Learning Deep Kernels for Non-Parametric Two-Sample Tests

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Abstract
We propose a class of kernel-based two-sample tests, which aim to determine whether two sets of samples are drawn from the same distribution. Our tests are constructed from kernels parameterized by deep neural nets, trained to maximize test power. These tests adapt to variations in distribution smoothness and shape over space, and are especially suited to high dimensions and complex data. By contrast, the simpler kernels used in prior kernel testing work are spatially homogeneous, and adaptive only in lengthscale. We explain how this scheme includes popular classifier-based two-sample tests as a special case, but improves on them in general. We provide the first proof of consistency for the proposed adaptation method, which applies both to kernels on deep features and to simpler radial basis kernels or multiple kernel learning. In experiments, we establish the superior performance of our deep kernels in hypothesis testing on benchmark and real-world data. The code of our deep-kernel-based two sample tests is available at github.com/fengliu90/DK-for-TST.

1. Introduction
Two sample tests are hypothesis tests aiming to determine whether two sets of samples are drawn from the same distribution. Traditional methods such as $t$-tests and Kolmogorov-Smirnov tests are mainstays of statistical applications, but require strong parametric assumptions about the distributions being studied and/or are only effective on data in extremely low-dimensional spaces. A broad set of recent work in statistics and machine learning has focused on relaxing these assumptions, with methods either generally applicable or specific to various more complex domains (Gretton et al., 2012a; Székely & Rizzo, 2013; Heller & Heller, 2016; Jitkrittum et al., 2016; Ramdas et al., 2017; Lopez-Paz & Oquab, 2017; Chen & Friedman, 2017; Gao et al., 2018; Ghoshdastidar et al., 2017; Ghoshdastidar & von Luxburg, 2018; Li & Wang, 2018; Kirchler et al., 2019). These tests have also allowed application in various machine learning problems such as domain adaptation, generative modeling, and causal discovery (Binkowski et al., 2018; Gong et al., 2016; Stojanov et al., 2019; Lopez-Paz & Oquab, 2017).

A popular class of non-parametric two-sample tests is based on kernel methods (Smola & Schölkopf, 2001): such tests construct a kernel mean embedding (Berlinet & Thomas-Agnan, 2004; Muandet et al., 2017) for each distribution, and measure the difference in these embeddings. For any characteristic kernel, two distributions are the same if and only if their mean embeddings are the same; the distance between mean embeddings is the maximum mean discrepancy (MMD) (Gretton et al., 2012a). There are also several closely related methods, including tests based on checking for differences in mean embeddings evaluated at specific locations (Chwialkowski et al., 2015; Jitkrittum et al., 2016) and kernel Fisher discriminant analysis (Harchaoui et al., 2007). These tests all work well for samples from simple distributions when using appropriate kernels.

Problems that we care about, however, often involve distributions with complex structure, where simple kernels will often map distinct distributions to nearby (and hence hard to distinguish) mean embeddings. Figure 1a shows an example of a multimodal dataset, where the overall modes align but the sub-mode structure varies differently at each mode. A translation-invariant Gaussian kernel only “looks at” the data uniformly within each mode (see Figure 1b), requiring many samples to correctly distinguish the two distributions. The distributions can be distinguished more effectively if we understand the structure of each mode, as with the more complex kernel illustrated in Figure 1c.

To model these complex functions, we adopt a deep kernel approach (Wilson et al., 2016; Sutherland et al., 2017; Li et al., 2017; Jean et al., 2018; Li et al., 2019), building a kernel with a deep network. In this paper, we use

$$k_\omega(x, y) = [(1 - \epsilon)\kappa(\phi_\omega(x), \phi_\omega(y)) + \epsilon]q(x, y), \quad (1)$$
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where the deep neural network $\phi_\omega$ extracts features of samples, and $\kappa$ is a simple kernel (e.g., a Gaussian) on those features, while $q$ is a simple characteristic kernel (e.g., Gaussian) on the input space. With an appropriate choice of $\phi_\omega$, this allows for extremely flexible kernels which can learn complex behavior very different in different parts of space. This choice is discussed further in Section 5.

These complex kernels, though, cannot feasibly be specified by hand or simple heuristics, as is typical practice in kernel methods. We select the parameters $\omega$ by maximizing the ratio of the MMD to its variance, which maximizes test power at large sample sizes. This procedure was proposed by Sutherland et al. (2017), but we establish for the first time that it gives consistent selection of the best kernel in the class, whether optimizing our deep kernels with hundreds of thousands of parameters or simply choosing lengthscales of a Gaussian as did Sutherland et al. Previously, there were no guarantees this procedure would yield a kernel which generalized at all from the training set to a test set.

Another way to compare distributions is to train a classifier between them, and evaluate its accuracy (Lopez-Paz & Oquab, 2017). We show, perhaps surprisingly, that our framework encompasses this approach, but deep kernels allow for more general model classes which can use the data more efficiently. We also train representations directly to maximize test power, rather than a cross-entropy surrogate.

We test our method on several simulated and real-world datasets, including complex synthetic distributions, high-energy physics data, and challenging image problems. We find convincingly that learned deep kernels outperform simple shallow methods, and learning by maximizing test power outperforms learning through a cross-entropy surrogate loss.

2. MMD Two-Sample Tests

Two-sample testing. Let $\mathcal{X}$ be a separable metric space – in this paper, typically a subset of $\mathbb{R}^d$ – and $P, Q$ be Borel probability measures on $\mathcal{X}$. We observe independent identically distributed (i.i.d.) samples $S_P = \{x_i\}_{i=1}^n \sim P^n$ and $S_Q = \{y_j\}_{j=1}^m \sim Q^m$. We wish to know whether $S_P$ and $S_Q$ come from the same distribution: does $P = Q$?

We use the null hypothesis testing framework, where the null hypothesis $H_0 : P = Q$ is tested against the alternative hypothesis $H_1 : P \neq Q$. We perform a two-sample test in four steps: select a significance level $\alpha \in [0, 1]$; compute a test statistic $\hat{t}(S_P, S_Q)$; compute the p-value $\hat{p} = P_{H_0}(T > \hat{t})$, the probability of the two-sample test returning a statistic as large as $t$ when $H_0$ is true; finally, reject $H_0$ if $\hat{p} < \alpha$.

Maximum mean discrepancy (MMD). We will base our two-sample test statistic on an estimate of a distance between distributions. Our metric, the MMD, is defined in terms of a kernel $k$ giving point-level “similarities” on $\mathcal{X}$.

**Definition 1** (Gretton et al., 2012a). Let $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be the kernel of a reproducing kernel Hilbert space $\mathcal{H}_k$, with feature maps $k(\cdot, x) \in \mathcal{H}_k$. Let $X, X' \sim P$ and $Y, Y' \sim Q$, and define the kernel mean embeddings $\mu_P := \mathbb{E}[k(\cdot, X)]$ and $\mu_Q := \mathbb{E}[k(\cdot, Y)]$. Under mild integrability conditions,

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

$$= \|\mu_P - \mu_Q\|_{\mathcal{H}_k} = \sqrt{\mathbb{E}[k(X,X') + k(Y,Y') - 2k(X,Y)]}.$$ 

For characteristic kernels, $\mu_P = \mu_Q$ implies $P = Q$, hence $\text{MMD}(P, Q; \mathcal{H}_k) = 0$ if and only if $P = Q$.

The first form shows that the MMD is an integral probability metric (Müller, 1997), along with such popular distances as the Wasserstein and total variation.

There are several natural estimators of the MMD from samples. We will assume $n = m$ and use the $U$-statistic estimator, which is unbiased for $\text{MMD}^2$ and has nearly minimal variance among unbiased estimators (Gretton et al., 2012a):

$$\widehat{\text{MMD}}_n^2(S_P, S_Q; k) = \frac{1}{n(n-1)} \sum_{i < j} \mathbb{H}_{ij}$$

$$H_{ij} = k(X_i, X_j) + k(Y_i, Y_j) - k(X_i, Y_j) - k(Y_i, X_j).$$

Figure 1. Blob dataset (a), with contours of Gaussian kernel (b) and deep kernel (c) evaluated at 9 locations (contour values are 0.7, 0.8 and 0.9). Each distribution has 9 modes; the central modes have the same shape, but $Q$ has a different shape at each other mode. A Gaussian kernel (b) compares points isotropically throughout the space; contours show $k(x, \mu)$ for each mode $\mu$. A deep kernel (c) learned by our methods compares points differently in different locations, allowing better identification of differences between $P$ and $Q$. 
The similar $\hat{\text{MMD}}_b^2 := \frac{1}{n^2} \sum_{ij} H_{ij}$ is the squared MMD between the empirical distributions of $S_P$ and $S_Q$.\(^1\)

**Testing with the MMD.** It can be shown that under $H_0$, $n \hat{\text{MMD}}_a^2$ converges to a distribution depending on $\mathbb{P}$ and $k$; we thus use this as our test statistic.

**Proposition 2 (Asymptotics of $\hat{\text{MMD}}_a^2$).** Under the null hypothesis, $H_0 : \mathbb{P} = \mathbb{Q}$, we have if $Z_i \sim \mathcal{N}(0, \sqrt{2})$,

$$n \hat{\text{MMD}}_a^2 \overset{d}{\to} \sum_i \lambda_i (Z_i^2 - 2);$$

where $\lambda_i$ are the eigenvalues of the $\mathbb{P}$-covariance operator of the centered centered kernel (Gretton et al., 2012a, Theorem 12).

Under the alternative, $H_1 : \mathbb{P} \neq \mathbb{Q}$, a standard central limit theorem holds (Serfling, 1980, Section 5.5.1):

$$\sqrt{n} (\text{MMD}_a^2 - \text{MMD}^2) \overset{d}{\to} \mathcal{N}(0, \sigma_{H_1}^2)$$

$$\sigma_{H_1}^2 := 4 \left( \mathbb{E}[H_{12}^2 H_{13}] - \mathbb{E}[H_{12}^2] \right).$$

Although it is possible to construct a test based on directly estimating this null distribution (Gretton et al., 2009), it is both simpler and, if implemented carefully, faster (Sutherland et al., 2017) to instead use a permutation test. This general method (Dwass, 1957; Alba Fernández et al., 2008) observes that under $H_0$, the samples from $\mathbb{P}$ and $\mathbb{Q}$ are interchangeable; we can therefore estimate the null distribution of our test statistic by repeatedly re-computing it with the samples randomly re-assigned to $S_P$ or $S_Q$.

**Test power.** The main measure of efficacy of a null hypothesis test is its power: the probability that, for a particular $\mathbb{P} \neq \mathbb{Q}$ and $n$, we correctly reject $H_0$. Proposition 2 implies, where $\Phi$ is the standard normal CDF, that

$$\Pr_{H_1} (n \hat{\text{MMD}}_a^2 > r) \to \Phi \left( \frac{\sqrt{n} \text{MMD}^2}{\sigma_{H_1}} - \frac{r}{\sqrt{n} \sigma_{H_1}} \right);$$

we can find the approximate test power by using the rejection threshold, found via (e.g.) permutation testing, as $r$. We also know via Proposition 2 that this $r$ will converge to a constant, and MMD, $\sigma_{H_1}$, are also constants. For reasonably large $n$, the power is dominated by the first term, and the kernel yielding the most powerful test will approximately maximize (Sutherland et al., 2017)

$$J(\mathbb{P}, \mathbb{Q}; k) := \frac{\text{MMD}_a^2(\mathbb{P}, \mathbb{Q}; k)}{\sigma_{H_1}(\mathbb{P}, \mathbb{Q}; k)}. \tag{3}$$

**Selecting a kernel.** The criterion $J(\mathbb{P}, \mathbb{Q}; k)$ depends on the particular $\mathbb{P}$ and $\mathbb{Q}$ at hand, and thus we typically will neither be able to choose a kernel *a priori*, nor exactly evaluate $J$ given samples. We can, however, estimate it with

$$\hat{J}_\lambda(\mathbb{P}, \mathbb{Q}; k) := \frac{\text{MMD}_a^2(\mathbb{P}, \mathbb{Q}; k)}{\hat{\sigma}_{H_1, \lambda}(\mathbb{P}, \mathbb{Q}; k)}, \tag{4}$$

where $\hat{\sigma}_{H_1, \lambda}^2$ is a regularized estimator of $\sigma_{H_1}^2$, given by

$$\frac{4}{n^3} \sum_{i=1}^n \left( \sum_{j=1}^n H_{ij} \right)^2 - \frac{4}{n^2} \left( \sum_{i=1}^n \sum_{j=1}^n H_{ij} \right) + \lambda. \tag{5}$$

Given $S_P$ and $S_Q$, we could construct a test by choosing $k$ to maximize $\hat{J}_\lambda(\mathbb{P}, \mathbb{Q}; k)$, then using a test statistic based on $\text{MMD}(S_P, S_Q; k)$. This sample re-use, however, violates the conditions of Proposition 2, and permutation testing would require repeatedly re-training $k$ with permuted labels.

Thus we split the data, get $k^{tr} \approx \max_k \hat{J}_\lambda(S_P^{tr}, S_Q^{tr}; k)$, then compute the test statistic and permutation threshold on $S_P^{tr}, S_Q^{tr}$ using $k^{tr}$. This procedure was proposed for $\hat{\text{MMD}}_a^2$ by Sutherland et al. (2017), but the same technique works for a variety of tests (Gretton et al., 2012b; Jitkrittum et al., 2016; 2017; Lopez-Paz & Oquab, 2017). Our paper adopts this framework (Section 5) and studies it further.

