A Riemannian–Stein Kernel Method

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October 16, 2018

Abstract

This paper presents a theoretical analysis of numerical integration based on interpolation with a Stein kernel. In particular, the case of integrals with respect to a posterior distribution supported on a general Riemannian manifold is considered and the asymptotic convergence of the estimator in this context is established. Our results are considerably stronger than those previously reported, in that the optimal rate of convergence is established under a basic Sobolev-type assumption on the integrand. The theoretical results are empirically verified on \(S^2\).

1 Introduction

The focus of this paper is the numerical approximation of an integral

\[ I(f) = \int_M f \, dP \]  \hspace{1cm} (1)

where \(P\) is a probability measure on a compact Riemannian manifold \(M\) and \(f \in L^1(P)\). The distribution \(P\) is assumed to admit a density \(p\) with respect to the natural volume measure on \(M\), specified only up to an unknown normalisation constant. It is assumed that direct computation of the normalisation constant is difficult and therefore precluded. This final point demands special consideration and prevents standard numerical integration method from being used. This situation is of course regularly encountered in Bayesian statistics, where \(P\) is a posterior distribution whose density \(p\) is specified in un-normalised form as the product of a prior and a likelihood. In general the direct computation of the normalisation constant is difficult in the Bayesian context (Gelman and Meng 1998).
Several approaches to approximation of Eqn. 1 have been developed. These range from heuristic approaches, such as variational inference (Kingma and Welling, 2014) and Laplace approximation (Rue et al., 2009), through to asymptotically exact approaches such as Markov chain Monte Carlo (MCMC; Gilks et al., 1995) and quasi Monte Carlo (Dick et al., 2016). Among asymptotically exact approaches, MCMC is most widely-used and its convergence theory is well-developed (Meyn and Tweedie, 2012). However, the absolute error of the ergodic average is gated at $O(n^{-1/2})$, where $n$ is the number of evaluations of the integrand. This rate is sub-optimal for an $s$-times weakly differentiable integrand when $s > \frac{d}{2}$ and $d$ is the intrinsic dimension of the manifold; a consequence of the fact that the ergodic average does not exploit smoothness properties of the integrand (Traub, 2003). In recent years, several alternatives to MCMC have been developed to address this convergence bottleneck, focussing on smooth integrals of low effective dimension for which sub-optimality of MCMC is most pronounced. These include transport maps (Marzouk et al., 2016), Riemann sums (Philippe and Robert, 2001), quasi Monte Carlo ratio estimators (Schwab and Stuart, 2012), minimum energy designs (Joseph et al., 2017), support points (Mak and Joseph, 2016) and estimators based on Stein’s method (Liu and Wang, 2016; Oates et al., 2017; 2018; Chen et al., 2018). The computational cost of some of these methods is higher than $O(n)$ and, for the method that we study in this work, the cost is $O(n^3)$. Thus any accelerated convergence being offered must be weighed against this increased computational overhead.

1.1 Context

The purpose of this paper is to present a novel theoretical analysis of numerical integration based on interpolation with a Stein kernel, an approach first proposed in Oates et al. (2017). To this end, we recall how Stein’s method (Stein, 1972) can be used in the numerical integration context. In what follows, continuity of the integrand $f$ will be assumed, so that in particular point evaluation is well-defined. Let $F(M, F)$ denote the vector space of $F$-valued integrable functions on $M$, where $F$ is a specified field, and let $P(M)$ denote the space of Borel distributions on $M$.

**Definition 1.** Consider a set $\mathcal{H} \subset F(M, F)$ and an operator $\tau : \mathcal{H} \to F(M, F)$ with the property that, for fixed $P \in P(M)$ and all $\tilde{P} \in P(M)$,

$$\tilde{P} = P \iff \int_M \tau h \, d\tilde{P} = 0 \in F \quad \forall h \in \mathcal{H}.$$  

Then $(\mathcal{H}, \tau)$ is said to be a Stein characterisation of $P$. In this case the set $\mathcal{H}$ is called a Stein class and the operator $\tau$ is called a Stein operator. If only the $\Rightarrow$ implication holds, so that $\mathcal{H}$ need not be rich enough to distinguish elements in $P(M)$, then we call $(\mathcal{H}, \tau)$ a Stein pair for $P$.

The definition of a Stein characterisation is classical, but in this paper only the (novel) definition of a Stein pair will be used. The reader is referred to Ley et al. (2017) for further background on Stein’s method.
For the moment, let us suppose that a Stein pair \((\mathcal{H}, \tau)\) for \(P\) can be found. Then Eqn. \[1\] can be approximated in direct a manner, that will now be explained: First, select a set of distinct locations \(X = \{x_i\}_{i=1}^n \subset M\) at which the integrand is to be evaluated. Then construct an estimator of the form

\[
I_X(f) = \arg \inf_{\xi \in \mathbb{R}} \inf_{h \in \mathcal{H}} \sum_{i=1}^n \left( \xi + \tau h(x_i) - f(x_i) \right)^2 + R_1(\xi) + R_2(h) \tag{2}
\]

where \(R_1\) and \(R_2\) are regularisation terms, whose purpose is to ensure that a (unique) minimum will exist. As explained in the original work of Oates et al. (2017), the form of Eqn. \[2\] can be motivated as constructing an approximation \(\hat{f}\) to the integrand \(f\), based on the data \(\{(x_i, f(x_i))\}_{i=1}^n\), in the class of functions of the form \(\hat{f} = \xi + h\), where \(\xi \in \mathbb{R}\) and \(h \in \mathcal{H}\). In particular, the definition of a Stein pair ensures that \(\int_M \tau h dP = 0\), so that Eqn. \[2\] can be interpreted as an integral \(I_X(f) = \xi = \int_M \hat{f} dP\) of an approximation \(\hat{f}\) to the integrand. From this perspective, Eqn. \[2\] is similar to classical numerical integration methods such as Gaussian cubatures or spline-based methods, in each case explicitly based on an interpolant of the integrand.

The properties of the numerical integration method depend on the Stein class \(\mathcal{H}\), the Stein operator \(\tau\), the point set \(X\) and the regularisation terms \(R_1, R_2\) and thus the above formulation is quite general. Some specific choices are discussed next.

### 1.2 Existing Work

Previous related work has focussed on the Euclidean context with \(M = \mathbb{R}^d\). In this paper \(\nabla\) denotes the gradient operator on \(M\), which for the Euclidean manifold is \(\nabla = [\partial_{x_1}, \ldots, \partial_{x_d}]\). In particular, Assaraf and Caffarel (1999); Mira et al. (2013) considered the case where \(\mathcal{H}\) is a space of low-degree polynomials under no regularisation, i.e. \(R_1, R_2 \equiv 0\). This was combined with the Stein operator \(\tau : \mathcal{H} \to \mathcal{F}(\mathbb{R}^d, \mathbb{R}), \tau h = \nabla \cdot (p \nabla h)/p\), a second-order differential operator that can be evaluated without access to the normalisation constant. This led to an over-constrained least-squares problem and \(I_X\) can be seen as a classical control variate method.

The innovation in Oates et al. (2017) was to consider instead an infinite-dimensional normed space for \(\mathcal{H}\). The operator in Oates et al. (2017) was \(\tau : \mathcal{H} \to \mathcal{F}(\mathbb{R}^d, \mathbb{R}), \) where \(\mathcal{H} \subset \mathcal{F}(\mathbb{R}^d, \mathbb{R})\) was a Cartesian product of reproducing kernel Hilbert spaces and \(\tau h = \nabla \cdot h + (h \cdot \nabla p)/p\) was a first-order differential operator that can again be evaluated without the normalisation constant. To complete the specification of the method, the following natural regularisation terms were proposed:

\[
R_1(\xi) = \sigma^{-2} \xi^2 \\
R_2(h) = \inf \{\|h'\|_\mathcal{H}^2 : h' \in \mathcal{H}, \tau(h' - h) = 0\} \tag{3}
\]

where \(\sigma > 0\) was a parameter to be specified and \(\|\cdot\|_\mathcal{H}\) denotes the norm associated to \(\mathcal{H}\). That the term \(R_2(h)\) should depend on \(h\) through \(\tau h\) is natural, since \(h\) enters into
the approximation \( \hat{f} \) only through \( \tau h \). The output \( I_X \) of this Stein kernel method can be computed in closed-form and was termed a control functional method.

In subsequent work, Liu and Lee (2017) considered adding additional regularisation to Eqn. 2 whilst in Belomestny et al. (2017) the authors proposed to replace the squared error objective in Eqn. 2 with an empirical variance estimator. This was shown, empirically, to improve estimator performance but at the cost of no longer having a closed-form expression for the estimator. In a different direction, Zhu et al. (2018) proposed to take \( \mathcal{H} \) to be a finite-dimensional parametric neural network and explored its potential through simulation experiment.

1.3 Our Contribution

The aim of the present paper is to present a comprehensive analysis of a particular, widely-applicable Stein kernel method. The method that we consider is of the form \( I_X \) in Eqn. 2 with regularisation terms of the form in Eqn. 3 for a particular choice of Stein pair \((\mathcal{H}, \tau)\).

The principle contributions are as follows:

- **Generalisation to a Riemannian manifold:** A particular Stein pair \((\mathcal{H}, \tau)\) is proposed for use with a general Riemannian manifold. Integrals on manifolds arise in many important applications of Bayesian statistics, most notably directional statistics (Mar-dia and Jupp, 2000) and modelling of functional data on the sphere \( S^2 \) (Porcu et al., 2016). In this context, MCMC methods have been developed to sample from distributions defined on a manifold (e.g. Diaconis et al., 2013; Byrne and Girolami, 2013; Lan et al., 2014; Holbrook et al., 2016). In this paper we complement this existing work by generalising the Stein kernel method to integrals defined on a Riemannian manifold.

- **Asymptotic theory:** The convergence of \( I_X \) to \( I \) is established in the standard Sobolev space context. In particular, this represents a considerable strengthening of the earlier results in Oates et al. (2018), which relied on a rather opaque assumption on the integrand. The optimal convergence rate is established, under appropriate regularity assumptions on the distribution \( P \) and the point set \( X \). A more explicit statement of the rate is presented in Thm. 1, our main result.

- **Error assessment:** A computable upper bound on (relative) integration error – a kernel Stein discrepancy (Chwialkowski et al., 2016; Liu et al., 2016; Gorham and Mackey, 2017) – is shown to be obtained as a by-product of approximating the integral. This extends the aforementioned earlier work to the manifold context.

