Minimum Kernel Discrepancy Estimators

Chris. J. Oates
Newcastle University, UK
August 24, 2023

Abstract

For two decades, reproducing kernels and their associated discrepancies have facilitated elegant theoretical analyses in the setting of quasi Monte Carlo. These same tools are now receiving interest in statistics and related fields, as criteria that can be used to select an appropriate statistical model for a given dataset. The focus of this article is on minimum kernel discrepancy estimators, whose use in statistical applications is reviewed, and a general theoretical framework for establishing their asymptotic properties is presented.

1 Introduction

The abstract problem tackled in quasi Monte Carlo is to construct an empirical distribution $P_n$ that provides an accurate approximation to a given probability distribution $P$ of interest. To make this problem well-defined a discrepancy is required, to precisely quantify the quality of the approximation $P_n$ to $P$. The mathematical tractability of the discrepancy is an important consideration, both for algorithmic design and for analysis of the error of the approximations $P_n$ that are produced. In a seminal paper, Hickernell (1998) advocated kernel discrepancies in this context, explaining how reproducing kernels can be used to construct explicit discrepancies with a range of favourable mathematical properties. Subsequent researchers have exploited kernel discrepancies to analyse a variety of modern and powerful quasi Monte Carlo methods (see e.g. Dick and Pillichshammer, 2010), and more recently also Markov chain Monte Carlo methods (see e.g. Gorham and Mackey, 2017).

The abstract problem tackled in statistics is to construct a probabilistic model $P$ for a population quantity of interest, given a finite sample from this population with empirical distribution $P_n$. Thus, on the face of it, the problems tackled in quasi Monte Carlo and in statistics are diametrically opposed. Nevertheless, an equally valid approach to the statistical problem is to first select a discrepancy and proceed to select a probabilistic model $P_\theta$ from a parametric set such that the discrepancy between $P_n$ and $P_\theta$ is minimised. It is well-known that maximum likelihood estimation asymptotically minimises the Kullback–Leibler divergence between $P$ and $P_\theta$ (Akaike, 1973), and as such the maximum likelihood estimator
can be acutely sensitive to the extent to which the model is misspecified, referring to the scenario in which $P$ and $P_\theta$ do not coincide for any value $\theta$ in the parameter set. Several more robust (i.e. less sensitive, in the sense just described) alternatives to maximum likelihood have been proposed, such as M-estimation (Huber, 1964) and the more general minimum distance estimation (Donoho and Liu, 1988), which remains an active research field (Basu et al., 2011; Pardo, 2018). More interestingly, as far as this article is concerned, minimum kernel discrepancy estimation has recently been proposed and studied. The use of kernel discrepancies in the statistical context can be traced back at least to Song et al. (2008), before receiving considerable attention in the machine learning community, where minimum kernel discrepancy estimation has been used to train machine learning models (Dziugaite et al., 2015; Li et al., 2015; Sutherland et al., 2017), to calibrate computer simulations (Park et al., 2016; Mitrovic et al., 2016; Dellaporta et al., 2022), and to facilitate goodness-of-fit testing (Key et al., 2021). It seems, to this author, that there could be a useful dialogue between the quasi Monte Carlo and the statistical communities, centring on whether the theoretical insight into kernel discrepancies gleaned in the former can be used to explain the remarkable success in applications achieved by the latter. This article serves as an introduction to minimum kernel discrepancy estimation, and along the way some opportunities for dialogue between the communities will be highlighted.

In Section 2 both kernel discrepancy and of minimum kernel discrepancy estimators are defined. The use of minimum kernel discrepancy estimators in statistics is described in Section 3. A concise set of theoretical results for minimum kernel discrepancy estimation are presented in Section 4. Some open questions and possible research directions are suggested in Section 5.

## 2 Kernels, Discrepancies, and Estimators

Section 2.1 introduces the set-up and notation that will be used. The role of kernel discrepancies in quasi Monte Carlo is reviewed in Section 2.2. Then, minimum kernel discrepancy estimators are defined in Section 2.3.

### 2.1 Set-Up and Notation

Our setting is a measurable space $\mathcal{X}$. A **kernel** is a function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, that is measurable, symmetric and positive semi-definite, meaning respectively that

- $k(\cdot, x)$ is measurable for all $x \in \mathcal{X}$
- $k(x, y) = k(y, x)$ for all $x, y \in \mathcal{X}$
- $\sum_{i=1}^n \sum_{j=1}^n w_i w_j k(x_i, x_j) \geq 0$ for all $w_1, \ldots, w_n \in \mathbb{R}$, $x_1, \ldots, x_n \in \mathcal{X}$, $n \in \mathbb{N}$.

The **reproducing kernel Hilbert space** associated to a kernel $k$ is a Hilbert space $\mathcal{H}(k)$ of real-valued functions on $\mathcal{X}$, such that
• \( k(\cdot, x) \in \mathcal{H}(k) \) for all \( x \in X \)

• \( \langle h, k(\cdot, x) \rangle_{\mathcal{H}(k)} = h(x) \) for all \( x \in X \), \( h \in \mathcal{H}(k) \).

The latter requirement is known as the reproducing property. It can be shown that \( \mathcal{H}(k) \) exists, that \( \mathcal{H}(k) \) is uniquely determined, and that the elements of \( \mathcal{H}(k) \) are measurable functions on \( X \) (see Chapter 4 of Steinwart and Christmann, 2008). Our interest in reproducing kernel Hilbert spaces derives from their suitability for constructing a discrepancy between probability distributions on \( X \), as explained next.

Let \( \mathcal{P}_k(X) \) be the set of probability distributions \( P \) on \( X \) for which \( P : \mathcal{H}(k) \to \mathbb{R} \), \( P(h) = \int h \ dP \), is a bounded linear functional. Sufficient conditions for \( P \in \mathcal{P}_k(X) \) are discussed in Appendix A. If \( P \in \mathcal{P}_k(X) \) then there exists a Riesz representer \( \mu_k(P) \in \mathcal{H}(k) \), called the kernel mean element, such that \( P(h) = \langle h, \mu_k(P) \rangle_{\mathcal{H}(k)} \) for all \( h \in \mathcal{H}(k) \). The kernel discrepancy on \( \mathcal{P}_k(X) \) is defined as

\[
D_k : \mathcal{P}_k(X) \times \mathcal{P}_k(X) \to [0, \infty) \quad (P, Q) \mapsto \|\mu_k(P) - \mu_k(Q)\|_{\mathcal{H}(k)},
\]

being the distance between the Riesz representatives \( \mu_k(P) \) and \( \mu_k(Q) \) in \( \mathcal{H}(k) \). It is immediate that \( D_k \) is a pseudo-metric on \( \mathcal{P}_k(X) \), meaning that \( D_k \) satisfies all the requirements of a metric on \( \mathcal{P}_k(X) \) except for the distinguishability requirement, since in general we may have \( D_k(P, Q) = 0 \) even if \( P \) and \( Q \) are distinct. The pseudo-metric \( D_k \) appears in several fields; in machine learning it is called the maximum mean discrepancy (Gretton et al., 2012; Muandet et al., 2017), in probability it is called an integral probability (pseudo-)metric (Muller, 1997), in statistics it is the discrepancy associated to the kernel scoring rule (Gneiting and Raftery, 2007; Dawid, 2007), and in quasi Monte Carlo it is called the worst case integration error (Dick and Pillichshammer, 2010). The popularity of kernel discrepancy is due in large part to a well-known explicit formula that enables it to be computed:

**Proposition 1.** For \( P, Q \in \mathcal{P}_k(X) \),

\[
D_k(P, Q) = \sqrt{\iint k_Q(x, y) dP(x) dP(y)},
\]

where

\[
k_Q(x, y) := k(x, y) - \int k(x, y) dQ(x) - \int k(x, y) dQ(y) + \iint k(x, y) dQ(x) dQ(y).
\]  

**Proof.** The reproducing property, together with the definition of \( \mu_k(P) \) as the Riesz representer of \( P \), leads to \( \mu_k(P)(y) = \langle \mu_k(P), k(\cdot, y) \rangle_{\mathcal{H}(k)} = P(k(\cdot, y)) = \int k(x, y) dP(x) \). Thus the kernel mean element is the weak (or Pettis) integral \( \mu_k(P)(\cdot) = \int k(x, \cdot) dP(x) \), for all \( P \in \mathcal{P}_k(X) \). In particular, \( \langle \mu_k(P), \mu_k(Q) \rangle_{\mathcal{H}(k)} = \int \mu_k(P)(y) dQ(y) = \iint k(x, y) dP(x) dQ(y) \) for all \( P, Q \in \mathcal{P}_k(X) \). Therefore, recalling that \( k \) is symmetric,

\[
D_k(P, Q)^2 = \langle \mu_k(P), \mu_k(P) \rangle_{\mathcal{H}(k)} - 2\langle \mu_k(P), \mu_k(Q) \rangle_{\mathcal{H}(k)} + \langle \mu_k(Q), \mu_k(Q) \rangle_{\mathcal{H}(k)}
\]

\[
= \iint k(x, y) dP(x) dP(x) - 2 \iint k(x, y) dP(x) dQ(y) + \iint k(x, y) dQ(x) dQ(y)
\]

\[
= \iint k_Q(x, y) dP(x) dP(y),
\]  

3
which completes the proof.

It can be verified that the map $k_Q : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ in (1) is a $Q$-dependent kernel, satisfying $\int k_Q(x, y) dP(x) = 0$ for all $y \in \mathcal{X}$ whenever $Q = P$. This presentation, which assigns different roles to $P$ and $Q$, is useful in our setting, where the first argument $P$ will be fixed and the second argument $Q$ will be varied.

### 2.2 Kernel Discrepancies in Quasi Monte Carlo

Classical analysis of quasi Monte Carlo focused on the design of point sets or sequences for which small values of a *figure of merit*, quantifying in a sense the uniformity of the points, is achieved. For simplicity the domain $\mathcal{X}$ is typically taken to be $[0, 1]^d$. Depending on the nature of the algorithm being considered, and the assumed regularity of the integrands involved, a different figure of merit was typically used. For example, the van der Corput–Halton and Sobol’ sequences were analysed using the *star discrepancy* figure of merit (Hlawka, 1961), while for lattice rules a figure of merit called $P_\alpha$ was used (Sloan and Kachoyan, 1987). A turning point came in Hickernell (1998), who observed that each of the above figures of merit can be recovered as a specific instance of a kernel discrepancy $D_k$ (i.e. corresponding to a particular choice of kernel $k$). Further, elementary properties of reproducing kernels give rise to a natural cubature error bound, involving simply the product of $D_k$ and the norm of the integrand in $\mathcal{H}(k)$. Since then, kernel discrepancies have been adopted for the analysis of a variety of modern and powerful quasi Monte Carlo methods. Indeed, many of the regularities that are exploited by modern quasi-Monte Carlo algorithms can be encoded directly at the level of the kernel.

Two examples in particular clearly illustrate the elegance of the kernel framework. First, the *dominating mixed smoothness* assumption, concerning the existence of mixed partial derivatives of order up to $s$ in each coordinate\(^1\), corresponds to a tensor product kernel

$$k(x, y) = \prod_{i=1}^{d} k_{1D}(x_i, y_i)$$

where $k_{1D}$ is a kernel reproducing $s$-times differentiable functions on $[0, 1]$ (see e.g. Dick and Pillichshammer, 2010, Section 14.6). Such assumptions have been used to prove arbitrarily fast convergence rates for quasi Monte Carlo based on *higher-order digital nets*, as the order of differentiability $s$ is increased (see e.g. Dick and Pillichshammer, 2010, Theorem 15.21). Tensor product kernels have the further advantage that computation of the kernel mean element $\mu_k(P)$ reduces to computation of $d$ univariate integrals whenever the components of a $P$-distributed random variable are independent, which is the case for the canonical choice of the uniform distribution on $[0, 1]^d$. Second, the *effective low dimension* assumption, which states that most of the variation in the output of a function occurs when only a small number

\(^1\)i.e. additional levels of differentiability in directions that are axis-aligned
of the inputs are varied, can be expressed using a weighted kernel

\[ k(x, y) = \sum_{u \subseteq \{1, \ldots, d\}} \gamma_u k_u(x_u, y_u), \]

(2)

where \( x_u = (x_i : i \in u) \) and \( k_u \) is a kernel on \([0, 1]^{|u|}\). The weights \( \gamma_u \geq 0 \) determine the extent to which variation in the coordinates indexed by \( u \) is permitted. The additive form of (2) enables the associated kernel discrepancy to be computed; indeed, \( D_k^2 = \sum_u \gamma_u D_{k_u}^2 \) follows from Proposition 1. The specification of suitable weights for the integration task at hand is an important factor in ensuring low cubature error (Kuo, 2003). In an extreme case the effective dimension, defined as \( \sum_u \gamma_u \), may remain finite as \( d \to \infty \) and one can obtain error bounds for quasi Monte Carlo that are dimension-independent (Sloan and Woźniakowski, 1998; Dick et al., 2013).

The author, in writing this article, is interested in whether the considerable theoretical and practical expertise in kernel discrepancies that has developed in the quasi Monte Carlo community can be brought to bear also on theoretical and practical aspects of minimum kernel discrepancy estimators, which are introduced next.

