which is equivalent to using a KL complexity penalty with regularisation controlled by  $\lambda$ , is strongly reminiscent of instead using *PAC-Bayesian* (Section 2) capacity control. The Donsker-Varadhan equality shows the equivalence of this regularisation-based approach with ours, and is used heavily in that literature, alongside a number of other techniques we adapt to our setting.

## 5. Theoretical Power of MMD-FUSE

In this section we outline possible sufficient conditions for our tests to obtain power at least  $1 - \beta$  at given level  $\alpha$ . The conditions will depend on a fixed data-independent “prior”  $\pi \in \mathcal{M}_+^1(\mathcal{K})$  and thus hold even without unsupervised parameter optimisation. They are stated as requirements for the *existence* of a “posterior”  $\rho \in \mathcal{M}_+^1(\mathcal{K})$  with corresponding mean kernel  $K_\rho$  as defined in Section 4.1. In the finite case  $K_\rho$  is simply a weighted sum of kernels, so these requirements are also satisfied under the same conditions for any single kernel, corresponding to the case where the posterior puts all its weight on a single kernel.

Technically, these results require that there is some constant  $\kappa$  upper bounding all of the kernels, and that  $n, m$  are within a constant multiple (*i.e.*  $n \leq m \leq cn$  for some  $c \geq 1$ , notated  $n \asymp m$ ). They hold when using randomised permutations provided  $B > c'\alpha^{-2} \log(\beta^{-1})$  for small constant  $c' > 0$ .

**Theorem 2** (FUSE-1 Power). *Fix prior  $\pi$  independently of the data. For the un-normalised test FUSE-1 with  $\lambda \asymp n/\kappa$  and  $n \asymp m$ , there exists a universal constant  $C > 0$  such that*

$$\exists \rho \in \mathcal{M}_+^1(\mathcal{K}) : \text{MMD}^2(p, q; K_\rho) > \frac{C\kappa}{n} \left( \frac{1}{\beta} + \log \frac{1}{\alpha} + \text{KL}(\rho, \pi) \right).$$

*is sufficient for a test with power  $\geq 1 - \beta$  at level  $\alpha$ .*

A similar result is obtained for FUSE-N under an assumption that the normalising term is well behaved. Specifically we require there for all  $k \in \text{supp}(\pi)$  the expectation  $\mathbb{E}_{\mathbf{Z} \sim p \times q} \left[ \widehat{N}_k(\mathbf{Z})^{-1} \right] < c/\kappa$  is bounded for some  $c < \infty$ . This requirement will be satisfied for kernels (including most common ones) that tend to zero only in the limit of the data being infinitely far apart.

**Theorem 3** (FUSE-N Power). *Fix prior  $\pi$  independently of the data. For the normalised test FUSE-N with  $\lambda \asymp n \asymp m$ , there exists universal constant  $C > 0$  such that*

$$\exists \rho \in \mathcal{M}_+^1(\mathcal{K}) : \text{MMD}^2(p, q; K_\rho) > \frac{C\kappa}{n} \left( \frac{1}{\beta^2} + \log \frac{1}{\alpha} + \text{KL}(\rho, \pi) \right).$$

*is sufficient for a test with power  $\geq 1 - \beta$  at level  $\alpha$ .*

**Discussion.** The conditions in Theorems 2 and 3 give the optimal  $\text{MMD}^2$  separation rate rate in  $n$  (Domingo-Enrich et al., 2023, Proposition 2). These results also imply

consistency if the prior  $\pi$  assigns non-zero weight to characteristic kernels.<sup>4</sup> Applying these results to uniform priors supported on  $r$  points, the KL penalty can be upper bounded as  $\text{KL}(\rho, \pi) \leq \log(r)$ . Thus in the *worst* case, where only a single kernel achieves large  $\text{MMD}^2(p, q; k)$ , the price paid for adaptivity is only  $\log(r)$ . In many cases, *most* of the kernels will give large  $\text{MMD}^2(p, q; k)$ . The posterior will then mirror the prior, and this KL penalty will be even smaller. Thus very large numbers of kernels could be considered, and if all give large MMD values the power would not be greatly affected.

**Additional Technical Results.** Aside from the presentation of our new statistics and tests, we make a number of technical contributions on the way to proving Theorem 2 and Theorem 3, as well as proving some additional results. In particular, we give exponential concentration bounds for our statistics under permutations and the null, which do not require bounded kernels. This refined analysis requires the construction of a coupled Rademacher chaos and concentration thereof. We obtain intermediate results using variances from the proofs of Theorems 2 and 3 that could be used in future work to obtain power guarantees under alternative assumptions such as Sobolev spaces (Schrab et al., 2021). Finally, we prove exponential concentration for  $\widehat{\text{FUSE}}_1$  under the alternative and bounded kernels, requiring the proof of a ‘‘PAC-Bayesian’’ bounded differences-type concentration inequality. For a more detailed overview see Section 7.

## 6. Experiments

We compare the test power of MMD-FUSE-N against various MMD-based kernel selective tests (see Section 1 for details) using: the median heuristic (MMD-Median; Gretton et al., 2012a), data splitting (MMD-Split; Sutherland et al., 2017), analytic Mean Embeddings and on the difference in Smooth Characteristic Functions (ME & SCF; Jitkrittum et al., 2016), the MMD Deep kernel (MMD-D; Liu et al., 2020), Automated Machine Learning (AutoML; Kübler et al., 2022b) kernel thinning to (Aggregate) Compress Then Test (CTT & ACTT; Domingo-Enrich et al., 2023), and MDD Aggregated (Incomplete) tests (MMDAgg & MMDAggInc; Schrab et al., 2021, 2022b). Additional details and code link for experimental reproducibility are provided in the appendix.

**Distribution on Kernels.** We choose our kernel prior distribution  $\pi$  as uniform over a collection of Gaussian,  $k_\gamma^g(x, y) = \exp(-\|x - y\|_2^2/2\gamma^2)$ , and Laplace,  $k_\gamma^l(x, y) = \exp(-\sqrt{2}\|x - y\|_1/\gamma)$ , kernels with various bandwidths  $\gamma > 0$ . These bandwidths are chosen as the uniform discretisation of the interval between half the 5% and twice the 95% quantiles (for robustness) of  $\{\|z - z'\|_r : z, z' \in \mathbf{Z}\}$ , with  $r \in \{1, 2\}$  respectively. This choice is similar to that of Schrab et al. (2021, Section 5.2), who empirically show that ten points for the discretisation is sufficient (Schrab et al., 2021, Figure 6). This set of distances is permutation-invariant so Theorem 1 guarantees a well-calibrated test even though the kernels are data-dependent.

**Mixture of Gaussians.** Our first experiments (Figure 1) consider multimodal distributions  $p$  and  $q$ , each a 2-dimensional mixture of four Gaussians with means  $(\pm\mu, \pm\mu)$  with  $\mu = 20$  and diagonal covariances. For  $p$ , the four components all have unit variances, while for  $q$  we vary the standard deviation  $\sigma$  of *one* of the Gaussians.  $\sigma = 1$  corresponds to the null hypothesis  $p = q$ . Intuitively, an appropriate kernel bandwidth to distinguish  $p$  from  $q$  would correspond to that separating Gaussians with standard deviations 1 and  $\sigma$ . This is significantly smaller than the *median* bandwidth which scales with the distance  $\mu$  between modes.

<sup>4</sup> Under this condition  $\text{KL}(\nu, \pi) < \infty$  with  $\nu$  the restriction of  $\pi$  to characteristic kernels.  $K_\nu$  is characteristic so  $\text{MMD}(p, q; K_\nu) > 0 \iff p \neq q$ , and our condition lower bound tends to zero with  $n \rightarrow \infty$ .

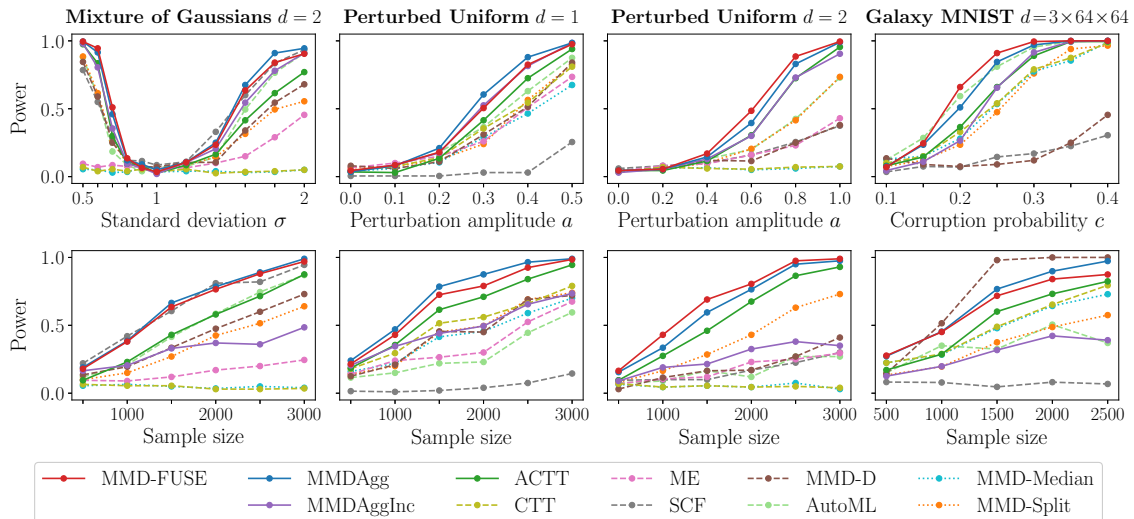


Figure 1: Power experiments. The four columns correspond to different settings: Mixture of Gaussians in two dimensions (null  $\sigma = 1$ ), Perturbed Uniform for  $d \in \{1, 2\}$  (null  $a = 0$ ), and Galaxy MNIST in dimension 12288 (null  $c = 0$ ). In the first row, the deviations away from the null are varied for fixed sample size  $m = n = 500$ . In the second row, the sample size varies while the deviations are fixed as  $\sigma = 1.3$ ,  $a = 0.2$ ,  $a = 0.4$ , and  $c = 0.15$ , for the four respective problems. The plots correspond to the rejections of the null averaged over 200 repetitions.

**Perturbed Uniform.** In Figure 1, we report test power for detecting perturbations on uniform distributions in one and two dimensions. We vary the amplitude  $a$  of two perturbations from  $a = 0$  (null) to  $a = 1$  (maximum value for the density to remain non-negative). A similar benchmark was first proposed by Schrab et al. (2021, Section 5.5) and considered in several other works (Schrab et al., 2022b; Hagrass et al., 2022; Chatterjee and Bhattacharya, 2023). Different bandwidths are required to detect different amplitudes of the perturbations.

**Galaxy MNIST.** We examine performance on real-world data in Figure 1, through satellite-captured galaxy images (Walmsley et al., 2022) in dimension  $d = 3 \times 64 \times 64 = 12288$ . These consist of four classes: ‘smooth and cigar-shaped’, ‘edge-on-disk’, ‘unbarred spiral’, and ‘smooth and round’. One distribution uniformly samples images from the first three categories, while the other does the same with probability  $1 - c$  and uniformly samples a ‘smooth and round’ galaxy image with probability of corruption  $c \in [0, 1]$ . The null hypothesis corresponds to the case  $c = 0$ .