MMD-GANs (Li et al., 2017; Binkowski et al., 2018) seek a model $\mathbb{Q}_\theta$ to matches a target $\mathbb{P}$ according to a kernel optimized to distinguish the two. For instance, if $\mathbb{Q}_\theta$ is quite far from $\mathbb{P}$, an MMD-GAN requires a “weak” kernel for $\mathbb{Q}_\theta$ to find a path for improvement (Arbel et al., 2018), while our ideal kernel is one which perfectly distinguishes $\mathbb{P}$ and $\mathbb{Q}$ and would likely give no signal for improvement. Our algorithm, theoretical guarantees, and empirical evaluations thus all differ significantly from those for MMD-GANs.

### 3. Limits of Simple Kernels

We can use the criterion $\hat{J}_\lambda$ of (4) even to select parameters among a simple family, such as the lengthscales of a Gaussian kernel. Doing so on the Blob problem of Figure 1 illustrates the limitations of using MMD with these kernels.

In Figure 2c, we show how the maximal value of $\hat{J}$ changes as we see more samples from $\mathbb{P}$ and $\mathbb{Q}$, for both a family of Gaussian kernels (green dashed line) and a family (1) of deep kernels (red line). The optimal $\hat{J}$ is always higher

\(^2\) This estimator, as a $V$-statistic, is biased even when $\lambda = 0$ (although this bias is only $O(1/N)$; see Lemma 15). Although Sutherland et al. (2017); Sutherland (2019) give a quadratic-time estimator unbiased for $\sigma_{H_1}^2$, it is much more complicated to implement and analyze, likely has higher variance, and (being unbiased) can be negative, especially e.g. when the kernel is poor.
for the deep kernels; as expected, the empirical test power (Figure 2a) is also higher for deep kernels.

Most simple kernels used for MMD tests, whether the Gaussian we use here or Laplace, inverse multiquadric, even automatic relevance determination kernels, are all translation invariant: $k(x, y) = k(x-t, y-t)$ for any $t \in \mathbb{R}^d$. (All kernels used by Sutherland et al. (2017), for instance, were of this type.) Hence the kernel behaves the same way across space, as in Figure 1b. This means that for distributions whose behavior varies through space, whether because principal directions change (as in Figure 1) so the shape should be different, or because some regions are much denser than others and so need a smaller lengthscale (e.g. Li et al., 2019, Figures 1 and 2), any single global choice is suboptimal.

Kernels which are not translation invariant, such as the deep kernels (1) shown in Figure 1c, can adapt to the different shapes necessary in different areas.

4. Relationship to Classifier-Based Tests

Another popular method for conducting two-sample tests is to train a classifier between $S_P^n$ and $S_Q^n$, then assess its performance on $S_P^n$, $S_Q^n$. If $P = Q$, the classification problem is impossible and performance will be at chance.

The most common performance metric is the accuracy (Lopez-Paz & Oquab, 2017); this scheme is fairly common among practitioners, and Ramdas & Wasserman (2016) showed it to be rate-optimal in one extremely limited setting (linear discriminant analysis between high-dimensional Gaussians with identical covariances). We will call this approach a Classifier Two-Sample Test based on Sign, C2ST-S.

Letting $f : X \to \mathbb{R}$ output classification scores, the C2ST-S statistic is $\hat{\text{acc}}(S_P, S_Q; f)$ given by

$$\frac{1}{2n} \sum_{x_i \in S_P} \mathbb{1}(f(x_i) > 0) + \frac{1}{2n} \sum_{y_i \in S_Q} \mathbb{1}(f(y_i) \leq 0).$$

Let $\text{acc}(P, Q; f) := \frac{1}{2} \text{Pr}(f(X) > 0) + \frac{1}{2} \text{Pr}(f(Y) \leq 0)$; $\hat{\text{acc}}$ is unbiased for $\text{acc}$ and has a simple asymptotically normal null distribution.

Although it is perhaps not immediately obvious this is the case, C2ST-S is almost a special case of the MMD. Let

$$k_f^{(S)}(x, y) = \frac{1}{4} \mathbb{1}(f(x) > 0) \mathbb{1}(f(y) > 0).$$

A C2ST-S with $f$ is equivalent to an MMD test with $k_f^{(S)}$.

**Proposition 3.** It holds that

$$\text{MMD}(P, Q; k_f^{(S)}) = \left| \text{acc}(P, Q; f) - \frac{1}{2} \right|$$

$$\overline{\text{MMD}}_b(S_P, S_Q; k_f^{(S)}) = \left| \hat{\text{acc}}(S_P, S_Q; f) - \frac{1}{2} \right|.$$

**Proof.** The mean embedding $\mu_2$ under $k_f^{(S)}$ is simply

$$\frac{1}{2} \mathbb{E} \mathbb{1}(f(X) > 0) = \frac{1}{2} \text{Pr}(f(X) > 0),$$

so the MMD is

$$\frac{1}{2} \left| \text{Pr}(f(X) > 0) - \text{Pr}(f(Y) > 0) \right| = \left| \text{acc}(P, Q; f) - \frac{1}{2} \right|.$$ 

Moreover, $\hat{\text{acc}}$ is unbiased on empirical distributions. $\square$

The C2ST-S, however, selects $f$ to maximize cross-entropy (approximately maximizing $\hat{\text{acc}}$), while we maximize $J_\lambda$ (4). Although $k_f^{(S)}$ is not differentiable, maximizing (3) would exactly maximize $\text{acc}$ and hence maximize test power (Lopez-Paz & Oquab, 2017, Theorem 1).

Accessing $f$ through its sign allows for a simple null distribution, but it ignores $f$’s measure of confidence: a highly confident output extremely far from the decision boundary is treated the same as being very uncertain one lying in an area of high overlap between $P$ and $Q$, dramatically increasing the variance of the statistic. A scheme we call C2ST-L instead tests difference in means of $f$ on $P$ and $Q$ (Chen & Cloninger, 2019). Let

$$k_f^{(L)}(x, y) = f(x)f(y).$$

A C2ST-L is equivalent to an MMD test with $k_f^{(L)}$.

**Proposition 4.** It holds that

$$\text{MMD}(P, Q; k_f^{(L)}) = \left| \mathbb{E} f(X) - \mathbb{E} f(Y) \right|$$

$$\overline{\text{MMD}}_b(S_P, S_Q; k_f^{(L)}) = \left| \frac{1}{n} \sum_{x_i \in S_P} f(x_i) - \frac{1}{n} \sum_{y_i \in S_Q} f(y_i) \right|.$$

**Proof.** This kernel’s feature map is $k_f^{(L)}(x, y) = f(x)$. $\square$

Now maximizing accuracy (or a cross-entropy proxy) no longer directly maximizes power. This kernel is differentiable, so we can directly compare the merits of maximizing (4) to maximizing cross-entropy; we will see in Section 7.2 that our more direct approach is empirically superior.

Compared to using $k_f^{(L)}$, however, Section 7.2 shows that learned MMD tests also obtain better performance using kernels like (1). This is analogous to a similar phenomenon observed in other problems by Binkowski et al. (2018) and Li et al. (2019): C2STs learn a full discriminator function on the training set, and then apply only that function to the test set. Learning a deep kernel like (1) corresponds to learning only a powerful representation on the training set, and then still learning $f$ itself from the test set – in a closed form that makes permutation testing simple.

One advantage of classifier-based methods is that they have computational cost linear in the sample size, rather than quadratic as for MMD. This problem, though, is less severe...
than it might appear: on a mini-batch we would use on a GPU anyway, the (quadratic) cost of $J_\lambda$ given $\phi$ is typically trivial compared to the (linear) cost of computing featureizations. Estimating the MMD with mini-batches corresponds to the block estimator approach of Zaremba et al. (2013). In our experiments (Section 7), there is very little difference in the runtime of our methods from C2STs.

5. Learning Deep Kernels

**Choice of kernel architecture.** Most previous work on deep kernels has used a kernel $k$ directly on the output of a featureization network $\phi$, $k_\omega(x, y) = \kappa(\phi_\omega(x), \phi_\omega(y))$. This is certainly also an option for us. Any such $k_\omega$, however, is characteristic if and only if $\phi_\omega$ is injective. If we select our kernel well, this is not really a concern. Even so, it would be reassuring to know that, even if the optimization goes awry, the resulting test will still be at least consistent. More importantly, it can be helpful in optimization to add a “safeguard” preventing the learned kernel from considering extremely far-away inputs as too similar. We can achieve these goals with the form (1), repeated here for reference:

$$k_\omega(x, y) = (1 - \epsilon)\kappa(\phi_\omega(x), \phi_\omega(y)) + \epsilon q(x, y).$$

Here $\phi_\omega$ is a deep network (with parameters $\omega$) that extracts features, and $\kappa$ is a kernel on those features; we use a Gaussian with lengthscale $\sigma_\phi$, $\kappa(a, b) = \exp \left(-\frac{1}{2\sigma_\phi^2} \|a - b\|^2\right)$. We choose $0 < \epsilon < 1$ and $q$ a Gaussian with lengthscale $\sigma_q$.

**Proposition 5.** Let $k_\omega$ be of the form (1) with $\epsilon > 0$ and $q$ characteristic. Then $k_\omega$ is characteristic.

**Learning the deep kernel.** The kernel optimization and testing procedure is summarized in Algorithm 1. For larger datasets, or when $n \neq n_0$, we use minibatches in the training procedure; for smaller datasets, we use full batches. We use the Adam optimizer (Kingma & Ba, 2015). Note that the parameters $\epsilon, \sigma_\phi$, and $\sigma_q$ are included in $\omega$, all parameterized in log-space (i.e. we optimize $\epsilon'$ where $\epsilon = \exp(\epsilon')$).

### Algorithm 1 Testing with a learned deep kernel

**Input:** $S_0, S_Q$, various hyperparameters used below; $\omega \leftarrow \omega_0; \lambda \leftarrow 10^{-8}$; Split the data as $S_0 = S_0^T \cup S_0^S$ and $S_Q = S_Q^T \cup S_Q^S$:

- **Phase 1:** train the kernel parameters $\omega$ on $S_0^T$ and $S_Q^T$
  - for $T = 1, 2, \ldots, T_{\text{max}}$ do
    - $X \leftarrow$ mini-batch from $S_0^T$; $Y \leftarrow$ mini-batch from $S_0^S$;
    - $k_\omega \leftarrow$ kernel function with parameters $\omega$;
    - $M(\omega) \leftarrow \text{MMD}_n^2(X, Y; k_\omega)$; # as in (1)
    - $V_\lambda(\omega) \leftarrow \sigma_{\text{est}}^2(X, Y; k_\omega)$; # using (2)
    - $\hat{J}_\lambda(\omega) \leftarrow M(\omega)/\sqrt{V_\lambda(\omega)}$; # as in (4)
  - $\omega \leftarrow \omega + \eta \hat{\nabla}_{\text{Adam}} \hat{J}_\lambda(\omega)$; # maximize $\hat{J}_\lambda(\omega)$
  - end for

- **Phase 2:** permutation test with $k_\omega$ on $S_0^T$ and $S_Q^T$
  - for $i = 1, 2, \ldots, n_{\text{perm}}$ do
    - Shuffle $S_0^T \cup S_Q^T$ into $X$ and $Y$
    - $\text{perm}_i \leftarrow \text{MMD}_n^2(X, Y; k_\omega)$
  - end for

**Output:** $k_\omega$, est, p-value $\frac{1}{n_{\text{perm}}} \sum_{i=1}^{n_{\text{perm}}} 1(\text{perm}_i \geq \text{est})$

6. Theoretical Analysis

We now show that optimizing the regularized test power criterion based on a finite number of samples works: as $n$ increases, our estimates converge uniformly over a ball in parameter space, and therefore if there is a unique best kernel, we converge to it. Sutherland et al. (2017) gave no such guarantees; this result allows us to trust that, at least for reasonably large $n$ and if our optimization process succeeds, we will find a kernel that generalizes nearly optimally rather than just overfitting to $S_T$.

**Theorem 6.** Take $k_\omega$ as in Section 5, with $\phi_\omega$ a fully-
connected ReLU network with \( \Omega \) layers and \( D \) total parameters. Let \( \Omega \) be a set of kernel parameters for which \( \sigma_{\Omega}^2 \geq s^2 > 0 \), and the operator norms of each weight matrix and \( L_2 \) norms of each bias vector are at most \( R_0 \). Suppose each \( x \in \mathcal{X} \) has \( \|x\| \leq R_X \). Take \( \lambda = n^{-1/3} \). Then, using \( \hat{O}_P \) to suppress logarithmic factors,

\[
\sup_{\omega \in \Omega} \left| \hat{J}_\lambda(S P, Q; k_\omega) - J(\mathcal{P}, \mathcal{Q}; k_\omega) \right|
= \hat{O}_P \left( \frac{1}{s^2 n^{1/3}} \left[ \frac{1}{s} + \sqrt{D} + \Lambda R_0^{\lambda-1} R_X + 1 \right] \right).
\]

If there is a unique best kernel \( \omega^* \), the maximizer of \( \hat{J}_\lambda \) converges in probability to \( \omega^* \) as \( n \to \infty \).

A more general version of the result, including explicit constants and detailed assumptions, is in Appendix A. Our main results (Theorem 8 and Corollary 9) allow for any kernel which changes smoothly with its parameterization in a Banach space, based on uniform convergence of the MMD and variance estimators using an \( \epsilon \)-net argument.

Proposition 20 establishes the result above for deep kernels.\(^4\) Our results also apply to other deep learning settings: Proposition 18 gives the rate \( \hat{O}_P \left( s^{-2} n^{-1/3} (s^{-1} + R_X) \right) \) for choosing the lengthscale of a single Gaussian, while Proposition 23 gives the rate \( \hat{O}_P \left( s^{-2} n^{-1/3} (s^{-1} + \sqrt{D}) \right) \) for learning a linear combination of \( D \) fixed base kernels.