### 2.3 Minimum Kernel Discrepancy Estimators

Consider data that are assumed to arise as a sequence of independent and identically distributed random variables \((x_n)_{n \in \mathbb{N}}\), with \( x_n \sim P \) and \( P \in \mathcal{P}_k(\mathcal{X}) \). Let \( P_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i} \) denote the empirical distribution of the first \( n \) terms in the dataset. A statistical model is a collection \( \{P_\theta\}_{\theta \in \Theta} \subset \mathcal{P}_k(\mathcal{X}) \), where the parameter \( \theta \) takes values in an index set \( \Theta \). Minimum kernel discrepancy estimators, if they exist, are defined as

\[ \theta_n \in \arg \min_{\theta \in \Theta} D_k(P_n, P_\theta), \]

as illustrated in Figure 1. The properties of such estimators depend on the choice of kernel \( k \) and the statistical model \( \{P_\theta\}_{\theta \in \Theta} \), but are independent of how the statistical model is parametrised (in \( \theta \)). Under regularity conditions, established in Section 4, the estimators \( \theta_n \) converge (in an appropriate sense) to a population minimiser

\[ \theta_* \in \arg \min_{\theta \in \Theta} D_k(P, P_\theta), \]

if these exist. Since in all cases we take \( Q = P_\theta \) in (1), we henceforth adopt the shorthand \( k_\theta \) for \( k_Q \). Through selection of the kernel \( k \), one can trade statistical efficiency with robustness to model misspecification, which is not possible within the classical framework of maximum likelihood; see Section 4.4. However, important aspects of kernel selection remains unsolved, for example it is unclear how to retain statistical efficiency when \( \mathcal{X} \) is high-dimensional. Such open challenges are highlighted in Section 5.
Figure 1: *Minimum kernel discrepancy estimation.* The distance, as measured in $\mathcal{H}(k)$, between the kernel mean element $\mu_k(P_{\theta})$ associated to the statistical model $P_{\theta}$ and the kernel mean element $\mu_k(P_n)$ associated to the dataset is minimised. Under conditions established in Section 4, a minimum kernel discrepancy estimator $\theta_n$ converges to a value $\theta_*$ that minimises the distance to the kernel mean element $\mu_k(P)$ associated to the true data-generating distribution $P$.

### 3 Applications

This section presents three distinct applications for minimum kernel discrepancy estimation: the generalised method of moments (Section 3.1), generative adversarial networks (Section 3.2), and energy-based models (Section 3.3).

#### 3.1 Generalised Method of Moments

Let $\phi : \mathcal{X} \to \mathbb{R}^p$ have components that are integrable with respect to each $\{P_{\theta}\}_{\theta \in \Theta}$, and let $\phi(P) := \int \phi dP_{\theta}$ denote a vector of summary statistics, meaning that this vector summarises some of the salient aspects of $P_{\theta}$. The *generalised method of moments* estimator, if it exists, is defined as

$$\theta_n \in \arg \min_{\theta \in \Theta} \| \phi(P_n) - \phi(P_{\theta}) \|,$$

being the parameter vector of a statistical model whose summary statistics agree most closely with the empirical summary statistics $\phi(P_n)$ calculated using the dataset (Hansen, 1982). This procedure can be cast as minimum kernel discrepancy estimation using a kernel $k(x, y) = \langle \phi(x), \phi(y) \rangle$. For this kernel, $\int k(x, y)dP_{\theta}(y) = \langle \phi(x), \phi(P_{\theta}) \rangle$ and $\int \int k(x, y)dP_{\theta}(x)dP_{\theta}(y) = \langle \phi(P_{\theta}), \phi(P_{\theta}) \rangle$. Then $k_{\theta}(x, y) = \langle \phi(x), \phi(y) \rangle - \langle \phi(x), \phi(P_{\theta}) \rangle - \langle \phi(P_{\theta}), \phi(y) \rangle + \langle \phi(P_{\theta}), \phi(P_{\theta}) \rangle$, so that $D_k(P_n, P_{\theta})^2 = \langle \phi(P_n), \phi(P_n) \rangle - \langle \phi(P_n), \phi(P_{\theta}) \rangle - \langle \phi(P_{\theta}), \phi(P_n) \rangle + \langle \phi(P_{\theta}), \phi(P_{\theta}) \rangle =$
\[ \|\phi(P_n) - \phi(P_0)\|^2. \] In contrast to minimum kernel discrepancy estimation in general, the generalised method of moments is mathematically transparent in the special case where we assume the statistical model \( P_\theta \) can be parametrised such that \( \theta = \phi(P_\theta) \) and \( \Theta = \mathbb{R}^p \).

Indeed, in this case \( D_k(P_n, P_\theta) = \|\theta_n - \theta\|, \) so the generalised method of moments estimator is

\[ \theta_n = \frac{1}{n} \sum_{i=1}^n \phi(x_i), \]

which converges to \( \theta_* = \phi(P) \) and satisfies the central limit \( \sqrt{n}(\theta_n - \theta_*) \overset{d}{\to} N(0, \mathbb{C}_{X \sim P}[\phi(X)]) \) whenever the associated covariance matrix is well-defined. This will provide a convenient opportunity to verify, in a concrete setting, the general theoretical results presented in Section 4.3.

Though originating as a statistically efficient and computationally favourable alternative to maximum likelihood, it has more recently been observed that, through careful selection of the summary statistics \( \phi \), one can usefully trade-off the efficiency and the robustness of the estimator. The related areas of approximate Bayesian computation (Beaumont, 2019) and Bayesian synthetic likelihood (e.g. Frazier and Drovandi, 2021) contain extensive practical guidance on how summary statistics can be selected. Indeed, the estimator \( \theta_n \) can be recognised as a maximum a posteriori estimator in an approximate Bayesian computation framework when a flat a priori distribution is employed.

### 3.2 Generative Adversarial Networks

A generative model consists of a measurable space \( \mathcal{Y} \), equipped with a probability measure \( \mathbb{P} \), and statistical model of the form

\[ P_\theta = G^\theta_\# \mathbb{P} \]  

(3)

where \( G^\theta : \mathcal{Y} \to \mathcal{X} \) is measurable for each \( \theta \in \Theta \). Here \( G^\theta_\# \mathbb{P} \) denotes the pushforward of \( \mathbb{P} \) through \( G^\theta \), meaning that samples \( X \sim P_\theta \) are generated by first sampling \( Y \sim \mathbb{P} \) and then setting \( X = G^\theta(Y) \). In the specific case where \( G^\theta \) is a (deep) neural network, we call \( P_\theta \) a (deep) neural network generative model. It is clear that many rich and interesting statistical models can be constructed in this manner, using arbitrarily large neural networks with a corresponding parameter vector \( \theta \) that is arbitrarily high-dimensional. However, conventional statistical wisdom suggests that such models may not be useful in practice, due to the prohibitively large number of parameters that will need to be estimated. Maximum likelihood estimation has shown to struggle when real data are used since, despite its flexibility, the statistical model will necessarily be misspecified (Theis et al., 2016). Alternative strategies have nevertheless been developed to estimate the parameters \( \theta \) of such models and – remarkably – these have demonstrated a high level of success provided one has access to a sufficiently rich training dataset. Here we focus on a line of research called generative adversarial networks (GANs) (Goodfellow et al., 2020), and specifically the so-called integral probability metric GANs. Let \( P_n \) denote the empirical distribution of the training dataset.
Then a GAN estimator for $\theta$, if one exists, is defined as

$$\theta_n \in \arg \min_{\theta \in \Theta} \max_{f \in F} \left| \int f dP_n - \int f dP_\theta \right|,$$

where $F$ is a set of test functions such that $F \subset L^1(P_\theta)$ for each $\theta \in \Theta$. The choice of $F$ determines the properties of the GAN estimator. The GAN nomenclature originates from the case where the elements of $F$ are also neural networks, so that the witness function or critic $f$ for which the maximum is realised can be interpreted as an adversarial neural network. Alternative choices of $F$ lead to so-called generative moment matching networks (Dziugaite et al., 2015; Li et al., 2015), MMD GANs (Li et al., 2017), Wasserstein GANs (Arjovsky et al., 2017), Mc GANs (Mroueh et al., 2017), Fisher GANs (Mroueh and Sercu, 2017), and Sobolev GANs (Mroueh et al., 2018). Here we focus on generative moment matching networks, which take $F$ to be the unit ball in a reproducing kernel Hilbert space $H(k)$ of real-valued functions on $X$; see Figure 2. It is a standard fact that this procedure can be cast as minimum kernel discrepancy estimation:

**Proposition 2.** The GAN estimator $\theta_n$ is a minimum kernel discrepancy estimator when $F$ is the set of $f \in H(k)$ such that $\|f\|_{H(k)} \leq 1$.

**Proof.** For $f \in F$, using Cauchy–Schwarz,

$$\left| \int f dP_n - \int f dP_\theta \right| = |\langle f, \mu_k(P_n) - \mu_k(P_\theta) \rangle| \leq \|f\|_{H(k)} \|\mu_k(P_n) - \mu_k(P_\theta)\|_{H(k)}$$

which shows that

$$0 \leq \max_{f \in F} \int f dP_n - \int f dP_\theta \leq D_k(P_n, P_\theta).$$

If $D_k(P_n, P_\theta) = 0$ then we must have equality, so suppose $D_k(P_n, P_\theta) \neq 0$. Then one can verify that $f = [\mu_k(P_n) - \mu_k(P_\theta)]/D_k(P_n, P_\theta)$ is the witness function for which equality is realised.

This class of GANs is appealing in the sense that the optimisation over $F$ can be explicitly solved, and the solution is the kernel discrepancy $D_k(P_n, P_\theta)$. Although the kernel mean element $\mu_k(P_\theta)$ is not closed-form in general, it can be consistently approximated using an empirical approximation to $P_\theta$; this is discussed further in Section 5. The performance of these GANs depends on the choice of kernel $k$, and methods have been proposed to flexibly learn a suitable $k$ based on the training dataset (Li et al., 2017). These methods have demonstrated remarkable performance on machine learning benchmarks, out-performing other forms of GAN (Bińkowski et al., 2018).

### 3.3 Energy-Based Models

An energy-based model on $X = \mathbb{R}^d$ is a statistical model $P_\theta$ with probability density function (PDF)

$$p_\theta(x) = \frac{\exp(-E_\theta(x))}{Z(\theta)},$$

where $Z(\theta)$ is the partition function.
Figure 2: Minimum kernel discrepancy estimation for generative models. The parameters $\theta$ of sophisticated generative models may be estimated by minimising the kernel discrepancy between the generative model $P_\theta$ and the empirical distribution of the dataset. Confidence sets $C^\gamma_n$ for $\theta^\star$ can be constructed to ensure the notional coverage of $100\gamma\%$ is asymptotically correct; see Section 4.

where $E_\theta : \mathcal{X} \to \mathbb{R}$ is a flexibly parametrised potential such that $x \mapsto \exp(-E_\theta(x))$ is integrable and $Z(\theta) := \int \exp(-E_\theta(x))dx > 0$. Energy-based models arise both in statistics, where they are referred to as an instance of intractable likelihood (Lyne et al., 2015), and in machine learning, where they provide an alternative to GANs that can be more convenient when an explicit PDF is required (LeCun et al., 2007). Similarly to GANs, maximum likelihood estimation has been shown to struggle in this setting, where, despite its flexibility, the statistical model will necessarily be misspecified. However, there is an additional barrier to application of minimum kernel discrepancy estimation to energy-based models; the challenge of approximating the kernel mean element $\mu_k(P_\theta)$. Indeed, due to the intractable normalisation constant $Z(\theta)$, sampling from an energy-based model is not straightforward and an algorithm such as Markov chain Monte Carlo (MCMC) is required to approximately sample from $P_\theta$ for each value of $\theta \in \Theta$. This can entail a prohibitive computational cost when attempting optimisation over $\Theta$ (Song and Kingma, 2021).

To address this computational challenge, we can employ a class of kernels $k$ introduced in Oates et al. (2017). These kernels $k$ solve the computational problem by ensuring that $\mu_k(P_\theta)$ is equal to 0 in $\mathcal{H}(k)$, and thus $\mu_k(P_\theta)$ can be trivially computed. To achieve this, the kernel $k$ must be allowed to depend on $\theta$, and in what follows we write $k(x, y; \theta)$ to make this dependence explicit. Before describing the kernels with this property, we first introduce some notation and assumptions. Let $\nabla f = (\partial_{x_1} f, \ldots, \partial_{x_d} f)^\top$ denote the gradient of a differentiable function $f : \mathbb{R}^d \to \mathbb{R}$ and let $\nabla \cdot f = \partial_{x_1} f_1 + \cdots + \partial_{x_d} f_d$ denote the divergence of a differentiable function $f : \mathbb{R}^d \to \mathbb{R}^d$. The presentation in the remainder of this section follows Barp et al. (2022):
Proposition 3. Let $g : \mathbb{R}^d \to \mathbb{R}^d$ satisfy $g, A_\theta g \in L^1(P_\theta)$ where

$$(A_\theta g)(x) := (\nabla \cdot g)(x) - \langle g(x), (\nabla E_\theta)(x) \rangle.$$ 

Then $\int A_\theta g \, dP_\theta = 0$.