**CIFAR 10 vs 10.1.** The aim of this experiment is to detect the difference between images from the CIFAR-10 (Krizhevsky, 2009) and CIFAR-10.1 (Recht et al., 2019) test sets. This is a challenging problem as CIFAR-10.1 was specifically created to consist of new samples from the CIFAR-10 distribution so that it can be used as an alternative test set for models trained on CIFAR-10. Samples from the two distributions are presented in Figure 6 in Appendix A.3 (Liu et al., 2020, Figure 5). This benchmark was proposed by Liu et al. (2020, Table 3) who introduced the deep MMD test MMD-D and the MMD-Split test (here referred to as MMD-O to point out that their implementation has been used rather than ours). They also compare to ME and SCF, as well as to C2ST-L and C2ST-S (Lopez-Paz and Oquab, 2017) which correspond to Classifier Two-Sample Tests based on Sign or Linear kernels. For the tests splitting the data, 1000 images from both datasets are used for parameter selection and/or model training, and 1021 other images from each

distributions are used for testing. Consequently, tests avoiding data splitting are given the full 2021 images from CIFAR-10.1 and 2021 images sampled from CIFAR-10.

**Experimental Results of Figure 1.** We observe similar trends in all eight experiments in Figure 1: **MMD-FUSE** *matches the power* of state-of-the-art MMDAgg while being computationally *faster* (both theoretically and practically). These two tests consistently obtain the highest power in every experiment, except when increasing the number of GalaxyMNIST images where MMD-D obtains higher power. However, we observe in Table 1 that MMD-FUSE outperforms MMD-D on another image data problem, also with large sample size. On synthetic data, the deep kernel test MMD-D surprisingly only obtains power similar to MMD-split in most experiments (even lower in the 2-dimensional perturbed uniform experiment). The two near-linear aggregated variants ACTT and MMDAggInc trade-off a small portion of test power for computational efficiency, with the former outperforming the latter for large sample sizes. The importance of kernel selection is emphasised by the fact the two tests using the median bandwidth (MMD-Median and CTT) achieve very low power. While the linear SCF test, based in the frequency domain, attains high power in the Mixture of Gaussians experiments, it has low power in the three other experiments. Its spatial domain variant ME performs better on Perturbed Uniform  $d \in \{1, 2\}$  experiments but in general still has reduced power compared to both linear and quadratic time alternatives. Finally, the AutoML test performs well for fixed sample size  $m = n = 500$  (first row of Figure 1), but its power compared to other tests considerably deteriorates as the sample size increases (second row of Figure 1). Overall, MMD-FUSE achieves *state-of-the-art performance* across our experiments on both low-dimensional synthetic data and high-dimensional real-world data.

**Experimental Results of Table 1.** We report in Table 1 the power achieved by each test on the CIFAR 10 vs 10.1 experiment, which is averaged over 1000 repetitions. We observe that MMD-FUSE performs the best and obtains power 0.937, which means that out of 1000 repetitions, it was 937 times able to distinguish between samples from CIFAR-10 and from CIFAR-10.1. This demonstrates that the images in CIFAR-10.1 do not come from the same distribution as those in CIFAR-10.

## 7. Conclusions

In this work, we propose MMD-FUSE, an MMD-based test which fuses kernels through a soft maximum and a method for learning general two-sample testing parameters in an unsupervised fashion. We demonstrate the empirical performance of MMD-FUSE and show that it achieves the optimal MMD separation rate guaranteeing high test power. This optimality holds with respect to the sample size and likely also for the logarithmic dependence in  $\alpha$ , but we believe the dependence on  $\beta$  could be improved in future work; a general question is whether lower bounds in terms of  $\alpha$  and  $\beta$  can be proved. Obtaining separation rates in terms of the  $L^2$ -norm between the densities (Schrab et al., 2021) may also be possible but challenging; unlike MMD, this distance is independent of the kernel.

An open question is in explaining the significant empirical power advantage of the normalised test over its un-normalised variant, which is currently not reflected in the derived rates. The importance of this normalisation is clear when considering kernels with different bandwidths, leading to vastly different scaling in the un-normalised permutation distributions. Work here could begin with finite-sample concentration guarantees for our normalised statistic or other “studentised” variants, some of which might obtain better performance.

Table 1: Test power for detecting the difference between CIFAR-10 and CIFAR-10.1 images with test level  $\alpha = 0.05$ . The averaged numbers of rejections over 1000 repetitions are reported.

Tests	Power
MMD-FUSE	<b>0.937</b>
MMDAgg	0.883
MMD-D	0.744
CTT	0.711
MMD-Median	0.678
ACTT	0.652
ME	0.588
AutoML	0.544
C2ST-L	0.529
C2ST-S	0.452
MMD-O	0.316
MMDAggInc	0.281
SCF	0.171

Future work could also examine computationally efficient variants of MMD-FUSE, by either relying on incomplete  $U$ -statistics (Schrab et al., 2022b) and leading to suboptimal rates, or by relying on recent ideas of kernel thinning (Domingo-Enrich et al., 2023) which can lead to the same optimal rate under stronger assumptions on the data distributions. Finally, our two-sample MMD fusing approach could be extended to the HSIC independence framework (Gretton et al., 2005, 2008; Albert et al., 2022) and to the KSD goodness-of-fit setting (Chwialkowski et al., 2016; Liu et al., 2016; Schrab et al., 2022a).

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## Overview of Appendices

**Appendix A** We give further experimental details, discuss time complexity of our results while graphing run-times. We also give additional results on an image benchmark (CIFAR-10 vs CIFAR-10.1), where we outperform other existing tests.

**Appendix B** We discuss how  $\widehat{\text{FUSE}}_1$  can be expressed in a simple form for certain uncountable priors.

**Appendix C** We prove exponential concentration bounds for both our statistics under the null and permutations.

**Appendix D** We prove exponential concentration bounds for the  $\widehat{\text{FUSE}}_1$  statistic under the alternative hypothesis.

**Appendix E** We prove the power results stated in Section 5 and other interesting intermediate results.

## A. Experiments

### A.1. Code and licenses

Our implementation of MMD-FUSE in Jax (Bradbury et al., 2018), as well as the code for the reproducibility of the experiments, are made publicly available at:

<https://github.com/antoninschrab/mmdfuse-paper>

Our code is under the MIT License, and we also implement ourselves the MMD-Median (Gretton et al., 2012a) and MMD-Split (Sutherland et al., 2017) tests. For ME & SCF (Jitkrittum et al., 2016), MMD-D (Liu et al., 2020), AutoML (Kübler et al., 2022b), CTT & ACTT (Domingo-Enrich et al., 2023), MMDAgg & MMDAggInc (Schrab et al., 2021, 2022b), we use the implementations of the respective authors, which are all under the MIT license.

The experiments were run on an AMD Ryzen Threadripper 3960X 24 Cores 128Gb RAM CPU at 3.8GHz and on an NVIDIA RTX A5000 24Gb Graphics Card, with a compute time of a couple of hours.

### A.2. Test parameters

In general, we use the default test parameters recommended by the authors of the tests (listed above). For the ME and SCF tests, ten test locations are chosen on half of the data. AutoML is run with the recommended training time limit of one minute.

**Kernels.** As explained in Section 6 (§Distribution on Kernels), for MMD-Fuse, we use Gaussian and Laplace kernels with bandwidths in  $\{q_{5\%}^r + i(q_{95\%}^r - q_{5\%}^r)/9 : i = 0, \dots, 9\}$  where  $q_{5\%}^r$  is half the 5% quantile of all the inter-sample distances  $\{\|z - z'\|_r : z, z' \in \mathbf{Z}\}$  with  $r = 1$  and  $r = 2$  for Laplace and Gaussian kernels, respectively. Similarly,  $q_{95\%}^r$  is twice the 95% quantile.

MMD-Split selects a Gaussian kernel on half of the data with bandwidth in  $\{q_{5\%}^r + i(q_{95\%}^r - q_{5\%}^r)/99 : i = 0, \dots, 99\}$  by maximizing a proxy for asymptotic power which is the ratio of the estimated MMD with its estimated standard deviation under the alternative (Liu et al., 2020, Equation 3). The MMD test is then run on the other half with the selected kernel.

CTT and MMD-Median both use a Gaussian kernel with bandwidth the median of  $\{\|z - z'\|_2 : z, z' \in \mathbf{Z}\}$ , while ACTT is run with Gaussian kernels with bandwidths in  $\{q_{5\%}^2 + i(q_{95\%}^2 - q_{5\%}^2)/9 : i = 0, \dots, 9\}$ .

The MMDAgg and MMDAggInc tests are run with their default implementations, which similarly use collections of 20 kernels split equally between Gaussian and Laplace kernels with ten bandwidths each, but they use a different (non-uniform) discretisation of the intervals  $[q_{95\%}^r, q_{5\%}^r]$ .

**Permutations.** For MMD-Median, MMD-Split, and MMD-FUSE, we use 2000 permutations to estimate the quantiles. MMDAgg and MMDAggInc use 2000 + 2000 and 500 + 500 permutations, respectively, to approximate the quantiles and the multiple testing correction. The CTT and ACTT tests are run with 39 and 299 + 200 permutations, respectively. AutoML uses 10000 permutations and MMD-D 100 of them. The ME and SCF tests use asymptotic quantiles. We recall that using a higher number of permutations for the quantile does not necessarily lead to a more powerful test (Rindt et al., 2021, Section 7).



### A.3. Details on the experiments of Section 6

In this section, we present figures illustrating the four experimental settings described in Section 6 with results in Figure 1: Mixture of Gaussians (Figure 2), Perturbed Uniform  $d = 1$  (Figure 3), Perturbed Uniform  $d = 2$  (Figure 4), Galaxy MNIST (Figure 5), and CIFAR 10 vs 10.1 (Figure 6).

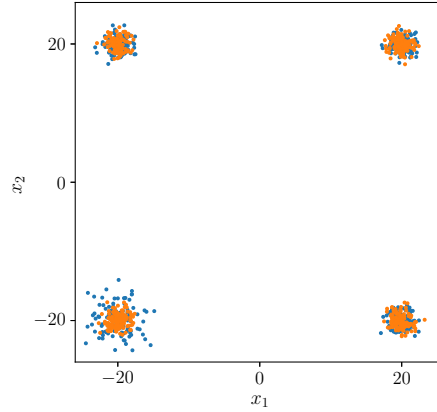


Figure 2: Mixture of Gaussians. Both distributions are mixtures of four 2-dimensional Gaussians with means  $(\pm 20, \pm 20)$  and standard deviations  $\sigma_1 = \sigma_2 = \sigma_3 = 1$ . Samples from  $p$  (orange) are drawn with  $\sigma_4 = 1$ , while samples from  $q$  (blue) are drawn with  $\sigma_4 = 2$ .

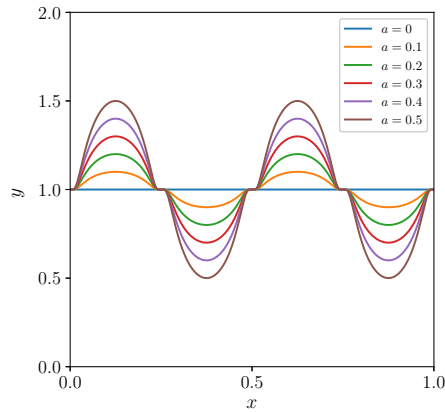


Figure 3: Perturbed Uniform  $d = 1$ . One-dimensional uniform densities with two perturbations are plotted for various amplitudes  $a$ .