The dependence on \( s \) is somewhat unfortunate, but the ratio structure of \( J \) means that otherwise, errors in very small variances can hurt us arbitrarily. Despite this, “near-perfect” kernels (with reasonably large MMD and very small variance) will likely still be chosen as the maximizer of the regularized criterion, even if we do not estimate the (extremely large) ratio accurately. Likewise, near-perfect kernels (with very small variance but still small \( J \)) will generally have their \( J \) underestimated, and so are unlikely to be selected when a better kernel is available. The \( \epsilon q \) component in (1) may also help avoid extremely small variances.

Given \( N \) data points, this result also gives insight into how many we should use to train the kernel and how many to test. With perfect optimization, Corollary 11 shows a bound on the asymptotic power of the test is maximized by training on \( \Theta \left( \left( N \sqrt{\log N} \right)^{1/3} \right) \) points, and testing on the remainder.

7. Experimental Results

7.1. Comparison on Benchmark Datasets

We compare the following tests on several datasets:

- \textbf{MMD-D:} \textit{MMD} with a deep kernel; our method described in Section 5.
- \textbf{MMD-O:} \textit{MMD} with a Gaussian kernel whose lengthscale is optimized as in Section 5. This gives better results than standard heuristics.
- \textbf{Mean embedding (ME):} a state-of-the-art test (Chwialkowski et al., 2015; Jitkrittum et al., 2016) based on differences in Gaussian kernel mean embeddings at a set of optimized points.
- \textbf{Smooth characteristic functions (SCF):} a state-of-the-art test (Chwialkowski et al., 2015; Jitkrittum et al., 2016) based on differences in Gaussian mean embeddings at a set of optimized frequencies.
- \textbf{Classifier two-sample tests,} including C2STS-S (Lopez-Paz & Oquab, 2017) and C2ST-L (Chen & Cloninger, 2019) as described in Section 4. We set the test thresholds via permutation for both.

For synthetic datasets, we take a single sample set for \( S_{\mathcal{P}}^r \) and \( S_{\mathcal{Q}}^r \) and learn a kernel/test locations/etc once for each method on that training set. We then evaluate its rejection rate on 100 new sample sets \( S_{\mathcal{P}}^r, S_{\mathcal{Q}}^r \) from the same distribution. For real datasets, we select a subset of the available data for \( S_{\mathcal{P}}^r \) and \( S_{\mathcal{Q}}^r \) and train on that; we then evaluate on 100 random subsets, disjoint from the training set, of the remaining data. We repeat this full process 10 times, and report the mean rejection rate of each test. Table 5 shows significance tests. Further details are in Appendix B.

**Blob dataset.** Blob-D is the dataset shown in Figure 1; Blob-S has \( \mathcal{Q} \) also equal to the distribution shown in Figure 1a, so that the null hypothesis holds. Details are given in Table 6 (Appendix B.1).

Results are shown in Figure 2. MMD-D and C2ST-L are the clear winners in power, with MMD-D better in the higher-sample regime, and MMD-D is more reliable than C2STs. Figure 2c shows that \( J \) is higher for MMD-D than MMD-O, in addition to the actual test power being better, as discussed in Section 3. All methods have expected Type I error rates.

**High-dimensional Gaussian mixtures.** Here we study bimodal Gaussian mixtures in increasing dimension. Each distribution has two Gaussian components; in HDGM-S, \( \mathcal{P} \) and \( \mathcal{Q} \) are the same, while in HDGM-D, \( \mathcal{P} \) and \( \mathcal{Q} \) differ in the covariance of a single dimension pair but are otherwise the same. Details are in Table 6 (Appendix B.1). We consider both increasing \( N \) while keeping \( d = 10 \) and increasing \( d \) while keeping \( N = 4000 \), with results shown in Figure 3. Again, MMD-D has generally the best test power across a range of problem settings, with reasonable type I error.

**Higgs dataset (Baldi et al., 2014).** We compare the jet \( \phi \)-momenta distribution (\( d = 4 \)) of the background process, \( \mathcal{P} \), which lacks Higgs bosons, to the corresponding...
distribution $\mathcal{Q}$ for the process that produces Higgs bosons, following Chwialkowski et al. (2015). As discussed in these previous works, $\phi$-momenta carry very little discriminating information for recognizing whether Higgs bosons were produced. We consider a series of tests with increased number of samples $N$.

We report average test power (comparing $\mathcal{P}$ to $\mathcal{Q}$) in Table 1, and average type-I error (comparing $\mathcal{P}$ to $\mathcal{P}$ or $\mathcal{Q}$ to $\mathcal{Q}$) in Table 7 (Appendix B.6). As before, MMD-D generally performs the best; although the improvement over MMD-O here is not dramatic, MMD-D does notably outperform C2ST. All methods maintain reasonable Type I errors.

**MNIST generative model.** The MNIST dataset contains 70,000 handwritten digit images (LeCun et al., 1998). We compare true MNIST data samples $\mathcal{P}$ to samples $\mathcal{Q}$ from a pretrained deep convolutional generative adversarial network (DCGAN) (Radford et al., 2016). Samples from both distributions are shown in Figure 4 (in Appendix B.2).

We consider tests for increasing numbers of samples $N$, and report average test power (for $\mathcal{P}$ to $\mathcal{Q}$) in Table 2 and average Type I error (for $\mathcal{P}$ to $\mathcal{P}$) in Table 8 (in Appendix B.6). MMD-D substantially outperforms its competitors in test power, with the desired Type I error. ME also does well in this case: it is perhaps particularly suited to this problem, since it is capable of identifying either modes dropped by the generative model or spurious modes it inserts.

**CIFAR-10 vs CIFAR-10.1.** CIFAR-10.1 (Recht et al., 2019) is an attempt to collect a new test set for the very popular CIFAR-10 image classification dataset (Krizhevsky, 2009). Normally, when evaluating a supervised model, we consider the test set an independent sample from the training distribution, ideally never-before-seen by the training algorithm. But modern computer vision model architectures and training procedures have been developed based on repeatedly evaluating on the CIFAR-10 test set ($\mathcal{P}$), so it is possible that current models themselves are dependent on $\mathcal{P}$. CIFAR-10.1 ($\mathcal{Q}$) is an attempt at an independent sample from this distribution, collected after the models were trained, so that they are truly independent of $\mathcal{Q}$. These models do obtain substantially lower accuracies on $\mathcal{Q}$ than on $\mathcal{P}$—but this drop is surprisingly consistent across models, which seems unlikely to be due to the expected overfitting. The main potential explanation proposed by Recht et al. is dataset shift, but their attempt (in their Appendix C.2.8) at what amounts to a C2ST-S did not reject $H_0$.\(^5\) Samples from each distribution are shown in Figure 5 (Appendix B.2).

We train on 1000 images from each dataset and test on 1031, so that we use the entirety of CIFAR-10.1 each time, and average over ten repetitions. These tests provide strong evidence (Table 3) that images in the CIFAR-10.1 test set are statistically different from the CIFAR-10 test set, with MMD-D again strongest and ME still performing well.

---

\(^{5}\)Assuming pretrained classifiers are independent of $\mathcal{P}$, Figure 1 of Recht et al. (2019) indicates that the joint (images, labels) distribution certainly differs between CIFAR-10 and CIFAR-10.1. We test here whether the marginal image distribution differs.
Table 2. MNIST ($\alpha = 0.05$): average test power $\pm$ standard error for comparing $N$ real images to $N$ DCGAN samples.

| $N'$ | ME  | SCF  | C2ST-S | C2ST-L | MMD-O  | MMD-D  |
|------|-----|------|--------|--------|--------|--------|
| 200  | 0.414±0.050 | 0.107±0.018 | 0.193±0.037 | 0.234±0.031 | 0.188±0.010 | 0.555±0.044 |
| 400  | 0.921±0.032 | 0.152±0.021 | 0.646±0.039 | 0.706±0.047 | 0.363±0.017 | 0.996±0.004 |
| 600  | 1.000±0.000 | 0.294±0.008 | 1.000±0.000 | 0.977±0.012 | 0.619±0.021 | 1.000±0.000 |
| 800  | 1.000±0.000 | 0.317±0.017 | 1.000±0.000 | 1.000±0.000 | 0.797±0.015 | 1.000±0.000 |
| 1000 | 1.000±0.000 | 0.346±0.019 | 1.000±0.000 | 1.000±0.000 | 0.894±0.016 | 1.000±0.000 |
| Avg. | 0.867 | 0.243 | 0.768 | 0.783 | 0.572 | 0.910 |

Table 3. CIFAR-10.1 ($\alpha = 0.05$): mean rejection rates.

| ME  | SCF  | C2ST-S | C2ST-L | MMD-O  | MMD-D  |
|-----|------|--------|--------|--------|--------|
| 0.588 | 0.171 | 0.452  | 0.529  | 0.316  | 0.744  |

Our learned kernel also helps provide some ability to interpret the difference between $I^p$ and $Q$, particularly if we use it for an ME test. Appendix C explores this.

Recht et al. (2019) also provide a new ImageNetV2 test set for the ImageNet dataset, with similar properties; we defer this more challenging problem to future work.

7.2. Detailed Comparison to Classifier Tests

We now study the behavior of MMD-D and C2STs. Recall from Section 4 that there are two main differences: first, using a “full” kernel $(1)$ rather than the sign-based kernel $(6)$ or the intermediate linear kernel $(7)$. Second, training to maximize $J_\alpha (4)$ rather than a cross-entry surrogate. MMD-D uses a full kernel $(1)$ trained for test power; C2ST-S effectively uses the sign kernel $(6)$ trained for cross entropy.

In this section, we consider the performance of several intermediate models empirically, demonstrating that both factors help in testing. All are based on the same feature extraction architecture $\phi_{\omega}$; some models add a classification layer with new parameters $w$ and $b$,

$$f_{\omega}(x) = w^T \phi_{\omega}(x) + b,$$

which is treated as outputting classification logits. The model variants we consider are

- **S** A kernel $I(f_{\omega}(x) > 0)I(f_{\omega}(y) > 0)$; corresponds to a test statistic of the accuracy of $f$ (Proposition 3).
- **L** A kernel $f_{\omega}(x)f_{\omega}(y)$; corresponds to a test statistic comparing the mean value of $f$ (Proposition 4).
- **G** A Gaussian kernel $\kappa(\phi_{\omega}(x), \phi_{\omega}(y))$.
- **D** The deep kernel $(1)$ based on $\phi_{\omega}$.

We combine these model variants with a suffix describing the optimization objective:

- **J** Choose $\omega$, including possibly $w$ and $b$, to optimize the approximate test power $(4)$.
- **C** Choose $\omega$, including $w$ and $b$, to optimize cross-entropy

Table 4 presents results for all of these methods (except for S+J, which is non-differentiable and hence difficult to optimize). Performance generally improves as we move from S to L to G to D, and from C to J.

8. Conclusions

The test power of MMD is limited by simple kernels (e.g., Gaussian kernel) when facing complex-structured distributions, but we can avoid this problem with richer deep kernels. We show that optimizing the parameters of these kernels to maximize the test power, as proposed by Sutherland et al. (2017), outperforms state-of-the-art alternatives even when considering large, deep kernels with hundreds of thousands of parameters, rather than the simple shallow kernels they considered. We provide theoretical guarantees that this process is reasonable to conduct on finite samples.

\[^{6}\text{G+C and D+C take the fixed } \phi_{\omega} \text{ embeddings, then find the optimal lengthscale/etc by optimizing } J_\lambda.\]
and asymptotically selects the most powerful kernel. We also give deeper insight into the relationship between this approach and classifier two-sample tests (Lopez-Paz & Oquab, 2017), explaining why this approach outperforms that one.

We thus recommend practitioners to use optimized deep kernel methods when they wish to check if two distributions are the same, rather than indirectly training a classifier.

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A. Theoretical analysis

Appendix A.2 proves the main results under some assumptions about the kernel parameterization, using intermediate results about uniform convergence of our estimators in Appendix A.3. Appendix A.4 then shows that these assumptions hold for different settings of kernel learning.

A.1. Preliminaries

Given a kernel \( k_\omega \) and sample sets \( \{X_i\}_{i=1}^n \sim P^n \), \( \{Y_i\}_{i=1}^n \sim Q^n \), define the \( n \times n \) matrix

\[
H_{ij}^{(\omega)} = k_\omega(X_i, X_j) + k_\omega(Y_i, Y_j) - k_\omega(X_i, Y_j) - k_\omega(X_j, Y_i);
\]

we will often omit \( \omega \) when it is clear from context. The \( U \)-statistic estimator of the squared MMD (2) is

\[
\hat{\eta}_\omega = \frac{1}{n(n-1)} \sum_{i \neq j} H_{ij}.
\]

The squared MMD is \( \eta_\omega = \mathbb{E}[H_{12}] \). The variance of \( \hat{\eta}_\omega \) is given by Lemma 7.