Proof. Let $\varphi_n : \mathbb{R}^d \to \mathbb{R}$ be a compactly supported function with $\varphi_n(x) = 1$ for $\|x\| \leq n$ and $\|\nabla \varphi_n\| < n^{-1}$, for each $n \in \mathbb{N}$. From the divergence theorem,

$$0 = \int (\nabla \cdot (\varphi_n p_\theta g))(x) \, dx = \int \langle \nabla \varphi_n(x), (p_\theta g)(x) \rangle \, dx + \int \varphi_n(x)(\nabla \cdot (p_\theta g))(x) \, dx.$$

Since $\varphi_n \to 1$ pointwise and $\nabla \cdot (p_\theta g) \in L^1(\mathbb{R}^d)$, from the dominated convergence theorem

$$\int \varphi_n(x)(\nabla \cdot (p_\theta g))(x) \, dx \to \int (\nabla \cdot (p_\theta g))(x) \, dx.$$

On the other hand, since $p_\theta g \in L^1(\mathbb{R}^d)$,

$$\left| \int \langle \nabla \varphi_n(x), (p_\theta g)(x) \rangle \, dx \right| \leq \|\nabla \varphi_n\| \int \|(p_\theta g)(x)\| \, dx \to 0.$$

Thus we have shown that

$$\int A_\theta g \, dP_\theta = \int \frac{1}{p_\theta} \nabla \cdot (p_\theta g) \, dP_\theta = \int (\nabla \cdot (p_\theta g))(x) \, dx = 0,$$

as claimed.

\[\Box\]

Proposition 4. Let $c : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ be a kernel with $c(\cdot, y), \nabla_y c(\cdot, y), A_\theta c(\cdot, y) 1_d, A_\theta \nabla_y c(\cdot, y) \in L^1(P_\theta)$ for each $y \in \mathbb{R}^d$. Then

$$k(x, y; \theta) = \nabla_x \cdot \nabla_y c(x, y) - \langle \nabla_x E_\theta(x), \nabla_y c(x, y) \rangle$$

$$- \langle \nabla_y E_\theta(y), \nabla_x c(x, y) \rangle + \langle \nabla_x E_\theta(x), \nabla_y E_\theta(y) \rangle c(x, y)$$

is a $\theta$-dependent kernel with $\mu_k(P_\theta) = 0$ for all $\theta \in \Theta$.

Proof. For the proof that $k(\cdot, \cdot; \theta)$ is indeed a kernel we refer to Barp et al. (2022, Theorem 2.6). For the final part, note that

$$k(x, y; \theta) = A_\theta g(x), \quad g(x) = \nabla_y c(x, y) + c(x, y) \nabla_y \log p_\theta(y)$$

where, under our assumptions, $g, A_\theta g \in L^1(P_\theta)$. Then we may apply Proposition 3 to deduce that $\mu_k(P_\theta)(y) = \int k(x, y; \theta) \, dP_\theta(x) = \int A_\theta g(x) \, dP_\theta(x) = 0$ for all $y \in X$, and thus $\mu_k(P_\theta) = 0$, as claimed. \[\Box\]
This construction enables minimum kernel discrepancy estimation to be applied to energy-based models, with positive initial result reported in a range of statistical applications (Barp et al., 2019; Matsubara et al., 2022a). Indeed, \( k(\cdot, \cdot; \theta) \) can be evaluated without the normalisation constant \( Z(\theta) \), and any kernel for which the conclusion of Proposition 4 holds satisfies \( k_\theta(\cdot, \cdot) = k(\cdot, \cdot; \theta) \). The discrepancy associated to \( k(\cdot, \cdot; \theta) \) is called a kernel Stein discrepancy (Liu et al., 2016; Chwialkowski et al., 2016; Gorham and Mackey, 2017); these kernelise the score-matching divergence of Hyvärinen and Dayan (2005) and have recently been applied to a variety of other tasks in statistics and machine learning (Anastasiou et al., 2023).

This completes our short tour of how minimum kernel discrepancy methods can be used. Next we turn our attention to the asymptotic properties of these estimators, aiming insofar as possible for a general framework.

4 Asymptotic Theory

The aim of this section is to present general asymptotic theory that is applicable to each of the applications we have just discussed. If the kernel is \( \theta \)-independent, the minimum kernel discrepancy estimator can be recognised as both an M-estimator and a minimum scoring rule estimator, so established asymptotic theory can be applied (Van der Vaart, 2000; Dawid et al., 2016). However, this identification does not hold when the kernel is \( \theta \)-dependent, and bespoke arguments are needed. To this end, conditions for strong consistency of the minimum kernel discrepancy estimator are established for a \( \theta \)-independent kernel in Section 4.1 and extended to the case of a \( \theta \)-dependent kernel in Section 4.2. Conditions for asymptotic normality in the case of a possibly \( \theta \)-dependent kernel are established in Section 4.3, and the strength of these conditions is examined in Appendix C. The presentation is intended to be self-contained; we relate our results to existing literature in Section 4.4.

To simplify the presentation, it will be assumed throughout that \( P \in \mathcal{P}_k(X) \) and \( \{P_\theta\}_{\theta \in \Theta} \subset \mathcal{P}_k(X) \), so that the kernel discrepancy is well-defined. It will also be assumed that the statistical model is parameterised in such a way that \( \theta_* \) and \( \theta_n \) actually exist, in the latter case for \( n \) sufficiently large (but in neither case is uniqueness assumed). Convergence in distribution, convergence in probability, and almost sure convergence will be respectively denoted \( \overset{d}{\rightarrow} \), \( \overset{p}{\rightarrow} \) and \( \overset{a.s.}{\rightarrow} \).

4.1 Strong Consistency

In this section we consider a topological space \( \Theta \); no additional structure on \( \Theta \) is required until Section 4.2. Our first task is to find weak sufficient conditions under which a.s. every sequence \( (\theta_n)_{n \in \mathbb{N}} \) of minimum kernel discrepancy estimators satisfies

\[
\{\text{accumulation points of } (\theta_n)_{n \in \mathbb{N}}\} \subseteq \arg \min_{\theta \in \Theta} D_k(P, P_\theta). \tag{4}
\]

That is, there is a probability 1 set on which all accumulation points of all sequences \( \theta_n \) of minimum kernel discrepancy estimators are minimisers \( \theta_* \) of the kernel discrepancy between
the distribution $P$, from which the data are sampled, and the statistical model $P_\theta$. To begin with we consider the case where the kernel $k$ does not depend on the parameter $\theta$ and standard arguments can be used; the case of a $\theta$-dependent kernel is treated in Section 4.2.

**Lemma 5** (Strong consistency of the kernel mean element). *Assume that*

\[ A1 \ H(k) \text{ is separable.} \]
\[ A2 \ \int \sqrt{k(x,x)} \ dP(x) < \infty. \]

*Then $\mu_k(P_n) \xrightarrow{a.s.} \mu_k(P)$.***

**Proof.** The random variables $\xi_i = k(\cdot, x_i)$ are independent, identically distributed, and satisfy $\mathbb{E}[\|k(\cdot, x_i)\|_{H(k)}] = \int \sqrt{k(x,x)} \ dP < \infty$ (from $A2$), so we may appeal to the strong law of large numbers (Theorem 18) in the separable (from $A1$) Banach space $B = H(k)$, to get

$$
\mu_k(P_n) = \frac{1}{n} \sum_{i=1}^{n} k(\cdot, x_i) \xrightarrow{a.s.} \int k(\cdot, x) \ dP(x) = \mu_k(P),
$$

which establishes the result. \qed

Note that $A2$ implies the weak integral $\mu_k(P) = \int k(\cdot, x) \ dP(x)$ is in fact a strong (or Bochner) integral.

**Lemma 6** (Uniform convergence in discrepancy). *Assume $A1$, $A2$. Then*

$$
\sup_{\theta \in \Theta} |D_k(P_n, P_\theta) - D_k(P, P_\theta)| \xrightarrow{a.s.} 0. \quad (5)
$$

**Proof.** Let $f(\theta) = D_k(P, P_\theta)$ and $f_n(\theta) = D_k(P_n, P_\theta)$. From the reverse triangle inequality and Lemma 5, we have that

$$
\sup_{\theta \in \Theta} |f_n(\theta) - f(\theta)| = \sup_{\theta \in \Theta} \left| \|\mu_k(P_n) - \mu_k(P_\theta)\|_{H(k)} - \|\mu_k(P) - \mu_k(P_\theta)\|_{H(k)} \right|
\leq \|\mu_k(P_n) - \mu_k(P)\|_{H(k)} \xrightarrow{a.s.} 0, \quad (6)
$$

which establishes the result. \qed

**Lemma 7** (Discrepancy is minimised). *Assume $A1$, $A2$. Then*

$$
D_k(P, P_{\theta*}) \xrightarrow{a.s.} \min_{\theta \in \Theta} D_k(P, P_\theta).
$$

**Proof.** Let $f$ and $f_n$ be as in the proof of Lemma 6. Let $\epsilon > 0$. Pick one element $\theta* \in \arg\min_{\theta \in \Theta} f(\theta)$. Then a.s. there exists $n_0$ such that for all $n > n_0$ we have that

$$
[f(\theta*) \xrightarrow{\text{def of } \theta*} f(\theta_n) \xrightarrow{\text{Lemma 6}} f_n(\theta_n) + \frac{\epsilon}{2} \xrightarrow{\text{def of } \theta*} f_n(\theta*) + \frac{\epsilon}{2} \xrightarrow{\text{Lemma 6}} f(\theta*) + \epsilon.]
$$

Since $\epsilon > 0$ was arbitrary, it follows that $f(\theta_n) \xrightarrow{a.s.} \min_{\theta \in \Theta} f(\theta)$. \qed
Using an additional assumption that there exists a unique and sufficiently distinct global minimum at the parameter level, we obtain a basic strong consistency result at the parameter level. The proof of the following result is immediate from Lemma 7:

**Theorem 8** (Strong consistency with unique minimum). Assume A1, A2. If \( \theta_* \in \Theta \) is such that for every open neighbourhood \( \theta_* \in N(\theta_*) \subset \Theta \) we have

\[
D_k(P, P_{\theta_*}) < \inf_{\theta \in \Theta \setminus N(\theta_*)} D_k(P, P_{\theta}),
\]

then \( \theta_n \xrightarrow{a.s.} \theta_* \).

In practice the uniqueness of a minimum is often difficult or impossible to check, since in general the statistical model will be misspecified. This motivates a more realistic analysis, which we state in two parts. The closure of a subset \( S \) of a topological space \( \Theta \) will be denoted \( \text{cl}(S) \), and we recall that a subset \( C \) of a topological space \( \Theta \) is sequentially compact if every sequence in \( C \) has an accumulation point in \( C \).

**Theorem 9** (Strong consistency with several minima, part I). Assume A1, A2, and assume that \( \theta \mapsto D_k(P, P_{\theta}) \) is a continuous function on \( \Theta \). Then any accumulation point of \( (\theta_n)_{n \in \mathbb{N}} \) is a.s. an element of \( \min_{\theta \in \Theta} D_k(P, P_{\theta}) \).

**Proof.** Let \( f \) be as in the proof of Lemma 6. Let \( \epsilon > 0 \) and let \( \theta_* \) be an accumulation point, meaning that there exists a subsequence with \( \theta_{n_m} \to \theta_* \) as \( m \to \infty \). Then a.s. there exists \( m_0 \) such that for all \( m > m_0 \) we have

\[
f(\theta_*) \xrightarrow{\text{cts at } \theta_*} f(\theta_{n_m}) + \epsilon.
\]

Taking the limit \( m \to \infty \) on both sides and using Lemma 7, we have that a.s.

\[
f(\theta_*) < \min_{\theta \in \Theta} f(\theta) + \epsilon.
\]

Since \( \epsilon > 0 \) was arbitrary, it follows that a.s. \( \theta_* \in \min_{\theta \in \Theta} f(\theta) \).

**Theorem 10** (Strong consistency with several minima, part II). Assume A1, A2, and assume there is an \( \epsilon > 0 \) for which

\[
C := \text{cl}\left\{ \theta \in \Theta : D_k(P, P_{\theta}) < \epsilon + \inf_{\theta \in \Theta} D_k(P, P_{\theta}) \right\}
\]

is sequentially compact. Then the sequence \( (\theta_n)_{n \in \mathbb{N}} \) has at least one accumulation point.

**Proof.** Let \( f \) and \( f_n \) be as in the proof of Lemma 6. From Lemma 6, there a.s. exists \( n_0 \) such that for all \( n > n_0 \) we have \( \sup_{\theta \in \Theta} |f_n(\theta) - f(\theta)| < \epsilon/2 \). In particular, there a.s. exists \( n_0 \) such that \( (\theta_n)_{n > n_0} \subset C \). Since the sequence \( (\theta_n)_{n \in \mathbb{N}} \) is a.s. eventually contained in \( C \), and \( C \) is sequentially compact, there a.s. exists an accumulation point.

For \( \Theta = \mathbb{R}^d \), the topological condition in Theorem 10 is satisfied when \( C \) is bounded.
4.2 Extension to $\theta$-Dependent Kernel

To accommodate also the $\theta$-dependent kernels $k(\cdot, \cdot; \theta)$ from Section 3.3, here we provide an alternative to Lemma 6.

**Lemma 11** (Uniform convergence in discrepancy; $\theta$-dependent kernel). Assume $A1$ for each $\theta \in \Theta$. Assume $\Theta \subset \mathbb{R}^p$ is open, convex and bounded, and that

$A3 \int \sqrt{k_\theta(x,x)} \, dP(x) < \infty$, for all $\theta \in \Theta$

$A4 \int \sup_{\theta \in \Theta} \| \partial_\theta k_\theta(x,x) \| \, dP(x) < \infty$

$A5 \iint \sup_{\theta \in \Theta} \| \partial_\theta k_\theta(x,y) \| \, dP(x) dP(y) < \infty$.