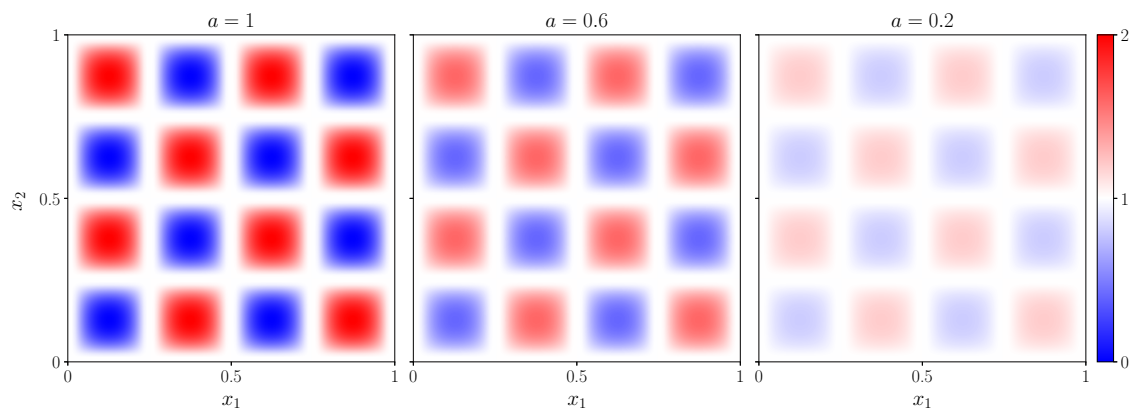
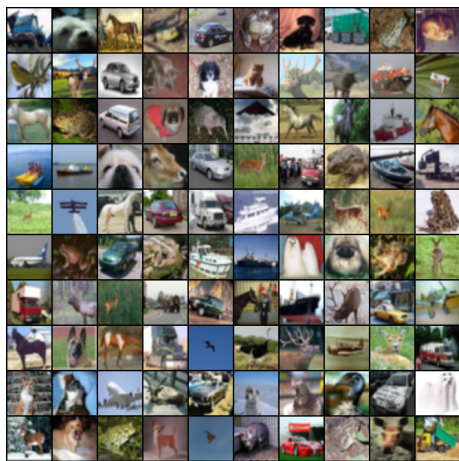


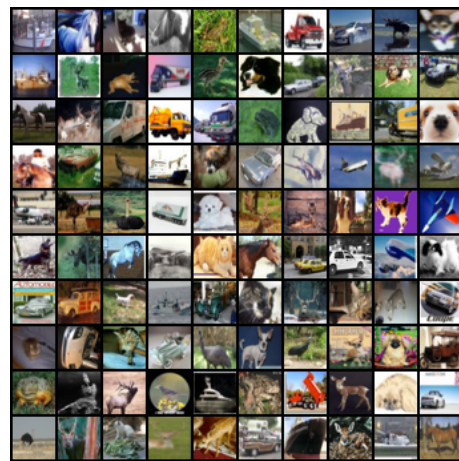
Figure 4: Perturbed Uniform  $d = 2$ . Two-dimensional uniform densities with two perturbations per dimension are plotted for various amplitudes  $a$ .



Figure 5: Galaxy MNIST (Walmsley et al., 2022) images in dimension  $3 \times 64 \times 64$  across four categories: ‘smooth cigar’ (first row), ‘edge on disk’ (second row), ‘unbarred spiral’ (third row), and ‘smooth round’ (fourth row).



(a) CIFAR-10 images



(b) CIFAR-10.1 images

Figure 6: Images from the CIFAR-10 (Krizhevsky, 2009) and CIFAR-10.1 (Recht et al., 2019) test sets. This figure corresponds to Figure 5 of Liu et al. (2020).

#### A.4. Time complexity and runtimes

The time complexity of MMD-FUSE is

$$\mathcal{O}\left(K B (m^2 + n^2)\right)$$

where  $m$  and  $n$  are the sizes of the two samples,  $K$  is the number of kernels fused, and  $B$  is the number of permutations to estimate the quantile. Note that this is an improvement over the time complexity of MMDAgg (Schrab et al., 2021)

$$\mathcal{O}\left(K (B + B') (m^2 + n^2)\right)$$

where the extra parameter  $B'$  corresponds to the number of permutations used to estimate the multiple testing correction, often set as  $B' = B$  in practice (Schrab et al., 2021, Section 5.2). We indeed observe in Figure 7 that MMD-FUSE runs twice as fast as MMDAgg.

While the runtimes of most tests should not depend on the type of data (only on the sample size and on the dimension), we note that the runtimes of tests relying on optimisation (e.g. ME & SCF) can be affected. In the experiment of Figure 7, we consider samples from multivariate Gaussians centred at zero with covariance matrices  $I_d$  and  $\sigma I_d$  with  $\sigma = 1.1$ . We vary both the sample sizes and the dimensions.

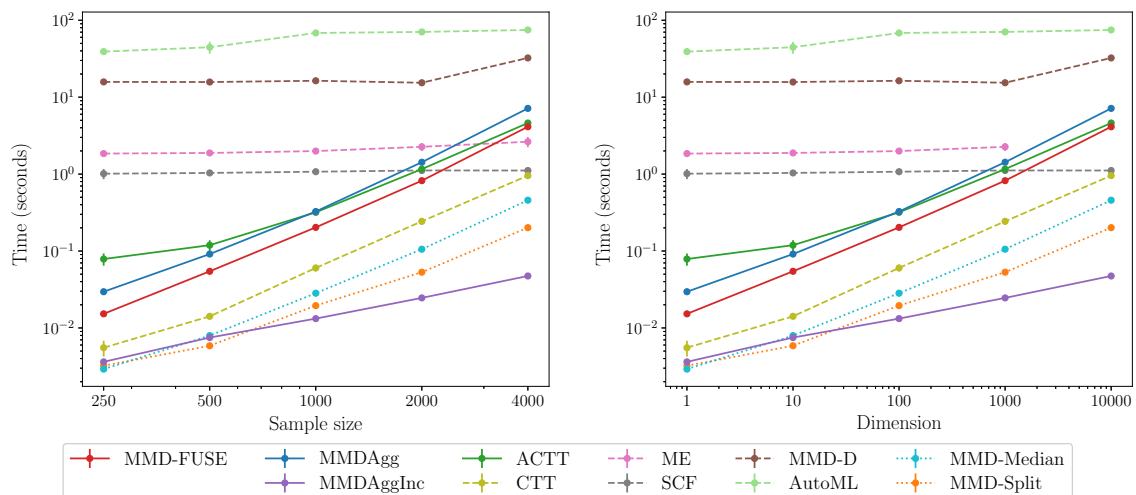


Figure 7: Test runtimes plotted using logarithmic scales. In the LHS figure, we vary the sample size for fixed dimension 10. In the RHS figure, we vary the dimension for fixed sample size 500. The mean and standard deviations of the test runtimes over ten repetitions are reported. Recall that the tests are run with their default parameters with different numbers of permutations, and that AutoML has a training time parameter which is set to 60 seconds by default, as described in Appendix A.2.

## B. Closed Form Mean Kernel

We have observed in the main text that in some cases where the prior has non-finite support,  $\widehat{\text{FUSE}}_1$  still gives a straightforwardly expressed statistic. This happens because for certain kernel choices, the expectation of the kernel with respect to some parameter is still a closed form kernel. We give one example of such a statistic here.

**Theorem 4.** *For any fixed  $\alpha > 0$ , the following is an example of a  $\widehat{\text{FUSE}}_1$  statistic:*

$$\widehat{\text{FUSE}}_1^{rq}(\mathbf{Z}) = \sup_{R>0} \widehat{\text{MMD}}_u^2(\mathbf{Z}; k_{rq(\alpha, \sqrt{R}\eta_0)}) - \alpha \cdot \frac{\log R + 1/R - 1}{\lambda}$$

where  $k_{rq(\alpha, \eta)} = (1 + \|x - y\|^2/2\eta^2)^{-\alpha}$  is a rational quadratic kernel, and  $\eta_0$  is the ‘‘prior’’ bandwidth (which can essentially be absorbed into the data scaling).

**Proof of Theorem 4.** Firstly, we define a general rational quadratic kernel

$$k_{rq(\alpha, \eta)}(x, y) = \left(1 + \frac{\|x - y\|^2}{2\eta^2}\right)^{-\alpha}.$$

Note that  $k_g(r) = e^{-\tau r^2/2}$  with  $r = \|x - y\|$  is a bounded kernel with parameter  $\tau$ . If we take the expectation of  $\tau$  with respect to a Gamma distribution,

$$\begin{aligned} \mathbb{E}_{\tau \sim \Gamma(\alpha, \beta)} e^{-\tau r^2/2} &= \frac{\beta^\alpha}{\Gamma(\alpha)} \int_{-\infty}^{\infty} \tau^{\alpha-1} \exp(-\tau\beta) \exp(-\tau r^2/2) d\tau \\ &= \frac{\beta^\alpha}{\Gamma(\alpha)} \Gamma(\alpha) \left(\beta + \frac{r^2}{2}\right)^{-\alpha} \\ &= \left(1 + \frac{r^2}{2\beta}\right)^{-\alpha} = k_{rq(\alpha, \sqrt{\beta})}(r). \end{aligned}$$

The KL divergence between Gamma distributions is

$$\text{KL}(\Gamma(\alpha, \beta), \Gamma(\alpha_0, \beta_0)) = (\alpha - \alpha_0)\psi(\alpha) + \log \frac{\Gamma(\alpha_0)}{\Gamma(\alpha)} + \alpha_0 \log R + \alpha \left(\frac{1}{R} - 1\right)$$

where  $R = \beta/\beta_0$ . Using the dual form of  $\widehat{\text{FUSE}}_1$  we find that

$$\widehat{\text{FUSE}}_1 = \sup_{\alpha>0, \beta>0} \widehat{\text{MMD}}^2(\mathbf{Z}; k_{rq(\alpha, \sqrt{\beta})}) - \frac{\text{KL}(\Gamma(\alpha, \beta), \Gamma(\alpha_0, \beta_0))}{\lambda}.$$

Restricting  $\alpha = \alpha_0$ , prior  $\beta_0 = \eta_0^2$  and setting  $\beta = R\eta_0^2$  gives the result.  $\square$

## C. Null and Permutation Concentration Results

In this section we prove the following concentration results under the null (or equivalently, under the permutation distribution). These results show that for appropriate choices of  $\lambda$ , both statistics converge to zero at rate at least  $\mathcal{O}(1/n)$  under the null or permutations. We recall that without loss of generality  $n \leq m$ .

**Theorem 5.** *If the kernels are bounded,  $k \leq \kappa < \infty$ , then with probability at least  $1 - \delta$  over either a sample  $\mathbf{Z}$  from the null,*

$$\widehat{\text{FUSE}}_1(\mathbf{Z}) \leq \frac{4\kappa^2\lambda}{n(n-1)} + \frac{\log \frac{1}{\delta}}{\lambda}$$

provided  $0 < \lambda < \sqrt{n(n-1)}/8\sqrt{2}\kappa$ , and

$$-\widehat{\text{FUSE}}_1(\mathbf{Z}) \leq \frac{4\kappa^2 t}{n(n-1)} + \frac{\log \frac{1}{\delta}}{t}$$

provided  $0 < t < \sqrt{n(n-1)}/8\sqrt{2}\kappa$ .

Also, under the null hypothesis with probability at least  $1 - \delta$ , and without the assumption of boundedness,

$$\widehat{\text{FUSE}}_N(\mathbf{Z}) \leq \frac{16\lambda}{n(n-1)} + \frac{\log \frac{1}{\delta}}{\lambda},$$

provided  $0 < \lambda < \sqrt{n(n-1)}/16\sqrt{2}$ , and

$$-\widehat{\text{FUSE}}_N(\mathbf{Z}) \leq \frac{16t}{n(n-1)} + \frac{\log \frac{1}{\delta}}{t},$$

provided  $0 < t < \sqrt{n(n-1)}/16\sqrt{2}$ .

The above bounds are also valid for  $\widehat{\text{FUSE}}_1(\sigma\mathbf{Z})$ ,  $\widehat{\text{FUSE}}_N(\sigma\mathbf{Z})$  and any fixed  $\mathbf{Z}$  (potentially non-null) under permutation by  $\sigma \sim \text{Uniform}(\mathfrak{S}_{n+m})$ .