**Lemma 7.** For a fixed kernel \( k_\omega \) and random sample sets \( \{X_i\}_{i=1}^n \), \( \{Y_i\}_{i=1}^n \), we have

\[
\text{Var}[\hat{\eta}_\omega] = \frac{4(n-2)}{n(n-1)} \xi_1^{(\omega)} + \frac{2}{n(n-1)} \xi_2^{(\omega)} = \frac{4}{n} \xi_1^{(\omega)} + \frac{2 \xi_2^{(\omega)} - 4 \xi_1^{(\omega)}}{n(n-1)},
\]

where

\[
\xi_1^{(\omega)} = \mathbb{E} \left[ H_{12}^{(\omega)} H_{13}^{(\omega)} \right] - \mathbb{E} \left[ H_{12}^{(\omega)} \right]^2, \quad \xi_2^{(\omega)} = \mathbb{E} \left[ \left( H_{12}^{(\omega)} \right)^2 \right] - \mathbb{E} \left[ H_{12}^{(\omega)} \right]^2.
\]

Thus as \( n \to \infty \),

\[n \text{ Var}[\hat{\eta}_\omega] \to 4 \xi_1^{(\omega)} =: \sigma_\omega^2.\]

**Proof.** Let \( U \) denote the pair \( (X, Y) \), and \( h_\omega(U, U') = k_\omega(X, X') + k_\omega(Y, Y') - k_\omega(X, Y') - k_\omega(X', Y) \), so that \( H_{ij}^{(\omega)} = h_\omega(U_i, U_j) \). Via Lemma A in Section 5.2.1 of Serfling (1980), we know that (8) holds with

\[
\xi_1^{(\omega)} = \text{Var}_{U, U'} \left[ \mathbb{E}_{U'} [h_\omega(U, U')] \right]
\]

\[= \mathbb{E}_{U, U'} \left[ \mathbb{E}_{U'} [h_\omega(U, U')] \mathbb{E}_{U''} [h_\omega(U, U'')] \right] - \mathbb{E}_{U, U'} [h_\omega(U, U')]^2 \]

and

\[
\xi_2 = \text{Var}_{U, U'} [h_\omega(U, U')] = \mathbb{E} \left[ \left( H_{12}^{(\omega)} \right)^2 \right] - \mathbb{E} \left[ H_{12}^{(\omega)} \right]^2.
\]

We use a \( V \)-statistic estimator (5) for \( \sigma_\omega^2 \):

\[
\tilde{\sigma}_\omega^2 = 4 \left( \frac{1}{n} \sum_{i=1}^n \left( \frac{1}{n} \sum_{j=1}^n H_{ij}^{(\omega)} \right)^2 - \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n H_{ij}^{(\omega)} \right).
\]

As a \( V \)-statistic, \( \tilde{\sigma}_\omega^2 \) is biased. In fact, Sutherland et al. (2017) and Sutherland (2019) provide an unbiased estimator of \( \text{Var}[\hat{\eta}_\omega] \) – including the terms of order \( \frac{1}{n(n-1)} \). Although this estimator takes the same quadratic time to compute as (5), it contains many more terms, which are cumbersome both for implementation and for analysis. (5) is also marginally more convenient in that it is always at least nonnegative. As we show in Lemma 15, the amount of bias is negligible as \( n \) increases. In practice, we expect the difference to be unimportant – or the \( V \)-statistic may in fact be beneficial, since underestimating \( \sigma^2 \) harms the estimate of \( \eta / \sigma^2 \) more than overestimating it does.

Similarly, although we use the \( U \)-statistic estimator (2), it would be very similar to use the biased estimator \( n^{-2} \sum_{ij} H_{ij} \), or the minimum variance unbiased estimator \( n^{-1} \sum_{i \neq j} (k(X_i, X_j) + k(Y_i, Y_j)) - 2n^{-2} \sum_{ij} k(X_i, Y_j) \). Showing comparable concentration behavior to Proposition 12 is trivially different, and in fact it is also not difficult to show \( \sigma_\omega^2 \) is the same for all three estimators (up to lower-order terms).
A.2. Main results

We will require the following assumptions. These are fairly agnostic as to the kernel form; Appendix A.4.2 shows that these assumptions hold (and gives the constants) for the kernels (1) we use in the paper.

(A) The kernels \( k_\omega \) are uniformly bounded:

\[
\sup_{\omega \in \Omega} \sup_{x \in \mathcal{X}} k_\omega(x, x) \leq \nu.
\]

For the kernels we use in practice, \( \nu = 1 \).

(B) The possible kernel parameters \( \omega \) lie in a Banach space of dimension \( D \). Furthermore, the set of possible kernel parameters \( \Omega \) is bounded by \( R_\omega, \Omega \subseteq \{ \omega \mid \|\omega\| \leq R_\Omega \} \).

Appendix A.4.2 builds this space and its norm for the kernels we use in the paper.

(C) The kernel parameterization is Lipschitz: for all \( x, y \in \mathcal{X} \) and \( \omega, \omega' \in \Omega \),

\[
|k_\omega(x, y) - k_{\omega'}(x, y)| \leq L_k \|\omega - \omega'\|.
\]

Proposition 20 in Appendix A.4.2 gives an expression for \( L_k \) for the kernels we use in the paper.

We will first show the main results under these general assumptions, using uniform convergence results shown in Appendix A.3, then show Assumptions (B) and (C) for particular kernels in Appendix A.4.2.

**Theorem 8.** Under Assumptions (A) to (C), let \( \Omega_\omega \subseteq \Omega \) be the set of kernel parameters for which \( \sigma_\omega^2 \geq s^2 \), and assume \( \nu \geq 1 \). Take \( \lambda = n^{-1/3} \). Then, with probability at least \( 1 - \delta \),

\[
\sup_{\omega \in \Omega_\omega} \left| \hat{\eta}_\omega - \frac{\eta_\omega}{\sigma_\omega} \right| \leq \frac{2\nu}{s^2 n^{1/3}} \left( \frac{1}{s} + \frac{2304\nu^2}{2304\nu^2 + 1024\nu} \right) \sqrt{L_k + \sqrt{\frac{2\log \frac{2}{\delta} + 2D(4R_\Omega\sqrt{n})}{2}}}.
\]

and thus, treating \( \nu \) as a constant,

\[
\sup_{\omega \in \Omega_\omega} \left| \hat{\eta}_\omega - \frac{\eta_\omega}{\sigma_\omega} \right| = \tilde{O}_\nu \left( \frac{1}{s^2 n^{1/3}} \left[ \frac{1}{s} + L_k + \sqrt{D} \right] \right).
\]

**Proof.** Let \( \sigma^2_{\omega, \lambda} := \sigma^2_\omega + \lambda \). Using \( |\hat{\eta}_\omega| \leq 4\nu \), we begin by decomposing

\[
\sup_{\omega \in \Omega_\omega} \left| \frac{\hat{\eta}_\omega - \eta_\omega}{\sigma_{\omega, \lambda}} \right| = \sup_{\omega \in \Omega_\omega} \left| \frac{\hat{\eta}_\omega - \eta_\omega}{\sigma_{\omega, \lambda}} \right| + \sup_{\omega \in \Omega_\omega} \left| \frac{\hat{\eta}_\omega - \eta_\omega}{\sigma_{\omega, \lambda}} \right| + \sup_{\omega \in \Omega_\omega} \left| \frac{\hat{\eta}_\omega - \eta_\omega}{\sigma_{\omega, \lambda}} \right|
\]

\[
= \sup_{\omega \in \Omega_\omega} \left| \frac{\hat{\eta}_\omega - \eta_\omega}{\sigma_{\omega, \lambda}} \right| + \sup_{\omega \in \Omega_\omega} \left| \frac{\hat{\eta}_\omega - \eta_\omega}{\sigma_{\omega, \lambda}} \right| + \sup_{\omega \in \Omega_\omega} \left| \frac{\hat{\eta}_\omega - \eta_\omega}{\sigma_{\omega, \lambda}} \right|
\]

\[
\leq \frac{4\nu}{s^2 \sqrt{\lambda}} \sup_{\omega \in \Omega_\omega} \left| \sigma^2_{\omega, \lambda} - \frac{\sigma^2_\omega}{\lambda} \right| + \frac{2\nu}{s^2 \lambda} + \frac{1}{s} \sup_{\omega \in \Omega_\omega} |\hat{\eta}_\omega - \eta_\omega|.
\]

Propositions 12 and 13 show uniform convergence of \( \hat{\eta}_\omega \) and \( \hat{\sigma}^2_\omega \), respectively. Thus, with probability at least \( 1 - \delta \), the error is at most

\[
\frac{2\nu}{s^3 \lambda} + \left[ \frac{8\nu}{s^2 n^{1/3}} + \frac{1792\nu}{s^2 n^{1/3}} \right] \sqrt{\frac{2\log \frac{2}{\delta} + 2D(4R_\Omega\sqrt{n})}{2\log \frac{2}{\delta} + 2D(4R_\Omega\sqrt{n})}} + \left[ \frac{8}{s^2 \sqrt{n}} + \frac{2048\nu^2}{s^2 \sqrt{n} s^2 \sqrt{\lambda}} \right] L_k + \frac{4608\nu^3}{s^2 n^{3/2}}.
\]

Taking \( \lambda = n^{-1/3} \) gives

\[
\frac{2\nu}{s^3 n^{1/3}} + \left[ \frac{8\nu}{s^2 n^{1/3}} + \frac{1792\nu}{s^2 n^{1/3}} \right] \sqrt{\frac{2\log \frac{2}{\delta} + 2D(4R_\Omega\sqrt{n})}{2\log \frac{2}{\delta} + 2D(4R_\Omega\sqrt{n})}} + \left[ \frac{8}{s^2 \sqrt{n}} + \frac{2048\nu^2}{s^2 n^{1/3}} \right] L_k + \frac{4608\nu^3}{s^2 n^{5/6}}.
\]
Using $1 \leq \nu$, $1792 < 2048$, we can get the slightly simpler upper bound
\[
\frac{2\nu}{s^3n^{1/3}} + \left[ \frac{8\nu}{s^3n} + \frac{2048\nu^2}{s^3n^{1/3}} \right] \left[ L_k + \sqrt{2\log \frac{2}{\delta} + 2D \log (4R\sqrt{n})} \right] + \frac{4608\nu^3}{n^{1/6}}.
\]

It is worth noting that, if we are particularly concerned about the $s$ dependence, we can make some slightly different choices in the decomposition to improve the dependence on $s$ while worsening the rate with $n$.

**Corollary 9.** In the setup of Theorem 8, additionally assume that there is a unique population maximizer $\omega^*$ of $J$ from (3), i.e. for each $t > 0$ we have
\[
\sup_{\omega \in \Omega_s \mid \|\omega - \omega^*\| > t} J(P, Q; k_\omega) < J(P, Q; k_{\omega^*}).
\]

For each $n$, let $S_p^{(n)}$ and $S_Q^{(n)}$ be sequences of sample sets of size $n$, let $\hat{J}_n(\omega)$ denote $J_{\lambda=n^{-1/3}}(S_p^{(n)}, S_Q^{(n)}; k_\omega)$, and take $\hat{\omega}_n^*$ to be a maximizer of $\hat{J}_n(\omega)$. Then $\hat{\omega}_n^*$ converges in probability to $\omega^*$.

**Proof.** By Theorem 8, $\sup_{\omega \in \Omega_s} \left| \hat{J}_n(\omega) - J(\omega) \right| \overset{P}{\to} 0$. Then the result follows by Theorem 5.7 of Van der Vaart (2000).

**Corollary 10.** In the setup of Theorem 8, suppose we use $n$ sample points to select a kernel $\hat{\omega}_n \in \arg \max_{\omega \in \Omega_s} \hat{J}_n(\omega)$ and $m$ sample points to run a test of level $\alpha$. Let $r_{\omega, n}^{(m)}$ denote the rejection threshold for a test with that kernel of size $m$. Define $J^* := \sup_{\omega \in \Omega_s} J(\omega)$, and constants $C, C', C''$, $N_0$ depending on $\nu, L_k, D, R_\Omega$ and $s$. For any $n \geq N_0$, with probability at least $1 - \delta$, this test procedure has power
\[
\Pr \left( m \hat{\eta}_{\omega} > r_{\omega, n}^{(m)} \right) \geq \Phi \left( \sqrt{mJ^*} - C\frac{\sqrt{m}}{n^{1/3}} \sqrt{\log \frac{n}{\delta}} - C'\sqrt{\log \frac{1}{\alpha}} \right) - C''.
\]

**Proof.** Let $\hat{\omega}_n \in \arg \max_{\omega \in \Omega_s} \hat{J}_n(\omega)$. By Theorem 8, there are some $N_0, C$ depending on $\nu, L_k, D, R_\Omega$, and $s$ such that as long as $n \geq N_0$, with probability at least $1 - \delta$ it holds that
\[
\sup_{\omega \in \Omega_s} \left| J_\lambda(\omega) - J(\omega) \right| \leq \frac{1}{2} Cn^{-1/3} \sqrt{\log \frac{n}{\delta}} =: \epsilon_n.
\]
Assume for the remainder of this proof that this event holds. Letting $\omega^* \in \arg \max J(\omega)$, we know because $\hat{\omega}_n$ maximizes $\hat{J}_n$ that $\hat{J}_n(\hat{\omega}_n) \geq \hat{J}_n(\omega^*)$. Using uniform convergence twice,
\[
J(\omega^*) - \epsilon_n \geq \hat{J}_n(\omega^*) - \epsilon_n \geq (J(\omega^*) - \epsilon_n) - \epsilon_n = J^* - 2\epsilon_n.
\]

Now, although Proposition 2 establishes that $r_{\omega, n}^{(m)} \to r_{\omega}$ and it is even known (Korolyuk & Borovskikh, 1988, Theorem 5) that $|r_{\omega, n}^{(m)} - r_{\omega}| = o(1/\sqrt{m})$, the constant in that convergence will depend on the choice of $\omega$ in an unknown way. It’s thus simpler to use the very loose but uniform (McDiarmid-based) bound given by Corollary 11 of Gretton et al. (2012a), which implies $r_{\omega, n}^{(m)} \leq 4\nu \sqrt{\log(\alpha^{-1})m}$ no matter the choice of $\omega$.