Then

$$\sup_{\theta \in \Theta} |D_\theta(P_n, P_\theta) - D_\theta(P, P_\theta)| \xrightarrow{a.s.} 0. \quad (8)$$

*Proof.* The aim is to establish the conditions for the uniform law of large numbers in Theorem 21. Let $g(\theta) = D_\theta(P, P_\theta)^2$ and $g_n(\theta) = D_\theta(P_n, P_\theta)^2$. From (1) and the fact that $k(\cdot, \cdot; \theta)$ is positive semi-definite,

$$k(x,x; \theta) \leq k_\theta(x,x) + 2 \int k(x,y; \theta) dP_\theta(y).$$

Taking the square root and integrating,

$$\int \sqrt{k(x,x; \theta)} dP(x) \leq \int \sqrt{k_\theta(x,x) + 2 \int k(x,y; \theta) dP_\theta(y)} \, dP(x)$$

$$\leq \int \sqrt{k_\theta(x,x)} dP(x) + \int \sqrt{2 \int k(x,y; \theta) dP_\theta(y)} \, dP(x) \quad (9)$$

$$\leq \int \sqrt{k_\theta(x,x)} dP(x) + \sqrt{2 \int \int k(x,y; \theta) dP_\theta(y) dP(x)}, \quad (10)$$

where (9) used the fact that $\sqrt{a + b} \leq \sqrt{a} + \sqrt{b}$, and (10) used Jensen’s inequality. The first integral in (10) exists from $A3$ and all other integrals exist as a consequence of the standing assumption that $P, P_\theta \in \mathcal{P}_{k(\cdot, \cdot; \theta)}(X)$. Thus $\int \sqrt{k(x,x; \theta)} \, dP(x) < \infty$. From this fact and $A1$, we can apply Lemma 5 to deduce that $g_n(\theta) \xrightarrow{a.s.} g(\theta)$ for each $\theta \in \Theta$. Thus the first condition in Theorem 21 is satisfied.

For the second condition in Theorem 21, we start by noting it is implicit in $A4$, $A5$ that $\partial_\theta k_\theta$ exists in $\Theta$ and thus $g_n$ is differentiable in $\Theta$. Let $\theta, \vartheta \in \Theta$. From the mean value theorem, and the fact that $\Theta$ is open and convex,

$$g_n(\theta) - g_n(\vartheta) = \langle \theta - \vartheta, \partial_\theta g_n(\vartheta) \rangle$$

14
for some $\phi \in \{t\theta + (1-t)\vartheta : 0 \leq t \leq 1\} \subset \Theta$. In particular,

$$|g_n(\theta) - g_n(\vartheta)| \leq \|\theta - \vartheta\| \sup_{\phi \in \Theta} \|\partial_\phi g_n(\phi)\| \leq \|\theta - \vartheta\| \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \sup_{\phi \in \Theta} \|\partial_\phi k_\theta(x_i, x_j)\| \cdot$$

Now, since we have a V-statistic, we use $A4$ and $A5$ to verify that

$$\int \int |v(x, y)|dP(x)dP(y) = \int \int \sup_{\theta \in \Theta} \|\partial_\theta k_\theta(x, y)\|dP(x)dP(y) < \infty$$

and thus from Theorem 19 we have that

$$B_n := \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \sup_{\theta \in \Theta} \|\partial_\theta k_\theta(x_i, x_j)\| \overset{a.s.}{\longrightarrow} \int \int \sup_{\theta \in \Theta} \|\partial_\theta k_\theta(x, y)\|dP(x)dP(y) < \infty.$$ 

Since in addition $\Theta$ is assumed to be bounded, the conditions of the uniform law of large numbers in Theorem 21 have now been established. Thus Theorem 21 gives that $\sup_{\theta \in \Theta} |g_n(\theta) - g(\theta)| \overset{a.s.}{\longrightarrow} 0$, as claimed. $\square$

The arguments of Lemma 7 and Theorems 8 to 10 all go through with $A3$, $A4$ and $A5$ in place of $A2$.

### 4.3 Asymptotic Normality

The last asymptotic result we present is to show that fluctuations of the minimum kernel discrepancy estimator are asymptotically normal. For a matrix $M \in \mathbb{R}^{p \times p}$, we write $M \succ 0$ to indicate that $M$ is positive definite; i.e. for all $0 \neq c \in \mathbb{R}^p$ we have $c^\top Mc > 0$.

**Theorem 12** (Asymptotic normality). Suppose $\theta_n \overset{a.s.}{\longrightarrow} \theta_\ast$. Let there exist an open set $S \subseteq \Theta \subseteq \mathbb{R}^p$ such that $\theta_\ast \in S$ and the following hold:

- **A6** $\int \sup_{\theta \in S} \|\partial_\theta k_\theta(x, y)\|dP(x)dP(y) < \infty$

- **A7** the functions $\{\theta \mapsto \partial_\theta k_\theta(x, y) : x, y \in X\}$ are differentiable on $S$

- **A8** the functions $\{\theta \mapsto \partial^2_\theta k_\theta(x, y) : x, y \in X\}$ are uniformly continuous at $\theta_\ast$

- **A9** $\int \|\partial_\theta k_\theta(x, y)\|^2dP(x)dP(y)_{\theta = \theta_\ast} < \infty$

- **A10** $\int \|\partial^2_\theta k_\theta(x, x)\|dP(x)_{\theta = \theta_\ast} < \infty$

- **A11** $\int \|\partial^2_\theta k_\theta(x, y)\|dP(x)dP(y)_{\theta = \theta_\ast} < \infty$

- **A12** $\Gamma := \frac{1}{2} \int \partial^2_\theta k_\theta(x, x)dP(x)dP(y)_{\theta = \theta_\ast} > 0$. 

15
\[
\sqrt{n}(\theta_n - \theta_\ast) \xrightarrow{d} N(0, \Gamma^{-1}\Sigma \Gamma^{-\top}), \quad \text{where } \Sigma := \mathbb{C}_{X \sim \mathcal{P}} \left[ \int \partial_\theta k_\theta(X, y) dP(y) \right]_{\theta = \theta_\ast}.
\]

**Proof.** For a function \( \theta \mapsto h(\theta) \), let \( h'(\theta) = \partial_\theta h(\theta) \), and let \( h''(\theta) = \partial^2 h(\theta) \). Let \( g \) and \( g_n \) be as in the proof of Lemma 11. From A7 there is a convex open set \( N(\theta_\ast) \subset \Theta \) with \( \theta_\ast \in N(\theta_\ast) \) on which the functions \( \theta \mapsto \partial_\theta k_\theta(x, y) \) are differentiable, and thus the map \( \theta \mapsto \partial_\theta g_n(\theta) \) is differentiable on \( N(\theta_\ast) \). Since we are assuming \( \theta_n \xrightarrow{a.s.} \theta_\ast \), there a.s. exists \( n_0 \in \mathbb{N} \) such that for all \( n \geq n_0 \) we have \( \theta_n \in N(\theta_\ast) \). Thus for each \( n \geq n_0 \) we can apply the mean value theorem on the convex open set \( N(\theta_\ast) \) to establish that there is a \( \tilde{\theta}_n = t_n \theta_n + (1 - t_n) \theta_\ast \), \( t_n \in [0, 1] \), for which

\[
0 = g_n'(\theta_n) = g_n'(\tilde{\theta}_n) + g_n''(\tilde{\theta}_n) \times (\theta_n - \theta_\ast).
\]

If \( g_n''(\tilde{\theta}_n) \) is non-singular (as will be established below by showing convergence to a matrix \( 2\Gamma \), assumed to be positive definite due to A12), then we can re-express this as

\[
\sqrt{n}(\theta_n - \theta_\ast) = -[g_n''(\tilde{\theta}_n)]^{-1}[\sqrt{n}g_n'(\tilde{\theta}_n)]
\]

The stated result follows from Slutsky’s lemma if we can show both that \( g_n''(\tilde{\theta}_n) \xrightarrow{p} 2\Gamma \) and \( \sqrt{n}g_n'(\tilde{\theta}_n) \xrightarrow{d} N(0, 4\Sigma) \). Both of these will now be established.

**Establishing** \( g_n''(\tilde{\theta}_n) \xrightarrow{p} 2\Gamma \). First we make the trivial algebraic observation that

\[
g_n''(\tilde{\theta}_n) = g_n''(\theta_\ast) + [g_n'(\tilde{\theta}_n) - g_n'(\theta_\ast)].
\]

From A10 and A11, for \( r, s \in \{1, \ldots, p\} \) we have that

\[
\int |\partial_{\theta_r} \partial_{\theta_s} k_\theta(x, x)| dP(x) \bigg|_{\theta = \theta_\ast}, \quad \int \int |\partial_{\theta_r} \partial_{\theta_s} k_\theta(x, y)| dP(x) dP(y) \bigg|_{\theta = \theta_\ast} < \infty
\]

and thus Theorem 19 on the consistency of V-statistics can be applied, establishing that

\[
[g_n''(\theta_\ast)]_{r,s} = \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \partial_{\theta_r} \partial_{\theta_s} k_\theta(x_i, x_j) \bigg|_{\theta = \theta_\ast} \xrightarrow{a.s.} \int \int \partial_{\theta_r} \partial_{\theta_s} k_\theta(x, y) dP(x) dP(y) \bigg|_{\theta = \theta_\ast} = 2\Gamma_{r,s},
\]

and in particular \( g_n''(\theta_\ast) \xrightarrow{p} 2\Gamma \). Next consider the second term in (12). For any \( \epsilon > 0 \), from A8 there exists a bounded open set \( N_\epsilon(\theta_\ast) \subset \Theta \) such that \( \theta_\ast \in N_\epsilon(\theta_\ast) \) and \( \|\partial^2 k_\theta(x, y) - \partial^2 k_\theta(x, y)|_{\theta = \theta_\ast}\| < \epsilon \) for all \( \theta \in N_\epsilon(\theta_\ast) \) and all \( x, y \in \mathcal{X} \). Since we are assuming \( \theta_n \xrightarrow{a.s.} \theta_\ast \), this means \( \theta_n \xrightarrow{a.s.} \theta_\ast \), and thus there a.s. exists \( n_\epsilon \in \mathbb{N} \) such that for all \( n \geq n_\epsilon \) we have \( \tilde{\theta}_n \in N_\epsilon(\theta_\ast) \). Thus, for all \( n \geq n_\epsilon \),

\[
\left\| g_n''(\tilde{\theta}_n) - g_n''(\theta_\ast) \right\| = \left\| \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \partial^2 k_\theta(x_i, x_j) \bigg|_{\theta = \tilde{\theta}_n} - \partial^2 k_\theta(x_i, x_j) \bigg|_{\theta = \theta_\ast} \right\|
\]

\[
\leq \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \left\| \partial^2 k_\theta(x_i, x_j) \bigg|_{\theta = \tilde{\theta}_n} - \partial^2 k_\theta(x_i, x_j) \bigg|_{\theta = \theta_\ast} \right\| < \epsilon
\]

which demonstrates that the second term in (12) a.s. vanishes.
Establishing \( \sqrt{n}g'_n(\theta_*) \overset{d}{\to} N(0,4\Sigma) \). Let \( 0 \neq c \in \mathbb{R}^p \). From \( \textbf{A6} \), the function \( h : S \times (\mathcal{X} \times \mathcal{X}) \to \mathbb{R}^p \) defined as \( h(\theta, (x, y)) = k_\theta(x, y) \) has \( \partial_\theta h \) locally uniformly integrably bounded in the sense of Definition 22, and thus the conditions of Lemma 23 hold in a neighbourhood of \( \theta_* \), permitting us to interchange \( \partial_\theta \) and the integral with respect to \( P \times P \). This, together with the fact that \( \theta_* \) is a minimiser of \( g(\theta) \), shows that

\[
\int \int c^\top \partial_\theta k_\theta(x, y) dP(x)dP(y)\bigg|_{\theta=\theta_*} = c^\top \partial_\theta \int \int k_\theta(x, y) dP(x)dP(y)\bigg|_{\theta=\theta_*} = c^\top g'(\theta_*) = 0. \tag{13}
\]

Further, from \( \textbf{A9} \) and Cauchy–Schwarz,

\[
\int \int (c^\top \partial_\theta k_\theta(x, y))^2 dP(x)dP(y)\bigg|_{\theta=\theta_*} \leq \|c\|^2 \int \int \|\partial_\theta k_\theta(x, y)\|^2 dP(x)dP(y)\bigg|_{\theta=\theta_*} < \infty.
\]

Thus we can appeal to asymptotic normality of V-statistics, using Theorem 20, to obtain that

\[
c^\top \sqrt{n}g'_n(\theta_*) = \sqrt{n} \left( \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} c^\top \partial_\theta k_\theta(x_i, x_j)\bigg|_{\theta=\theta_*} - 0 \right) \overset{d}{\to} N(0,4\sigma_c^2)
\]

where

\[
\sigma_c^2 = \mathbb{V}_{X \sim P} \left[ \int c^\top \partial_\theta k_\theta(X, y) dP(y)\bigg|_{\theta=\theta_*} \right] = c^\top \Sigma c.
\]

Since \( c \neq 0 \) was arbitrary, it follows that \( \sqrt{n}g'_n(\theta_*) = \sqrt{n}[g'_n(\theta_*) - g'(\theta_*)] \overset{d}{\to} N(0,4\Sigma) \), as required.