Note that, while the upper bounds depend critically upon our choice of  $\lambda$ , the lower bounds instead hold for any  $t$  that satisfy the requisite conditions. Note also that choosing  $\lambda \asymp \sqrt{n(n-1)} \asymp n$  indeed gives the desired rates  $\mathcal{O}(1/n)$ .

### C.1. Sub-Gaussian Chaos Theorem

**Theorem 6** (Sub-Gaussian Chaos; adapted from [Rudelson and Vershynin, 2013](#)). *Let  $X_i$  be mean-zero 1-sub-Gaussian variables, such that  $\log \mathbb{E}_X \exp(tX) \leq \frac{1}{2}t^2$  for every  $t \in \mathbb{R}$ . Let  $A \in \mathbb{R}^{n \times n}$  be a real symmetric matrix with zeros on the diagonal and we define the sub-Gaussian chaos*

$$W := \sum_{i=1}^n \sum_{j=1}^n A_{ij} X_i X_j.$$

For all  $|t| \leq (4\sqrt{2}\|A\|)^{-1}$ ,

$$\mathbb{E}_X \exp(tW) \leq \exp(16t^2\|A\|_F^2).$$

**Proof.** This proof is closely adapted from [Rudelson and Vershynin \(2013\)](#) with some modifications which reflect the desire for the tightest possible bound on the moment generating function.

Let  $X_i$  be mean-zero 1-sub-Gaussian variables, such that  $\log \mathbb{E}_X \exp(tX) \leq \frac{1}{2}t^2$  for every  $t \in \mathbb{R}$ . We are considering

$$W := \sum_{i,j} A_{ij} X_i X_j$$

where  $A_{ij}$  has zeros on the diagonal. We introduce independent Bernoulli random variables  $\delta_i \in \{0, 1\}$  with  $\mathbb{E}\delta_i = 1/2$  and define the matrix  $A^\delta$  with entries  $(A^\delta)_{ij} = \delta_i(1 - \delta_j)A_{ij}$ . Note that  $\mathbb{E}_\delta A^\delta = \frac{1}{4}A$ , since  $\mathbb{E}\delta_i(1 - \delta_j)$  equals  $1/4$  for  $i \neq j$ .

Writing the set of indices  $\Lambda_\delta = \{i \in [n] : \delta_i = 1\}$ , we introduce

$$W_\delta := \sum_{i,j} A_{ij}^\delta X_i X_j = \sum_{i \in \Lambda_\delta, j \in \Lambda_\delta^c} A_{ij} X_i X_j = \sum_{j \in \Lambda_\delta^c} X_j \left( \sum_{i \in \Lambda_\delta} A_{ij} X_i \right).$$

By Jensen's inequality,

$$\mathbb{E}_X \exp(tW) \leq \mathbb{E}_{X,\delta} \exp(4tW_\delta).$$

Conditioned on  $\delta$  and  $(X_i)_{i \in \Lambda_\delta}$ ,  $W_\delta$  is a linear combination of the mean-zero sub-gaussian random variables  $X_j$ ,  $j \in \Lambda_\delta^c$ . It follows that this conditional distribution of  $W_\delta$  is sub-gaussian, and so

$$\mathbb{E}_{(X_j)_{j \in \Lambda_\delta^c}} \exp(4tW_\delta) \leq \exp \left( \frac{1}{2}(4t)^2 \sum_{j \in \Lambda_\delta^c} \left( \sum_{i \in \Lambda_\delta} A_{ij} X_i \right)^2 \right).$$

Now introduce  $g = (g_1, \dots, g_n) \sim N(0, 1)$  i.i.d. draws from a normal and note that the above can also arise directly as the moment generating function of these Normal variables, so we make the further equality (for fixed  $X$  and  $\delta$ ),

$$\exp \left( \frac{1}{2}(4t)^2 \sum_{j \in \Lambda_\delta^c} \left( \sum_{i \in \Lambda_\delta} A_{ij} X_i \right)^2 \right) = \mathbb{E}_g \exp \left( 4t \sum_{j \in \Lambda_\delta^c} g_j \left( \sum_{i \in \Lambda_\delta} A_{ij} X_i \right)^2 \right).$$

Rearranging the terms, and using that the resulting term is a linear combination of the sub-Gaussian  $X_i$ ,  $i \in \Lambda_\delta$ , we find that

$$\begin{aligned} \mathbb{E}_{X,g} \exp \left( 4t \sum_{j \in \Lambda_\delta^c} g_j \left( \sum_{i \in \Lambda_\delta} A_{ij} X_i \right)^2 \right) &= \mathbb{E}_{X,g} \exp \left( 4t \sum_{i \in \Lambda_\delta} X_i \left( \sum_{j \in \Lambda_\delta^c} A_{ij} g_j \right) \right) \\ &\leq \mathbb{E}_{X,g} \exp \left( \frac{1}{2}(4t)^2 \sum_{i \in \Lambda_\delta} \left( \sum_{j \in \Lambda_\delta^c} A_{ij} g_j \right)^2 \right) \\ &\leq \mathbb{E}_{X,g} \exp \left( 8t^2 \sum_i \left( \sum_j \delta_i(1 - \delta_j) A_{ij} g_j \right)^2 \right) \\ &\leq \mathbb{E}_{X,g} \exp \left( 8t^2 \|A^\delta g\|_2^2 \right). \end{aligned}$$

Now, by the rotation invariance of the distribution of  $g$ , the random variable  $\|A^\delta g\|_2^2$  is distributed identically with  $\sum_i s_i^2 g_i^2$  where  $s_i$  denote the singular values of  $A^\delta$ , so by independence

$$\mathbb{E}_{X,g} \exp \left( 8t^2 \|A^\delta g\|_2^2 \right) = \mathbb{E}_g \exp \left( 8t^2 \sum_i s_i^2 g_i^2 \right)$$

$$\begin{aligned}
&= \prod_i \mathbb{E}_g \exp(8t^2 s_i^2 g_i^2) \\
&\leq \prod_i \exp(16t^2 s_i^2)
\end{aligned}$$

where the last inequality holds if  $8t^2 \max_i s_i^2 \leq \frac{1}{4}$  and arises since the MGF of a Chi-squared variable,  $\mathbb{E}e^{tg^2} \leq e^{2t}$  for  $0 \leq t \leq \frac{1}{4}$ .

Since  $\max_i s_i = \|A_\delta\| \leq \|A\|$  and  $\sum_i s_i^2 = \|A_\delta\|_F^2 \leq \|A\|_F$ , we combine the above steps to find that

$$\mathbb{E}_X \exp(tW) \leq \exp(16t^2 \|A\|_F^2) \quad \text{for } |t| \leq (4\sqrt{2}\|A\|)^{-1}.$$

□

## C.2. Permutation Bounds for Two-Sample U-Statistics

The main technical result we use for the null bounds is the following. Here we assume the permutation-invariance property of the U statistic kernel that  $h(x_1, x_2; y_1, y_2) = h(x_2, x_1; y_1, y_2) = h(x_1, x_2; y_2, y_1)$ . This can always be ensured by symmetrizing the kernel, and is satisfied by the kernel used by  $\widehat{\text{MMD}}^2$  which we consider in this paper.

**Theorem 7.** *Fix combined sample  $\mathbf{Z}$  of size  $n + m$  with  $n \leq m$  and let  $h(x_1, x_2; y_1, y_2)$  be a two-sample U-statistic kernel as described above. Define*

$$U(\mathbf{Z}) := \frac{1}{n(n-1)m(m-1)} \sum_{(i,i') \in [n]_2} \sum_{(j,j') \in [m]_2} h(Z_i, Z_{i'}; Z_{n+j}, Z_{n+j'}).$$

and

$$\bar{U}(\mathbf{Z}) = \frac{1}{n(n-1)m(m-1)} \sup_{\sigma \in \mathfrak{S}_{n+m}} \sqrt{\sum_{(i,i') \in [n]_2} \left( \sum_{(j,j') \in [m]_2} h(Z_{\sigma(i)}, Z_{\sigma(i')}; Z_{\sigma(n+j)}, Z_{\sigma(n+j')}) \right)^2}.$$

If  $\sigma \in \text{Uniform}(\mathfrak{S}_{n+m})$  is a random permutation of the dataset, then then for all  $|t| < (4\sqrt{2}\bar{U}(\mathbf{Z}))^{-1}$ ,

$$\mathbb{E}_\sigma \exp(tU(\sigma\mathbf{Z})) \leq \exp(t^2 \bar{U}^2(\mathbf{Z})).$$

**Theorem 8** (Normaliser Bound). *If  $h(x, x'; y, y') = k(x, x') + k(y, y') - k(x, y') - k(x', y)$  then*

$$\bar{U}(\mathbf{Z})^2 \leq \frac{16}{n(n-1)} \hat{N}(\mathbf{Z})$$

where  $n \leq m$  and

$$\hat{N}(\mathbf{Z}) = \frac{1}{n(n-1)} \sum_{(i,j) \in [n+m]_2} k(Z_i, Z_j)^2.$$

Additionally, if  $0 \leq k(x, x') \leq \kappa$  for all  $x, x'$ , then

$$\bar{U}^2(\mathbf{Z}) \leq \frac{4\kappa^2}{n(n-1)}.$$

**Proof of Theorem 7.** Firstly, we make the following definitions based on the work of [Kim et al. \(2022\)](#): let  $L = \{l_1, \dots, l_n\}$  be an  $n$ -tuple drawn uniformly without replacement from  $[m]$ . Then for any fixed  $\mathbf{Z}$

$$\mathbb{E}_L[\tilde{U}^L(\mathbf{Z})] = U(\mathbf{Z}) \tag{5}$$



where we define

$$\tilde{U}^L(\mathbf{Z}) := \frac{1}{n(n-1)} \sum_{(i,j) \in [n]_2} h(Z_i, Z_j; Z_{n+l_i}, Z_{n+l_j}).$$

Note that in the above we have used the invariance  $h(x_1, x_2; y_1, y_2) = h(x_1, x_2; y_2, y_1)$ .

Now additionally define  $\zeta_i$  as i.i.d. Rademacher variables, and let  $\sigma \sim \text{Uniform}(\mathfrak{S}_{n+m})$ . For any fixed  $\mathbf{Z}$

$$\tilde{U}^L(\sigma \mathbf{Z}) =^d \tilde{U}^{L,\zeta}(\sigma \mathbf{Z}) \quad (6)$$

where we have defined

$$\tilde{U}^{L,\zeta}(\mathbf{Z}) := \frac{1}{n(n-1)} \sum_{(i,j) \in [n]_2} \zeta_i \zeta_j h(Z_i, Z_j; Z_{n+l_i}, Z_{n+l_j}).$$

This works because we can first define  $\tilde{Z}_i = Z_i$  or  $\tilde{Z}_i = Z_{n+l_i}$ , each with probability  $\frac{1}{2}$ . The distribution of  $\tilde{U}^L(\sigma \mathbf{Z}) =^d \tilde{U}^{L,\zeta}(\sigma \mathbf{Z})$ , and then using the symmetry of  $k(x, y)$  in its arguments gives the equivalence Equation (6) (c.f. eq. 28, Kim et al., 2022).