We will now need a more precise characterization of the power than that provided by the central limit theorem of Proposition 2. Callaert & Janssen (1978) provide such a result, a Berry-Esseen bound on $U$-statistic convergence: there is some absolute constant $C_{BS} = 2^{14}3^4 C_{BS}$ such that
\[
\sup_t \left| \Pr_{H_1} \left( \frac{\hat{\eta}_{\omega} - \eta_\omega}{\sigma_\omega^2} \leq t \right) - \Phi(t) \right| \leq \frac{C_{BS} \mathbb{E} |H_{12}|^3}{(\sigma_\omega/2)^3 \sqrt{m}} \leq \frac{C_{BS} \nu^3}{\sigma_\omega \sqrt{m}}.
\]

\footnote{In fact, it suffices for the $\hat{\omega}_n^*$ to only approximately maximize $\hat{J}_n$, as long as their suboptimality is $o_P(1)$.}
Letting $r^{(m)}_\omega$ be the appropriate rejection threshold for $k_\omega$ with $m$ samples, the power of a test with kernel $k_\omega$ is
\[
\Pr \left( m\tilde{\eta}_\omega > r^{(m)}_\omega \right) = \Pr \left( \sqrt{m} \tilde{\eta}_\omega - \frac{r^{(m)}_\omega}{\sigma_\omega} > \frac{r^{(m)}_\omega}{\sqrt{m}\sigma_\omega} \right)
\geq \Phi \left( \sqrt{m} J(\omega) - \frac{r^{(m)}_\omega}{\sigma_\omega} \right) - \frac{C_{BS}\nu^3}{\sigma_\omega^3 \sqrt{m}}
\geq \Phi \left( \sqrt{m} J(\omega) - \frac{r^{(m)}_\omega}{s\sqrt{m}} \right) - C'' \frac{1}{\sqrt{m}}
\]
using a new constant $C'' := C_{BS}\nu^3/s^3$. Combining the previous results on $J(\tilde{\omega}_n)$ and $r^{(m)}_\omega$ yields the claim.

**Corollary 11.** In the setup of Corollary 10, suppose we are given $N$ data points to divide between $n$ training points and $m = N - n$ testing points. Ignoring the Berry-Esseen convergence term outside of $\Phi$, the asymptotic power upper bound
\[
\Phi \left( \sqrt{m} J^* - C \frac{\sqrt{m}}{n^3} \sqrt{\log \frac{n}{\delta}} - C' \sqrt{\log \frac{1}{\alpha}} \right)
\]
is maximized by choosing, as $N \to \infty$ and other quantities remain constant,
\[
n \sim \left( \frac{C}{J^* N} \left( \frac{1}{3}\log N \right) \right)^{\frac{2}{3}}.
\]

**Proof.** Because the $C'$ term is constant, we wish to choose
\[
\arg \max_{0 < n < N} \frac{J^*}{C} \sqrt{N - n} - \sqrt{\frac{N - n}{n^4}} \sqrt{\log \frac{n}{\delta}}.
\]
Clearly neither endpoint is optimal, so the optimum must be achieved at a stationary point, which implies
\[
\frac{-J^*}{2C\sqrt{N - n}} + \frac{\sqrt{\log \frac{n}{\delta}}^{\frac{2}{3}}}{2\sqrt{N - n}} + \frac{1}{3} \sqrt{N - n} - n^{-\frac{2}{3}} \sqrt{\log \frac{n}{\delta}} - \frac{1}{2} \sqrt{N - n} - n^{-\frac{2}{3}} \left( \log \frac{n}{\delta} \right)^{-\frac{2}{3}} = 0
\]
\[
D := -\frac{J^*}{C} n^{\frac{4}{3}} \sqrt{\log \frac{n}{\delta}} + n \log \frac{n}{\delta} + (N - n) \left[ \frac{2}{3} \log \frac{n}{\delta} - 1 \right] = 0.
\]
Suppose briefly that $n = \tilde{\Theta}(N^p)$. Then
\[
D = \tilde{\Theta} \left( -N^{\frac{2}{3}p} + N^p + N - N^p \right).
\]
Thus, if $n = \tilde{\omega} \left( N^{\frac{2}{3}} \right)$, then $D = -\tilde{\omega}(N)$. But this precludes $D = 0$, a contradiction. On the other hand, if $n = \tilde{\omega} \left( N^{\frac{2}{3}} \right)$, we’d have $D = \tilde{\omega}(N)$, also a contradiction. Thus $n = \tilde{\Theta} \left( N^{\frac{2}{3}} \right)$. The two $n \log \frac{n}{\delta}$ terms are thus lower-order, so that
\[
D \sim \frac{2}{3} N \log n - \frac{J^*}{C} n^{\frac{4}{3}} \sqrt{\log n}.
\]
As $n = \tilde{\Theta} \left( N^{\frac{2}{3}} \right)$, there are $A, q$ such that $n \sim AN^{\frac{2}{3}}(\log N)^q$. Here $\log n \sim \log A + \frac{3}{4} \log N + q \log \log N \sim \frac{3}{4} \log N$, so
\[
D \sim \frac{1}{2} N \log N - \frac{J^*}{C} A^\frac{2}{3} N (\log N)^{\frac{3}{4}q} \sqrt{\frac{3}{4} \log N} = \frac{1}{2} N \log N - \frac{J^*}{2C} A^\frac{2}{3} N (\log N)^{\frac{3}{4}q + \frac{1}{2}}.
\]
To achieve $D = \Theta(1)$, we need $\frac{3}{4}q + \frac{1}{2} = 1$, so that $q = \frac{3}{8}$. Then for $D \to 0$ to be possible, we need
\[
\frac{1}{2} = \frac{J^*}{2C} A^\frac{2}{3} \quad \text{i.e.} \quad A = \left( \frac{C}{\sqrt{3}J^*} \right)^{\frac{3}{2}}.
\]
\[\square\]
A.3. Uniform convergence results

These results, on the uniform convergence of \( \hat{\eta} \) and \( \hat{\sigma}^2 \), were used in the proof of Theorem 8.

**Proposition 12.** Under Assumptions (A) to (C), we have that with probability at least \( 1 - \delta \),

\[
\sup_\omega |\hat{\eta}_\omega - \eta_\omega| \leq \frac{8}{\sqrt{n}} \left[ \nu \sqrt{2 \log \frac{2}{\delta} + 2D \log (4R_\Omega \sqrt{n})} + L_k \right].
\]

**Proof.** Theorem 7 of Sriperumbudur et al. (2009) gives a similar bound in terms of Rademacher chaos complexity, but for ease of combination with our bound on convergence of the variance estimator, we use a simple \( \epsilon \)-net argument instead.

We study the random error function

\[
\Delta(\omega) := \hat{\eta}_\omega - \eta_\omega.
\]

First, we place \( T \) points \( \{\omega_i\}_{i=1}^T \) such that for any point \( \omega \in \Omega \), \( \min_i \|\omega - \omega_i\| \leq q \); Assumption (B) ensures this is possible with at most \( T = (4R_\Omega/q)^D \) points (Cucker & Smale, 2001, Proposition 5).

Now, \( \Delta = 0 \), because \( \hat{\eta} \) is unbiased. Recall that \( \hat{\eta} = \frac{1}{n(n-1)} \sum_{i \neq j} H_{ij} \), and via Assumption (A) we know \( |H_{ij}| \leq 4\nu \). This \( \hat{\eta} \), and hence \( \Delta \), satisfies bounded differences: if we replace \( (X_1, Y_1) \) with \( (X'_1, Y'_1) \), obtaining \( \hat{\eta}' = \frac{1}{n(n-1)} \sum_{i \neq j} F_{ij} \) where \( F \) agrees with \( H \) except when \( i \) or \( j \) is 1, then

\[
|\hat{\eta} - \hat{\eta}'| \leq \frac{1}{n(n-1)} \sum_{i \neq j} |H_{ij} - F_{ij}| = \frac{1}{n(n-1)} \sum_{i>1} |H_{i1} - F_{i1}| + \frac{1}{n(n-1)} \sum_{j>1} |H_{1j} - F_{1j}|
\]

\[
\leq \frac{2}{n(n-1)} \sum_{i>1} 8\nu = \frac{16\nu}{n}.
\]

Using McDiarmid’s inequality for each \( \Delta(\omega_i) \) and a union bound, we then obtain that with probability at least \( 1 - \delta \),

\[
\max_{i \in \{1, \ldots, T\}} |\Delta(\omega_i)| \leq \frac{16\nu}{\sqrt{2n}} \sqrt{\log \frac{2T}{\delta}} \leq \frac{8\nu}{\sqrt{n}} \sqrt{2 \log \frac{2}{\delta} + 2D \log \frac{4R_\Omega}{q}}.
\]

We also have via Assumption (C), for any two \( \omega, \omega' \in \Omega \),

\[
|\hat{\eta}_\omega - \hat{\eta}_{\omega'}| \leq \frac{1}{n(n-1)} \sum_{i \neq j} |H_{ij}^{(\omega)} - H_{ij}^{(\omega')}| \leq \frac{1}{n(n-1)} \sum_{i \neq j} 4L_k \|\omega - \omega'\| = 4L_k \|\omega - \omega'\|
\]

\[
|\eta_\omega - \eta_{\omega'}| = \left| \mathbb{E} \left[ H_{12}^{(\omega)} \right] - \mathbb{E} \left[ H_{12}^{(\omega')} \right] \right| \leq \left| \mathbb{E} \left[ H_{12}^{(\omega)} - H_{12}^{(\omega')} \right] \right| \leq 4L_k \|\omega - \omega'\|
\]

so that \( \|\Delta\|_L \leq 8L_k \). Combining these two results, we know that with probability at least \( 1 - \delta \)

\[
\sup_\omega |\Delta(\omega)| \leq \max_{i \in \{1, \ldots, T\}} |\Delta(\omega_i)| + 8L_k q \leq \frac{8\nu}{\sqrt{n}} \sqrt{2 \log \frac{2}{\delta} + 2D \log \frac{4R_\Omega}{q}} + 8L_k q;
\]

setting \( q = 1/\sqrt{n} \) yields the desired result. \( \Box \)

**Proposition 13.** Under Assumptions (A) to (C), with probability at least \( 1 - \delta \),

\[
\sup_{\omega \in \Omega} |\hat{\sigma}^2_\omega - \sigma^2_{\omega}| \leq \frac{64}{\sqrt{n}} \left[ 7 \sqrt{2 \log \frac{2}{\delta} + 2D \log (4R_\Omega \sqrt{n})} + \frac{18\nu^2}{\sqrt{n}} + 8L_k \nu \right].
\]

**Proof.** We again use an \( \epsilon \)-net argument on the (random) error function

\[
\Delta(\omega) := \hat{\sigma}^2_\omega - \sigma^2_\omega.
\]
First, choose \( T \) points \( \{\omega_i\}_{i=1}^T \) such that for any point \( \omega \in \Omega, \min_i \|\omega - \omega_i\| \leq q \); again, via Assumption (B) and Proposition 5 of Cucker & Smale (2001) we have \( T \leq (4R_\Omega/q)^D \). By Lemmas 14 and 15 and a union bound, with probability at least \( 1 - \delta \),

\[
\max_{i \in \{1, \ldots, T\}} |\Delta(\omega)| \leq 448 \sqrt{\frac{2}{n} \log \frac{2T}{\delta} + \frac{1152\nu^2}{n}} \leq 448 \sqrt{\frac{2}{n} \log \frac{2}{\delta} + \frac{2}{n} D \log \frac{4R_\Omega}{q} + \frac{1152\nu^2}{n}}.
\]

Lemma 16 shows that \( \|\Delta\|_L \leq 512Lk\nu \), which means that with probability at least \( 1 - \delta \),

\[
\sup_{\omega \in \Omega} |\Delta(\omega)| \leq 448 \sqrt{\frac{2}{n} \log \frac{2}{\delta} + \frac{2}{n} D \log \frac{4R_\Omega}{q} + \frac{1152\nu^2}{n} + 512Lk\nu q}.
\]

Taking \( q = 1/\sqrt{n} \) gives the desired result.