The assumptions of Theorem 12 will be discussed in Appendix C, but we briefly remark that \( \textbf{A5} \) implies \( \textbf{A6} \) and that, due to the crude way it appears in the proof, \( \textbf{A8} \) can likely be weakened. The conclusion of Theorem 12 agrees with our discussion of the generalised method of moments in Section 3.1; in this case \( \partial_\theta k_\theta(x, y) = -\phi(x) - \phi(y) + 2\theta \) and \( \partial_\theta^2 k_\theta(x, y) = 2I \), so \( \Gamma = I \) and \( \Sigma = \mathbb{C}_{X \sim P}[\phi(X)] \), and Theorem 12 gives \( \sqrt{n}(\theta_n - \theta_*) \overset{d}{\to} N(0,\mathbb{C}_{X \sim P}[\phi(X)]) \), in agreement. Finally, we note that Theorem 12 gives rise to a consistent sandwich estimator \( \Gamma_n^{-1}\Sigma_n\Gamma_n^{-1} \) for the asymptotic covariance \( \Gamma^{-1}\Sigma\Gamma^{-1} \) of the minimum kernel discrepancy estimator, where \( \Gamma_n \) and \( \Sigma_n \) are obtained by substituting \( \theta_n \) \textit{in lieu} of \( \theta_* \) into the definitions of \( \Gamma \) and \( \Sigma \); see Freedman (2006). The resulting 100\( \gamma \)% confidence sets for \( \theta_* \) are illustrated in Figure 2.

### 4.4 Related Work

The theoretical properties of minimum kernel discrepancy estimators have been studied by a number of authors since 2015, but our analysis is arguably the most general to have appeared. Indeed, as we will discuss, previous work focused on either the case where \( k \) does not depend on \( \theta \), or on the case where \( k \) has a specific form of dependence on \( \theta \).
In the case where $k$ does not depend on $\theta$, the original work of Dziugaite et al. (2015) focused on obtaining non-asymptotic concentration inequalities at the level of the kernel discrepancy. Although not discussed in that work, these guarantees can be extended to guarantees at the level of the parameter under further assumptions similar to those in Theorem 8. These non-asymptotic results were extended to the regression context, where data $x_1, \ldots, x_n$ are non-independent, in Alquier and Gerber (2023); Chérif-Abdellatif and Alquier (2022). Both a non-asymptotic analysis and an asymptotic analysis were presented in Briol et al. (2019), where strong consistency was established under assumptions that include (1) a unique $\theta^*$, and (2) for all $n$, there exists $\epsilon_n > 0$ such that \( \{ \theta \in \Theta : D_k(P_n, P_{\theta}) < D_k(P, P_{\theta^*}) + \epsilon_n \} \) is a.s. bounded. The latter paper is comprehensive and includes also a discussion of the important issues of estimator robustness, the geometry induced by kernel discrepancy, and computational aspects of minimum kernel discrepancy estimation (a point we return to in Section 5). A Bayesian interpretation of minimum discrepancy estimation was proposed in Chérif-Abdellatif and Alquier (2020).

The case where $k$ depends on $\theta$ was first studied in Barp et al. (2019). There the authors focus on asymptotic analysis and a specific form of $k$ derived from Stein’s method, the canonical form of which we discussed in Section 3.3. Strong consistency of the minimum kernel Stein discrepancy estimator was established under assumptions that include (1) the statistical model is well-specified (i.e. $P = P_{\theta^*}$), (2) $\theta^*$ is unique, (3) $\theta \mapsto P_{\theta}$ is injective, and either (4a) $\Theta$ is compact, or (4b) the maps $\theta \mapsto D_k(P_n, P_{\theta})$ are a.s. convex. Sufficient conditions for asymptotic normality are also provided, and the important issues of estimator robustness, the geometry induced by kernel discrepancy, and computational aspects of minimum kernel Stein discrepancy estimation were discussed. Closest in spirit to our analysis is Matsubara et al. (2022b), who endowed the minimum kernel Stein discrepancy estimator with a Bayesian interpretation. The present analysis aims to be more concise, and also more general in the senses that: (1) uniqueness of $\theta^*$ is not assumed, and (2) existence of third derivatives $\partial^3 \theta k_{\theta}$ is not assumed. The aforementioned authors also discussed estimator robustness and computational aspects of minimum kernel Stein discrepancy estimation in detail.

Naturally, many alternatives to kernel discrepancy exist and have been explored in the parameter inference context; to limit scope these have not been discussed. However, we note that kernel discrepancies form a large class, some of which can be viewed as the limit of entropy-regularised optimal transport (Genevay et al., 2018), some of which offer control over smoothed Wasserstein distances (Nietert et al., 2021), and some of which metrise weak convergence on compact domains (Simon-Gabriel et al., 2023).

5 Open Research Directions

This paper was intended to serve both as a self-contained exposition of minimum kernel discrepancy estimation and as an invitation to contribute to this nascent research field. Accordingly, in this section we present a non-exhaustive list of open research questions that could be addressed:
1. **Computing the kernel mean element.** An important issue which we have not yet discussed is how to compute the kernel mean element $\mu_k(P_\theta)$, given that for general choices of $k$ and $P_\theta$ there will not be a closed-form solution to this integral. In the machine learning community, a Monte Carlo approximation of $P_\theta$ is typically used, often in tandem with stochastic gradient-based optimisation over $\theta \in \Theta$. However, in some situations one might expect to do better: In the context of generative models (3), one has $\mu_k(P_\theta) = \int k(G^\theta(x), \cdot) dP(x)$ where $P$ is a user-specified reference measure, typically the uniform measure on $[0, 1]^d$. This raises the possibility of using quasi Monte Carlo methods to approximate the kernel mean element. A preliminary investigation in Niu et al. (2023) established the $O(n^{-1+\epsilon})$ rate, but it remains an open problem to obtain explicit conditions on $G^\theta$ and $k$ that ensure higher-order quasi Monte Carlo convergence rates hold. Related, although the kernel mean element $\mu_k(P_n)$ is explicit, it is sometimes prohibitive to work with a very large dataset. In these circumstances, methods have been proposed to select a representative subset of data such that the kernel mean element associated to this subset is close to that of the full dataset (Cortes and Scott, 2016; Teymur et al., 2021). However, the interaction between computational approximations and the performance of the minimum kernel discrepancy estimator have yet to be studied, beyond the Monte Carlo case in Briol et al. (2019).

2. **Selecting a kernel.** Beyond the basic requirement that the estimator is consistent, further guidance on the application-specific selection of the kernel $k$ is needed. The choice of $k$ engenders an efficiency-robustness trade-off, so one must speculate about the extent to which a statistical model is likely to be misspecified. Further, the efficiency of minimum kernel discrepancy estimation in high-dimensional domains $\mathcal{X}$ is yet to be explored. It is typical to encounter $P$ whose mass is concentrated around a subset of $\mathcal{X}$, often a low-dimensional linear subspace or a sub-manifold. In such circumstances it would be desirable to select a kernel $k$ that is appropriately adapted to this low-dimensional set, perhaps as described in Section 2.2, to improve the dimension dependence of the estimator. Insight may be gained by considering the case where $\mathcal{X}$ is infinite-dimensional; kernel discrepancies are well-defined in this context (Wynne and Duncan, 2022; Wynne et al., 2022) but minimum kernel discrepancy estimation is yet to be explored. On the other hand, the case where $\mathcal{X}$ is discrete raises a different set of challenges, since selection of a natural kernel in the discrete context can be difficult. Both settings are further complicated by the fact that minimum kernel discrepancy estimation is not invariant to how the data are represented, i.e. the choice of $\mathcal{X}$ itself, and both theoretical and practical guidance is needed.

3. **Insight into machine learning.** Progress in machine learning is rapid, and in 2021 it was demonstrated that GANs are out-performed by so-called *diffusion models* on a range of image-generation tasks (Dhariwal and Nichol, 2021). Such applications are characterised by large training datasets, so $P_n$ is approximately equal to $P$, and high-dimensional $\mathcal{X}$, so there is a loose analogy to the setting where quasi Monte Carlo is studied. One might speculate on whether insights from quasi Monte Carlo might help
to explain the limited performance of GANs on such high-dimensional imaging tasks, or even suggest ways in which GANs might be improved.

4. **Probability in Hilbert spaces.** The strong consistency of the minimum kernel discrepancy estimator was established, for a $\theta$-independent kernel $k$, as a consequence of the strong law of large numbers in $\mathcal{H}(k)$. For a $\theta$-independent kernel it may also be possible also to establish asymptotic normality from the Hilbert space version of the central limit theorem. This approach would arguably be more elegant than the one we presented, avoiding the need to deal with V-statistics. However, it is not clear to this author whether such a strategy can be applied in the case of a $\theta$-dependent kernel.

5. **Confidence sets.** An estimate $\theta_n$ for a parameter of interest $\theta_*$ is only useful if the precision of $\theta_n$ can be estimated. Theorem 12 suggests the asymptotically valid $100\gamma\%$ confidence set

$$C^\gamma_n := \{\theta \in \Theta : \|\Sigma_n^{-1/2}\Gamma_n(\theta - \theta_n)\|_2^2 \leq F_{\chi^2_p}(\gamma)\},$$

where for simplicity here we assume that $\Theta = \mathbb{R}^p$ and $\Sigma \succ 0$, and we use $F$ notation to denote the cumulative probability distribution, here of a chi-squared distribution with $p$ degrees of freedom, $\chi^2_p$. However, at finite sample sizes $n$, the coverage of these confidence sets could be far from the notional $100\gamma\%$ due to the variance of the plug-in estimators $\Sigma_n$ and $\Gamma_n$ for $\Sigma$ and $\Gamma$. This problem is exacerbated when $\theta$ is high-dimensional, since these matrices are of dimension $p \times p$ where $p = \dim(\Theta)$.

A variety of strategies for regularised estimation exist and could be explored in this context (Lam, 2020).

**Acknowledgements** The author wishes to thank Alessandro Barp, François-Xavier Briol, Andrew Duncan, Jeremias Knoblauch, Lester Mackey, Takuo Matsubara, and an anonymous reviewer for comments on an earlier version of this manuscript, and financial support from EP/W019590/1 and EP/N510129/1.

**Appendices**

Appendix A discusses sufficient conditions for $P \in \mathcal{P}_k(\mathcal{X})$. Appendix B contains auxiliary results from probability and calculus that we used. Appendices C and D unpack and verify theoretical assumptions for the exponential family model.

## A Kernel Mean Embedding

In this section, $P$ is a distribution on a measurable space $\mathcal{X}$, and $k$ is a measurable and symmetric positive definite kernel with reproducing kernel Hilbert space denoted $\mathcal{H}(k)$. The central issue considered here is when $P(h) = \int h \, dP$ is a bounded linear functional on $\mathcal{H}(k)$. Our presentation here follows Barp et al. (2022, Appendix C).
**Definition 13** (Scalarly integrable). A map $\Phi : \mathcal{X} \to \mathcal{H}(k)$ is said to be scalarly $P$-integrable if \( \{ x \mapsto \langle h, \Phi(x) \rangle_{\mathcal{H}(k)} : h \in \mathcal{H}(k) \} \subset L^1(P) \).

The argument used in the following proof can be traced back to Dunford (1937), with our account based on Schwabik and Ye (2005, Lemma 2.1.1).

**Proposition 14.** If $\Phi : \mathcal{X} \to \mathcal{H}(k)$ is scalarly $P$-integrable, then

\[
P_\Phi : \mathcal{H}(k) \to \mathbb{R}
\]

\[
h \mapsto \int \langle h, \Phi(x) \rangle_{\mathcal{H}(k)} \, dP(x)
\]

is a bounded linear functional.

**Proof.** First we claim that the graph of the linear map

\[
T : \mathcal{H}(k) \to L^1(P)
\]

\[
h \mapsto (x \mapsto \langle h, \Phi(x) \rangle_{\mathcal{H}(k)}).
\]

is closed. To see this, let $h_n \to h$ in $\mathcal{H}(k)$ and suppose that $T(h_n) \to g$ in $L^1(P)$. The claim is that $g$ and $T(h)$ are equal in $L^1(P)$. Since every sequence converging in $L^1(P)$ has an almost surely converging subsequence, there is a subsequence $(h_{n_i})_{i \in \mathbb{N}}$ such that

\[
\langle h_{n_i}, \Phi(x) \rangle_{\mathcal{H}(k)} \to g(x)
\]

for $P$-almost all $x \in \mathcal{X}$. Since $\langle h_{n_i}, \Phi(x) \rangle_{\mathcal{H}(k)} \to \langle h, \Phi(x) \rangle_{\mathcal{H}(k)}$ for all $x \in \mathcal{X}$, it follows that $g(x) = \langle h, \Phi(x) \rangle_{\mathcal{H}(k)} = T(h)(x)$ for $P$-almost all $x \in \mathcal{X}$. Thus $g$ and $T(h)$ are equal in $L^1(P)$ and the graph of $T$ is indeed closed. The conditions of the closed graph theorem, which states that a linear map $T$ between Banach spaces is bounded if and only if its graph is closed, have now been verified. Thus $T$ is bounded and we denote

\[
\|T\| := \sup_{\|h\|_{\mathcal{H}(k)} \leq 1} \int |T(h)| \, dP < \infty.
\]

This allows us to conclude that $P_\Phi$ is a bounded linear functional, since

\[
|P_\Phi(h)| = \left| \int \langle h, \Phi(x) \rangle_{\mathcal{H}(k)} \, dP(x) \right| \leq \int |\langle h, \Phi(x) \rangle_{\mathcal{H}(k)}| \, dP(x) = \int |T(h)| \, dP \leq \|T\| \|h\|_{\mathcal{H}(k)},
\]

as required. \(\square\)

**Corollary 15** (Characterisation of $\mathcal{P}_k(\mathcal{X})$). $P \in \mathcal{P}_k(\mathcal{X})$ if and only if $\mathcal{H}(k) \subset L^1(P)$.