Now for fixed  $\mathbf{Z}$ , combining Equations (5) and (6) and Jensen's inequality we gives

$$\begin{aligned} \mathbb{E}_\sigma \exp(tU(\sigma \mathbf{Z})) &= \mathbb{E}_\sigma \exp(t\mathbb{E}_L[\tilde{U}^L(\sigma \mathbf{Z})|\sigma]) \\ &= \mathbb{E}_\sigma \exp(t\mathbb{E}_{L,\zeta}[\tilde{U}^{L,\zeta}(\sigma \mathbf{Z})|\sigma]) \\ &\leq \mathbb{E}_{\sigma,\zeta} \exp \left( t\mathbb{E}_L \left[ \frac{1}{n(n-1)} \sum_{(i,j) \in [n]_2} \zeta_i \zeta_j h(Z_{\sigma(i)}, Z_{\sigma(j)}; Z_{\sigma(n+l_i)}, Z_{\sigma(n+l_j)}) \middle| \sigma \right] \right) \\ &= \mathbb{E}_{\sigma,\zeta} \exp \left( t \frac{1}{n(n-1)} \sum_{(i,j) \in [n]_2} \zeta_i \zeta_j \mathbb{E}_L \left[ h(Z_{\sigma(i)}, Z_{\sigma(j)}; Z_{\sigma(n+l_i)}, Z_{\sigma(n+l_j)}) \middle| \sigma \right] \right) \\ &=: \mathbb{E}_{\sigma,\zeta} \exp \left( t \sum_{i=1}^n \sum_{j=1}^n \zeta_i \zeta_j A_{ij}^\sigma \right). \end{aligned}$$

In the final step we have defined the matrix  $A^\sigma$ , with entries  $A_{ij}^\sigma = (n(n-1))^{-1} \mathbb{E}_L \left[ h(Z_{\sigma(i)}, Z_{\sigma(j)}; Z_{\sigma(n+l_i)}, Z_{\sigma(n+l_j)}) \right]$  for  $i \neq j$  and  $A_{ii} = 0$  for all  $i$ .

We note that  $\zeta$  is independent of  $\sigma$  and satisfies the conditions of Theorem 6, so applying this theorem we obtain that

$$\begin{aligned} \mathbb{E}_{\sigma,\zeta} \exp \left( t \sum_{i=1}^n \sum_{j=1}^n \zeta_i \zeta_j A_{ij}^\sigma \right) &\leq \mathbb{E}_\sigma \exp \left( 16t^2 \|A^\sigma\|_F^2 \right) && \text{for } |t| < (4\sqrt{2} \|A^\sigma\|)^{-1} \\ &\leq \mathbb{E}_\sigma \exp \left( 16t^2 \|A^\sigma\|_F^2 \right) && \text{for } |t| < (4\sqrt{2} \|A^\sigma\|_F)^{-1} \\ &\leq \exp \left( 16t^2 \sup_{\sigma \in \mathfrak{S}_{n+m}} \|A^\sigma\|_F^2 \right) && \text{for } |t| < (4\sqrt{2} \sup_{\sigma \in \mathfrak{S}_{n+m}} \|A^\sigma\|_F)^{-1} \end{aligned}$$

where in the second line we have used that  $\|M\| \leq \|M\|_F$  for any matrix  $M$ .

Now note that

$$\|A^\sigma\|_F^2 = \sum_{i=1}^n \sum_{i'=1}^n (A_{ii'}^\sigma)^2$$

$$\begin{aligned}
&= \frac{1}{n^2(n-1)^2} \sum_{(i,i') \in [n]_2} (\mathbb{E}_L [h(Z_{\sigma(i)}, Z_{\sigma(i')}); Z_{\sigma(n+l_i)}, Z_{\sigma(n+l_{i'})}] | \sigma])^2 \\
&= \frac{1}{n^2(n-1)^2} \sum_{(i,i') \in [n]_2} \left( \frac{1}{m(m-1)} \sum_{(j,j') \in [m]_2} h(Z_{\sigma(i)}, Z_{\sigma(i')}); Z_{\sigma(n+j)}, Z_{\sigma(n+j')}) \right)^2.
\end{aligned}$$

We complete the proof by noting that  $\bar{U}(\mathbf{Z})^2 = \sup_{\sigma \in \mathfrak{S}_{n+m}} \|A^\sigma\|_F^2$ .  $\square$

**Proof of Theorem 8.** We have

$$\begin{aligned}
\bar{U}^2(\mathbf{Z}) &= \frac{1}{n^2(n-1)^2} \sum_{(i,i') \in [n]_2} \left( \frac{1}{m(m-1)} \sum_{(j,j') \in [m]_2} h(Z_{\sigma(i)}, Z_{\sigma(i')}); Z_{\sigma(n+j)}, Z_{\sigma(n+j')}) \right)^2 \\
&\leq \frac{1}{n^2(n-1)^2 m(m-1)} \sum_{(i,i') \in [n]_2} \sum_{(j,j') \in [m]_2} h(Z_{\sigma(i)}, Z_{\sigma(i')}); Z_{\sigma(n+j)}, Z_{\sigma(n+j')})^2 \\
&\leq \frac{4}{n^2(n-1)^2 m(m-1)} \sum_{(i,i') \in [n]_2} \sum_{(j,j') \in [m]_2} \left( k(Z_{\sigma(i)}, Z_{\sigma(i')})^2 + k(Z_{\sigma(n+j)}, Z_{\sigma(n+j')})^2 \right. \\
&\quad \left. + k(Z_{\sigma(i)}, Z_{\sigma(n+j')})^2 + k(Z_{\sigma(i')}, Z_{\sigma(n+j)})^2 \right) \\
&= \frac{4}{n^2(n-1)^2 m(m-1)} \left( m(m-1) \sum_{(i,i') \in [n]_2} k(Z_{\sigma(i)}, Z_{\sigma(i')})^2 \right. \\
&\quad \left. + n(n-1) \sum_{(j,j') \in [m]_2} k(Z_{\sigma(n+j)}, Z_{\sigma(n+j')})^2 \right. \\
&\quad \left. + (m-1)(n-1) \sum_{1 \leq i \leq n} \sum_{1 \leq j \leq m} k(Z_{\sigma(i)}, Z_{\sigma(n+j)})^2 \right. \\
&\quad \left. + (m-1)(n-1) \sum_{1 \leq i \leq n} \sum_{1 \leq j \leq m} k(Z_{\sigma(i')}, Z_{\sigma(n+j)})^2 \right) \\
&\leq \frac{16}{n^2(n-1)^2} \sum_{(i,j) \in [n+m]_2} k(Z_i, Z_j)^2 \\
&= \frac{16}{n(n-1)} \widehat{N}(\mathbf{Z})
\end{aligned}$$

where the first inequality holds by Jensen's inequality, the second by convexity (so that  $(a+b+c+d)^2 \leq 4(a^2+b^2+c^2+d^2)$ ) and the third inequality using  $n \leq m$  to upper bound each of the four scalars inside the parentheses by  $m(m-1)$ , and we also upper bounded each of sums over subsets of terms by the sum over all possible terms.

For the second part note that since  $h \in [-2\kappa, 2\kappa]$

$$\begin{aligned}
\bar{U}^2(\mathbf{Z}) &= \frac{1}{n^2(n-1)^2} \sum_{(i,i') \in [n]_2} \left( \frac{1}{m(m-1)} \sum_{(j,j') \in [m]_2} h(Z_{\sigma(i)}, Z_{\sigma(i')}); Z_{\sigma(n+j)}, Z_{\sigma(n+j')}) \right)^2 \\
&\leq \frac{1}{n^2(n-1)^2} \sum_{(i,i') \in [n]_2} (2\kappa)^2 \\
&\leq \frac{4\kappa^2}{n(n-1)}.
\end{aligned}$$

$\square$

### C.3. Bounds for MMD-Fuse under Null: Proof of Theorem 5

**Proof of Theorem 5.** Note under the null  $\mathbf{Z}$  is permutation invariant. We will use Theorem 7 with  $h$  as the MMD 2-statistic kernel, so that  $U(\mathbf{Z}) = \widehat{\text{MMD}}^2(\mathbf{Z})$  (for fixed  $k$ ). We will use the notation  $\leq_{1-\delta}$  to denote that the inequality holds with probability at least  $1 - \delta$  over the random variables being considered.

Note that  $\bar{U}^2 \leq 4\kappa^2/n(n-1)$  so that

$$\begin{aligned}
& \log \mathbb{E}_{k \sim \pi(\langle \mathbf{Z} \rangle)} \exp\left(t \widehat{\text{MMD}}_k^2(\mathbf{X}, \mathbf{Y})\right) \\
& \leq_{1-\delta} \frac{1}{t} \log \mathbb{E}_{\mathbf{Z}} \mathbb{E}_{k \sim \pi(\langle \mathbf{Z} \rangle)} \exp\left(t \widehat{\text{MMD}}_k^2(\mathbf{X}, \mathbf{Y})\right) + \log \frac{1}{\delta} && \text{Markov} \\
& = \log \mathbb{E}_{\sigma} \mathbb{E}_{\mathbf{Z}} \mathbb{E}_{k \sim \pi(\langle \mathbf{Z} \rangle)} \exp\left(t \widehat{\text{MMD}}_k^2(\sigma \mathbf{Z})\right) + \log \frac{1}{\delta} && \text{Null Permutation-Free} \\
& = \log \mathbb{E}_{\mathbf{Z}} \mathbb{E}_{k \sim \pi(\langle \mathbf{Z} \rangle)} \mathbb{E}_{\sigma} \exp\left(t \widehat{\text{MMD}}_k^2(\sigma \mathbf{Z})\right) + \log \frac{1}{\delta} && \text{Prior Permutation-Free} \\
& \leq \log \mathbb{E}_{\mathbf{Z}} \mathbb{E}_{k \sim \pi(\langle \mathbf{Z} \rangle)} \mathbb{E}_{\sigma} \exp\left(t^2 \bar{U}_k^2\right) + \log \frac{1}{\delta} \\
& \leq \frac{4\kappa^2 t^2}{n(n-1)} + \log \frac{1}{\delta},
\end{aligned}$$

where the penultimate result holds provided  $|t| < (4\sqrt{2} \sup_k \bar{U}_k(\mathbf{Z}))^{-1}$ . By dividing  $\widehat{\text{MMD}}^2$  by the permutation invariant  $\widehat{N}_k$  in every one of the above, we also find that

$$\log \mathbb{E}_{k \sim \pi(\langle \mathbf{Z} \rangle)} \exp\left(t \frac{\widehat{\text{MMD}}_k^2(\mathbf{X}, \mathbf{Y})}{\sqrt{\widehat{N}_k(\langle \mathbf{Z} \rangle)}}\right) \leq \frac{16t^2}{n(n-1)} + \log \frac{1}{\delta},$$

in the final step using that  $\bar{U}^2 \leq 16\widehat{N}_k/n(n-1)$ . The upper tail bounds for  $\widehat{\text{FUSE}}_N$  and  $\widehat{\text{FUSE}}_1$  immediately follow from their definitions and  $t = \lambda$ .

**Lower Bounds.** For the lower tails, we note that for any function  $f(\mathbf{Z}, k)$  and  $s > 0$ ,

$$\begin{aligned}
\log \mathbb{E}_{k \sim \pi(\langle \mathbf{Z} \rangle)} \exp(\lambda f(\mathbf{Z}, k)) & \geq \sup_{\rho} \rho[f(\mathbf{Z}, k)] - \frac{\text{KL}(\rho, \pi)}{\lambda} \\
& \geq \mathbb{E}_{k \sim \pi(\langle \mathbf{Z} \rangle)}[f(\mathbf{Z}, k)] = \frac{1}{s} \mathbb{E}_{k \sim \pi(\langle \mathbf{Z} \rangle)} \exp(sf(\mathbf{Z}, k)).
\end{aligned}$$

Combining this with the above results and  $t = -s$  gives

$$\begin{aligned}
-\widehat{\text{FUSE}}_1(\mathbf{Z}) & \leq_{1-\delta} \frac{4\kappa^2 t^2}{n(n-1)} + \log \frac{1}{\delta}, \\
-\widehat{\text{FUSE}}_N(\mathbf{Z}) & \leq_{1-\delta} \frac{16t^2}{n(n-1)} + \log \frac{1}{\delta}.
\end{aligned}$$

Unlike the upper bounds, where rates depend on setting  $\lambda \asymp n$ , we can freely choose  $s$  here to optimise the lower bounds.