The remainder of the paper proceeds as follows: In Sec. 2 we provide a brief mathematical background and state our main result. In Sec. 3 we discuss implementation of the Stein kernel method and explain how its error can be assessed based on kernel Stein discrepancy. The method is empirically assessed in Sec. 4 where our theoretical results are verified on \( S^2 \). The proof of our main theoretical result is contained in Sec. 5 Further discussion of the approach is provided in Sec. 6.
2 Main Result

This section establishes notation (Sec. 2.1), then presents our main result (Sec. 2.2) and its corollaries (Sec. 2.3).

2.1 Mathematical Background

The purpose of this section is to introduce the mathematical tools that are needed for our development.

2.1.1 Riemannian Manifold

A $d$-dimensional manifold $M$, $d \in \mathbb{N}$, is a Hausdorff topological space for which every point $x \in M$ has an open neighbourhood $U_x$ homeomorphic to an open subset of $\mathbb{R}^d$. If $\phi : U \rightarrow \mathbb{R}^d$ is a homeomorphism (onto its image) with $x \in U \subset M$, we say $(U, \phi)$ is a coordinate patch around $x$. This defines coordinates functions $q_j := \pi_j \circ \phi$ over $U$, where $\pi_j : \mathbb{R}^d \rightarrow \mathbb{R}$ are the canonical projections and $\circ$ denotes composition of functions. Let $C^l(\mathbb{F})$ denote the set of all $l$-times continuously differentiable functions of the form $\mathbb{F} \rightarrow \mathbb{R}$. A $C^l$ atlas is a collection of charts $(U_i, \phi_i)$ that cover $M$ such that the transition functions $\phi_j \circ \phi_i^{-1}$ are $C^l(\mathbb{R}^d)$ whenever they are defined. The tangent space $T_xM$ at $x$ is the vector space of linear functionals over $C^\infty(M)$ satisfying Leibniz rule. If $q_j$ are coordinates on a patch $(U, \phi)$ containing $x$, the coordinate vectors $\partial q_j \big|_x : f \mapsto \partial f/\partial q_j \big|_{\phi(x)}$ define a basis of $T_xM$. We say $(M, g)$ is a Riemannian manifold if $M$ has a metric tensor $g$, i.e., a smooth map $x \mapsto g_x$ such that $g_x$ is an inner product on $T_xM$. It will be convenient to represent the metric tensor $g_x$ as a matrix $G(x)$ with coordinates $G_{ij}(x) := g_x(\partial_i \big|_x, \partial_j \big|_x)$.

It will be assumed that $M$ is a smooth (i.e. in particular we assume a $C^\infty$ atlas), compact and connected manifold, that is either closed or is a manifold with boundary $\partial M$ (see p25 of [Lee, 2013]. In the latter case, the outward-pointing unit normal $n$ to the boundary $\partial M$ of the manifold can be defined via the fact that, if $(M, g|_{\partial M})$ is a Riemannian submanifold of $(M, g)$, then for each $x \in \partial M$, the metric $g_x$ of $M$ splits the tangent space $T_xM$ into $T_x\partial M$ and its orthogonal complement $N_x$; i.e. $T_xM = T_x\partial M \oplus N_x$. Elements of $N_x$ are normal vectors to $M$. See e.g. [Bachman, 2006].

The geodesic distance $d_M(x, y)$ on a Riemannian manifold is defined as the infimum of the length $\int_0^1 \sqrt{g(\dot{\gamma}(t), \dot{\gamma}(t))}dt$ over all $C^1$-curves $\gamma : [0, 1] \rightarrow M$ with $\gamma(0) = x$ and $\gamma(1) = y$, where $\dot{\gamma}$ is the tangent vector to $\gamma$.

Example 1. The sphere $S^2$ is a 2-dimensional Riemannian manifold. The coordinate patch $\phi$ with $\phi^{-1}(q) = (\cos q_1 \sin q_2, \sin q_1 \sin q_2, \cos q_2)$, with local coordinates $q_1 \in (0, 2\pi)$, $q_2 \in (0, \pi)$, holds for almost all $x \in S^2$ (it does not cover the half great circle that passes through both poles and the point $(1, 0, 0)$). The tangent space is spanned by $\partial_{q_1} = (-\sin q_1 \sin q_2, \cos q_1 \sin q_2, 0)$ and $\partial_{q_2} = (\cos q_1 \cos q_2, \sin q_1 \cos q_2, -\sin q_2)$. Let $s = s_1 \partial_{q_1} + s_2 \partial_{q_2} \in T_xM$ be associated with the coefficient vector $s^\top = [s_1, s_2]$ and similarly for $t^\top = [t_1, t_2]$. Taking the Euclidean inner product of these vectors shows that $g_x(s, t) := \langle s, t \rangle_G = s^\top G t$ where $G_{1,1} = \sin^2 q_2$, $G_{2,2} = 1$, $G_{1,2} = G_{2,1} = 0$. 

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2.1.2 Geometric Measure Theory

Any oriented Riemannian manifold has a natural measure $V$ over its Borel algebra, called the Riemannian volume measure, with infinitesimal volume element denoted $dV$. In a coordinate patch $U_i \subset \mathbb{R}^d$, this measure can be expressed in terms of the Lebesgue measure: $dV = \sqrt{\text{det}(G(x))} \lambda^d(dx)$. In particular when $M$ is the Euclidean space, this is just the Lebesgue measure, and when $M$ is an embedded manifold in $\mathbb{R}^m$, $V$ is the Hausdorff measure (Federer, 1969). A technical point is that we restrict attention to Riemannian manifolds that are oriented. This is equivalent to assuming that the volume form $dV$ is coordinate-independent.

To define a natural volume form $i_n dV$ on $\partial M$, note that $\partial M$ is a submanifold of $M$ and the restriction $g|_{\partial M}$ of the metric $g$ induces a Riemannian manifold $(\partial M, g|_{\partial M})$. Then $i_n dV$ can be seen as the natural volume form on the induced manifold.

**Example 2.** For the sphere $S^2$, $dV = \sin q_2 dq_1 dq_2$, where $\sin q_2$ is the area of the parallelogram spanned by $\partial q_1, \partial q_2$.

2.1.3 Calculus on a Riemannian Manifold

To present a natural, coordinate-independent construction of differential operators on manifolds would require either exterior calculus or the concept of a covariant derivative. To limit scope, we present two important differential operators in local coordinates and merely comment that the associated operators are in fact coordinate-independent; full details can be found in Bachman (2006). To this end, denote the gradient of a function $f : M \to \mathbb{R}$, assumed to exist, as

$$\nabla f = \sum_{i,j=1}^{d} [G^{-1}]_{ij} \frac{\partial f}{\partial q_j} \partial q_i.$$ 

Likewise, define the divergence of a vector field $s = s_1 \partial_{q_1} + \cdots + s_d \partial_{q_d}$ with $s_i = s_i(x)$, assumed to exist, as

$$\nabla \cdot s = \sum_{i=1}^{d} \frac{\partial s_i}{\partial q_i} + s_i \frac{\partial}{\partial q_i} \log \sqrt{\text{det}(G)}.$$ 

These two differential operators are sufficient for our work; for instance, they can be combined to obtain the Laplace-Beltrami operator $\Delta f := \nabla \cdot \nabla f$.

2.1.4 Reproducing Kernel Hilbert Spaces

A reproducing kernel Hilbert space (RKHS) $\mathcal{H}$ of functionals on $M$ is a Hilbert space which is a vector subspace of $\mathcal{F}(M, \mathbb{R})$ for which the evaluation functionals $E_x : \mathcal{H} \to \mathbb{R}$, $E_x(f) := f(x)$, are continuous for each $x \in M$. The dual space of bounded linear operators is denoted $\mathcal{H}^*$ and the norm of $\mathcal{H}^*$ is denoted

$$\|E\|_{\mathcal{H}}^* = \sup \{Ef : \|f\|_\mathcal{H} \leq 1\}.$$
The Riesz-representation theorem implies that $\mathcal{H}$ is isomorphic to $\mathcal{H}^*$ and we can thus associate a vector $k_x \in \mathcal{H}$ to $E_x$ which satisfies $f(x) = \langle f, k_x \rangle_{\mathcal{H}}$. The symmetric function $k(x, y) := k_x(y)$ is called the reproducing kernel for $\mathcal{H}$ and we denote this as $\mathcal{H}(k)$ in the sequel. It can also be checked $k$ is a semi-positive definite function on $\mathcal{X}$. Moore’s theorem states the converse is also true; any semi-positive function on $M$ defines an RKHS $\mathcal{H}(k)$ of functionals on $M$ with $k$ as its reproducing kernel.

2.1.5 Sobolev Norm on a Riemannian Manifold

Let $\Omega \subset \mathbb{R}^d$ and recall that the standard Sobolev space $W^{s}_2(\Omega)$ is defined as the set of equivalence classes $f \in L^2(\Omega)$ such that the weak derivatives $D^\alpha f := \partial_{x_1}^{\alpha_1} \cdots \partial_{x_d}^{\alpha_d} f \in L^2(\Omega)$ for all $|\alpha| := \alpha_1 + \cdots + \alpha_d \leq s$. The set $W^{s}_2(\Omega)$, for $s > \frac{d}{2}$, becomes a RKHS when equipped with the norm

$$\|f\|_{W^{s}_2(\Omega)} := \left( \sum_{|\alpha| \leq s} \|D^\alpha f\|_{L^2(\Omega)}^2 \right)^{\frac{1}{2}}.$$

In order to define a Sobolev space on a Riemannian manifold $(M, g)$, let $(U_i, \phi_i)$ be an open cover of $M$ and $(\rho_i)$ a partition of unity subordinate to $(U_i)$. Then let $W^{s}_2(M)$ be the set of functions in $F(M, \mathbb{R})$ for which the following norm is finite:

$$\|f\|_{W^{s}_2(M)}^2 = \sum_{i} \| (\rho_i f) \circ \phi_i^{-1} \|^2_{W^{s}_2(\mathbb{R}^d)}.$$

It can be shown that $W^{s}_2(M)$ is a RKHS. Note that the norm depends on the choice of atlas and partition of unity. Different choices lead to different norms, however these are all equivalent (Fuselier and Wright, 2012). To avoid confusion, we fix a specific atlas and partition of unity in the sequel.

2.2 Statement of Result

In this section our main result is stated. This concerns the convergence of the estimator $I_X$ in Eqn. 2 with regularisation terms in Eqn. 3 for a particular choice of Stein pair $(\mathcal{H}, \tau)$, defined in the sequel. Recall that all details on how the estimator can be implemented are reserved for Sec. 3.2. First in this section, we present and discuss the technical conditions that will be assumed.

Two normed spaces $(X, \| \cdot \|_X)$, $(Y, \| \cdot \|_Y)$ are said to be norm-equivalent if the sets $X$ and $Y$ are identical and if there exists $0 < C < \infty$ such that $C^{-1}\|x\|_X \leq \|x\|_Y \leq C\|x\|_X$ for all $x \in X$.