**Proof.** Take $\Phi(x) = k(\cdot, x)$ to be the canonical feature map, so that $k$ being measurable implies the scalar functions $x \mapsto \langle h, \Phi(x) \rangle = h(x)$ are measurable and $P = P_\Phi$. If $\mathcal{H}(k) \subset L^1(P)$ then $x \mapsto k(\cdot, x)$ is scalarly $P$-integrable, and Proposition 14 shows that $P$ is a bounded linear functional. Conversely, if $\mathcal{H}(k) \not\subset L^1(P)$ then it is clear that $P$ is not bounded and thus $P \notin \mathcal{P}_k(\mathcal{X})$. \(\square\)
The question then reduces to when $\mathcal{H}(k) \subset L^1(P)$.

**Proposition 16.** If $\int \sqrt{k(x, x)} dP(x) < \infty$ then $\mathcal{H}(k) \subset L^1(P)$.

**Proof.** For $h \in \mathcal{H}(k)$, from the reproducing property and Cauchy–Schwarz,

$$\int |h(x)| dP(x) = \int |\langle h, k(\cdot, x) \rangle| dP(x) \leq \|h\|_{\mathcal{H}(k)} \int \|k(\cdot, x)\|_{\mathcal{H}(k)} dP(x),$$

where the reproducing property again yields $\|k(\cdot, x)\|_{\mathcal{H}(k)} = \sqrt{k(x, x)}$, as required. \qed

One can weaken the above integrability condition under mild assumptions on $k$ and $X$:

**Proposition 17.** If $k$ is continuous, $X$ is separable, and $\iint |k(x, y)| dP(x) dP(y) < \infty$, then $\mathcal{H}(k) \subset L^1(P)$.

**Proof.** Since $k$ is measurable and real-valued, $k$ is strongly measurable in the sense of Carmeli et al. (2006, Section 3.1). Further, since $k$ is strongly measurable and $\iint |k(x, y)| dP(x) dP(y) < \infty$, then $k$ is $\infty$-bounded in the sense of Carmeli et al. (2006, Definition 4.1); see Carmeli et al. (2006, Corollary 4.3). Since $k$ is continuous and $X$ is separable, it follows that $\mathcal{H}(k)$ is separable (Carmeli et al., 2006, Corollary 5.2). Since $\mathcal{H}(k)$ is separable, $k$ being $\infty$-bounded is equivalent to $\mathcal{H}(k) \subset L^1(P)$ (Carmeli et al., 2006, Proposition 4.4). \qed

## B Auxiliary Results

The following auxiliary results were used for the proofs in the main text:

**Theorem 18** (Strong law of large numbers in a Banach space). Let $B$ be a separable Banach space and let $(\zeta_n)_{n \in \mathbb{N}}$ be a sequence of independent and identically distributed random variables taking values in $B$ such that $E[\|\zeta_n\|_B] < \infty$ and $E[\zeta_n] = 0$. Then

$$\frac{1}{n} \sum_{i=1}^{n} \zeta_i \xrightarrow{a.s.} 0.$$

**Proof.** See Ledoux and Talagrand (1991, Corollary 7.10). \qed

**Theorem 19** (Strong law of larger numbers for V-statistics). Let $P$ be a distribution on a measurable space $\mathcal{X}$, and let $(x_n)_{n \in \mathbb{N}}$ be a sequence of independent draws from $P$. Let $v: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be a measurable symmetric function with $\iint |v(x, y)| dP(x) dP(y) < \infty$ and $\int |v(x, x)| dP(x) < \infty$. Then

$$\frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} v(x_i, x_j) \xrightarrow{a.s.} \iint v(x, y) dP(x) dP(y).$$
Proof. Let

\[ V_n := \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} v(x_i, x_j), \quad U_n := \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j \neq i}^{n} v(x_i, x_j), \quad R_n := \sum_{i=1}^{n} v(x_i, x_i). \]

From the usual strong law of large numbers, we have that \( n^{-1} R_n \xrightarrow{\text{a.s.}} \int \int v(x, x) \, dP(x) < \infty \) and thus \( n^{-2} R_n \xrightarrow{\text{a.s.}} 0 \). From the strong law of large numbers for U-statistics, due to Hoeffding (1948), we have that \( U_n \xrightarrow{\text{a.s.}} \int \int v(x, y) \, dP(x) \, dP(y) \). Thus

\[ V_n = \frac{n-1}{n} U_n + \frac{1}{n^2} R_n \xrightarrow{\text{a.s.}} 1 \times \int \int v(x, y) \, dP(x) \, dP(y) + 0, \]

which completes the argument. \( \square \)

**Theorem 20** (Asymptotic normality of V-statistics). Let \( P \) be a distribution on a measurable space \( \mathcal{X} \), and let \( (x_n)_{n \in \mathbb{N}} \) be a sequence of independent draws from \( P \). Let \( v : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \) be a measurable symmetric function with \( \int \int v(x, y)^2 \, dP(x) \, dP(y) < \infty \). Let \( \sigma^2 = \mathbb{V}_{X \sim P} [\int \int v(X, Y) \, dP(Y)] \). Then

\[ \sqrt{n} \left( \frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} v(x_i, x_j) - \int \int v(x, y) \, dP(x) \, dP(y) \right) \xrightarrow{\text{d}} \mathcal{N}(0, 4\sigma^2), \]

where we interpret \( \mathcal{N}(0, 0) \) as a point mass \( \delta_0 \) at \( 0 \in \mathcal{X} \).

Proof. This proof uses the same notation as the proof of Theorem 19. From Hoeffding (1948), since \( \int \int v(x, y)^2 \, dP(x) \, dP(y) < \infty \), we have asymptotic normality of the U-statistic

\[ \sqrt{n} \left( U_n - \int \int v(x, y) \, dP(x) \, dP(y) \right) \xrightarrow{\text{d}} \mathcal{N}(0, 4\sigma^2) \]

(see also Section 5.5.1 of Serfling (2009)). From Theorem 1 of Bonner and Kirschner (1977), since \( \int \int v(x, y) \, dP(x) \, dP(y) < \infty \), we have that \( \sqrt{n}(V_n - U_n) \xrightarrow{p} 0 \) (see also Section 5.7.3 of Serfling (2009)). From Slutsky’s theorem, we can combine these facts to arrive at the required result. \( \square \)

**Theorem 21** (Uniform law of large numbers). Let \( \Theta \subset \mathbb{R}^p \) be bounded. Let \( f : \Theta \to \mathbb{R} \) be fixed and consider a sequence \( (f_n)_{n \in \mathbb{N}} \) of stochastic functions \( f_n : \Theta \to \mathbb{R} \). Suppose that

1. \( f_n(\theta) \xrightarrow{\text{a.s.}} f(\theta) \) for all \( \theta \in \Theta \)
2. \( |f_n(\theta) - f_n(\vartheta)| \leq B_n \|\theta - \vartheta\| \) for all \( \theta, \vartheta \in \Theta \), where \( B_n \) does not depend on \( \theta, \vartheta \) and \( \text{a.s.} \limsup B_n < \infty \).

Then \( \sup_{\theta \in \Theta} |f_n(\theta) - f(\theta)| \xrightarrow{\text{a.s.}} 0 \).

Proof. This follows as a combination of Theorem 21.8 and Theorem 21.10 from Davidson (1994). \( \square \)
Definition 22. Let $P$ be a distribution on a measurable space $\mathcal{X}$. A function $f : \Theta \times \mathcal{X} \to \mathbb{R}^p$ is locally uniformly integrably bounded with respect to $P$ if, for every $\theta \in \Theta$, there is a non-negative function $b_\theta : \mathcal{X} \to \mathbb{R}$ that is integrable with respect to $P$, and an open neighbourhood $U_\theta$ of $\theta$, such that $\|f(\vartheta, x)\| \leq b_\theta(x)$ for all $\vartheta \in U_\theta$.

Lemma 23 (Differentiate under the Lebesgue integral). Let $P$ be a distribution on a measurable space $\mathcal{X}$. Let $\Theta \subseteq \mathbb{R}^p$ be an open set. Let $h : \Theta \times \mathcal{X} \to \mathbb{R}$ be such that $\partial_\theta h$ is locally uniformly integrably bounded with respect to $P$. Then

$$\partial_\theta \int h(\theta, x) dP(x) = \int \partial_\theta h(\theta, x) dP(x).$$

Proof. See, for example, Aliprantis and Burkinshaw (1998, Theorem 24.5, p.193), Billingsley (1979, Theorem 16.8, pp.181-182). $\square$

C Assumptions for the Exponential Family Model

To better understand A1-A12, we consider the consequences of these assumptions in the setting of canonical exponential family statistical model

$$p_\theta(x) = \exp(\langle \theta, t(x) \rangle - a(\theta) + b(x))$$

where $x \in \mathcal{X} = \mathbb{R}^d$, whose parameter $\theta \in \Theta \subset \mathbb{R}^p$ is estimated using either the generalised method of moments (Appendix C.1) or using a kernel Stein discrepancy (Appendix C.2).

C.1 Estimation via Generalised Method of Moments

Consider the generalised method of moments from Section 3.1, which uses a finite rank kernel of the form $k(x, y) = \langle \phi(x), \phi(y) \rangle$. To simplify the following discussion we focus on the well-specified case where there is a unique $\theta_* \in \Theta = \mathbb{R}^p$ with $P = P_{\theta_*}$ and seek conditions under which the generalised moment matching estimator is consistent, with fluctuations that are asymptotically normal. In this context there are essentially two important conditions that must be satisfied:

- **B1** $\phi$ is uniformly continuous and bounded
- **B2** $M_{i,j} := \int \phi_j(x) [t_i(x) - \partial_\theta a(\theta)] dP(x)|_{\theta = \theta_*}$ has full row rank.

The first part, **B1**, is satisfied by (for example) the Fourier features popularised in Rahimi and Recht (2007), while **B2** ensures that the set of features is rich enough to identify the correct model. In addition to these two main conditions, we require sufficient regularity that, in a bounded open neighbourhood $S$ of $\theta_*$:

- **B3** $\theta \mapsto \int \phi dP_\theta$ is continuous at each $\theta \in S$
- **B4** $\theta \mapsto \int t dP_\theta$ and $\int tt^\top dP_\theta$ are continuous at $\theta_*$. 

24
\[ \sup_{\theta \in S} \int \|t\|^2 \, dP_\theta < \infty \]

**B6** for each \( \theta \in S \), there exists \( \gamma_\theta > 0 \) such that \( \int (1 + \|t\|^2) \exp(\gamma_\theta \|t\|) \, dP_\theta < \infty \)

**B7** \( \partial^2 \alpha(\theta) \) exists for each \( \theta \in S \) and is continuous at \( \theta_* \),

which are all reasonably mild. Collectively **B1-B7** imply **A1-A2** and **A6-A12**, so that the generalised moment matching estimator is both consistent and asymptotically normal. Full derivations are reserved for Appendix D.1.

### C.2 Estimation via Kernel Stein Discrepancy

Consider the minimum kernel Stein discrepancy estimator from Section 3.3. Here we suppose that \( \Theta \) is an open, convex and bounded subset of \( \mathbb{R}^p \) but, in contrast to the last section, we do not assume here the statistical model is well-specified. For \( f : \mathbb{R}^d \to \mathbb{R}^d \), the convention \( [\nabla f]_{i,j} = \partial_{x_i} f_j(x) \) will be used. In this application, there are three main conditions to be satisfied:

**C1** \( c(x,y), \nabla_x c(x,y), \nabla_y c(x,y) \) are bounded over \( x, y \in \mathbb{R}^d \)

**C2** \( \nabla E, \nabla t, \nabla b \) and \( x \mapsto \nabla_x \cdot \nabla_y c(x,y), \ y \in \mathbb{R}^d \), are in \( L^1(P_\theta) \) for each \( \theta \in \Theta \)

**C3** \( \int c(x,y)[\nabla t(x)]^T [\nabla t(y)] \, dP(x)dP(y) > 0 \)

The requirements **C1-C2** ensure the integrability conditions of Proposition 4 are satisfied, while **C3** is analogous to **B2**, ensuring that the optimal statistical model can be identified. In addition, the following regularity is required:

**C4** \( (x,y) \mapsto c(x,y), \nabla_x c(x,y), \nabla_y c(x,y), \nabla_x \cdot \nabla_y c(x,y) \) are continuous

**C5** \( \nabla t \) and \( \nabla b \) are continuous

**C6** \( \int \|\nabla t\|^4 \, dP, \int \|\nabla t\|^3 \|\nabla b\| \, dP, \int \|\nabla t\|^2 \|\nabla b\|^2 \, dP, \int \|\nabla b\| \, dP < \infty \),

which are again reasonably mild. Collectively **C1-C6** imply **A1** and **A3-A12**, so that the minimum kernel Stein discrepancy estimator is both consistent and asymptotically normal. Full derivations are reserved for Appendix D.2

### D Proofs for the Exponential Family Model

This appendix contains full details on how our theoretical assumptions were verified for the canonical exponential family statistical model in Appendix C.
D.1 Estimation via Generalised Method of Moments

In this section we verify that collectively B1-B7 imply A1-A2 and A6-A12, so that the generalised moment matching estimator is both consistent and asymptotically normal. The matrix norm \( \| M \|^2 = \sum M_{ij}^2 \) will be used. From B1, we have \( |k(x, y)| \leq k_{\text{max}} \) for all \( x, y \in \mathbb{R}^p \) where \( k_{\text{max}} \) is a positive constant.

Verify A1: The space \( \mathcal{H}(k) \) is separable whenever \( k \) is continuous and \( \mathcal{X} \) is separable (which is the case for \( \mathcal{X} = \mathbb{R}^d \)), and thus B1 implies A1.

Verify A2: B1 immediately implies A2.