**Under Permutation.** To prove the equivalent result for  $\sigma \mathbf{Z}$  under permutations, we replace  $\mathbf{Z}$  by  $\sigma \mathbf{Z}$  and our application of Markov's inequality introducing an expectation over  $\mathbf{Z}$  with one over  $\sigma$ . This changes nothing else in the derivations.  $\square$

## D. Concentration under the alternative

We give the exponential convergence bounds for  $\widehat{\text{FUSE}}_1$  under the alternative and relate it to its mean. In the following we will assume that  $\mathcal{K}$  is a class of kernels bounded by  $0 < \kappa < \infty$ , so that  $\widehat{\text{FUSE}}_1 \in [-2\kappa, 2\kappa]$ . We also introduce the following quantity (for fixed, data-free prior  $\pi$ ) which is closely related to the expectation of  $\widehat{\text{FUSE}}_1$ ,

$$\text{FUSE}_1 := \sup_{\rho \in \mathcal{M}_+^1(\mathcal{K})} \text{MMD}^2(p, q; K_\rho) - \frac{\text{KL}(\rho, \pi)}{\lambda}.$$

**Theorem 9.** *FUSE<sub>1</sub> is bounded in the following ways:*

$$\text{FUSE}_1 \leq \mathbb{E}_{\mathbf{Z}} \widehat{\text{FUSE}}_1(\mathbf{Z}) \leq \text{FUSE}_1 + 8\kappa^2 \lambda \left( \frac{1}{n} + \frac{1}{m} \right),$$

and

$$\text{MMD}^2(p, q; K_\pi) \leq \text{FUSE}_1 \leq \sup_{\rho \in \mathcal{M}_+^1(\mathcal{K}) : \text{KL}(\rho, \pi) < \infty} \text{MMD}^2(p, q; K_\rho) \leq \sup_{k \in \text{supp}(\pi)} \text{MMD}^2(p, q; k).$$

Under the null hypothesis  $\text{FUSE}_1 = 0$ .

We can now state concentration results for  $\widehat{\text{FUSE}}_1$  in terms of  $\text{FUSE}_1$ .

**Theorem 10.** *With probability at least  $1 - \delta$  over the sample*

$$\widehat{\text{FUSE}}_1(\mathbf{Z}) - \text{FUSE}_1 \leq 8\kappa^2 \lambda \left( \frac{1}{n} + \frac{1}{m} \right) + \frac{\log \delta^{-1}}{\lambda}$$

and with the same probability,

$$\text{FUSE}_1 - \widehat{\text{FUSE}}_1(\mathbf{Z}) \leq \kappa \sqrt{8 \left( \frac{1}{n} + \frac{1}{m} \right) \log \delta^{-1}}.$$

### D.1. Proofs

We begin with the following lemma.

**Theorem 11** (Bounded Difference Lemma). *A function  $f$  has the bounded difference property there exist constants  $L_\ell < \infty, \ell \in [n]$  such that*

$$|f(z_1, \dots, z_k, \dots, z_n) - f(z_1, \dots, z'_\ell, \dots, z_n)| \leq L_\ell$$

for any choices of  $z_1, \dots, z_n, z'_\ell$ , and  $\ell \in [n]$ .

For such a function and any independent random variables  $Z_1, \dots, Z_n$  and  $t \in \mathbb{R}$  (subject to appropriate measurability restrictions)

$$\mathbb{E} \exp(t(f(Z_1, \dots, Z_n) - \mathbb{E}f(Z_1, \dots, Z_n))) \leq \exp\left(\frac{1}{8}t^2 \sum_{\ell=1}^n L_\ell^2\right).$$

**Proof of Theorem 11.** We introduce the Doob construction, defining

$$D_\ell = \mathbb{E}[f(Z_1, \dots, Z_n) | Z_1, \dots, Z_\ell] - \mathbb{E}[f(Z_1, \dots, Z_n) | Z_1, \dots, Z_{\ell-1}]$$

This is a martingale difference sequence with

$$\sum_{\ell=1}^n D_\ell = f(Z_1, \dots, Z_n) - \mathbb{E}f(Z_1, \dots, Z_n).$$

It is shown by (for example) [Wainwright \(2019, Ch. 2.2, p.37\)](#) that  $D_\ell$  lies in an interval of length at most  $L_\ell$  by the bounded differences assumption. Thus, applying iterated expectation and Hoeffding's lemma for the MGF of bounded random variables,

$$\begin{aligned} \mathbb{E} \exp(t(f(Z_1, \dots, Z_n) - \mathbb{E}f(Z_1, \dots, Z_n))) &= \mathbb{E} \exp\left(\lambda \sum_{\ell=1}^n D_\ell\right) \\ &= \mathbb{E} \left[ \exp\left(\lambda \sum_{\ell=1}^{n-1} D_\ell\right) \mathbb{E}[\exp(\lambda D_n) | Z_1, \dots, Z_{n-1}] \right] \\ &\leq \mathbb{E} \left[ \exp\left(\lambda \sum_{\ell=1}^{n-1} D_\ell\right) \right] \exp\left(\frac{1}{8} \lambda^2 L_n^2 D_n\right) \\ &\leq \exp\left(\frac{1}{8} t^2 \sum_{\ell=1}^n L_\ell^2\right). \end{aligned}$$

□

The MGF of  $\widehat{\text{MMD}}^2$  can then be bounded using the following result, proved via the above.

**Theorem 12.** *For bounded kernel  $k \leq \kappa$ ,  $t \in \mathbb{R}$  and sample sizes  $m, n$ ,*

$$\mathbb{E} \exp(t(\widehat{\text{MMD}}^2(X, Y; k) - \text{MMD}^2(p, q; k))) \leq \exp\left(8t^2 \kappa^2 \left(\frac{1}{m} + \frac{1}{n}\right)\right).$$

**Proof of Theorem 12.** We show that  $\widehat{\text{MMD}}^2(x, y; k)$  has the bounded differences property and then apply Theorem 11. Denote by  $x^{\setminus \ell}$  for  $\ell \in [n]$  that the  $\ell$ -th example in the  $x$  sample is changed. Then

$$\begin{aligned} &|\widehat{\text{MMD}}^2(x, y; k) - \widehat{\text{MMD}}^2(x^{\setminus \ell}, y; k)| \\ &= \left| \frac{2}{n(n-1)} \sum_{i \in [n] \setminus \{\ell\}} (k(x_\ell, x_i) - k(x'_\ell, x_i)) - \frac{2}{mn} \sum_{j=1}^m (k(x_\ell, y_j) - k(x'_\ell, y_j)) \right| \\ &\leq \frac{2}{n(n-1)} \sum_{i \in [n] \setminus \{\ell\}} |k(x_\ell, x_i) - k(x'_\ell, x_i)| + \frac{2}{mn} \sum_{j=1}^m |k(x_\ell, y_j) - k(x'_\ell, y_j)| \\ &\leq \frac{2}{n(n-1)} (n-1) \cdot 2\kappa + \frac{2}{mn} m \cdot 2\kappa \\ &= \frac{8\kappa}{n}. \end{aligned}$$

A similar process for the  $y$  sample gives bounds of  $8\kappa/m$ , so that  $\widehat{\text{MMD}}^2$  has the bounded differences property with

$$\sum_{\ell=1}^{n+m} L_\ell^2 \leq n \cdot \left(\frac{8\kappa}{n}\right)^2 + m \cdot \left(\frac{8\kappa}{m}\right)^2 = 64\kappa^2 \left(\frac{1}{n} + \frac{1}{m}\right).$$

□

**Proof of Theorem 9.** For the first lower bound, note

$$\mathbb{E}_{\mathbf{Z}} \widehat{\text{FUSE}}_1(\mathbf{Z}) = \mathbb{E}_{\mathbf{Z}} \sup_{\rho} \mathbb{E}_{\rho} [\widehat{\text{MMD}}_k^2] - \frac{\text{KL}}{\lambda} \geq \sup_y \mathbb{E}_{\mathbf{Z}, \rho} [\widehat{\text{MMD}}_k^2] - \frac{\text{KL}}{\lambda} = \text{FUSE}_1.$$

For the upper bound, note that

$$\begin{aligned} \mathbb{E}_{\mathbf{Z}} \widehat{\text{FUSE}}_1(\mathbf{Z}) &\leq \left[ \frac{1}{\lambda} \log \left( \mathbb{E}_{\mathbf{Z}} \mathbb{E}_{k \sim \pi} \left[ e^{\lambda \widehat{\text{MMD}}_k^2} \right] \right) \right] && \text{Jensen} \\ &\leq \left[ \frac{1}{\lambda} \log \left( \mathbb{E}_{k \sim \pi} \mathbb{E}_{\mathbf{Z}} \left[ e^{\lambda \widehat{\text{MMD}}_k^2} \right] \right) \right] && \text{Independence of } \pi \text{ from } \mathbf{Z} \\ &\leq \frac{1}{\lambda} \log \left( \mathbb{E}_{k \sim \pi} \left[ e^{\lambda \text{MMD}_k^2 + 8\lambda^2 \kappa^2 / N} \right] \right) && \text{Theorem 12} \\ &= \text{FUSE}_1 + 8\kappa^2 \lambda \left( \frac{1}{n} + \frac{1}{m} \right). \end{aligned}$$

The lower bound on  $\text{FUSE}_1$  is obtained by relaxing the supremum with  $\rho = \pi$ . The upper bounds come since the supremum over  $\rho \in \mathcal{M}_+^1(\mathcal{K}) : \text{KL}(\rho, \pi) < \infty$  of  $\text{MMD}^2$  is clearly greater than the KL-regularised version. Under the null hypothesis,  $\text{MMD}(p, q; k) = 0$  for every kernel (regardless of them being characteristic or not), so  $\text{FUSE}_1 = 0$ . □

**Proof of Theorem 10.** For the upper bound,

$$\begin{aligned} \widehat{\text{FUSE}}_1(\mathbf{Z}) &= \left[ \frac{1}{\lambda} \log \left( \mathbb{E}_{k \sim \pi} \left[ e^{\lambda \widehat{\text{MMD}}_k^2} \right] \right) \right] \\ &\leq_{1-\delta} \left[ \frac{1}{\lambda} \log \left( \mathbb{E}_{\mathbf{Z}} \mathbb{E}_{k \sim \pi} \left[ e^{\lambda \widehat{\text{MMD}}_k^2} \right] \right) \right] + \frac{\log \delta^{-1}}{\lambda} && \text{Markov} \\ &\leq \left[ \frac{1}{\lambda} \log \left( \mathbb{E}_{k \sim \pi} \mathbb{E}_{\mathbf{Z}} \left[ e^{\lambda \widehat{\text{MMD}}_k^2} \right] \right) \right] + \frac{\log \delta^{-1}}{\lambda} && \text{Independence of } \pi \text{ from } \mathbf{Z} \\ &\leq \frac{1}{\lambda} \log \left( \mathbb{E}_{k \sim \pi} \left[ e^{\lambda \text{MMD}_k^2 + 8\lambda^2 \kappa^2 (m^{-1} + n^{-1})} \right] \right) + \frac{\log \delta^{-1}}{\lambda} && \text{Theorem 12} \\ &= \text{FUSE}_1 + 8\kappa^2 \lambda \left( \frac{1}{n} + \frac{1}{m} \right) + \frac{\log \delta^{-1}}{\lambda}. \end{aligned}$$