**Lemma 14.** For any kernel \( k \) bounded by \( \nu \) (Assumption (A)), with probability at least \( 1 - \delta \),

\[
|\hat{\sigma}_k^2 - \mathbb{E}[\hat{\sigma}_k^2]| \leq 448 \sqrt{\frac{2}{n} \log \frac{2}{\delta}}.
\]

**Proof.** We simply apply McDiarmid’s inequality to \( \hat{\sigma}_k^2 \). Suppose we change \((X_1, Y_1)\) to \((X'_1, Y'_1)\), giving a new \( H \) matrix \( F \) which agrees with \( H \) on all but the first row and column. Note that \( |H_{ij}| \leq 4\nu \), and recall

\[
\hat{\sigma}_k^2 = 4 \left( \frac{1}{n^3} \sum_i \left( \sum_j H_{ij} \right)^2 - \left( \frac{1}{n^2} \sum_{ij} H_{ij} \right)^2 \right).
\]

The first term in the parentheses of \( \hat{\sigma}_k^2 \) changes by

\[
\left| \frac{1}{n^3} \sum_i \left( \sum_j H_{ij} \right)^2 - \frac{1}{n^3} \sum_i \left( \sum_j F_{ij} \right)^2 \right| \leq \frac{1}{n^3} \sum_{ij\ell} |H_{ij}H_{i\ell} - F_{ij}F_{i\ell}|.
\]

In this sum, if none of \( i, j, \) or \( \ell \) are one, the term is zero. The \( n^2 \) terms for which \( i = 1 \) are each upper-bounded by \( 32\nu^2 \), simply bounding each \( H \) or \( F \) by \( 4\nu \). Of the remainder, there are \((n - 1) \) terms where \( j = \ell = 1 \), each \( |H_{11}^2 - F_{11}^2| \leq 16\nu^2 \). We are left with \( 2(n - 1)^2 \) terms which have exactly one of \( j \) or \( \ell \) equal to \( 1 \); the \( j = 1 \) terms are \( |H_{1i}H_{i1} - F_{1i}F_{i1}| \leq |H_{1i} - F_{1i}| |H_{i1}| \leq (8\nu)(4\nu), \) so each of these terms is at most \( 32\nu^2 \). The total sum is thus at most

\[
\frac{1}{n^3} \left( n^2 32\nu^2 + (n - 1)16\nu^2 + 2(n - 1)^2 32\nu^2 \right) = \left( \frac{6}{n} - \frac{7}{n^2} + \frac{3}{n^3} \right) 16\nu^2.
\]

The remainder of the change in \( \hat{\sigma}_k^2 \) can be determined by bounding

\[
\sum_{ij} |H_{ij} - F_{ij}| \leq \sum_j |H_{ij} - F_{ij}| = \sum_j |H_{1j} - F_{1j}| + \sum_{i>1} |H_{i1} - F_{i1}| \leq n(8\nu) + (n - 1)(8\nu) = (8\nu)(2n - 1),
\]

which then gives us

\[
\left| \left( \frac{1}{n^2} \sum_{ij} H_{ij} \right)^2 - \left( \frac{1}{n^2} \sum_{ij} F_{ij} \right)^2 \right| = \left| \frac{1}{n^2} \sum_{ij} H_{ij} + \frac{1}{n^2} \sum_{ij} F_{ij} \right| \left| \frac{1}{n^2} \sum_{ij} H_{ij} - \frac{1}{n^2} \sum_{ij} F_{ij} \right| \leq (2 \cdot 4\nu) \frac{2n - 1}{n^2} (8\nu) = 64\nu^2 \left( \frac{2}{n} - \frac{1}{n^2} \right).
\]
Thus
\[ |\hat{\sigma}^2_k - \sigma^2_k| \leq 4 \left[ \frac{6}{n^2} + \frac{3}{n^2} \right] 16\nu^2 + \left( \frac{2}{n} - \frac{1}{n^2} \right) 64\nu^2 \] \[ = \frac{64\nu^2}{n^3} [14n^2 - 11n + 3] \leq \frac{896\nu^2}{n}. \]

Because the same holds for changing any of the \((X_i, Y_i)\) pairs, the result follows by McDiarmid’s inequality.

**Lemma 15.** For any kernel \(k\) bounded by \(\nu\) (Assumption (A)), the estimator \(\hat{\sigma}^2_k\) satisfies
\[ |E \hat{\sigma}^2_k - \sigma^2_k| \leq \frac{1152\nu^2}{n}. \]

**Proof.** We have that
\[ E \hat{\sigma}^2_k = 4 \left( \frac{1}{n^3} \sum_{ij\ell} E[H_{ij}H_{\ell}] - \frac{1}{n^4} \sum_{ijab} E[H_{ij}H_{ab}] \right). \]

Most terms in these sums have their indices distinct; these are the ones that we care about. (We could evaluate the expectations of the other terms exactly, but it would be tedious.) We can thus break down the first term as
\[ \frac{1}{n^3} \sum_{ij\ell} E[H_{ij}H_{\ell}] = \frac{1}{n^3} \sum_{ij: |(i,j)\ell| = 3} E[H_{ij}H_{\ell}] + \frac{1}{n^3} \sum_{ij\ell: |(i,j)\ell| < 3} E[H_{ij}H_{\ell}] \]
\[ = \frac{n(n-1)(n-2)}{n^3} E[H_{12}H_{13}] + \left( 1 - \frac{n(n-1)(n-2)}{n^3} \right) q, \]
where \(q\) is the appropriately-weighted mean of the various \(E[H_{ij}H_{\ell}]\) terms for which \(i, j, \ell\) are not mutually distinct. Since \(|H_{ij}| \leq 4\nu, E[H_{ij}H_{\ell}] < 16\nu^2\) and so \(|q| \leq 16\nu^2\) as well. Noting that
\[ \frac{n(n-1)(n-2)}{n^3} = 1 - \frac{3}{n^2} + \frac{2}{n^2}, \]
we obtain
\[ \left| \frac{1}{n^3} \sum_{ij\ell} E[H_{ij}H_{\ell}] - E[H_{12}H_{13}] \right| = \left( \frac{3}{n} - \frac{2}{n^2} \right)|E[H_{12}H_{13}] + q| \leq \left( \frac{3}{n} - \frac{2}{n^2} \right) 32\nu^2. \tag{10} \]

The second term can be handled similarly:
\[ \frac{1}{n^4} \sum_{ijab} E[H_{ij}H_{ab}] = \frac{1}{n^4} \sum_{ijab: |(i,j,a,b)| = 4} E[H_{ij}H_{ab}] + \frac{1}{n^4} \sum_{ijab: |(i,j,a,b)| < 4} E[H_{ij}H_{ab}] \]
\[ = \frac{n(n-1)(n-2)(n-3)}{n^4} E[H_{ij}H_{ab}] + \left( 1 - \frac{n(n-1)(n-2)(n-3)}{n^4} \right) r, \]
where \(r\) is the appropriately-weighted mean of the non-distinct terms, \(|r| \leq 16\nu^2\). For \(i, j, a, b\) all distinct, \(E[H_{ij}H_{ab}] = E[H_{12}]^2\). Here
\[ \frac{n(n-1)(n-2)(n-3)}{n^4} = \frac{(n-1)(n^2 - 5n + 6)}{n^3} = 1 - \frac{6}{n} + \frac{11}{n} - \frac{6}{n^3}, \]
and so
\[ \left| \frac{1}{n^4} \sum_{ijab} E[H_{ij}H_{ab}] - E[H_{12}]^2 \right| \leq \left( \frac{6}{n} - \frac{11}{n^2} + \frac{6}{n^3} \right) 32\nu^2. \tag{11} \]

Recalling \(\sigma^2_k = 4[E[H_{12}H_{13}] - E[H_{12}]^2]\),
\[ |E \hat{\sigma}^2_k - \sigma^2_k| \leq 128\nu^2 \left( \frac{9}{n} - \frac{13}{n^2} + \frac{6}{n^3} \right), \]
and since \(n \geq 1\), we have \(13/n^2 > 6/n^3\), yielding the result. \(\square\)
Lemma 16. Under Assumptions (A) and (C), we have

\[
\sup_{\omega, \omega' \in \Omega} \left| \hat{\sigma}_\omega^2 - \hat{\sigma}_{\omega'}^2 \right| \leq 256 L_k \nu \quad \text{and} \quad \sup_{\omega, \omega' \in \Omega} \frac{|\sigma_\omega^2 - \sigma_{\omega'}^2|}{\|\omega - \omega'\|} \leq 256 L_k \nu.
\]

Proof. We first handle the change in \( \hat{\sigma}_k \):

\[
\left| \hat{\sigma}_k^2 - \hat{\sigma}_k'^2 \right| = \frac{4}{n^2} \sum_{ij} \left| H_{ij}^{(\omega)} H_{ij}^{(\omega')} - \frac{1}{n^3} \sum_{ij} H_{ij}^{(\omega)} H_{ij}^{(\omega')} - \frac{1}{n^3} \sum_{ij} H_{ij}^{(\omega)} H_{ij}^{(\omega')} + \frac{1}{n^3} \sum_{ij} H_{ij}^{(\omega)} H_{ij}^{(\omega')} \right|
\]

\[
\leq \frac{4}{n^3} \sum_{ij} \left| H_{ij}^{(\omega)} H_{ij}^{(\omega')} - H_{ij}^{(\omega')} H_{ij}^{(\omega)} \right| + \frac{4}{n^3} \sum_{ij} \left| H_{ij}^{(\omega)} H_{ij}^{(\omega')} - H_{ij}^{(\omega')} H_{ij}^{(\omega)} \right|.
\]

We can bound both terms by bounding

\[
\left| H_{ij}^{(\omega)} H_{ij}^{(\omega')} - H_{ij}^{(\omega')} H_{ij}^{(\omega)} \right| \leq \left| H_{ij}^{(\omega)} H_{ij}^{(\omega')} - H_{ij}^{(\omega)} H_{ij}^{(\omega')} \right| + \left| H_{ij}^{(\omega)} H_{ij}^{(\omega')} - H_{ij}^{(\omega)} H_{ij}^{(\omega')} \right|
\]

\[
= \left| H_{ij}^{(\omega)} \right| \left| H_{ij}^{(\omega')} - H_{ij}^{(\omega)} \right| + \left| H_{ij}^{(\omega)} - H_{ij}^{(\omega')} \right| \left| H_{ij}^{(\omega)} \right|
\]

\[
\leq 4 \nu \left( \left| H_{ij}^{(\omega)} - H_{ij}^{(\omega')} \right| + \left| H_{ij}^{(\omega)} - H_{ij}^{(\omega')} \right| \right).
\]

Using Assumption (C) and the definition of \( H \),

\[
\left| H_{ij}^{(\omega)} - H_{ij}^{(\omega')} \right| \leq 4L_k \|\omega - \omega'\|
\]

so

\[
\left| H_{ij}^{(\omega)} H_{ij}^{(\omega')} - H_{ij}^{(\omega')} H_{ij}^{(\omega)} \right| \leq 32 \nu L_k \|\omega - \omega'\| \tag{12}
\]

and hence

\[
\left| \hat{\sigma}_\omega^2 - \hat{\sigma}_{\omega'}^2 \right| \leq 256 \nu L_k \|\omega - \omega'\|.
\]

Again using (12), we also have

\[
\left| \sigma_\omega^2 - \sigma_{\omega'}^2 \right| \leq 4 \left( \left| H_{12}^{(\omega)} H_{13}^{(\omega')} \right| - \left| H_{12}^{(\omega')} H_{13}^{(\omega')} \right| \right) + 4 \left( \left| H_{12}^{(\omega)} \right|^2 - \left| H_{12}^{(\omega')} \right|^2 \right)
\]

\[
\leq 4 \| H_{12}^{(\omega)} H_{13}^{(\omega')} - H_{12}^{(\omega')} H_{13}^{(\omega')} \| + 4 \left( \left| H_{12}^{(\omega)} \right|^2 - \left| H_{12}^{(\omega')} \right|^2 \right)
\]

\[
\leq 256 \nu L_k \|\omega - \omega'\|.
\]

A.4. Constructing appropriate kernels

We now show that Assumption (C) is satisfied by various choices of kernel: Gaussian bandwidth selection (Appendix A.4.1), deep kernels (Appendix A.4.2), and classic multiple kernel learning (Appendix A.4.3). The following assumption will be useful for different kernel schemes.

(1) The domain \( \mathcal{X} \) is Euclidean and bounded, \( \mathcal{X} \subseteq \{ x \in \mathbb{R}^d : \|x\| \leq R_X \} \) for some constant \( R_X < \infty \).

We begin by recalling a well-known property of the Gaussian kernel, useful for both Gaussian bandwidth selection and deep kernels. A proof is in Appendix A.5.

Lemma 17. The Gaussian kernel \( \kappa(a, b) = \exp \left( -\frac{\|a-b\|^2}{2\sigma^2} \right) \) satisfies

\[
|\kappa(a, b) - \kappa(a', b')| \leq \frac{1}{\sigma \sqrt{e}} (\|a - b\| + \|a' - b'\|) \leq \frac{1}{\sigma \sqrt{e}} (\|a - a'\| + \|b - b'\|).
\]
A.4.1. Gaussian bandwidth selection

Lemma 17 immediately gives us Assumption (C) when we chose among Gaussian kernels:

**Proposition 18.** Define a one-dimensional Banach space for inverse lengthscales of Gaussian kernels $\gamma > 0$, so that $k_\gamma(x, y) = \kappa_{1 / \gamma}(x, y)$, with standard addition and multiplication and norms defined by the absolute value, and $k_0$ taken to be the constant 1 function. Let $\Omega$ be any subset of this space. Under Assumption (I), Assumption (C) holds: for any $x, y \in \mathcal{X}$ and $\gamma, \gamma' \in \Gamma$,

$$|k_\gamma(x, y) - k_{\gamma'}(x, y)| \leq \frac{2R}{\sqrt{e}}|\gamma - \gamma'|.$$

**Proof.**

$$|k_\gamma(x, y) - k_{\gamma'}(x, y)| = |\kappa_1(\gamma x, \gamma y) - \kappa_1(\gamma' x, \gamma' y)| \leq \frac{1}{\sqrt{e}}\|x - y\| = \frac{1}{\sqrt{e}}|\gamma - \gamma'|.$$

A.4.2. Deep kernels

To handle the deep kernel case, we will need some more assumptions on the form of the kernel.

(II) $\phi_\omega(x) = \phi_\omega^{(A)}$ is a feedforward neural network with $A$ layers given by

$$\phi_\omega^{(0)}(x) = x \quad \phi_\omega^{(A)}(x) = \sigma^{(A)} \left( W_\omega^{(A)} \phi_\omega^{(A-1)}(x) + b_\omega^{(A)} \right),$$

where the network parameter $\omega$ consists of all the weight matrices $W_\omega^{(A)}$ and biases $b_\omega^{(A)}$, and the activation functions $\sigma^{(A)}$ are each 1-Lipschitz, $\|\sigma^{(A)}(x) - \sigma^{(A)}(y)\| \leq \|x - y\|$, with $\sigma^{(A)}(0) = 0$ so that $\|\sigma^{(A)}(x)\| \leq \|x\|$. Define a Banach space on $\omega$, with addition and scalar multiplication componentwise, and

$$\|\omega\| = \max_{A \in \{1, \ldots, A\}} \max \left( \|W_\omega^{(A)}\|, \|b_\omega^{(A)}\| \right),$$

where the matrix norm denotes operator norm $\|W\| = \sup_x \|Wx\| / \|x\|$. (For convolutional networks, see Remark 22.)