**Assumption 1.** Let $\mathcal{H}(k)$ be norm-equivalent to $W^{s+2}_2(M)$, for some $s > \frac{d}{2}$.

Recall that a density $p$ for the distribution $P$ with respect to the Riemannian volume measure $V$ is required to exist and that the derivatives of $\log p$ can be computed without access to the normalisation constant.
Assumption 2. The function \( \log p : M \to \mathbb{R} \) is \( C^{s+1}(M) \), for the same exponent \( s \) introduced in Assumption 1.

The first-order differential operator used in Oates et al. (2017, 2018) cannot be generalised to the manifold context (see the discussion of this point in Liu and Zhu (2017)) and we therefore consider a different, second-order Stein operator. In fact, the differential operator that we consider is the Riemannian manifold generalisation of the original operator considered in Assaraf and Caffarel (1999):

Assumption 3. The operator \( \tau : \mathcal{H}(k) \to \mathcal{F}(M, \mathbb{R}) \) is the second differential order operator

\[
\tau h = \nabla \cdot (p \nabla h)/p.
\]

In Appendix we suggest other choices of differential operator that can be used in the manifold context, thought these were not the subject of our theoretical development.

In what follows, the operator in Assumption 3 will be called the Riemannian–Stein operator due to its suitability for Stein’s method on a Riemannian manifold. Note that by the product rule

\[
\tau h = \frac{p \nabla \cdot \nabla h + g(\nabla p, \nabla h)}{p} = \Delta h + g(\nabla \log p, \nabla h).
\]

Assumption 4. If \((M, g)\) is a Riemannian manifold with boundary \( \partial M \), then

\[
\int_{\partial M} g(p \nabla h, n) \ i_n \ dV = 0 \quad \forall h \in \mathcal{H}(k).
\]

For a manifold with boundary, the boundary condition in Assumption 4 is either automatically satisfied if \( p \) vanishes on \( \partial M \) or must be enforced through a suitable restriction on \( \mathcal{H}(k) \). On the other hand, if \( M \) is a closed manifold, then no assumption is required. This fact allows the Riemannian–Stein kernel method to be flexibly and widely used compared to the Euclidean case studied in Oates et al. (2017, 2018), where non-trivial boundary conditions could not be avoided.

The purpose of Assumptions 2–4, which are presumed to hold throughout the sequel, is made clear in the following result:

Proposition 1. \((\mathcal{H}(k), \tau)\) is a Stein pair for \( P \).

Proof. For all \( h \in \mathcal{H}(k) \), using the above assumptions and the divergence theorem on a Riemannian manifold (see Szekeres 2004), we find

\[
\int_M \tau h \ dP = \int_M \nabla \cdot (p \nabla h) \ dV
\]

\[= \begin{cases} 
\int_{\partial M} g(p \nabla h, n) \ i_n \ dV & \text{if } M \text{ is a manifold with boundary} \\
0 & \text{if } M \text{ is a closed manifold.}
\end{cases} \]

From Assumption 4 the boundary integral is zero, as required.

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Next, the formulation of our main result requires that the quality of a point set \( X = \{ x_i \}_{i=1}^n \) is quantified. For the purposes of this work, we require that \( X \) in some sense covers the manifold \( M \) (see e.g. Scheuerer et al., 2013):

**Definition 2.** The fill distance of the point set \( X = \{ x_i \}_{i=1}^n \subset M \) is defined as

\[
h_X = \sup_{x \in M} \min_{i = 1, \ldots, n} d_M(x, x_i),
\]

where \( d_M \) is the geodesic distance on the Riemannian manifold.

Note that the supremum in the definition of \( h_X \) is finite due to compactness of the manifold.

The main result of this work can now be stated. As both \( I \) and \( I_X \) are linear functionals on \( \mathcal{H}(k) \) (c.f. Sec. 3.2 for an explicit linear representation of \( I_X \)), it is natural to assess convergence of \( I_X \) to \( I \) in terms of the norm dual to the space of the integrand:

**Theorem 1 (Main result).** Under our stated assumptions, which include \( s > \frac{d}{2} \), the estimator \( I_X \) is a consistent approximation to the true integral operator \( I \), in the sense that

\[
\| I_X - I \|_{W^s_2(M)} \leq C_s h_X^s
\]

for some \( C_s \), a generic finite constant dependant on \( s \) but independent of the point set \( X \).

Thus when the points in \( X \) cover the manifold \( M \), in the sense that the fill distance \( h_X \) is small, the estimator \( I_X \) is an accurate approximation to the true integration operator \( I \). From the definition of the dual norm, an equivalent statement of Thm. 1 is that

\[
| I_X(f) - I(f) | \leq C_s h_X^s \| f \|_{W^s_2(M)}
\]

whenever the integrand \( f \in W^s_2(M) \). This should be contrasted with earlier work in Oates et al. (2018), where convergence was assessed in the Euclidean context and quantified in terms of a norm on \( f \) that was rather non-standard. In particular, it was not straightforward to characterise the integrands \( f \) for which the result in Oates et al. (2018) applied. In comparison, if \( f \) has weak derivatives of up to order \( s \) on \( M \), then \( \| f \|_{W^s_2(M)} < \infty \) and our result can be used.

**Remark 1 (Optimal rate of convergence).** For \( P \) equivalent (in the sense of measures) to the natural volume measure \( V \), an information-theoretic lower bound on any estimator \( I_X \), based on a size \( n \) point set \( X \), is \( C n^{-\frac{s}{2}} \leq \| I_X - I \|_{W^s_2(M)}^* \), for some \( C > 0 \) (Brandolini et al., 2014). This shows that our estimator \( I_X \) is rate-optimal whenever the point set \( X \) is selected such that the fill-distance is asymptotically minimised, i.e. \( h_X = O(n^{-\frac{1}{2}}) \). This is in principle a weak requirement, as under suitable conditions even a random point set with \( x_i \overset{i.i.d.}{\sim} \bar{V} \), where \( \bar{V} \) denotes the normalised Riemannian measure on the compact manifold, achieves this rate up to a logarithmic factor; see Reznikov and Saff (2015, Thm. 3.2, Cor. 3.3) and Ehler et al. (2017).

In Sec. 2.3 we specialise Thm. 1 to the case where the point set \( X = \{ x_i \}_{i=1}^n \) arises as \( x_i \overset{i.i.d.}{\sim} P \); see Cor. 1. However, for applications in Bayesian statistics, points in the set \( X \) will typically not be independent, arising instead as the output from an MCMC method. The second result, Cor. 2 in the next section, aims to understand the asymptotic convergence of \( I_X \) to \( I \) in the MCMC context.
2.3 Extension to MCMC

The most popular approaches to Bayesian computation are based on sampling, in particular MCMC. In this section we therefore present the consequences of Thm. 1 in the case where the point set \( X \) arises from a Monte Carlo sampling method.

**Corollary 1.** Suppose that \((x_i)_{i \in \mathbb{N}}\) is a sequence of independent samples from the distribution \( P \). Let \( X = \{x_i\}_{i=1}^n \) and denote expectation with respect to the sampling distribution of \( X \) as \( \mathbb{E}_X \). Then

\[
\mathbb{E}_X \| I_X - I\|_{W^s_2(M)} \leq C'_s n^{-\frac{s}{d}} \log(n)^{\frac{s}{d}}
\]

for some \( C'_s \), a generic finite \( s \)-dependant constant.

Note that the constant \( C'_s \) is dependent on \( P \) through the infimum of \( p(x) \) on \( x \in M \).

Our final result allows for points in the set \( X \) to be correlated. Recall that notions of geometric and uniform ergodicity coincide on a compact state space when the invariant measure \( P \) is equivalent (in the sense of measures) to \( \bar{V} \); we therefore describe a Markov chain \((x_i)_{i \in \mathbb{N}}\) with \( n \)th step transition kernel \( P^n \) and invariant distribution \( P \) simply as *ergodic* if there exists a finite constant \( C \) and a number \( 0 \leq \rho < 1 \) such that

\[
|P^n(x_1, A) - P(A)| \leq C \rho^n
\]

for all \( x_1 \in M \) and all measurable \( A \subseteq M \). The reader is referred to Meyn and Tweedie (2012) for background.

**Corollary 2.** The conclusion of Cor. 1 continues to hold if we instead suppose that \((x_i)_{i \in \mathbb{N}}\) is an ergodic Markov chain with invariant distribution \( P \), initialised at an arbitrary point \( x_0 \in M \).

3 Implementation and Error Assessment

The purpose of this section is to expand on how the proposed method can be implemented. From Assumption 1, the set \( \mathcal{H}(k) \) is a RKHS and it is therefore not a surprise that the computation of \( I_X \) reduces to manipulation of a reproducing kernel. Sec. 3.1 is devoted to a discussion of the choice of kernel \( k \), whilst Sec. 3.2 explains how exact computation is performed and Sec. 3.3 describes an approach to error assessment.

3.1 Extrinsic vs Intrinsic Kernels

The performance of the Stein kernel method depends, of course, on the selection of a reproducing kernel \( k \) to define the space \( \mathcal{H}(k) \). For standard manifolds, such as the sphere \( M = \mathbb{S}^2 \), several function spaces and their reproducing kernels have been studied (e.g. Porcu et al., 2016). For more general manifolds, an extrinsic kernel can be induced from restriction...
under embedding into an ambient space (Lin et al., 2017), or the stochastic partial differential approach (Fasshauer and Ye, 2011; Lindgren et al., 2011; Niu et al. 2017) can be used to numerically approximate a suitable intrinsic kernel. The choice of kernel will be explored in detail for the case of the sphere $S^2$ in Sec. 4.2. Note that none of the theoretical development in this paper relies on an embedding of $M$ into an ambient space; all of our analysis is intrinsic to the manifold. Next we address the practical matter of how the estimator can be computed.

3.2 Computation of $I_X(f)$

The aim of this section is to spell out exactly how the estimator $I_X(f)$ is computed. The computations are analogous to those of traditional kriging, albeit based on a non-standard, non-radial kernel (Stein, 2012). It will be assumed that the point set $X \subset M$ has already been generated. No specific requirements are needed on $X$ in order for the estimator to be computed, however it will be assumed that its elements are distinct.