For the lower bound, let  $\rho^*$  be the value of  $\rho$  achieving the supremum in the dual form of  $\text{FUSE}_1$  (which we note is independent of the sample), so that

$$\begin{aligned} \text{FUSE}_1 - \widehat{\text{FUSE}}_1(\mathbf{Z}) &= \sup_{\rho} \left\{ \mathbb{E}_{\rho^*} [\text{MMD}_k^2] - \frac{\text{KL}(\rho, \pi)}{\lambda} \right\} - \sup_{\rho} \left\{ \mathbb{E}_{\rho} [\widehat{\text{MMD}}_k^2] - \frac{\text{KL}(\rho, \pi)}{\lambda} \right\} \\ &= \mathbb{E}_{\rho^*} [\text{MMD}_k^2] - \frac{\text{KL}(\rho^*, \pi)}{\lambda} - \sup_{\rho} \left\{ \mathbb{E}_{\rho} [\widehat{\text{MMD}}_k^2] - \frac{\text{KL}(\rho, \pi)}{\lambda} \right\} \\ &\leq \mathbb{E}_{\rho^*} [\text{MMD}_k^2] - \frac{\text{KL}(\rho^*, \pi)}{\lambda} - \left( \mathbb{E}_{\rho^*} [\widehat{\text{MMD}}_k^2] - \frac{\text{KL}(\rho^*, \pi)}{\lambda} \right) \\ &= \mathbb{E}_{\rho^*} [\text{MMD}_k^2 - \widehat{\text{MMD}}_k^2] \\ &= \text{MMD}^2(p, q; K_{\rho^*}) - \widehat{\text{MMD}}_k^2(\mathbf{X}, \mathbf{Y}; K_{\rho^*}). \end{aligned}$$

This is of the form with an MGF that can be bounded by Theorem 12, so we apply Chernoff's exponential inequality to obtain the final result (since  $K_{\rho^*}$  is independent of the sample). □

## E. Power Analysis

### E.1. General Recipe for Power Analysis of Permutation Tests

The general outline for power analysis consists of the following: First we start with the Type II error probability. Then we attempt to upper bound it by iteratively applying the following simple lemma to the different terms.

**Monotonicity in High Probability.** Let  $X, Y$  be r.v.s, such that  $X \leq Y$  w.p.  $\geq 1 - \delta$ . Then  $\mathbb{P}(X \geq c) \leq \mathbb{P}(Y \geq c) + \delta$ . This result can be applied both when  $X \leq Y$  a.s. giving  $\delta = 0$ , or if  $Y = a$  is constant.

Iteratively applying this lemma gives  $\mathbb{P}(\text{Type II}) \leq N\delta$ , and then we set  $N\delta = \beta$ .

As a first step in the above process we will use the following useful result (adapted from [Kim et al., 2022](#)) to convert from the random permutations we use in practice to the full set of permutation. This result shows that when  $B$  is taken sufficiently large (roughly  $\Omega(\alpha^{-2} \log(\beta^{-1}))$ ), the only changes to the final power results will be in constants multiplying  $\alpha$  and  $\beta$ .

**Theorem 13** (From Randomised to Deterministic Permutations). *Suppose  $G = (g_1, \dots, g_{B+1})$  consists of  $B$  uniformly drawn permutations from  $\mathcal{G}$ , plus the identity permutation as  $g_{B+1}$ . Then*

$$\mathbb{P}\left(\tau(\mathbf{Z}) \leq \text{quantile}_{1-\alpha, G}\tau(g\mathbf{Z})\right) \leq \mathbb{P}\left(\tau(\mathbf{Z}) \leq \text{quantile}_{1-\alpha_B, \mathcal{G}}\tau(g\mathbf{Z})\right) + \delta$$

where  $1 - \alpha_B = \frac{B+1}{B}(1 - \alpha) + \sqrt{\frac{\log(2/\delta)}{2B}}$ .

We note that provided  $B \geq 8\alpha^{-2} \log(2/\delta)$ , then  $1 - \alpha_B \leq 1 - \alpha/2$ .

**Proof.** We note the Dvoretzky–Kiefer–Wolfowitz inequality [Dvoretzky et al. \(1956\)](#); [Massart \(1990\)](#) for empirical CDF  $F_n$  of  $n$  samples from original CDF  $F$ :

$$\mathbb{P}\left(\sup_x |F_n(x) - F(x)| \geq t\right) \leq 2e^{-2nt^2} \quad (7)$$

for every  $t > 0$ .

The permutation CDF for a group  $\mathcal{G}$  take the form

$$F_{\mathcal{G}}(x) = \frac{1}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} \mathbf{1}\{\tau(g\mathbf{Z}) \leq x\}$$

and given sample  $\tilde{G} = (g_1, \dots, g_B)$  i.i.d. uniformly from  $\mathcal{G}$  (this excludes the identity permutation added to  $G$ ), the empirical CDF is

$$\hat{F}_{\tilde{G}}(x) = \frac{1}{B} \sum_{g \in \tilde{G}} \mathbf{1}\{\tau(g\mathbf{Z}) \leq x\}$$

We can also write  $\hat{F}_{\tilde{G}}(x)$  including the identity permutation as  $g_{B+1}$ , and note that  $\hat{F}_G(x) =$   
Define the good event

$$\mathcal{A} = \left\{ \sup_x |F_{\tilde{G}}(x) - F_{\mathcal{G}}(x)| \leq \sqrt{\frac{\log(2/\delta)}{2B}} \right\}$$

which holds with probability at least  $1 - \delta$  by Equation (7). Given  $\mathcal{A}$ , we have

$$\begin{aligned}
q_G &:= \underset{1-\alpha, g \in G}{\text{quantile}} \tau(g\mathbf{Z}) = \inf\left\{r \in \mathbb{R} : \frac{1}{B+1} \sum_{g \in G} \mathbf{1}\{\tau(g\mathbf{Z}) \leq r\} \geq 1 - \alpha\right\} \\
&\leq \inf\left\{r \in \mathbb{R} : \frac{1}{B+1} \sum_{g \in G} \mathbf{1}\{\tau(g\mathbf{Z}) \leq r\} \geq 1 - \alpha\right\} \\
&= \inf\left\{r \in \mathbb{R} : \widehat{F}_{\tilde{G}}(r) \geq \frac{B+1}{B}(1 - \alpha)\right\} \\
&\leq \inf\left\{r \in \mathbb{R} : \widehat{F}_G(r) \geq \frac{B+1}{B}(1 - \alpha) + \sqrt{\frac{\log(2/\delta)}{2B}}\right\} \\
&= \underset{1-\alpha_B, g \in \mathcal{G}}{\text{quantile}} \tau(g\mathbf{Z}) =: q
\end{aligned}$$

where we have defined  $\alpha_B$  as above.

$$\mathbb{P}(\tau \leq q_G) \leq \mathbb{P}(\tau \leq q_G | \mathcal{A}) + \mathbb{P}(\mathcal{A}^c) \leq \mathbb{P}(\tau \leq q) + \delta. \quad \square$$

## E.2. Variance of $\widehat{\text{MMD}}^2$

In proving our power results it is necessary to upper bound the variance of  $\widehat{\text{MMD}}^2$ .

**Theorem 14.** *For any kernel  $k$  upper bounded by  $\kappa$ , if  $n \leq m \leq cn$  for  $c \geq 1$ , there exists universal constant  $C > 0$  depending only on  $c$ , such that*

$$\mathbb{V}[\widehat{\text{MMD}}^2] \leq C \left( \frac{4\kappa \text{MMD}^2}{n} + \frac{\kappa^2}{n^2} \right)$$

**Proof.** We define

$$\begin{aligned}
\sigma_{10}^2 &= \mathbb{V}_X(\mathbb{E}_{X', Y, Y'}[h(X, X', Y, Y')]) \\
\sigma_{01}^2 &= \mathbb{V}_Y(\mathbb{E}_{X, X', Y'}[h(X, X', Y, Y')]) \\
\sigma_{11}^2 &= \max\{\mathbb{E}[k^2(X, X')], \mathbb{E}[k^2(X, Y)], \mathbb{E}[k^2(Y, Y')]\}.
\end{aligned}$$

From a well-known bound (based on Lee, 1990, Equation 2, p.38; see also Kim et al., 2022, Appendix F, Equation 59 or Schrab et al., 2021, Proposition 3),

$$\begin{aligned}
\mathbb{V}[\widehat{\text{MMD}}^2] &\leq C \left( \frac{\sigma_{10}^2}{m} + \frac{\sigma_{01}^2}{n} + \sigma_{11}^2 \left( \frac{1}{m} + \frac{1}{n} \right)^2 \right) \\
&\leq C \left( \frac{\sigma_{10}^2}{n} + \frac{\sigma_{01}^2}{n} + \frac{\sigma_{11}^2}{n^2} \right)
\end{aligned}$$

where we used that  $n \leq m \leq cn$ . and the result in red above, and the boundedness of the kernel for the final term. This gives the further bound

$$\mathbb{V}[\widehat{\text{MMD}}^2] \leq C \left( \frac{4\kappa \text{MMD}^2}{n} + \frac{\kappa^2}{n^2} \right)$$

$$\begin{aligned}
\sigma_{10}^2 &= \text{var}_X(\mathbb{E}_{X', Y, Y'}[h(X, X', Y, Y')]) \\
&= \mathbb{E}_X \left[ (\mathbb{E}_{X', Y, Y'}[h(X, X', Y, Y')])^2 \right]
\end{aligned}$$



$$\begin{aligned}
&= \mathbb{E}_X \left[ \langle \phi(X) - \phi(Y), \phi(X') - \phi(Y') \rangle^2 \right] \\
&\leq \left( \mathbb{E}_X \left[ \|\phi(X) - \mu_Q\|^2 \right] \right) \|\mu_P - \mu_Q\|^2 \\
&\leq 2\kappa \|\mu_P - \mu_Q\|^2 \\
&= 2\kappa \text{MMD}^2,
\end{aligned}$$

a similar result for  $\sigma_{01}$ , and the simple bound  $\sigma_{11}^2 \leq \kappa^2$ .  $\square$

### E.3. Proof of Theorem 2

**Proof.** For any  $\rho$ , we define

$$S_\rho = \text{MMD}^2(p, q; K_\rho) - \frac{\text{KL}(\rho, \pi)}{\lambda} - \text{quantile}_{1-\alpha_B, \mathcal{G}} \widehat{\text{FUSE}}_1(\sigma \mathbf{Z})$$

and note that  $1 - \alpha_B < 1 - \alpha/2$  under the assumption  $B \geq 8\alpha^{-2} \log(4/\beta)$ .