(III) $k_\omega$ is a kernel of the form (1),

$$k_\omega(x, y) = [(1 - \epsilon)\kappa(\phi_\omega(x), \phi_\omega(y)) + \epsilon] q(x, y),$$

with $0 \leq \epsilon \leq 1$, $\kappa$ a kernel function, and $q(x, y)$ a kernel with $\sup_x q(x, x) \leq Q$.

Note that this includes kernels of the form $k_\omega(x, y) = \kappa(\phi_\omega(x), \phi_\omega(y))$, take $\epsilon = 0$ and $q(x, y) = 1$.

(IV) $\kappa$ in Assumption (III) is a kernel function satisfying

$$|\kappa(a, b) - \kappa(a', b')| \leq L_\kappa \|a - a'\| + \|b - b'\|.$$ 

This holds for a Gaussian $\kappa$ via Lemma 17.

We now turn to proving Assumption (C) for deep kernels. First, we will need some smoothness properties of the network $\phi$.

**Lemma 19.** Under Assumption (II), suppose $\omega, \omega'$ have $\|\omega\| \leq R$, $\|\omega'\| \leq R$, with $R \neq 1$. Then, for any $x$,

$$\|\phi_\omega(x)\| \leq R^A \|x\| + \frac{R^A}{R - 1} (R^A - 1) \quad (13)$$

$$\|\phi_\omega(x) - \phi_{\omega'}(x)\| \leq (A R^A - 1) \left( \|x\| + \frac{R}{R - 1} - \frac{R^A - 1}{(R - 1)^2} \right) \|\omega - \omega'\|. \quad (14)$$

If $R \geq 2$, we furthermore have

$$\|\phi_\omega(x)\| \leq R^A (\|x\| + 2) \quad (15)$$

$$\|\phi_\omega(x) - \phi_{\omega'}(x)\| \leq A R^A - 1 (\|x\| + 2) \|\omega - \omega'\|. \quad (16)$$
The proof, by recursion, is given in Appendix A.5. We are now ready to prove Assumption (C) for deep kernels.

**Proposition 20.** Make Assumptions (I) to (IV) and Assumption (B), with $R \geq 2$. Then Assumption (C) holds: for any $x, y \in X$ and $\omega, \omega' \in \Omega$,

$$|k_\omega(x, y) - k_{\omega'}(x, y)| \leq 2Q(1 - \epsilon)L_\kappa \Lambda R_{\Omega}^{\lambda - 1}(R_X + 2) \|\omega - \omega'\|.$$  

**Proof.**

$$|k_\omega(x, y) - k_{\omega'}(x, y)| = (1 - \epsilon) |\kappa(\phi_\omega(x), \phi_\omega(y)) - \kappa(\phi_{\omega'}(x), \phi_{\omega'}(y))| q(x, y)$$

$$\leq Q(1 - \epsilon)L_\kappa (|\phi_\omega(x) - \phi_{\omega'}(x)| + |\phi_\omega(y) - \phi_{\omega'}(y)|)$$

$$\leq Q(1 - \epsilon)L_\kappa \Lambda R_{\Omega}^{\lambda - 1}(\|x\| + \|y\| + 4) \|\omega - \omega'\|$$

$$\leq 2Q(1 - \epsilon)L_\kappa \Lambda R_{\Omega}^{\lambda - 1}(R_X + 2) \|\omega - \omega'\|.$$

**Remark 21.** For the deep kernels we use in the paper (Assumptions (II) to (IV)) on bounded domains (Assumption (I)), we know $L_\kappa$ via Proposition 20; Theorem 6 combines Theorem 8, Corollary 9, and Proposition 20. If we further use a Gaussian kernel $q$ of bandwidth $\sigma_\omega$, the last bracketed term in the error bound of Theorem 8 becomes

$$\frac{2(1 - \epsilon)}{\sigma_\omega \sqrt{c}} \Lambda R_{\Omega}^{\lambda - 1}(R_X + 2) + \sqrt{2 \log \frac{2}{\delta} + 2D \log (4R_\Omega \sqrt{n})}.$$  

The component $R_{\Omega}^{\lambda - 1}(R_X + 2)$, from (15), is approximately the largest that $\phi_\omega$ could make its outputs’ norms; $\sigma_\omega$ will generally be on a comparable scale to the norm of the actual outputs of the network, so their ratio is something like the “unused capacity” of the network to blow up its inputs. This term is weighted about equally in the convergence bound with the square root of the total number of parameters in the network.

**Remark 22.** We can handle convolutional networks as follows. We define $\Omega$ in essentially the same way, letting $W_{\omega}^{(f)}$ denote the convolutional kernel (the set of parameters being optimized), but define $\|\omega\|$ in terms of the operator norm of the linear transform corresponding to the convolution operator. This is given in terms of the operator norm of various discrete Fourier transforms of the kernel matrix by Lemma 2 of Bibi et al. (2019); see also Theorem 6 of Sedghi et al. (2019). The number of parameters $D$ is then the actual number of parameters optimized in gradient descent, but the radius $R_{\Omega}$ is computed differently.

### A.4.3. Multiple kernel learning

Multiple kernel learning (Gönen & Alpaydün, 2011) also falls into our setting. A special case of this family of kernels was studied for the (easier to analyze) “streaming” MMD estimator by Gretton et al. (2012b).

(V) Let $\{k_i\}_{i=1}^D$ be a set of base kernels, each satisfying $\sup_{x \in X} k_i(x, x) \leq K$ for some finite $K$. Define $k_\omega$ as

$$k_\omega(x, y) = \sum_{i=1}^D \omega_i k_i(x, y).$$

Define the norm of a kernel parameter by the norm of the corresponding vector $\omega \in \mathbb{R}^D$. Let $\Omega$ be a set of possible parameters such that for each $\omega \in \Omega$, $k_\omega$ is positive semi-definite, and $\|\omega\| \leq R_{\Omega}$ for some $R_{\Omega} < \infty$.

Not only does learning in this setting work (Proposition 23), it is also – unlike the deep setting – efficient to find an exact maximizer of $J_\lambda$ (Proposition 24).

**Proposition 23.** Assumption (V) implies Assumptions (A) to (C). In particular,

$$\sup_{\omega \in \Omega} \sup_{x \in X} k_\omega(x, x) \leq KR_{\Omega} \sqrt{D}$$

$$|k_\omega(x, y) - k_{\omega'}(x, y)| \leq K \sqrt{D} \|\omega - \omega'\|.$$  

\(^8\)Of course, if we know a bound of $R < 2$, the result will still hold using $R = 2$. It is also possible to show a tighter result, via (13) and (14) or their analogue for $R = 1$; the expression is simply less compact.
A maximizer of \( \hat{\omega} \) as long as Lemma 17. The Gaussian kernel \( \kappa(x, y) = \exp \left( -\frac{\|x - y\|^2}{2\sigma^2} \right) \) satisfies
\[
|\kappa(a, b) - \kappa(a', b')| \leq \frac{1}{\sigma \sqrt{\epsilon}} (\|a - b\| + \|a' - b'\|) \leq \frac{1}{\sigma \sqrt{\epsilon}} (\|a - a'\| + \|b - b'\|).
\]

**Proof.** We have that
\[
|\kappa(a, b) - \kappa(a', b')| = \left| \exp \left( -\frac{\|a - b\|^2}{2\sigma^2} \right) - \exp \left( -\frac{\|a' - b'\|^2}{2\sigma^2} \right) \right|
\leq \left\| x \mapsto \exp \left( -\frac{x^2}{2\sigma^2} \right) \right\|_L \|a - b\| - \|a' - b'\|.
\]

**A.5. Miscellaneous Proofs**

The following lemma was used for Propositions 18 and 20.

**Lemma 17.** The Gaussian kernel \( \kappa(a, b) = \exp \left( -\frac{\|a - b\|^2}{2\sigma^2} \right) \) satisfies
\[
|\kappa(a, b) - \kappa(a', b')| \leq \frac{1}{\sigma \sqrt{\epsilon}} (\|a - b\| + \|a' - b'\|) \leq \frac{1}{\sigma \sqrt{\epsilon}} (\|a - a'\| + \|b - b'\|).
\]
We can bound the Lipschitz constant as its maximal derivative norm,
\[
\sup_x \left| \frac{x}{\sigma^2} \exp \left( -\frac{x^2}{2\sigma^2} \right) \right|
\]
Noting that
\[
\frac{d}{dx} \log \left( \frac{|x|}{\sigma^2} \exp \left( -\frac{x^2}{2\sigma^2} \right) \right) = \frac{1}{x} - \frac{x}{\sigma^2}
\]
vanishes only at \( x = \pm \sigma \), the supremum is achieved by using that value, giving
\[
\left\| x \mapsto \exp \left( -\frac{x^2}{2\sigma^2} \right) \right\|_L = \frac{1}{\sqrt{\sigma^2}}
\]
The result follows from
\[
\|a - b\| - \|a' - b'\| \leq \|a - b - a' + b'\| \leq \|a - a'\| + \|b - b'\|
\]
This next lemma was used in Proposition 20.

**Lemma 19.** Under Assumption (II), suppose \( \omega, \omega' \) have \( \|\omega\| \leq R, \|\omega'\| \leq R \), with \( R \neq 1 \). Then, for any \( x \),
\[
\| \phi_\omega(x) \| \leq R^\Lambda \|x\| + \frac{R}{R^R - 1} (R^\Lambda - 1)
\]
\[
\| \phi_\omega(x) - \phi_{\omega'}(x) \| \leq \left( \Lambda R^{\Lambda-1} \left( \|x\| + \frac{R}{R^R - 1} \right) - \frac{R^\Lambda - 1}{(R - 1)^2} \right) \|\omega - \omega'\|.
\]
If \( R \geq 2 \), we furthermore have
\[
\| \phi_\omega(x) \| \leq R^\Lambda (\|x\| + 2)
\]
\[
\| \phi_\omega(x) - \phi_{\omega'}(x) \| \leq R^{\Lambda-1} (\|x\| + 2) \|\omega - \omega'\|.
\]

**Proof.** First, \( \| \phi_\omega^{(0)}(x) \| = \|x\| \), showing (13) when \( \Lambda = 0 \). In general,
\[
\| \phi_\omega^{(\ell)}(x) \| = \| \sigma^{(\ell)} \left( W_\omega^{(\ell)} \phi_\omega^{(\ell-1)}(x) + b_\omega^{(\ell)} \right) \|
\leq \| W_\omega^{(\ell)} \phi_\omega^{(\ell-1)}(x) + b_\omega^{(\ell)} \|
\leq \| W_\omega^{(\ell)} \| \| \phi_\omega^{(\ell-1)}(x) \| + \| b_\omega^{(\ell)} \|
\leq R \| \phi_\omega^{(\ell-1)}(x) \| + R,
\]
and expanding this recursion gives
\[
\| \phi_\omega^{(\ell)}(x) \| \leq R^\ell \|x\| + \sum_{m=1}^\ell R^m = R^\ell \|x\| + \frac{R}{R^\ell - 1} (R^\ell - 1).
\]
Now, we have (14) for \( \Lambda = 0 \) because \( \phi_\omega^{(0)}(x) - \phi_{\omega'}^{(0)}(x) = 0 \). For \( \ell \geq 1 \), we have
\[
\| \phi_\omega^{(\ell)}(x) - \phi_{\omega'}^{(\ell)}(x) \| = \| \sigma^{(\ell)} \left( W_\omega^{(\ell)} \phi_\omega^{(\ell-1)}(x) + b_\omega^{(\ell)} \right) - \sigma^{(\ell)} \left( W_{\omega'}^{(\ell)} \phi_{\omega'}^{(\ell-1)}(x) - b_{\omega'}^{(\ell)} \right) \|
\leq \| W_\omega^{(\ell)} \phi_\omega^{(\ell-1)}(x) - W_{\omega'}^{(\ell)} \phi_{\omega'}^{(\ell-1)}(x) \| + \| W_\omega^{(\ell)} \phi_\omega^{(\ell-1)}(x) - W_{\omega'}^{(\ell)} \phi_{\omega'}^{(\ell-1)}(x) \| + \| b_\omega^{(\ell)} - b_{\omega'}^{(\ell)} \|
\leq \| W_\omega^{(\ell)} - W_{\omega'}^{(\ell)} \| \| \phi_\omega^{(\ell-1)}(x) \| + \| W_\omega^{(\ell)} \| \| \phi_{\omega'}^{(\ell-1)}(x) \| + \| \omega - \omega' \|
\leq \| \omega - \omega' \| \left( R^{\ell-1} \|x\| + \frac{R}{R^{\ell-1} - 1} (R^{\ell-1} - 1) + 1 \right) + R \| \phi_\omega^{(\ell-1)}(x) - \phi_{\omega'}^{(\ell-1)}(x) \|. \]
Expanding the recursion yields
\[
\left\| \phi^{(t)}_\omega(x) - \phi^{(t)}_{\omega'}(x) \right\| \leq \sum_{m=0}^{\ell-1} R^m \left( \frac{R^{\ell-1-m} \left\| x \right\|}{R - 1} + \frac{R}{R - 1} \right) \left( R^{\ell-m-1} - 1 \right) \left\| \omega - \omega' \right\|
\]
\[
= \sum_{m=0}^{\ell-1} \left( R^{\ell-1} \left\| x \right\| + \frac{R^\ell}{R - 1} - \frac{R^{m+1}}{R - 1} + R^m \right) \left\| \omega - \omega' \right\|
\]
\[
= \left( \ell R^{\ell-1} \left\| x \right\| + \frac{\ell R^\ell}{R - 1} - \frac{R^\ell}{R - 1} - \frac{1}{R - 1} R^{\ell-1} \right) \left\| \omega - \omega' \right\|
\]

When \( R \geq 2 \), we have that \( R/(R - 1) \leq 2 \) and \( R^\ell > 1 \), giving (15) and (16).