First, for $\sigma > 0$ a function $k_{P,\sigma} : M \times M \to \mathbb{R}$ is defined as

$$k_{P,\sigma}(\mathbf{x}, \mathbf{x}') = \sigma^2 + \tau'\tau k(\mathbf{x}, \mathbf{x}')$$

where the Riemannian–Stein operators $\tau$ and $\tau'$ act, respectively, on the first and second argument of the kernel. Note that this is well-defined, as Assumption 3 implies that $\tau$ is a second-order differential operator (so that $\tau\tau'$ is a fourth order differential operator) and Assumption 1 implies, from the Sobolev embedding theorem, that $k \in C^4(M \times M)$. Moreover, in Sec. 3.1 it is established that $k_P(\mathbf{x}, \mathbf{x}') := \tau\tau'k(\mathbf{x}, \mathbf{x}')$ is symmetric positive definite, and hence $k_{P,\sigma}$ is also symmetric and positive definite, each on $M \times M$.

The calculations in Oates et al. (2017) established that

$$I_X(f) = \sigma^2 1^\top K_P^{-1} f$$

where

$$K_{P,\sigma} = \begin{bmatrix}
    k_{P,\sigma}(x_1, x_1) & \ldots & k_{P,\sigma}(x_1, x_n) \\
    \vdots & \ddots & \vdots \\
    k_{P,\sigma}(x_n, x_1) & \ldots & k_{P,\sigma}(x_n, x_n)
\end{bmatrix}, \quad f = \begin{bmatrix}
    f(x_1) \\
    \vdots \\
    f(x_n)
\end{bmatrix}.$$

The requirement that elements of $X$ are distinct, together with the fact that $k_{P,\sigma}$ is positive definite, ensure that $K_{P,\sigma}^{-1}$ is well-defined. Note that the computation of $I_X(f)$ is associated with a $O(n^3)$ cost. As mentioned in Sec. 1 an increased cost (relative to MCMC) is typical for methods with accelerated convergence and can be justified when the convergence rate is sufficiently fast.

Remark 2. From Eqn. 4, the operator $I_X$ is seen to be linear, as earlier claimed. In particular, it is recognised as a weighted cubature rule $I_X(f) = \sum_{i=1}^n w_i f(x_i)$ with weights $w = [w_1, \ldots, w_n]^\top$ the solution to $K_{P,\sigma} w = \sigma^2 1$. 

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In practice, the parameter $\sigma$ can either be set in a data-driven manner or eliminated altogether. Indeed, we have the following result:

**Proposition 2.** Let $K_P$ denote the $n \times n$ matrix with entries $k_P(x_i, x_j)$. Then

$$\lim_{\sigma \to \infty} I_X(f) = \left( \frac{K_P^{-1}1}{1^\top K_P^{-1}1} \right)^\top f.$$  \hfill (5)

*Proof.* Note that $K_{P,\sigma} = \sigma^211^\top + K_P$. The proof is then an application of the Woodbury matrix inversion formula, which can be used to deduce that

$$I_X(f) = \sigma^21^\top(\sigma^211^\top + K_P)^{-1}f = \frac{1^\top K_P^{-1}f}{\sigma^{-2} + 1^\top K_P^{-1}1}$$

from which the result is immediately established. \hfill \Box

Due to its simplicity, the estimator in Eqn. 5 is the one that we recommend and the one that is experimentally tested in Section 4. In addition, this estimator has the desirable property that constant functions are exactly integrated. This follows since the limiting integration weights sum to one; indeed, a similar limit was studied in Karvonen et al. (2018) for standard kernel cubature, where further details are provided. Alternative kernel estimators, such as estimators that enforce non-negativity of the weights $w_i$, could also be considered (c.f. Liu and Lee, 2017; Ehler et al., 2017).

### 3.3 Error Assessment

In addition to returning an estimate for the integral, the Riemannian–Stein kernel method is accompanied by a parsimonious error assessment, which is now described. The expression $(1^\top K_P^{-1}1)^{-1/2}$, which is obtained as a by-product when the estimator is computed, can be interpreted as a kernel Stein discrepancy (KSD; Chwialkowski et al., 2016; Liu et al., 2016; Gorham and Mackey, 2017)

$$\text{KSD} \left( \sum_{i=1}^n w_i \delta(x_i), P \right) = \sqrt{\sum_{i,j=1}^n w_i w_j k_P(x_i, x_j)}$$ \hfill (6)

for the specific choice of weights

$$w = \frac{K_P^{-1}1}{1^\top K_P^{-1}1}$$ \hfill (7)

that arise in Prop. 2. Indeed, minimisation of Eqn. 6 over the weights $w$ subject to the non-degeneracy constraint $1^\top w = 1$ leads to Eqn. 7 so that these weights are in a sense optimal. From the Moore–Aronszajn theorem, the kernel $k_P$ induces a RKHS, denoted $\mathcal{H}(k_P)$. In
more traditional numerical integration terminology, the KSD is identical to the worst case error of the cubature rule in Eqn. 5 in the unit ball of $\mathcal{H}(k_P)$:

$$
(1^T K_P^{-1} 1)^{-1/2} = \sup \left\{ \left| I(f) - \lim_{\sigma \to \infty} I_X(f) \right| : \|f\|_{\mathcal{H}(k_P)} \leq 1 \right\}
$$

(8)

Of course, the space $\mathcal{H}(k_P)$ is somewhat artificial due to its dependence on $P$. However, under certain conditions on $P$ and $k$, the kernel Stein discrepancy can in turn control the standard notion of weak convergence of the weighted empirical measure $\sum_{i=1}^{n} w_i \delta(x_i)$ to the target $P$. Sufficient conditions for the Euclidean manifold and a first order differential operator were established in [Gorham and Mackey (2017); Chen et al. (2018)]; the extension of these results to a general Riemannian manifold should be natural, but is beyond the scope of the present paper, since we are focussing on an integral approximation method and not on a distributional approximation method.

## 4 Numerical Assessment

In this section we report experiments designed to assess the performance of the proposed Riemannian–Stein kernel method. For this purpose we considered arguably the most important compact manifold; the sphere $\mathbb{S}^2$.

### 4.1 Differential Operator

The coordinate patch $\phi$ from Ex. 1 in Sec. 2.1 can be used to compute the metric tensor

$$
G = \begin{pmatrix}
\sin^2 q_2 & 0 \\
0 & 1
\end{pmatrix}
$$

and a natural volume element $dV = \sin q_2 dq_1 dq_2$. It follows that, for a function $h: \mathbb{S}^2 \to \mathbb{R}$, we have the gradient differential operator

$$
\nabla h = \frac{1}{\sin^2 q_2} \frac{\partial h}{\partial q_1} \partial_{q_1} + \frac{\partial h}{\partial q_2} \partial_{q_2}.
$$

Similarly, for a vector field $s = s_1 \partial_{q_1} + s_2 \partial_{q_2}$, we have the divergence operator

$$
\nabla \cdot s = \frac{\partial s_1}{\partial q_1} + \frac{\partial s_2}{\partial q_2} + \frac{\cos q_2}{\sin q_2} s_2.
$$

Thus the Riemannian–Stein operator $\tau$ is:

$$
\tau h = \frac{\cos q_2}{\sin q_2} \frac{\partial h}{\partial q_2} + \frac{1}{\sin^2 q_2} \left\{ \frac{1}{p} \frac{\partial p}{\partial q_1} \frac{\partial h}{\partial q_1} + \frac{\partial^2 h}{\partial q_1^2} \right\} + \left\{ \frac{1}{p} \frac{\partial p}{\partial q_2} \frac{\partial h}{\partial q_2} + \frac{\partial^2 h}{\partial q_2^2} \right\}.
$$

(9)

Turning this into expressions in terms of $x$ requires that we notice

$$
\frac{\cos q_2}{\sin q_2} = \frac{x_3}{\sqrt{1 - x_3^2}}, \quad \frac{1}{\sin^2 q_2} = \frac{1}{1 - x_3^2}
$$

and use chain rule for partial differentiation.
4.2 Choice of Kernel

To proceed, we require a reproducing kernel. On non-Euclidean spaces the choice of the kernel is somewhat subtle and we therefore dedicate a substantial portion of the remainder to a discussion of kernel choice on $S^d$ in general. In particular, we consider three qualitatively different choices of kernel and explore, empirically, how the choice of the kernel influences the performance of the Riemannian–Stein kernel method on $S^2$.

It is important to distinguish between the geodesic distance $d_M(x, y) = \arccos(x \cdot y)$ on $S^d$ and the chordal distance $d_C(x, y) = \|x - y\|_2$, which is induced by the restriction of Euclidean distance in $\mathbb{R}^{d+1}$ to $S^d$. Of course, the two are related via $d_C = 2 \sin(\frac{d}{2} d_M)$, but from a mathematical perspective $d_M$ is more natural. Indeed, there has been substantial criticism on the chordal distance and the reader is referred to Banerjee (2005); Porcu et al. (2018). Although our focus is on $S^2$, for generality the remainder of this section discusses kernels on $S^d$.

A kernel on $S^d$ is characterised by a scalar $\sigma > 0$ and a sequence $(b_{n,d})_{n=0}^{\infty}$ of $d$-Schoenberg coefficients, such that $0 \leq b_{n,d}$ and $\sum_{n=0}^{\infty} b_{n,d} = 1$, in the sense that

$$k(x, y) = \sigma^2 \sum_{n=0}^{\infty} b_{n,d} \frac{C_n^{(d-1)/2}(x \cdot y)}{C_n^{(d-1)/2}(1)}, \quad x, y \in S^d$$

where $C_n^\lambda$ are the Geigenbauer polynomials of degree $n$ and order $\lambda > 0$ (Bingham, 1973; Marinucci and Peccati, 2011; Dai and Xu, 2013; Gneiting, 2013; Daley and Porcu, 2013). It is known that $b_{n,d} \asymp n^{-2\alpha}$ if and only if $H(k)$ is norm-equivalent to the Sobolev space $W_2^{\alpha}(S^d)$ (Daley and Porcu, 2013). Thus in principle one has much scope to design an appropriate kernel whilst also ensuring that Assumption 1 is satisfied. Therefore we need to elicit some additional desiderata (D) to constrain ourselves to those kernels which are most useful:

Desiderata 1. The kernel should have an explicit form that can be easily differentiated.

Desiderata 2. The kernel should be intrinsic, based directly on $d_M$.

Desiderata 3. The kernel should have easily customisable smoothness.

For the Riemannian–Stein kernel method to be practical, D1 must hold. It could be expected than improved empirical performance is associated with D2. For the Stein kernel method to be flexibly used, D3 must hold.