By Theorem 13 we can consider the full permutation set as

$$\mathbb{P}_{p \times q, \mathcal{G}} \left( \widehat{\text{FUSE}}_1(\mathbf{Z}) \leq \text{quantile}_{1-\alpha, \mathcal{G}} \widehat{\text{FUSE}}_1(\sigma \mathbf{Z}) \right) \leq \mathbb{P}_{p \times q} \left( \widehat{\text{FUSE}}_1(\mathbf{Z}) \leq \text{quantile}_{1-\alpha_B, \mathcal{G}} \widehat{\text{FUSE}}_1(\sigma \mathbf{Z}) \right) + \beta/2.$$

Next, Type II under the full permutation set can be bounded as

$$\begin{aligned}
&\mathbb{P}_{p \times q} \left( \widehat{\text{FUSE}}_1(\mathbf{Z}) \leq \text{quantile}_{1-\alpha_B, \mathcal{G}} \widehat{\text{FUSE}}_1(\sigma \mathbf{Z}) \right) \\
&= \mathbb{P} \left( \text{MMD}^2(p, q; K_\rho) - \frac{1}{\lambda} \text{KL}(\rho, \pi) - \widehat{\text{FUSE}}_1(\mathbf{Z}) \geq S_\rho \right) \\
&= \mathbb{P} \left( \text{MMD}^2(p, q; K_\rho) - \frac{1}{\lambda} \text{KL}(\rho, \pi) - \sup_{\rho'} \left( \widehat{\text{MMD}}^2(\mathbf{Z}; K_\rho) - \frac{1}{\lambda} \text{KL}(\rho', \pi) \right) \geq S_\rho \right) \\
&\leq \mathbb{P} \left( \text{MMD}^2(p, q; K_\rho) - \widehat{\text{MMD}}^2(\mathbf{Z}; K_\rho) \geq S_\rho \right) \\
&= \frac{1}{S_\rho^2} \mathbb{V}_{p \times q} \left[ \widehat{\text{MMD}}^2(\mathbf{Z}; K_\rho) \right] \\
&\leq \frac{C_1}{S_\rho^2} \left( \frac{4\kappa \text{MMD}^2}{n} + \frac{\kappa^2}{n^2} \right),
\end{aligned}$$

where the inequalities are  $\sup f(\rho') \geq f(\rho)$ , Chebyshev's, and Theorem 14. This term is upper bounded by  $\beta/2$  if we set

$$S_\rho^2 > \frac{2C_1}{\beta} \left( \frac{4\kappa \text{MMD}^2}{n} + \frac{\kappa^2}{n^2} \right).$$

We also recall that from Theorem 5 when  $\lambda = cn/\kappa$ ,

$$\text{quantile}_{1-\alpha_B, \mathcal{G}} \widehat{\text{FUSE}}_1(\sigma \mathbf{Z}) \leq \frac{C_2 \kappa (1 + \log \alpha^{-1})}{n}.$$

We also note that for  $a, b, x$  all non-negative, if  $x^2 > a^2 + 2b$ , then  $x^2 > ax + b$ . This works because  $x^2 > ax + b$  is equivalent to  $x^2 > \left(\frac{a}{2} + \sqrt{\frac{a^2}{4} + b}\right)^2$  by taking the positive root, and

$$\left(\frac{a}{2} + \sqrt{\frac{a^2}{4} + b}\right)^2 = \frac{a^2}{2} + b + 2\frac{a}{2}\sqrt{\frac{a^2}{4} + b} \leq a^2 + 2b$$

using Young's inequality  $2AB \leq A^2 + B^2$ .

Combining the above the Type II error rate is controlled by  $\beta$  provided any of the following statements are true for any  $\rho$  (with each new result implying the former):

$$\begin{aligned} \text{MMD}^2(p, q; K_\rho) &> \frac{\text{KL}(\rho, \pi)}{\lambda} + \frac{C_2\kappa(1 + \log \alpha^{-1})}{n} + \sqrt{\frac{2C_1}{\beta} \left(\frac{4\kappa \text{MMD}^2}{n} + \frac{\kappa^2}{n^2}\right)} \\ \text{MMD}^2(p, q; K_\rho) &> \frac{\text{KL}(\rho, \pi)}{\lambda} + \frac{C_2\kappa(1 + \log \alpha^{-1})}{n} + \sqrt{\frac{8C_1\kappa}{n\beta} \text{MMD}} + \frac{\sqrt{2C_1\kappa}}{n\sqrt{\beta}} \\ \text{MMD}^2(p, q; K_\rho) &> \frac{2\text{KL}(\rho, \pi)}{\lambda} + \frac{2C_2\kappa(1 + \log \alpha^{-1})}{n} + \frac{8C_1\kappa}{n\beta} + \frac{2\sqrt{2C_1\kappa}}{n\sqrt{\beta}} \\ \text{MMD}^2(p, q; K_\rho) &> \frac{C\kappa}{n} \left(\frac{1}{\beta} + \log \frac{1}{\alpha} + \text{KL}(\rho, \pi)\right) \end{aligned}$$

where we used that  $\sqrt{x+y} \leq \sqrt{x} + \sqrt{y}$ , the result above, and  $\lambda = cn/\kappa$ .  $\square$

#### E.4. Power for $\widehat{\text{FUSE}}_N$

The proof of this statement proceeds similarly to the proof of Theorem 2. We assume that  $n \leq m \leq cn$  for some  $c \geq 1$ . Based on this, note that  $N_k \leq \kappa^2/C_1^2$  for  $C_1$  depending only on  $m/n \in [1, c]$ .

For any  $\rho : \text{KL}(\rho, \pi) < \infty$  we define

$$\begin{aligned} T_\rho &= \frac{C_1}{\kappa} \cdot \text{MMD}_{K_\rho}^2 \\ S_\rho &= T_\rho - \frac{1}{\lambda} \text{KL}(\rho, \pi) - \text{quantile}_{1-\alpha_B, \mathcal{G}} \widehat{\text{FUSE}}_N(\sigma \mathbf{Z}). \end{aligned}$$

Note that (since  $\text{MMD}^2 \geq 0$  is strictly non-negative, unlike  $\widehat{\text{MMD}}^2$  which can be negative),

$$-\mathbb{E}_\rho \left[ \frac{\text{MMD}_k^2}{\sqrt{\widehat{N}_k(\mathbf{Z})}} \right] \leq -\frac{C_1}{\kappa} \mathbb{E}_{k \sim \rho} [\text{MMD}_k^2] = -T_\rho. \quad (8)$$

Now we bound the type II under the full set of permutations as

$$\begin{aligned} &\mathbb{P} \left( \widehat{\text{FUSE}}_N(\mathbf{Z}) \leq \text{quantile}_{1-\alpha_B, \mathcal{G}} \widehat{\text{FUSE}}_N(\sigma \mathbf{Z}) \right) \\ &= \mathbb{P} \left( T_\rho - \frac{1}{\lambda} \text{KL}(\rho, \pi) - \widehat{\text{FUSE}}_N(\mathbf{Z}) \geq S_\rho \right) \\ &= \mathbb{P} \left( T_\rho - \frac{1}{\lambda} \text{KL}(\rho, \pi) - \sup_{\rho'} \left( \mathbb{E}_{k \sim \rho'} \left[ \frac{\widehat{\text{MMD}}^2(\mathbf{Z}; k)}{\sqrt{\widehat{N}_k(\mathbf{Z})}} \right] - \frac{1}{\lambda} \text{KL}(\rho', \pi) \right) \geq S_\rho \right) \end{aligned}$$

$$\begin{aligned}
&\leq \mathbb{P} \left( T_\rho - \mathbb{E}_{k \sim \rho} \left[ \frac{\widehat{\text{MMD}}^2(\mathbf{Z}; k)}{\sqrt{\widehat{N}_k(\mathbf{Z})}} \right] \geq S_\rho \right) && \sup f(\rho') \geq f(\rho) \\
&= \mathbb{P} \left( T_\rho - \mathbb{E}_{k \sim \rho} \left[ \frac{\text{MMD}_k^2}{\sqrt{\widehat{N}_k(\mathbf{Z})}} - \frac{\text{MMD}_k^2}{\sqrt{\widehat{N}_k(\mathbf{Z})}} + \frac{\widehat{\text{MMD}}^2(\mathbf{Z}; k)}{\sqrt{\widehat{N}_k(\mathbf{Z})}} \right] \geq S_\rho \right) \\
&= \mathbb{P} \left( T_\rho - \mathbb{E}_{k \sim \rho} \left[ \frac{\text{MMD}_k^2}{\sqrt{\widehat{N}_k(\mathbf{Z})}} \right] + \mathbb{E}_{k \sim \rho} \left[ \frac{\text{MMD}_k^2 - \widehat{\text{MMD}}^2(\mathbf{Z}; k)}{\sqrt{\widehat{N}_k(\mathbf{Z})}} \right] \geq S_\rho \right) \\
&= \mathbb{P} \left( T_\rho - \mathbb{E}_{k \sim \rho} \left[ \frac{\text{MMD}_k^2}{\sqrt{\widehat{N}_k(\mathbf{Z})}} \right] + \mathbb{E}_{k \sim \rho} \left[ \frac{\text{MMD}_k^2 - \widehat{\text{MMD}}^2(\mathbf{Z}; k)}{\sqrt{\widehat{N}_k(\mathbf{Z})}} \right] \geq S_\rho \right) \\
&\leq \mathbb{P} \left( \mathbb{E}_{k \sim \rho} \left[ \frac{\text{MMD}_k^2 - \widehat{\text{MMD}}^2(\mathbf{Z}; k)}{\sqrt{\widehat{N}_k(\mathbf{Z})}} \right] \geq S_\rho \right) && \text{by Equation (8)} \\
&\leq \mathbb{P} \left( \left| \mathbb{E}_{k \sim \rho} \left[ \frac{\text{MMD}_k^2 - \widehat{\text{MMD}}^2(\mathbf{Z}; k)}{\sqrt{\widehat{N}_k(\mathbf{Z})}} \right] \right| \geq S_\rho \right) && x \leq |x| \\
&\leq \mathbb{P} \left( \mathbb{E}_{k \sim \rho} \left[ \left| \frac{\text{MMD}_k^2 - \widehat{\text{MMD}}^2(\mathbf{Z}; k)}{\sqrt{\widehat{N}_k(\mathbf{Z})}} \right| \right] \geq S_\rho \right) && |x| \text{ convex, Jensen} \\
&= \mathbb{P} \left( \mathbb{E}_{k \sim \rho} \left[ \frac{|\text{MMD}_k^2 - \widehat{\text{MMD}}^2(\mathbf{Z}; k)|}{\sqrt{\widehat{N}_k(\mathbf{Z})}} \right] \geq S_\rho \right) && N_k \text{ non-neg.} \\
&\leq \frac{1}{S_\rho} \mathbb{E}_{\mathbf{Z}} \mathbb{E}_{k \sim \rho} \left[ \frac{|\text{MMD}_k^2 - \widehat{\text{MMD}}^2(\mathbf{Z}; k)|}{\sqrt{\widehat{N}_k(\mathbf{Z})}} \right] && N_k \text{ non-neg, Markov} \\
&\leq \frac{1}{S_\rho} \sqrt{\mathbb{E}_{\mathbf{Z}} \mathbb{E}_{k \sim \rho} \left[ |\text{MMD}_k^2 - \widehat{\text{MMD}}^2(\mathbf{Z}; k)|^2 \right] \mathbb{E}_{\mathbf{Z}} \mathbb{E}_{k \sim \rho} \left[ \frac{1}{\widehat{N}_k(\mathbf{Z})} \right]} && \text{Cauchy-Schwarz.}
\end{aligned}$$

Thus, combining with Theorem 13, our true type II error will be controlled by  $\beta$  if for any  $\rho$

$$S_\rho > \frac{2}{\beta} \sqrt{\mathbb{E}_{\mathbf{Z}} \mathbb{E}_{k \sim \rho} \left[ |\text{MMD}_k^2 - \widehat{\text{MMD}}^2(\mathbf{Z}; k)|^2 \right] \mathbb{E}_{\mathbf{Z}} \mathbb{E}_{k \sim \rho} \left[ \frac{1}{\widehat{N}_k(\mathbf{Z})} \right]}.$$

Provided there is a  $c > 0$  with

$$\mathbb{E}_{p \times q} \left[ \frac{1}{\widehat{N}_k(\mathbf{Z})} \right] \leq c$$

for all  $k$ , use  $\lambda = cn$  and Theorem 5 to reduce this to the condition

$$\text{MMD}^2(p, q; K_\rho) > C_2 \kappa \left( \frac{\log \alpha^{-1}}{n} + \frac{1}{\beta} \sqrt{\mathbb{E}_\rho \mathbb{V}_{p \times q} \left[ \widehat{\text{MMD}}^2(\mathbf{Z}; k) \right]} + \frac{\text{KL}(\rho, \pi)}{n} \right).$$

Applying Theorem 14, the proof is completed in essentially the same way as in the result for FUSE<sub>1</sub> (with slightly different  $\beta$  dependence).