Verify A6 and A9: At each \( \theta \in S \), we claim the functions \( x \mapsto k(x, y)\partial_\theta p_\theta(x) \) and \( x \mapsto \int k(x, y)\partial_\theta p_\theta(x)\,dP_\theta(y) \) are locally uniformly integrably bounded with respect to the Lebesgue measure on \( \mathbb{R}^p \). Indeed, for the first of these functions we have a bound

\[
\int \sup_{\theta \in S_{\gamma, \theta}} \| k(x, y)\partial_\theta p_\theta(x) \| \,dx \leq k_{\text{max}} \int \sup_{\theta \in S_{\gamma, \theta}} \| t(x) - \partial_\theta a(\theta) \| p_\theta(x) \,dx
\]

\[
= k_{\text{max}} \int \sup_{\theta \in S_{\gamma, \theta}} \| t(x) - \partial_\theta a(\theta) \| \frac{p_\theta(x)}{p_\theta(\theta)} dP_\theta(x),
\]

where \( S_{\gamma, \theta} = S \cap \{ \theta \in \mathbb{R}^p : \| \theta - \theta \| < \gamma \} \). An identical bound holds also for the second function considered. Now,

\[
\sup_{\theta \in S_{\gamma, \theta}} \| t(x) - \partial_\theta a(\theta) \| \leq \| t(x) \| + C_1
\]

\[
\frac{p_\theta(x)}{p_\theta(\theta)} = \exp \left( (\theta - \theta, t(x)) - [a(\theta) - a(\theta)] \right) \leq \exp \left( C_2 \| t(x) \| + C_3 \right)
\]

where \( C_1 = \sup_{\theta \in S_{\gamma, \theta}} \| \partial_\theta a(\theta) \|, \ C_2 = \sup_{\theta \in S_{\gamma, \theta}} \| \theta - \theta \| \) and \( C_3 = \sup_{\theta \in S_{\gamma, \theta}} |a(\theta) - a(\theta)| \).

From B7, we have \( C_1, C_3 < \infty \), and \( C_2 < \infty \) holds since \( S \) is bounded. Thus

\[
\int \sup_{\theta \in S_{\gamma, \theta}} \| k(x, y)\partial_\theta p_\theta(x) \| \,dx \leq k_{\text{max}} \int \left[ \| t(x) \| + C_1 \right] \exp \left( C_2 \| t(x) \| + C_3 \right) dP_\theta(x) < \infty,
\]

where the final integral is finite due to B6. Thus we have established the conditions of Lemma 23 and we may interchange \( \partial_\theta \) with integration with respect to \( dx \) and \( dy \):

\[
\partial_\theta k_\theta(x, y) = - \int k(x, y)\partial_\theta p_\theta(x)\,dx - \int k(x, y)\partial_\theta p_\theta(y)\,dy + \int \int k(x, y)\partial_\theta [p_\theta(x)p_\theta(y)] dxdy
\]

\[
= - \int k(x, y)[t(x) - \partial_\theta a(\theta)] dP_\theta(x) - \int k(x, y)[t(y) - \partial_\theta a(\theta)] dP_\theta(y)
\]

\[
+ \int \int k(x, y)[t(x) + t(y) - 2\partial_\theta a(\theta)] dP_\theta(x)dP_\theta(y)
\]

so, using the triangle inequality and Jensen’s inequality,

\[
\frac{\| \partial_\theta k_\theta(x, y) \|}{k_{\text{max}}} \leq 4 \int \| t(x) \| dP_\theta(x) + 4\| \partial_\theta a(\theta) \|.
\]
From $B5$ we have that $\sup_{\theta \in S} |t|dP_\theta < \infty$ and, since $S$ is bounded, $B7$ implies that $\sup_{\theta \in S} \|\partial_\theta a(\theta)\| < \infty$. Thus $\sup_{x,y \in \mathcal{X}} \|\partial_\theta k_\theta(x,y)\| < \infty$ and, in particular, $A6$ and $A9$ hold.

**Verify A7:** An argument analogous to the previous argument shows that $B6$ is sufficient to allow a second interchange of $\partial_\theta$ with integration with respect to $dx$ and $dy$:

$$
\partial^2_\theta k_\theta(x,y) = [\partial^2_\theta a(\theta)] \int k(x,y)dP_\theta(x) - \int k(x,y)[t(x) - \partial_\theta a(\theta)][t(x) - \partial_\theta a(\theta)]^T dP_\theta(x) \\
+ [\partial^2_\theta a(\theta)] \int k(x,y)dP_\theta(y) - \int k(x,y)[t(y) - \partial_\theta a(\theta)][t(y) - \partial_\theta a(\theta)]^T dP_\theta(y) \\
- 2[\partial^2_\theta a(\theta)] \int k(x,y)dP_\theta(x)dP_\theta(y) + \int k(x,y)[t(x) + t(y) - 2\partial_\theta a(\theta)][t(x) + t(y) - 2\partial_\theta a(\theta)]^T dP_\theta(x)dP_\theta(y)
$$

(14)

where the quantities exist on $\theta \in S$ due to $B5$ and $B7$, showing that $A7$ is satisfied.

**Verify A8:** Since (14) takes the form

$$
\partial^2_\theta k_\theta(x,y) = \int k(x,u)f(u,\theta) du + \int k(y,u)f(u,\theta) du - \int k(u,v)g(u,v,\theta) duv \\
f(u,\theta) := \{[\partial^2_\theta a(\theta)] - [t(u) - \partial_\theta a(\theta)][t(u) - \partial_\theta a(\theta)]^T\} p_\theta(u) \\
g(u,v,\theta) = \{2[\partial^2_\theta a(\theta)] - [t(u) + t(v) - 2\partial_\theta a(\theta)][t(u) + t(v) - 2\partial_\theta a(\theta)]^T\} p_\theta(u)p_\theta(v),
$$

we have that

$$
\sup_{x,y \in \mathcal{X}} \|\partial^2_\theta k_\theta(x,y) - [\partial^2_\theta k_\theta(x,y)]\|_{\theta = \theta_*} \leq 2 \int |f(u,\theta) - f(u,\theta_*)| du \\
+ \int g(u,v,\theta) - g(u,v,\theta_*)| duv
$$

Since $\partial^2_\theta a(\theta)$ is continuous at $\theta_*$ from $B7$ and $\int t dP_\theta$ and $\int tt^T dP_\theta$ are continuous at $\theta_*$ from $B4$, it follows that both integrals on the right hand side vanish as $\theta \to \theta_*$, meaning $A8$ is established.

**Verify A10 and A11:** Application of the triangle inequality to (14), and collecting together terms, yields

$$
\frac{\|\partial^2_\theta k_\theta(x,y)\|}{k_{\max}} \leq 4 \int \|t(x)\|^2 dP_\theta(x) + 12\|\partial_\theta a(\theta)\| \int \|t(x)\| dP_\theta(x) \\
+ 4\|\partial^2_\theta a(\theta)\| + 6\|\partial_\theta a(\theta)\|^2 + 2 \left( \int \|t(x)\| dP_\theta(x) \right)^2.
$$

Thus $B5$ and $B7$ imply $\sup_{x,y \in \mathcal{X}} \left[\|\partial^2_\theta k_\theta(x,y)\|_{\theta = \theta_*}\right] < \infty$, so $A10$ and $A11$ hold.
Verify A12: Integrating both arguments of (14) with respect to $P = P_{\theta_*}$, we obtain
\[
\Gamma = \frac{1}{2} \iint \partial^2_{\theta} k_\theta(x, y) dP(x) dP(y) \bigg|_{\theta = \theta_*} \\
= \int \int k(x, y) [t(x) - \partial_\theta a(\theta)] [t(y) - \partial_\theta a(\theta)]^T \, dP(x) dP(y) = MM^T \succ 0,
\]
where the final equality uses the definition of $M$ and the fact that $k(x, y) = \langle \phi(x), \phi(y) \rangle$, and the positive definiteness follows from B2.

Verify $\theta_n \overset{a.s.}{\rightarrow} \theta_*$: Through the above, we have proven that if $\theta_n \overset{a.s.}{\rightarrow} \theta_*$, then the fluctuations of $\theta_n$ are asymptotically normal. However, we have not yet commented on whether $\theta_n \overset{a.s.}{\rightarrow} \theta_*$. Since we are in the well-specified regime, we have from (14)
\[
\partial^2_{\theta} D_k(P, P_\theta) \bigg|_{\theta = \theta_*} = \iint \partial^2_{\theta} k_\theta(x, y) dP(x) dP(y) \bigg|_{\theta = \theta_*} = 2\Gamma \succ 0,
\]
showing that $\theta_*$ is a local minimum of the kernel discrepancy. Since we assumed $\theta_*$ is unique, and from B3 the map $\theta \mapsto D_k(P, P_\theta)$ is continuous, the conditions of Theorem 8 are satisfied, establishing that $\theta_n \overset{a.s.}{\rightarrow} \theta_*$.

D.2 Estimation via Kernel Stein Discrepancy

In this section we verify that collectively C1-C6 imply A1 and A3-A12, so that the minimum kernel Stein discrepancy estimator is both consistent and asymptotically normal. From C1, we have $|c(x, y)|, \|\nabla_x c(x, y)\|, \|\nabla_y c(x, y)\| \leq c_{\text{max}}$ for all $x, y \in \mathbb{R}^d$ where $c_{\text{max}}$ is a positive constant. From C2 the integrability conditions of Proposition 4 are satisfied, so that $k(., .; \theta) = k_\theta(., .)$ for each $\theta \in \Theta$.

Verify A1: From C4 and C5, $(x, y) \mapsto k(x, y; \theta) = k_\theta(x, y)$ is continuous, since
\[
k_\theta(x, y) = \nabla_x \cdot \nabla_y c(x, y) + \langle \nabla_x c(x, y), \nabla t(y) \theta + \nabla b(y) \rangle \\
+ \langle \nabla_y c(x, y), \nabla t(x) \theta + \nabla b(x) \rangle + c(x, y) \langle \nabla t(x) \theta + \nabla b(x), \nabla t(y) \theta + \nabla b(y) \rangle.
\]
The space $\mathcal{H}(k)$ is separable whenever $k$ is continuous and $\mathcal{X}$ is separable (which is the case for $\mathcal{X} = \mathbb{R}^d$), and thus $\mathcal{H}(k)$ is separable and we have A1.

Verify A7: First we compute
\[
\partial_\theta k_\theta(x, y) = \langle \nabla_x c(x, y), [\nabla t(y)]_{,i} \rangle + \langle \nabla_y c(x, y), [\nabla t(x)]_{,i} \rangle \\
+ c(x, y) \langle [\nabla t(x)]_{,i}, \nabla t(y) \theta + \nabla b(y) \rangle + c(x, y) \langle [\nabla t(x) \theta + \nabla b(x), [\nabla t(y)]_{,i} \rangle,
\]
which is a linear function of $\theta$, so that we trivially have A7.
Verify A4, A5, A6, A9: The triangle and Cauchy–Schwarz inequalities applied to (15) yield
\[
\frac{\| \partial_{\theta_i} k_{\theta}(x,y) \|}{c_{\text{max}}} \leq \| \nabla t(x) \| + \| \nabla t(y) \| + \| \nabla t(x) \| \sup_{\theta \in \Theta} \| \theta \| + \| \nabla b(x) \| \\
+ \| \nabla t(y) \| \left( \| \nabla t(x) \| \sup_{\theta \in \Theta} \| \theta \| + \| \nabla b(x) \| \right),
\]
where \(\sup_{\theta \in \Theta} \| \theta \| < \infty\) since we assumed that \(\Theta\) was bounded. Thus A4 holds from C6, and both A5 and A6 hold from C6. Squaring, we see also that A9 holds from C6.

Verify A8, A10, A11: Differentiating (15) again,
\[
\partial_{\theta_i} \partial_{\theta_j} k_{\theta}(x,y) = 2c(x,y) \langle [\nabla t(x)]_{,i}, [\nabla t(y)]_{,j} \rangle
\]
so A8 holds trivially, since these functions are constant in \(\theta\). Further,
\[
\frac{\| \partial_{\theta_i} \partial_{\theta_j} k_{\theta}(x,y) \|}{c_{\text{max}}} \leq 2 \| \nabla t(x) \| \| \nabla t(y) \|
\]
so A10 and A11 hold from C6.

Verify A12: Finally,
\[
\Gamma = \frac{1}{2} \iint \partial_{\theta}^2 k_{\theta}(x,y) \, dP(x)dP(y) \bigg|_{ \theta = \theta^* } = \iint c(x,y) [\nabla t(x)]^\top [\nabla t(y)] \, dP(x)dP(y) > 0
\]
from C3, establishing A12.

Verify \(\theta_n \overset{a.s.}{\longrightarrow} \theta^*\): Since we have verified A3, A4 and A5, we have from Lemma 11 and an essentially identical argument to Lemma 7 that \(D_k(P,P_{\theta_n}) \overset{a.s.}{\longrightarrow} D_k(P,P_{\theta^*})\). Since the squared kernel Stein discrepancy
\[
\theta \mapsto D_k(P,P_{\theta})^2 = \iint k_{\theta}(x,y) \, dP(x)dP(y)
\]
is a quadratic with minimum \(\theta^*\) and Hessian at \(\theta^*\) equal to \(2\Gamma > 0\), it is necessarily the case that \(\theta_n \overset{a.s.}{\longrightarrow} \theta^*\) in the \(n \to \infty\) limit.

References

H. Akaike. Information theory and an extension of the likelihood principle. In Proceedings of the Second International Symposium of Information Theory, 1973.