Note that one cannot, for example, just restrict the Matérn kernel on $\mathbb{R}^3$ to $S^2$; in order that the restriction is positive definite we require a strong condition $\nu \in (0, \frac{1}{2}]$ on the smoothness parameter (Gneiting, 2013). This fact makes this approach not suitable for our work, where higher order derivatives of the kernel are needed. In what follows, three different kernels that each reproduce Sobolev spaces are presented:

Kernel 1 (Brauchart and Dick (2013)). For $\alpha + \frac{1}{2} - \frac{d}{2} \in \mathbb{N}$ and $\alpha > \frac{d}{2}$, the kernel

$$k_1(x, y) = C^{(1)}_{d/2} \binom{1/2}{d/2} \binom{d/2 + 1/2 - \alpha}{d/2 + 1 - \alpha} \frac{1}{\Gamma(1/2)} \frac{\Gamma(d/2 + 1/2 - \alpha)}{\Gamma(d/2 + 1/2)} - \frac{1}{\Gamma(d/2 + 1/2 - \alpha)} \frac{\Gamma(d/2 + 1/2)}{\Gamma(d/2 + 1/2 - \alpha)} \left(1 - \frac{d}{2} x \cdot y \right) + C^{(2)} \|x - y\|_2^{2\alpha - 2},$$

(11)
therefore is extrinsic, so that D2 is not satisfied. In this paper, \( pF_q \) is the generalised hypergeometric function. The constant terms in the kernel in Eqn. (11) are as follows:

\[
C^{(1)} = \frac{2^{2\alpha - 2} \left( \frac{d}{2} \right)^{2\alpha - 2}}{2\alpha - d} \\
C^{(2)} = (-1)^{\alpha - \frac{d}{2} + \frac{1}{2}} 2^{2\alpha - 2 - \alpha} \Gamma\left( \alpha - \frac{d}{2} + \frac{1}{2} \right) \Gamma\left( \alpha - \frac{d}{2} + \frac{1}{2} \right) \sqrt{\pi} \Gamma\left( \frac{d}{2} \right) \Gamma\left( \frac{d}{2} + \frac{1}{2} \right) \gamma\left( \alpha - \frac{d}{2} + \frac{1}{2} \right) \gamma\left( \alpha - \frac{d}{2} + \frac{1}{2} \right)
\]

where \((z)_n := \Gamma(z + n)/\Gamma(z)\) is the Pochhammer symbol. From properties of hypergeometric functions, this kernel has an explicit closed form when \( \alpha + \frac{d}{2} - \frac{d}{2} \in \mathbb{N} \), so that D1 is satisfied. Moreover, D3 holds for this kernel. However this kernel is not intrinsic, due to the explicit presence of both the manifold and chordal distances, so that D2 is violated.

**Kernel 2** (Alegría et al. (2018)). Consider the kernel

\[
k_2(x, y) = \frac{\Gamma\left( \frac{x}{\lambda} + \frac{1}{2} + \alpha \right) \Gamma\left( \frac{y}{\lambda} + \alpha \right)}{\Gamma\left( \frac{x}{\lambda} + \frac{1}{2} + \alpha \right) \Gamma\left( \frac{y}{\lambda} + \alpha \right)} 2F_1\left( \frac{1}{\lambda}, \frac{1}{\lambda} + \frac{1}{2}; \frac{2}{\lambda} + \frac{1}{2} + \alpha; x \cdot y \right)
\]

(12)
defined for \( x, y \in \mathbb{S}^2 \). From properties of hypergeometric functions, this kernel has an explicit closed form when \( \alpha + \frac{1}{2} - \frac{d}{2} \in \mathbb{N} \), so that D1 is satisfied. The parameter \( \lambda > 0 \) represents the correlation length. Moreover, the kernel is based on the geodesic distance so that, for this kernel, D2 is satisfied.

However, the asymptotics of the Schoenberg coefficients appear difficult to establish for this kernel, so at present the associated RKHS has not been characterised. Thus, although the Riemannian–Stein kernel method can be implemented with this kernel, the main result in this paper cannot directly be applied. It is nevertheless possible to show that \( k_2 \in C^{2\nu}(\mathbb{S}^2 \times \mathbb{S}^2) \) whenever \( \nu < \alpha \), so that D3 is partially satisfied. This allows us to obtain a weaker result for this kernel through Sobolev embedding, which we present as Lem. 6 in Appendix A.

**Kernel 3** (Wendland (1995)). Consider the compact support positive definite functions due to Wendland (1995)

\[
\phi_{i,j}(r) = \begin{cases} 
p_{i,j}(r) & \text{if } r \leq 1 \\
0 & \text{if } r > 1
\end{cases},
\]

defined for \( r \geq 0 \) where \( p_{i,j} : [0, \infty) \to \mathbb{R} \) is a particular polynomial selected such that \( \phi_{i,j} \) is positive definite and \( \phi_{i,j} \in C^2 \). The radial basis function

\[
k_3(x, y) = \phi_{i,j}\left( \frac{\|x - y\|_2}{\lambda} \right),
\]

for \( \lambda > 0 \) reproduces \( W_2^{j+\frac{d+1}{2}}(\mathbb{R}^d) \) on \( x, y \in \mathbb{R}^d \) (see e.g. Thm. 2.1 in Wendland, 1998). In the particular case where \( i = d + 1 \), the restriction of \( k_3 \) to \( x, y \in \mathbb{S}^d \) reproduces \( W_2^\alpha(\mathbb{S}^d) \) with \( \alpha = j + \frac{1}{2} \); see Thm. 4.1 of Narcowich et al. (2007). See also Gneiting (2002); Narcowich and Ward (2002); Zastavnyi (2006); Bevilacqua et al. (2017). Desiderata D3 is therefore satisfied and in particular our convergence analysis will hold. Moreover, this kernel has a closed form so that D1 is satisfied. Finally, this kernel is based on chordal distance and therefore is extrinsic, so that D2 is not satisfied.
4.3 Assessment

To numerically assess the convergence of the Riemannian–Stein kernel method, consider the von Mises-Fisher distribution $P$ whose density with respect to $V$ is

$$p(x) = \frac{\|c\|_2^2}{4\pi \sinh(\|c\|_2^2)} \exp(c^\top x).$$

For illustration, we suppose that the normalisation constant is unknown and we are told only that $p(x) \propto \exp(c^\top x)$. This is sufficient to construct the differential operator operator $\tau$ as previously described. Our aim in what follows is to validate our theoretical analysis; for this reason in all experiments we fixed $\lambda = 1$ for $k_2$ and $\lambda = 2$ for $k_3$ as a convenient default. Further theoretical work will be needed to understand the properties of the Riemannian–Stein kernel method when kernel parameters are adaptively estimated (Stein, 2012).

In what follows we first considered point sets $X = \{x_i\}_{i=1}^n$ whose elements were quasi-uniformly distributed on $S^2$, being obtained by minimising a generalised electrostatic potential energy (Reisz’s-energy; Semechko, 2015). Note that these points, being uniform, do not arise as an approximation to $P$; rather, they are intended to asymptotically minimise $h_X$ as motivated by Thm. 1.

First, explicit function approximations are presented based on $k_1$, $k_2$, $k_3$ respectively in Figs. 1a, 1b, 1c. These function approximations are $\hat{f} = \xi + \tau h$ where $(\xi, h)$ solve Eqn. 2. Here the integrand $f(x)$ was based on a Rosenbrock function and represents a modest challenge to an interpolation-based integration method. It was observed that all kernels provided an accurate approximation when a large number of points were used ($n = 200$), with the most agreement observed for smoother kernels ($\alpha = 5.5$).

Next, for various values of $n$, we computed the worst case integration error in Eqn. 8 (i.e. the KSD). Results in Figs. 2a, 2b, 2c show that, for kernels $k_1$ and $k_3$, convergence of the KSD occurred at the rate that was theoretically predicted. Our theoretical analysis of kernel $k_2$ provided only a lower bound on the convergence rate, but this bound was seen to be attained. Note that numerical instabilities were observed when computing with kernel $k_2$ for $n \geq 400$ in that the matrices $K_P$ became numerically singular. This in turn led to the KSD being inaccurately computed, as is clear from Fig. 2b. In this work we did not consider extensions or modifications to mitigate numerical issues, since our focus was principally on verification of our theoretical result.

Finally, we re-evaluated the worst case integration error (i.e. the KSD), based instead on a point set $X$ generated as the realisation of an MCMC sample path. Here we employed a Metropolis-Hastings Markov chain with the normalised Riemannian measure $\bar{V}$ as the proposal. Results are presented in Figs. 3a, 3b, 3c where again the theoretically obtained convergence rate was validated.
Figure 1: Function approximation with the Riemannian–Stein kernel method. In each of (a-c), $f$ represents the exact integrand. Each panel represents a kernel (a) $k_1$, (b) $k_2$, (c) $k_3$, varying both the smoothness $\alpha$ of these kernel and the number $n$ of evaluations of the integrand. The point set was quasi-uniform over $S^2$. 
Figure 2: The worst case integration error (i.e., kernel Stein discrepancy; KSD) of the Riemann–Stein kernel method was plotted for three different kernels, (a) $k_1$, (b) $k_2$, (c) $k_3$, varying both the smoothness $\alpha$ of these kernels and the number $n$ of evaluations of the integrand. The point set was quasi-uniform over $S^2$. Dashed lines represent the slope of the convergence rates that we have theoretically established. (Note that in the case of kernel $k_2$ our theoretical analysis provides only a lower bound on the rate and not the rate itself. Moreover, numerical instability was observed for this kernel in computation of KSD for $n \geq 400$.)
Figure 3: The worst case integration error (i.e. kernel Stein discrepancy; KSD) of the Riemann–Stein kernel method was plotted for three different kernels, (a) $k_1$, (b) $k_2$, (c) $k_3$, varying both the smoothness $\alpha$ of these kernels and the number $n$ of evaluations of the integrand. The point set was obtained as the realisation of a Markov chain whose invariant distribution was $P$. Here the arithmetic mean estimator is presented along with standard error bars, averaged over multiple realisations of the Markov chain. Dashed lines represent the slope of the convergence rates that we have theoretically established. (Note that in the case of kernel $k_2$ our theoretical analysis provides only a lower bound on the rate and not the rate itself. Moreover, numerical instability was observed for this kernel in computation of KSD for $n \geq 400$.)
5 Proofs

This section contains proofs of the theoretical results presented in Sec. 2. To this end, there are two main theoretical challenges to be addressed: First, it is necessary to establish that \( k_{P,\sigma} \) is a valid kernel so that, from the Moore-Aronszajn theorem, \( k_{P,\sigma} \) defines a RKHS. This is addressed in Sec. 5.1. The RKHS will be called the Stein RKHS. This is norm-equivalent to the Sobolev space \( W^s_2(M) \). This is performed in two parts, with a Sobolev embedding of the Stein RKHS performed in Sec. 5.2 and a Stein embedding of the Sobolev RKHS performed in Sec. 5.3. For both parts we leverage results from the analysis of partial differential equations on a Riemannian manifold and our main reference is Grosse and Nistor (2017). From this point onward, our interpolation error bounds are standard in the Sobolev space context and the reminder of the proof for Thm. II is contained in Sec. 5.4. Corollaries for MCMC are established in Sec. 5.5.