## B. Experimental Details

### B.1. Details of synthetic datasets

Table 6 shows details of four synthetic datasets. *Blob* datasets are often used to validate two-sample test methods (Gretton et al., 2012b; Jitkrittum et al., 2016; Sutherland et al., 2017), although we rotate each blob to show the benefits of non-homogeneous kernels. *HDGM* datasets are first proposed in this paper. *HDGM-D* can be regarded as *high-dimension Blob-D* which contains two modes with the same variance and different covariance.

| Datasets        | \( p \)                                                                 | \( q \)                                                                 |
|-----------------|---------------------------------------------------------------------------|---------------------------------------------------------------------------|
| *Blob-S*        | \( \sum_{i=1}^{9} \frac{1}{9} \mathcal{N}(\mu_i^b, 0.03 \times I_2) \)    | \( \sum_{i=1}^{9} \frac{1}{9} \mathcal{N}(\mu_i^b, 0.03 \times I_2) \)    |
| *Blob-D*        | \( \sum_{i=1}^{9} \frac{1}{9} \mathcal{N}(\mu_i^b, 0.03 \times I_2) \)    | \( \sum_{i=1}^{9} \frac{1}{9} \mathcal{N} \left( \mu_i^b, \begin{bmatrix} \Delta_i^b \\ 0.03 \end{bmatrix} \right) \) |
| *HDGM-S*        | \( \sum_{i=1}^{2} \frac{1}{2} \mathcal{N}(\mu_i^h, I_d) \)               | \( \sum_{i=1}^{2} \frac{1}{2} \mathcal{N}(\mu_i^h, I_d) \)               |
| *HDGM-D*        | \( \sum_{i=1}^{2} \frac{1}{2} \mathcal{N}(\mu_i^h, I_d) \)               | \( \sum_{i=1}^{2} \frac{1}{2} \mathcal{N} \left( \mu_i^h, \begin{bmatrix} \Delta_i^h \Delta_i^h \end{bmatrix} \right) \) |

### B.2. Dataset visualization

Figure 4 shows images from real-*MNIST* and “fake”-*MNIST*, while Figure 5 shows samples from *CIFAR-10* and *CIFAR-10.1*.

### B.3. Configurations

We implement all methods on Python 3.7 (Pytorch 1.1) with a NVIDIA Titan V GPU. We run ME and SCF using the official code (Jitkrittum et al., 2016), and implement C2ST-S, C2ST-L, MMD-D and MMD-O by ourselves. We use permutation test to compute \( p \)-values of C2ST-S and C2ST-L, MMD-D, MMD-O and tests in Table 4. We set \( \alpha = 0.05 \) for all experiments. Following Lopez-Paz & Oquab (2017), we use a deep neural network \( F \) as the classifier in C2ST-S and C2ST-L, and train the \( F \) by minimizing cross entropy. To fairly compare MMD-D with C2ST-S and C2ST-L, the network \( \phi_\omega \) in MMD-D has the same architecture with feature extractor in \( F \). Namely, \( F = g \circ \phi_\omega \), where \( g \) is a two-layer fully-connected network. The network \( g \) is a simple binary classifier that takes extracted features (through \( \phi_\omega \)) as input. For test methods shown in Table 4, the network \( \phi_\omega \) in them also has the same architecture with that in MMD-D.

For *Blob*, *HDGM* and *Higgs*, \( \phi_\omega \) is a five-layer fully-connected neural network. The number of neurons in hidden and
output layers of $\phi_\omega$ are set to 50 for Blob, $3 \times d$ for HDGM and 20 for Higgs, where $d$ is the dimension of samples. These neurons are with softplus activation function, i.e., $\log(1 + \exp(x))$. For MNIST and CIFAR, $\phi_\omega$ is a convolutional neural network (CNN) that contains four convolutional layers and one fully-connected layer. The structure of the CNN follows the structure of the feature extractor in the discriminator of DCGAN (Radford et al., 2016) (see Figures 6 and 8 for the structure of $\phi_\omega$ in MMD-D, and Figures 7 and 9 for the structure of classifier $F$ in C2ST-S and C2ST-L). The link of DCGAN code is https://github.com/eriklindernoren/PyTorch-GAN/blob/master/implementations/dcgan/dcgan.py.

We use Adam optimizer (Kingma & Ba, 2015) to optimize 1) parameters of $F$ in C2ST-S and C2ST-L, 2) parameters of $\phi_\omega$ in MMD-D and 3) kernel lengthscales in MMD-O. We set drop-out rate to zero when training C2ST-S, C2ST-L and MMD-D on all datasets.
Figure 6. The structure of $\phi_M$ in MMD-D on MNIST. The kernel size of each convolutional layer is 3; stride (S) is set to 2; padding (P) is set to 1. We do not use dropout. Best viewed zoomed in.

Figure 7. The structure of classifier $F$ in C2ST-S and C2ST-L on MNIST. The kernel size of each convolutional layer is 3; stride (S) is set to 2; padding (P) is set to 1. We do not use dropout. In the first layer, we will convert the CIFAR images from $32 \times 32 \times 3$ to $64 \times 64 \times 3$. Best viewed zoomed in.

Figure 8. The structure of $\phi_M$ in MMD-D on CIFAR. The kernel size of each convolutional layer is 3; stride (S) is set to 2; padding (P) is set to 1. We do not use dropout in all layers. In the first layer, we will convert the CIFAR images from $32 \times 32 \times 3$ to $64 \times 64 \times 3$. Best viewed zoomed in.

Figure 9. The structure of classifier $F$ in C2ST-S and C2ST-L on CIFAR. The kernel size of each convolutional layer is 3; stride (S) is set to 2; padding (P) is set to 1. We do not use dropout. Best viewed zoomed in.

B.4. Detailed parameters of all test methods

In this subsection, we demonstrate detailed parameters of all test methods. Except for learning rate of Adam optimizer, we use default parameters of Adam optimizer provided by Pytorch. We use one validation set (with the same size of training set) to roughly search these parameters. Using these parameters, we compute test power of each test method on 100 test sets (with the same size of training set).

For ME and SCF, we follow Chwialkowski et al. (2015) and set $J = 10$ for Higgs. For other datasets, we set $J = 5$.

For C2ST-S and C2ST-L, we set batchsize to $\min\{2 \times n_b, 128\}$ for Blob, 128 for HDGM and Higgs, and 100 for MNIST and CIFAR. We set the number of epochs to $500 \times 18 \times n_b$/batchsize for Blob, 1,000 for HDGM, Higgs and CIFAR, and 2,000 for MNIST. We set learning rate to 0.001 for Blob, HDGM and Higgs, and 0.0002 for MNIST and CIFAR (following Radford et al. (2016)).

For MMD-O, we use full batch (i.e., all samples) to train MMD-O. We set the number of epochs to 1,000 for Blob, HDGM, Higgs and CIFAR, and 2,000 for MNIST. We set learning rate to 0.0005 for Blob, MNIST and CIFAR, and 0.001 for HDGM.

For MMD-D, we use full batch (i.e., all samples) to train MMD-D with samples from Blob, HDGM and Higgs. We use mini-batch (batchsize is 100) to train MMD-D with samples from MNIST and CIFAR. We set the number of epochs to 1,000 for Blob, HDGM, Higgs and CIFAR, and 2,000 for MNIST. We set learning rate to 0.0005 for Blob and Higgs, $10^{-5}$ for HDGM, 0.001 for MNIST and 0.0002 for and CIFAR (following Radford et al. (2016)).

B.5. Links to datasets

Higgs dataset can be downloaded from UCI Machine Learning Repository. The link is https://archive.ics.uci.edu/ml/datasets/HIGGS.

MNIST dataset can be downloaded via Pytorch. See the code in https://github.com/eriklindernoren/PyTorch-GAN/blob/master/ implementations/dcgan/dcgan.py.

CIFAR-10.1 is available from https://github.com/modestyachts/CIFAR-10.1/tree/master/
Table 7. Results on Higgs ($\alpha = 0.05$). We report average Type I error on Higgs dataset when increasing number of samples ($N$). Note that, in Higgs, we have two types of Type I errors: 1) Type I error when two samples drawn from $P$ (no Higgs bosons) and 2) Type I error when two samples drawn from $Q$ (having Higgs bosons). Type I reported here is the average value of 1) and 2). Since Type I error reported here is the average value of two average Type I errors, we do not report standard errors of the average Type I error in this table.

| $N$  | ME  | SCF | C2ST-S | C2ST-L | MMD-O | MMD-D |
|------|-----|-----|--------|--------|-------|-------|
| 1000 | 0.048 | 0.040 | 0.043 | 0.048 | 0.059 | 0.037 |
| 2000 | 0.043 | 0.032 | 0.060 | 0.056 | 0.055 | 0.053 |
| 3000 | 0.049 | 0.043 | 0.046 | 0.053 | 0.051 | 0.069 |
| 5000 | 0.056 | 0.035 | 0.052 | 0.065 | 0.049 | 0.062 |
| 8000 | 0.050 | 0.034 | 0.065 | 0.067 | 0.056 | 0.037 |
| 10000 | 0.059 | 0.032 | 0.057 | 0.058 | 0.045 | 0.048 |

Avg.  | 0.051 | 0.036 | 0.054 | 0.058 | 0.050 | 0.051 |

Table 8. Results on MNIST given $\alpha = 0.05$. We report average Type I error±standard errors on real-MNIST vs. real-MNIST when increasing number of samples ($N$).

| $N$  | ME  | SCF | C2ST-S | C2ST-L | MMD-O | MMD-D |
|------|-----|-----|--------|--------|-------|-------|
| 2000 | 0.076±0.011 | 0.075±0.010 | 0.035±0.006 | 0.045±0.005 | 0.068±0.004 | 0.056±0.003 |
| 4000 | 0.062±0.010 | 0.056±0.007 | 0.044±0.006 | 0.040±0.004 | 0.053±0.005 | 0.056±0.005 |
| 6000 | 0.051±0.003 | 0.049±0.009 | 0.039±0.005 | 0.054±0.007 | 0.066±0.008 | 0.056±0.008 |
| 8000 | 0.054±0.006 | 0.046±0.006 | 0.043±0.005 | 0.042±0.007 | 0.051±0.005 | 0.054±0.007 |
| 10000 | 0.047±0.006 | 0.045±0.010 | 0.038±0.006 | 0.046±0.005 | 0.041±0.007 | 0.062±0.006 |

Avg.  | 0.058 | 0.054 | 0.040 | 0.045 | 0.056 | 0.057 |

Datasets (we use cifar10_1_v4_data.npy). This new test set contains 2,031 images from TinyImages (Torralba et al., 2008).

B.6. Type I errors on Higgs and MNIST

Table 7 shows average Type I error on Higgs dataset when increasing number of samples ($N$). Table 8 shows average Type I error on real-MNIST vs. real-MNIST when increasing number of samples ($N$).

C. Interpretability on CIFAR-10 vs CIFAR-10.1

In Section 7.1, we have shown that images in CIFAR-10 and CIFAR-10.1 are not from the same distribution. Thus, it is interesting to try to understand the major difference between the datasets. Mean Embedding tests (Chwialkowski et al., 2015) compare the mean embeddings $\mu_P$ and $\mu_Q$ at test locations $v_1, \ldots, v_L$, rather than through their overall norm. The test statistic is

$$\hat{\Lambda} = n \bar{z}_n^T S^{-1} \bar{z}_n,$$

$$z_i = (k(x_i, v_j) - k(y_i, v_j))_{j=1}^L \in \mathbb{R}^L,$$

$$\bar{z}_n = \frac{1}{n} \sum_{i=1}^n z_i,$$

$$S_n = \frac{1}{n-1} \sum_{i=1}^n (z_i - \bar{z}_n)(z_i - \bar{z}_n)^T;$$

the asymptotic null distribution of $\hat{\Lambda}$ is $\chi^2_L$, and the estimator is computable in linear time rather than $\hat{\text{MMD}}_U$’s quadratic time.

Jitkrittum et al. (2017) jointly learn the parameters $v_j$ and kernel parameters to optimize test power. The best such test locations ($L = 1$) for a Gaussian kernel (with learned bandwidth) are shown in Figure 10. We could also try optimizing a deep kernel (1) and the test locations together; this procedure, however, failed to find a useful test. We can find a better test, though, with a two-stage scheme: first, learn a deep kernel to maximize $J_\lambda$, then choose $v_i$ to maximize $\hat{\Lambda}$ with that kernel fixed. Results are shown in Figure 11.

Although these approaches give nontrivial test power, it is hard to interpret either set of images, as the test locations have moved far outside the set of natural images. We can instead constrain $v_i \in S_P \cup S_Q$, simply picking the single point from the dataset which maximizes $\hat{\Lambda}$ (shown in Figure 12). This achieves similar test power, but lets us see that the difference might lie in images with smaller objects of interest than the mean for CIFAR-10.
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Figure 10. The best test locations (learned by an ME test with $L = 1$) from 10 experiments on CIFAR-10 vs CIFAR-10.1. Average rejection rate is 0.415.

Figure 11. The best test locations (learned by an ME test, $L = 1$, with a deep kernel optimized for an MMD test) from 10 experiments on CIFAR-10 vs CIFAR-10.1. Average rejection rate is 0.637.

Figure 12. The best test locations (selected among existing images with our learned deep kernel, $L = 1$) from 10 experiments on CIFAR-10 vs CIFAR-10.1. Average rejection rate is 0.653.