C. D. Aliprantis and O. Burkinshaw. Principles of Real Analysis. Academic Press, 1998.
P. Alquier and M. Gerber. Universal robust regression via maximum mean discrepancy. *Biometrika*, 2023. To appear.

A. Anastasiou, A. Barp, F.-X. Briol, B. Ebner, R. E. Gaunt, F. Ghaderinezhad, J. Gorham, A. Gretton, C. Ley, Q. Liu, L. Mackey, C. J. Oates, G. Reinert, and Y. Swan. Stein’s method meets statistics: A review of some recent developments. *Statistical Science*, 38(1): 120–139, 2023.

M. Arjovsky, S. Chintala, and L. Bottou. Wasserstein generative adversarial networks. In *Proceedings of the 34th International Conference on Machine Learning*, 2017.

A. Barp, F.-X. Briol, A. Duncan, M. Girolami, and L. Mackey. Minimum Stein discrepancy estimators. In *Proceedings of the 33rd Conference on Neural Information Processing Systems*, 2019.

A. Barp, C.-J. Simon-Gabriel, M. Girolami, and L. Mackey. Targeted separation and convergence with kernel discrepancies. *arXiv:2209.12835*, 2022.

A. Basu, H. Shioya, and C. Park. *Statistical Inference: The Minimum Distance Approach*. CRC Press, 2011.

M. A. Beaumont. Approximate bayesian computation. *Annual Review of Statistics and its Application*, 6:379–403, 2019.

P. Billingsley. *Probability and Measure*. John Wiley and Sons, 1979.

M. Bińkowski, D. J. Sutherland, M. Arbel, and A. Gretton. Demystifying MMD GANs. In *Proceedings of the 6th International Conference on Learning Representations*, 2018.

N. Bonner and H.-P. Kirschner. Note on conditions for weak convergence of von Mises’ differentiable statistical functions. *The Annals of Statistics*, 5(2):405–407, 1977.

F.-X. Briol, A. Barp, A. B. Duncan, and M. Girolami. Statistical inference for generative models with maximum mean discrepancy. *arXiv:1906.05944*, 2019.

C. Carmeli, E. De Vito, and A. Toigo. Vector valued reproducing kernel Hilbert spaces of integrable functions and Mercer theorem. *Analysis and Applications*, 4(04):377–408, 2006.

B.-E. Chérif-Abdellatif and P. Alquier. MMD-Bayes: Robust Bayesian estimation via maximum mean discrepancy. In *Symposium on Advances in Approximate Bayesian Inference*, pages 1–21. PMLR, 2020.

B.-E. Chérif-Abdellatif and P. Alquier. Finite sample properties of parametric MMD estimation: Robustness to misspecification and dependence. *Bernoulli*, 28(1):181–213, 2022.

K. Chwialkowski, H. Strathmann, and A. Gretton. A kernel test of goodness of fit. In *Proceedings of the 33rd International Conference on Machine Learning*, 2016.
E. C. Cortes and C. Scott. Sparse approximation of a kernel mean. *IEEE Transactions on Signal Processing*, 65(5):1310–1323, 2016.

J. Davidson. *Stochastic Limit Theory: An Introduction for Econometricians*. OUP Oxford, 1994.

A. P. Dawid. The geometry of proper scoring rules. *Annals of the Institute of Statistical Mathematics*, 59(1):77–93, 2007.

A. P. Dawid, M. Musio, and L. Ventura. Minimum scoring rule inference. *Scandinavian Journal of Statistics*, 43(1):123–138, 2016.

C. Dellaporta, J. Knoblauch, T. Damoulas, and F.-X. Briol. Robust Bayesian inference for simulator-based models via the MMD posterior bootstrap. In *Proceedings of the 25th International Conference on Artificial Intelligence and Statistics*, 2022.

P. Dhariwal and A. Nichol. Diffusion models beat GANs on image synthesis. In *Proceedings of the 35th Conference on Neural Information Processing Systems*, 2021.

J. Dick and F. Pillichshammer. *Digital Nets and Sequences: Discrepancy Theory and Quasi-Monte Carlo integration*. Cambridge University Press, 2010.

J. Dick, F. Y. Kuo, and I. H. Sloan. High-dimensional integration: The quasi-Monte Carlo way. *Acta Numerica*, 22:133–288, 2013.

D. L. Donoho and R. C. Liu. The “automatic” robustness of minimum distance functionals. *The Annals of Statistics*, 16(2):552–586, 1988.

N. Dunford. Integration of vector-valued functions. *Bulletin of the American Mathematical Society*, page 43, 1937.

G. K. Dziugaite, D. M. Roy, and Z. Ghahramani. Training generative neural networks via maximum mean discrepancy optimization. In *Proceedings of the 31st Conference on Uncertainty in Artificial Intelligence*, 2015.

D. T. Frazier and C. Drovandi. Robust approximate Bayesian inference with synthetic likelihood. *Journal of Computational and Graphical Statistics*, 30(4):958–976, 2021.

D. A. Freedman. On the so-called “Huber sandwich estimator” and “robust standard errors”. *The American Statistician*, 60(4):299–302, 2006.

A. Genevay, G. Peyré, and M. Cuturi. Learning generative models with sinkhorn divergences. In *Proceedings of the 21st International Conference on Artificial Intelligence and Statistics*, 2018.

T. Gneiting and A. E. Raftery. Strictly proper scoring rules, prediction, and estimation. *Journal of the American statistical Association*, 102(477):359–378, 2007.
I. Goodfellow, J. Pouget-Abadie, M. Mirza, B. Xu, D. Warde-Farley, S. Ozair, A. Courville, and Y. Bengio. Generative adversarial networks. *Communications of the ACM*, 63(11): 139–144, 2020.

J. Gorham and L. Mackey. Measuring sample quality with kernels. In *Proceedings of the 34th International Conference on Machine Learning*, 2017.

A. Gretton, K. M. Borgwardt, M. J. Rasch, B. Schölkopf, and A. Smola. A kernel two-sample test. *The Journal of Machine Learning Research*, 13(1):723–773, 2012.

L. P. Hansen. Large sample properties of generalized method of moments estimators. *Econometrica*, pages 1029–1054, 1982.

F. Hickernell. A generalized discrepancy and quadrature error bound. *Mathematics of Computation*, 67(221):299–322, 1998.

E. Hlawka. Funktionen von beschränkter variatiou in der theorie der gleichverteilung. *Annali di Matematica Pura ed Applicata*, 54(1):325–333, 1961.

W. Hoeffding. A class of statistics with asymptotically normal distribution. *The Annals of Mathematical Statistics*, 19(3):293–325, 1948.

W. Hoeffding. The strong law of large numbers for U-statistics. Technical report, North Carolina State University. Dept. of Statistics, 1961.

P. J. Huber. Robust estimation of a location parameter. *The Annals of Mathematical Statistics*, pages 73–101, 1964.

A. Hyvärinen and P. Dayan. Estimation of non-normalized statistical models by score matching. *Journal of Machine Learning Research*, 6(4), 2005.

O. Key, T. Fernandez, A. Gretton, and F.-X. Briol. Composite goodness-of-fit tests with kernels. *arXiv:2111.10275*, 2021.

F. Y. Kuo. Component-by-component constructions achieve the optimal rate of convergence for multivariate integration in weighted Korobov and Sobolev spaces. *Journal of Complexity*, 19(3):301–320, 2003.

C. Lam. High-dimensional covariance matrix estimation. *Wiley Interdisciplinary Reviews: Computational Statistics*, 12(2):e1485, 2020.

Y. LeCun, S. Chopra, R. Hadsell, M. Ranzato, and F. Huang. A tutorial on energy-based learning. In B. Schölkopf, A. J. Smola, B. Taskar, and S. Vishwanathan, editors, *Predicting Structured Data*. 2007.

M. Ledoux and M. Talagrand. *Probability in Banach Spaces: Isoperimetry and Processes*. Springer Science & Business Media, 1991.
C.-L. Li, W.-C. Chang, Y. Cheng, Y. Yang, and B. Póczos. MMD GAN: Towards deeper understanding of moment matching network. In Proceedings of the 31st Conference on Neural Information Processing Systems, 2017.

Y. Li, K. Swersky, and R. Zemel. Generative moment matching networks. In Proceedings of the 32nd International Conference on Machine Learning, 2015.

Q. Liu, J. Lee, and M. Jordan. A kernelized Stein discrepancy for goodness-of-fit tests. In Proceedings of the 33rd International Conference on Machine Learning, 2016.

A.-M. Lyne, M. Girolami, Y. Atchadé, H. Strathmann, and D. Simpson. On Russian roulette estimates for Bayesian inference with doubly-intractable likelihoods. Statistical Science, 30(4):443–467, 2015.

T. Matsubara, J. Knoblauch, F.-X. Briol, and C. J. Oates. Robust generalised bayesian inference for intractable likelihoods. Journal of the Royal Statistical Society, Series B, 84(3):997–1022, 2022a.

T. Matsubara, J. Knoblauch, F.-X. Briol, and C. J. Oates. Robust generalised Bayesian inference for intractable likelihoods. Journal of the Royal Statistical Society: Series B, 84(3):997–1022, 2022b.

J. Mitrovic, D. Sejdinovic, and Y.-W. Teh. DR-ABC: Approximate Bayesian computation with kernel-based distribution regression. In Proceedings of the 33rd International Conference on Machine Learning, 2016.

Y. Mroueh and T. Sercu. Fisher GAN. In Proceedings of the 31st Conference on Neural Information Processing Systems, 2017.

Y. Mroueh, T. Sercu, and V. Goel. McGAN: Mean and covariance feature matching GAN. In Proceedings of the 34th International Conference on Machine Learning, 2017.

Y. Mroueh, C.-L. Li, T. Sercu, A. Raj, and Y. Cheng. Sobolev GAN. In Proceedings of the 6th International Conference on Learning Representations, 2018.

K. Muandet, K. Fukumizu, B. Sriperumbudur, and B. Schölkopf. Kernel mean embedding of distributions: A review and beyond. Foundations and Trends® in Machine Learning, 10(1-2):1–141, 2017.

A. Müller. Integral probability metrics and their generating classes of functions. Advances in Applied Probability, 29(2):429–443, 1997.

S. Nietert, Z. Goldfeld, and K. Kato. Smooth $p$-wasserstein distance: Structure, empirical approximation, and statistical applications. In Proceedings of the 38th International Conference on Machine Learning, 2021.
Z. Niu, J. Meier, and F.-X. Briol. Discrepancy-based inference for intractable generative models using quasi-Monte Carlo. *Electronic Journal of Statistics*, 17(1):1411–1456, 2023.

C. J. Oates, M. Girolami, and N. Chopin. Control functionals for Monte Carlo integration. *Journal of the Royal Statistical Society, Series B*, 79:695–718, 2017.

L. Pardo. *Statistical Inference Based on Divergence Measures*. Chapman and Hall/CRC, 2018.

M. Park, W. Jitkrittum, and D. Sejdinovic. K2-ABC: Approximate Bayesian computation with kernel embeddings. In *Proceedings of the 18th International Conference on Artificial Intelligence and Statistics*, 2016.

A. Rahimi and B. Recht. Random features for large-scale kernel machines. In *Proceedings of the 21st Conference on Neural Information Processing Systems*, 2007.

S. Schwabik and G. Ye. *Topics in Banach Space Integration*. World Scientific, 2005.

R. J. Serfling. *Approximation Theorems of Mathematical Statistics*. John Wiley & Sons, 2009.

C.-J. Simon-Gabriel, A. Barp, and L. Mackey. Metrizing weak convergence with maximum mean discrepancies. *Journal of Machine Learning Research*, 24:1–20, 2023.

I. H. Sloan and P. J. Kachoyan. Lattice methods for multiple integration: Theory, error analysis and examples. *SIAM Journal on Numerical Analysis*, 24(1):116–128, 1987.

I. H. Sloan and H. Woźniakowski. When are quasi-Monte Carlo algorithms efficient for high dimensional integrals? *Journal of Complexity*, 14(1):1–33, 1998.

L. Song, X. Zhang, A. Smola, A. Gretton, and B. Schölkopf. Tailoring density estimation via reproducing kernel moment matching. In *Proceedings of the 25th International Conference on Machine Learning*, 2008.

Y. Song and D. P. Kingma. How to train your energy-based models. *arXiv:2101.03288*, 2021.

I. Steinwart and A. Christmann. *Support Vector Machines*. Springer Science & Business Media, 2008.

D. J. Sutherland, H.-Y. Tung, H. Strathmann, S. De, A. Ramdas, A. J. Smola, and A. Gretton. Generative models and model criticism via optimized maximum mean discrepancy. In *Proceedings of the 5th International Conference on Learning Representations*, 2017.

O. Teymur, J. Gorham, M. Riabiz, and C. J. Oates. Optimal quantisation of probability measures using maximum mean discrepancy. In *Proceedings of the 24th International Conference on Artificial Intelligence and Statistics*, 2021.
L. Theis, A. van den Oord, and M. Bethge. A note on the evaluation of generative models. In *Proceedings of the 4th International Conference on Learning Representations*, 2016.

A. W. Van der Vaart. *Asymptotic Statistics*. Cambridge University Press, 2000.

G. Wynne and A. B. Duncan. A kernel two-sample test for functional data. *Journal of Machine Learning Research*, 23(73):1–51, 2022.

G. Wynne, M. Kasprzak, and A. B. Duncan. A spectral representation of kernel Stein discrepancy with application to goodness-of-fit tests for measures on infinite dimensional Hilbert spaces. *arXiv:2206.04552*, 2022.