5.1 Characterisation of the Stein RKHS

The first result establishes how the kernel \( k_{P} \) can be computed:

**Lemma 1.** Let \( \langle \cdot, \cdot \rangle_{\mathcal{H}(k)} \) denote the inner product in \( \mathcal{H}(k) \). Then \( k_{P}(x, x') := \tau' \tau k(x, x') = \langle \tau k(x, \cdot), \tau' k(x', \cdot) \rangle_{\mathcal{H}(k)} \). In particular, \( k_P \) is symmetric and semi-positive definite; i.e. \( k_P \) is a kernel.

*Proof.* Since \( k \) reproduces \( W^s_2(M) \) for \( \alpha = s + 2 > s' + 2 \), it follows from the Sobolev embedding theorem that \( k(x, \cdot) \in C^2(M) \). Thus second order differential operators, such as \( \tau \), can be applied to this function (Lem. 4.34 of Steinwart and Christmann 2008).

Let \( g^{-1} \) be the metric tensor on differential forms associated to \( g \) by the musical isomorphism (Gallot et al. 1990). Then \( g(\nabla f, \nabla h) = g^{-1}(df, dh) \) where \( dh \) is the linear functional on \( T_xM \) such that \( dh(v) = v(h) \). Recall that \( \tau' \) is used to denote the action of a differential operator \( \tau \) on \( x' \). It follows that,

\[
g(\nabla' \log p, \nabla' g(\nabla \log p, \nabla k)) = g^{-1}\big(d' \log p, d' g^{-1}(d \log p, dk)\big)
= \sum_{i,j,r,l} g^{ij}(y)g^{rl}(x)\partial_{y^i} \log p(y)\partial_{x^r} \log p(x)\partial_{y^j} \partial_{x^l} k(x, y)
= \nabla \log p \nabla' \log p(k).
\]

Here \( \nabla \log p(k) \) is the function on \( M \) which maps \( x \) to \( \nabla_x \log p(k) \in \mathbb{R} \), where \( \nabla_x \log p \in T_xM \) is the gradient vector. Thus \( \nabla \log p \nabla' \log p(k) = \nabla \log p(\nabla' \log p(k)) \) is defined. Thus

\[
\tau' \tau k(x, x') = \nabla \log p \nabla' \log p(k) + g^{-1}(d \log p, d\Delta' k) + g^{-1}(d' \log p, d' \Delta k) + \Delta \Delta' k
= \langle \tau k(x, \cdot), \tau' k(x', \cdot) \rangle_{\mathcal{H}(k)}
\]

where local coordinates verify that the last equality is established.
Finally, observe that the map \( \phi : M \to \mathcal{H}(k) \), defined as \( \phi(x) := \tau k(x, \cdot) \), is a feature map for \( k_P \), meaning that \( k_P(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{H}(k)} \) for all \( x, x' \in M \). It follows that \( k_P \) is symmetric and semi-positive definite; indeed if \( \{w_i\}^n_{i=1} \subset \mathbb{R} \) and \( \{x_i\}^n_{i=1} \subset M \) then \( \sum_{i=1}^n \sum_{j=1}^n w_i w_j k_P(x_i, x_j) = \langle \sum_{i=1}^n w_i \phi(x_i), \sum_{j=1}^n w_j \phi(x_j) \rangle_{\mathcal{H}(k)} = \| \sum_{i=1}^n w_i \phi(x_i) \|^2_{\mathcal{H}(k)} \geq 0 \) as required.

**Lemma 2.** \( k_{P,\sigma} \) is symmetric and semi-positive definite; i.e. \( k_{P,\sigma} \) is a kernel.

**Proof.** Let \( \Phi := \mathbb{R} \times \mathcal{H}(k) \) denote the Hilbert space with inner product \( \langle (c_1, h_1), (c_2, h_2) \rangle_{\Phi} := c_1 c_2 + \langle h_1, h_2 \rangle_{\mathcal{H}(k)} \) for all \( c_1, c_2 \in \mathbb{R} \) and all \( h_1, h_2 \in \mathcal{H}(k) \). Denote the associated norm \( \| \cdot \|_{\Phi} \). Then the map \( \phi : M \to \Phi \), defined as \( \phi(x) := [\sigma, \tau k(x, \cdot)] \), is a feature map for \( k_{P,\sigma} \), meaning that \( k_{P,\sigma}(x, x') = \langle \phi(x), \phi(x') \rangle_{\Phi} \) for all \( x, x' \in M \). It follows that \( k_{P,\sigma} \) is symmetric and semi-positive definite, as explained in the proof of Lem. 1. \( \square \)

The Stein RKHS \( \mathcal{H}(k_{P,\sigma}) \) has the form \( \mathcal{H}(\sigma^2) \oplus \mathcal{H}(k_P) \) where \( \mathcal{H}(\sigma^2) \) is the RKHS with constant kernel \( \sigma^2 \). Moreover, from Thm. 4.21 of Steinwart and Christmann (2008), for \( \zeta \in \mathcal{H}(k_P) \)

\[
\| \zeta \|_{\mathcal{H}(k_P)} = \inf \{ \| h \|_{\mathcal{H}(k)} : h \in \mathcal{H}, \tau h = \zeta \}.
\]

Thus, from Thm. 5 of Berlinet and Thomas-Agnan (2011),

\[
\| f \|_{\mathcal{H}(k_{P,\sigma})}^2 = \inf \{ \sigma^{-2} \xi^2 + \| \zeta \|^2_{\mathcal{H}(k_P)} : f = \xi + \zeta, \xi \in \mathbb{R}, \zeta \in \mathcal{H}(k_P) \}
\]

\[= \inf \{ \sigma^{-2} \xi^2 + \| h \|^2_{\mathcal{H}(k)} : f = \xi + \tau h, \xi \in \mathbb{R}, h \in \mathcal{H}(k) \}. \tag{13}\]

Note that, since the only constant function in \( \mathcal{H}(k_P) \) is the zero function, the set over which the infimum is sought in Eqn. 13 in fact contains a single element. Let \( \hat{f} = \hat{\xi} + \tau \hat{h} \) where

\[
(\hat{\xi}, \hat{h}) = \arg \inf_{\xi \in \mathbb{R}, h \in \mathcal{H}(k)} \sum_{i=1}^n (\xi + \tau h(x_i) - f(x_i))^2 + R_1(\xi) + R_2(h) \tag{15}\]

and \( R_1, R_2 \) are the particular choice of regularisation terms in Eqn. 3. The \( (\hat{\xi}, \hat{h}) \) exist and are unique from the representer theorem [Schölkopf et al. 2001]. To understand the kernel Stein method it suffices to study the convergence of \( f \) to \( \hat{f} \) in the Stein RKHS. To this end, note at this point that the proof of the representer theorem shows that \( \hat{f} \) is the orthogonal projection of \( f \) onto the span of \( \{k_{P,\sigma}(\cdot, x_1), \ldots, k_{P,\sigma}(\cdot, x_n)\} \) in \( \mathcal{H}(k_{P,\sigma}) \), and thus we have

\[
\| f - \hat{f} \|_{\mathcal{H}(k_{P,\sigma})} \leq \| f \|_{\mathcal{H}(k_{P,\sigma})}, \tag{16}\]

the so-called best approximation property.

Our strategy in the remainder is to establish conditions for which the Stein RKHS is isomorphic to a standard Sobolev space, and then to leverage existing theoretical results on interpolation in Sobolev spaces.
5.2 Sobolev Embedding of the Stein RKHS

To establish a Sobolev embedding of the Stein RKHS we require a derivative counting argument. This is now established:

**Lemma 3.** The space $\mathcal{H}(k_{P,\sigma})$ is continuously embedded in $W^s_2(M)$. i.e. for some finite constant $C$, \[ \|f\|_{W^s_2(M)} \leq C\|f\|_{\mathcal{H}(k_{P,\sigma})}. \]

**Proof.** The elements of $\mathcal{H}(k_{P,\sigma})$ are all of the form $f = \xi + \tau h$ for $\xi \in \mathbb{R}$, $h \in \mathcal{H}(k)$, and therefore it is sufficient to show that there is a finite constant $C$ such that $\|\xi + \tau h\|_{W^s_2(M)} \leq C\|f\|_{\mathcal{H}(k_{P,\sigma})}$. From the triangle inequality and the definition of Sobolev norm, $\|\xi + \tau h\|_{W^s_2(M)} \leq C_1(\|\xi\|_{W^s_2(M)} + \|\tau h\|_{W^s_2(M)})$, where the constant $C_1$ depends on the volume of $M$. Now, we also know that $\|f\|_{\mathcal{H}(k_{P,\sigma})}^2 = \sigma^s \|\xi\|^2 + \|h\|^2_{\mathcal{H}(k)}$ where $h'$ is the element of $\mathcal{H}(k)$ that minimises $\|h\|_{\mathcal{H}(k)}$ subject to $\tau(h' - h) = 0$. The result therefore follows if $\|\tau h'\|_{W^s_2(M)} \leq C\|h'\|_{W^{s+2}_2(M)}$. This is a consequence of Lemma 2.4 in Grosse and Nistor (2017), and holds for the differential operator $\tau = \frac{1}{p} D_a$ whenever the section $a = pg(\cdot, \cdot)$ belongs to $W^{s}_\infty(M, T^* M \otimes T^* M)$ (see Baez and Munian (1994)).

Here $D_a := \nabla \cdot (p \nabla)$ is the differential operator associated to $a$, and $a$ is defined as the map that sends a point $x \in M$ to the bilinear form $p(x) g_x : T_x M \times T_x M \rightarrow \mathbb{R}$. The set $W^s_\infty(M, T^* M \otimes T^* M)$ contains sections such that when a pseudodifferential operator $L$ of order $s$ is applied, then $L[a]$ is bounded. Since $M$ is compact and $g$ is a smooth section, this holds for example whenever $p \in C^{s+1}(M)$. The final condition is implied by Assumption 2.

A result weaker than Lem. 3 analogous to Lem. 6 in Appendix A was established for the Euclidean manifold in Thm. 1 of Oates et al. (2018). On the other hand, in that work a converse result such as Lem. 4 presented next, was not established.

5.3 Stein Embedding of the Sobolev RKHS

In this section the converse of Lem. 6 is established:

**Lemma 4.** The space $W^s_2(M)$ is continuously embedded in $\mathcal{H}(k_{P,\sigma})$. i.e. for some finite constant $C$, \[ \|f\|_{\mathcal{H}(k_{P,\sigma})} \leq C\|f\|_{W^s_2(M)}. \]

**Proof.** Let $f \in W^s_2(M)$ and consider solutions $\xi \in \mathbb{R}$, $h \in W^{s+2}_2(M)$ to the partial differential equation

\begin{equation}
\begin{aligned}
\tau h + \xi &= f & \text{in } M \\
g(\nabla h, n) &= 0 & \text{on } \partial M,
\end{aligned}
\end{equation}

sometimes called the *Stein equation* (Ley et al., 2017). Note that for any solution pair $(\xi, h)$ we have $\xi = I(f)$ due to Assumption 4. In what follows we exploit Thm. 1.2 in Grosse and Nistor (2017) with pure Neumann boundary conditions and the operator $D_a : h \mapsto \nabla \cdot (p \nabla h)$,
associated to the strongly coercive bilinear form $a := pg$, which is in divergence form\footnote{Note it is also possible to redefine the Sobolev norm on manifold to include the factor $p$ in the volume form so that $\tau$ is in divergence form. This was not pursued.}. To use the results from \cite{Grosse2017}, we note that $D_a$ acts on functions, that is sections of the trivial line bundle $E = M \times \mathbb{R}$, so that sections $M \to M \times \mathbb{R}$ may be identified with smooth functions $M \to \mathbb{R}$, and $T^*M \otimes E \cong T^*M \cong TM$, where the last identification follows from the musical isomorphism, $v \in TM \leftrightarrow g(v, \cdot) \in T^*M$. Then setting $a = pg$ we can follow the derivation of $D_a$ in \cite{Grosse2017} and use the fact that the $L^2$ adjoint of the gradient is the divergence (see chapter 14 of \cite{Frankel2011}).

Thm. 1 in \cite{Grosse2017} implies that a solution $h$ to the Stein equation exists and satisfies, for some finite constants $C_i$,

$$
\|h\|_{W^{k+2}_2(M)} \leq C_1 \|p(f - \xi)\|_{W^2_2(M)} \\
\leq C_2 \|f - \xi\|_{W^2_2(M)} \\
\leq C_2 \left( \|f\|_{W^2_2(M)} + \|\xi\|_{W^2_2(M)} \right)
$$

where in a small abuse of notation $\xi$ denotes also the constant function with value $\xi$ and we have used the fact that the density $p$ is bounded above on $M$. Using Jensen inequality $\|\xi\|_{W^2_2(M)} \leq C_3 |\xi| \leq C_3 \|f\|_{L^1(M)} \leq C_4 \|f\|_{L^2(M)} \leq C_5 \|f\|_{W^2_2(M)}$. Thus $\|h\|_{W^{k+2}_2(M)} \leq C_6 \|f\|_{W^2_2(M)}$.

To complete the proof, we have from Eqn. \ref{eq:14} that

$$
\|f\|_{H(k,p,a)}^2 \leq \sigma^{-2} I(f)^2 + \|h\|_{H(k)}^2
$$

where $h$ is the unique element in $\mathcal{H}(k)$ that satisfies Eqn. \ref{eq:17}. Now, from Jensen’s inequality $I(f)^2 \leq I(f^2)$ and from the definition of the Sobolev norm (again using the fact the density $p$ is bounded above) $\|f\|_{L^2(p)} \leq C_7 \|f\|_{W^2_2(M)}$. Moreover, by hypothesis $\mathcal{H}(k)$ is norm-equivalent to $W^{k+2}_2(M)$; i.e. $\|h\|_{H(k)} \leq C_8 \|h\|_{W^{k+2}_2(M)}$ for some finite constant $C_8$. Thus

$$
\|f\|_{H(k,p,a)}^2 \leq (\sigma^{-2} C_7^2 + C_6^2 C_8^2) \|f\|_{W^2_2(M)}^2
$$

as required, with $C = (\sigma^{-2} C_7^2 + C_6^2 C_8^2)^{\frac{1}{2}}$.

\section{Proof of Theorem \ref{thm:1}}

The remainder of the proof of Thm. \ref{thm:1} is relatively standard. Indeed, from Lem. \ref{lem:3} and Lem. \ref{lem:4} we have established that $\mathcal{H}(k,p,a) \cong W^2_2(M)$ are norm-equivalent. Thus the convergence of $f$ to $f$ can be studied in the standard Sobolev space context.

The following Lem. \ref{lem:5} follows immediately from Prop. 7 and Thm. 8 in \cite{Fuselier2012}, together with the fact all Riemannian metrics (and their induced norms) are equivalent on a compact manifold, see page 22 of \cite{Hebey2000}.
Lemma 5. Let $M$ be a smooth, compact $d$-dimensional Riemannian manifold. Then there exists an atlas $\{\Psi_j, U_j\}$ on $M$ and constants $C_1, C_2 > 0$ such that, if $x, y \in U_j$ for some $j$, then
\[
C_1 \|\Psi_j(x) - \Psi_j(y)\|_2 \leq d_M(x, y) \leq C_2 \|\Psi_j(x) - \Psi_j(y)\|_2
\]
Moreover, let $h_{X \cap U_j}|_{U_j} := \sup_{x \in U_j} \min_{y \in X \cap U_j} d_M(x, y)$ denote the fill distance restricted to $U_j$. Then, if we choose an atlas as above, there exists finite constants $h_0, C$ such that, if $X \subset M$ is a finite point set with $h_X < h_0$, then for all $U_j$
\[
h_{X \cap U_j}|_{U_j} \leq Ch_X.
\]

The output of the Stein kernel method satisfies $I_X(f) = I(\hat{f})$ and in particular this means that
\[
|I(f) - I_X(f)| = |I(f - \hat{f})| = \left| \int_M (f - \hat{f}) dP \right| \leq \|f - \hat{f}\|_{L_2(P)}
\]
Using Lem. 5 and following the argument used in Thm. 10 of Fuselier and Wright (2012), we have that
\[
\|f - \hat{f}\|_{L_2(P)} \leq Ch_X^s \|f - \hat{f}\|_{W^2_+(M)}
\]
Hence, for some finite constants $C_i$,
\[
\|f - \hat{f}\|_{W^2_+(M)} \leq C_1 \|f - \hat{f}\|_{H(k_p, s)} \quad \text{(Lem. 3)}
\leq C_1 \|f\|_{H(k_p, s)} \quad \text{(best approximation property; Eqn. 16)}
\leq C_2 \|f\|_{W^2_+(M)} \quad \text{(Lem. 4)}
\]
Thus $|I(f) - I_X(f)| \leq C_3 h_X^s \|f\|_{W^2_+(M)}$, as required. This completes the proof of Thm. 1.

5.5 Proof of Corollaries for MCMC

Proof of Cor. 4 First, let $(Y_i : \Omega \rightarrow M)_{i \in \mathbb{N}}$ be a sequence of i.i.d. random variables distributed according to the normalised Riemannian measure $\bar{V}$, i.e., $P \circ Y^{-1} = \bar{V}$, where $P$ is the probability measure on $\Omega$. Let $Y^n = \{Y_i\}_{i=1}^n$ and denote expectation with respect to the sampling distribution of $Y$ as $E_Y$. From Reznikov and Saff (2015, Thm. 3.2, Cor. 3.3) we have that
\[
E_Y[h_X^s] \leq C_s^n n^{-\frac{s}{2}} \log(n)^{\frac{s^2}{2}}
\] (20)
for some $C_s^n$ a finite $s$-dependant constant. Now, since $M$ is compact and $p$ is continuous (Assumption 2), the Radon-Nikodym derivative $\frac{dP}{dV} \geq w > 0$ can be bounded away from
zero almost everywhere on $M$. Without loss of generality we can assume that the constant $w < 1$. It follows that $P$ can be represented as a bivariate mixture, one of whose components is $\bar{V}$. Specifically, $P = w\bar{V} + (1 - w)Q$, where $Q$ has density

$$\frac{dQ}{d\bar{V}} = \frac{1}{1 - w} \left( \frac{dP}{d\bar{V}} - w \right).$$

Let us introduce the Bernoulli random variables $B \overset{i.i.d.}{\sim} \text{Bernoulli}(w)$, and a random variable $Z$ with conditional distributions

$$Z|B \sim \begin{cases} \bar{V} & \text{if } B = 1 \\ Q & \text{if } B = 0 \end{cases}$$

It follows that the law of $Z$ is $P$, since

$$\mathbb{P}(Z^{-1}(A) = \mathbb{P}(Z \in A|B = 1)\mathbb{P}(B = 1) + \mathbb{P}(Z \in A|B = 0)\mathbb{P}(B = 0)$$

$$= \bar{V}(A)w + Q(A)(1 - w)$$

$$= P(A),$$

where $w = \mathbb{P}(B = 1)$. Consider then such a sequence $(Z_i)_{i \in \mathbb{N}}$ of i.i.d. random variables with the same law as $Z$, and let $Z_n = \{Z_i : 1 \leq i \leq n\}$. We set $|Y_n|$ to be the random variable corresponding to the number of samples of $Z_n$ that can be viewed as samples of $Y^m$. More precisely, if $\{z_i : 1 \leq i \leq n\}$ are samples from $Z_n$, of which $m$ were obtained by sampling from $Y_i$ (which arise whenever the Bernoulli random variable takes the value $B = 1$), then $|Y_n| = m$, and without loss of generality $Z_n|m = (Y_1, \ldots, Y_m, W_{m+1}, \ldots, W_n)$, where $W_i \sim Q$.

From the law of conditional expectation, the fact that $h_{Z_n}^{s}|m \leq h_{Y}^{s}|m$ and Eqn. 20

$$\mathbb{E}[h_{X}^{s}] = \mathbb{E}\mathbb{E}[h_{X}^{s}|m]$$

$$\leq \mathbb{E}\mathbb{E}[h_{Y}^{s}|m]$$

$$= \mathbb{E}\mathbb{E}[\min(\text{diam}(M), h_{Y}^{s}) | m]$$

$$\leq \mathbb{E}[\min(\text{diam}(M), C'' m^{-\frac{s}{2}} \log(m)^{\frac{s}{2}})].$$
Fix $0 < \epsilon < w$. From the law of total expectation, for $n > 1$:

\[
\begin{align*}
\mathbb{E}[\min(\text{diam}(M), C''_s m^{-\frac{1}{2}} \log(m)^{\frac{1}{2}})] \\
\frac{1}{n^{-\frac{1}{2}} \log(n)^{\frac{1}{2}}} \mathbb{P}(m = 0) \\
\frac{1}{n^{-\frac{1}{2}} \log(n)^{\frac{1}{2}}} \mathbb{E}[\min(\text{diam}(M), C''_s m^{-\frac{1}{2}} \log(m)^{\frac{1}{2}})|0 < m \leq \epsilon n] \mathbb{P}(0 < m \leq \epsilon n) \\
\frac{1}{n^{-\frac{1}{2}} \log(n)^{\frac{1}{2}}} \sum_{\tilde{m} > \epsilon n} \mathbb{E}[\min(\text{diam}(M), C''_s \tilde{m}^{-\frac{1}{2}} \log(\tilde{m})^{\frac{1}{2}})|m = \tilde{m}] \mathbb{P}(m = \tilde{m})
\end{align*}
\]

The first term is seen to vanish as $n \to \infty$:

\[(*) = \text{diam}(M)n^{\frac{1}{2}} \log(n)^{-\frac{1}{2}} (1 - w)^n \to 0\]

Since $m \sim \text{Binomial}(n, w)$, we have that $\log(m)/\log(n) \leq 1$ and moreover from Hoeffding’s inequality we have that

\[\mathbb{P}(m \leq \epsilon n) \leq \exp(-2(w - \epsilon)^2 n).\]

Thus, letting $C'''_s = \max(\text{diam}(M), C''_s)$, the second term is also seen to vanish as $n \to \infty$:

\[(**) \leq \mathbb{E}\left[\min\left(\text{diam}(M), C''_s \left(\frac{m}{n}\right)^{-\frac{1}{2}}\right)\right] \mathbb{P}(0 < m \leq \epsilon n) \\
\leq C'''_s n^{\frac{1}{2}} \mathbb{P}(0 < m \leq \epsilon n) \\
\leq C'''_s n^{\frac{1}{2}} \exp(-2(w - \epsilon)^2 n) \to 0\]

For the final term, let $g : [0, 1] \to \mathbb{R}$ be defined as

\[g(x) = \begin{cases} 
\epsilon^{-\frac{1}{2}} & x \leq \epsilon \\
\epsilon^{-\frac{1}{2}} & x > \epsilon
\end{cases}\]

which is observed to be a continuous and bounded. From the strong law of large numbers, $\frac{m}{n}$ converges a.e. to $w$, and thus in distribution to $\delta_w$. From the Portmanteau theorem we have that $\mathbb{E}[g(\frac{m}{n})] \to g(w) = w^{-\frac{1}{2}}$. Thus the third term is bounded as $n \to \infty$:

\[(***) \leq \sum_{\tilde{m} > \epsilon n} \min\left(\text{diam}(M), C''_s \left(\frac{\tilde{m}}{n}\right)^{-\frac{1}{2}}\right) \mathbb{P}(m = \tilde{m}) \\
\leq C'''_s \sum_{\tilde{m} > \epsilon n} \left(\frac{\tilde{m}}{n}\right)^{-\frac{1}{2}} \mathbb{P}(m = \tilde{m}) \\
\leq C'''_s \mathbb{E}\left[g\left(\frac{m}{n}\right)\right] \to C'''_s w^{-\frac{1}{2}} < \infty\]
Together with Thm. 1, the result is now established.

Proof of Cor. 2. The proof focuses on \((x_{in})_{i \in \mathbb{N}}\), which is sometimes referred to as the \(n\)-step jump chain and \(P^n\) is its transition kernel. Since \(M\) is compact and \(P\) is continuous (Assumption 2), the \(n\)th step transition distributions initialised from \(x_{in} \in M\), denoted \(P_{n,i}(\cdot) := P^n(x_{in}, \cdot)\), are absolutely continuous with respect to \(P\) and therefore admit Radon-Nikodym derivatives \(\frac{dP_{n,i}}{dP}\). Since the Markov chain is ergodic,

\[
\left| \frac{dP_{n,i}}{dP} - 1 \right| \leq C \rho^n
\]

and we can select a value \(n_0 \in \mathbb{N}\) independent of the \(i\) index such that, for some \(w < 1\) and all \(n \geq n_0\), it holds almost everywhere that \(\frac{dP_{n_0,i}}{dP} \geq w > 0\). It follows that \(P_{n_0,i}\) can be represented as a bivariate mixture, one of whose components is \(P\). Specifically, \(x_{in_0} \overset{d}{=} z_i\), where

\[
z_i | z_{i-1}, B_i \sim \begin{cases} P & \text{if } B_i = 1 \\ Q_i & \text{if } B_i = 0 \end{cases}, \quad B_i \overset{i.i.d.}{\sim} \text{Bernoulli}(w), \quad \frac{dQ_i}{dP} = \frac{1}{1 - w} \left( \frac{dP_{n_0,i-1}}{dP} - w \right).
\]

Consider then such a sequence \((z_i)_{i \in \mathbb{N}}\) and let \(Z = \{z_i : 1 \leq i \leq \lfloor \frac{n}{n_0} \rfloor \}\) and \(Y = \{z_i : B_i = 1, 1 \leq i \leq \lfloor \frac{n}{n_0} \rfloor \}\). The elements of \(Y\) are independent samples from \(P\) and \(m := |Y| \sim \text{Binomial}(\lfloor \frac{n}{n_0} \rfloor)\). The remainder of the proof is identical to that used for Cor. 1.

### 6 Discussion

This paper adds to the growing literature on Stein’s method in computational statistics, of which some contributions include Gorham et al. (2016); Liu and Wang (2016); Liu et al. (2016); Oates et al. (2017); Gorham and Mackey (2017); Liu and Zhu (2017); Liu and Lee (2017); Oates et al. (2018); Huggins and Mackey (2018); Chen et al. (2018); Detommaso et al. (2018); Zhu et al. (2018). Our contribution provides a formal theoretical analysis of the Stein kernel method proposed in Oates et al. (2017) and our results are stronger than those reported in Oates et al. (2018). Moreover, the method has been formalised for the case of a general oriented compact Riemannian manifold.

Two limitations of our analysis are acknowledged: First, the restriction to compact manifolds was fundamental to our analysis, as Sobolev norms on general manifolds are not equivalent to each other (since the Riemannian metrics are not equivalent), and in general there exist no finite patch cover of the manifold. Second, the novel Riemannian–Stein kernel method was numerically illustrated only on test problems on \(S^2\); as usual, the case of high-dimensional manifolds (i.e. \(d\) large) is likely to challenge any regression-based method unless strong assumptions can be made on the integrand. This second limitation will be the focus of our attention in subsequent work.

Topical extensions of this work could include a generalisation to non-stationary kernels (Paciorek, 2003), additional constructions to circumvent the need for gradient information.
on the target (Han and Liu, 2018), the simplification of computation when the density \( p \) can be factorised (Zhuo et al., 2018), the use of Riemannian–Stein kernels as a generalisation of score-matching in the manifold context (Mardia et al., 2016) and an extension of our methods to high- or infinite-dimensional spaces such as the Hilbert sphere \( S^\infty \) for functional data analysis on a manifold.

Acknowledgements

CJO and MG were supported by the Lloyd’s Register Foundation programme on Data-Centric engineering at the Alan Turing Institute, UK. AB was supported by a Roth scholarship from the Department of Mathematics at Imperial College London, UK. EP was partially supported by FONDECYT Grant [1170290], Chile, and by Iniciativa Científica Milenio - Minecon Nucleo Milenio MESCD. MG was supported by the EPSRC grants [EP/K034154/1, EP/R018413/1, EP/P020720/1, EP/L014165/1], an EPSRC Established Career Fellowship [EP/J016934/1] and a Royal Academy of Engineering Research Chair in Data Centric Engineering. The authors are grateful for discussions with Andrew Duncan, Toni Karvonen, Chang Liu, Gustav Holzegel, Julio Delgado and Andrew Stuart.

References


**A An Embedding Result**

The kernel of Alegria et al. (2018) has not been shown to reproduce a Sobolev space, and hence the convergence analysis in the main text cannot be applied. However, we are still able to make some theoretical progress for this kernel, and we present the following result:

**Lemma 6.** Let $M$ be compact and let $k \in C^{2\nu}(M \times M)$, $\nu > \frac{d}{2}$, be an arbitrary kernel. Then the associated space $H(k)$ is continuously embedded in $W^{\nu}_{2}(M)$. i.e. for some finite constant $C$, $\|f\|_{W^{\nu}_{2}(M)} \leq C\|f\|_{H(k)}$.

**Proof.** Set $\frac{\partial^j f}{\partial q^j} \phi^{-1}(x)$, on a coordinate patch where $\phi$ are the charts. If $k$ is a kernel on $M$, then its pullback $k \circ \phi^{-1}$ is a kernel on $\phi(U) \subset \mathbb{R}^d$, and $f \circ \phi^{-1}$ belongs to the RKHS generated by this pullback. It follows that $\frac{\partial^j f}{\partial q^j} \phi^{-1}(x) = \langle f \circ \phi^{-1}, \frac{\partial^j k \circ \phi^{-1}}{\partial x^j} \rangle_{H(k \circ \phi^{-1})}$. Recall here that $k \circ \phi^{-1}(a,b) := k(\phi^{-1}(a),\phi^{-1}(b))$, and $k \circ \phi^{-1} := k(\phi^{-1}(x),\cdot)$. By the Cauchy-Schwartz inequality we have $\langle f \circ \phi^{-1}, \frac{\partial^j k \circ \phi^{-1}}{\partial x^j} \rangle_{H(k)} \leq \|f \circ \phi^{-1}\|_{H(k \circ \phi^{-1})}\|\frac{\partial^j k \circ \phi^{-1}}{\partial x^j}\|_{H(k \circ \phi^{-1})}$. Then let $(U_b, \phi_b)$ be the open cover and $(\rho_b)$ the partition of unity subordinate to $(U_b)$ used in the definition of the Sobolev norm in Sec. 2.1.5.
From the Heine-Borel theorem we can assume this cover is finite. Moreover \( \text{supp}(\rho_b) \subset M \) is compact, since it is a closed subset of a compact manifold. Let us set \( \hat{f} := f \circ \phi_b^{-1} \). Then

\[
\|f\|_{W^2_2(M)}^2 = \sum_b \|(\rho_b f) \circ \phi_b^{-1}\|_{W^2_2(\mathbb{R}^n)}^2 \\
= \sum_b \sum_a \| \partial^a (\rho_b f) \circ \phi_b^{-1}\|_2^2 \\
= \sum_b \sum_a \int |\partial^a (\hat{\rho}_b(x) \hat{f}(x))|^2 \text{d}x \\
= \sum_b \sum_a \int \left( (\hat{f}(x) \partial^a \hat{\rho}_b(x))^2 + 2 \hat{\rho}_b(x) \hat{f}(x) \partial^a \hat{\rho}_b(x) \partial^a \hat{f}(x) + (\hat{\rho}_b(x) \partial^a \hat{f}(x))^2 \right) \text{d}x.
\]

Next we use that \( \hat{\rho}_b \leq 1 \) and \( \partial^a \hat{\rho}_b(x) |\text{supp}(\hat{\rho}_b) \leq D \) are compactly supported, \( \frac{\partial^a f_\phi^{-1}}{\partial q} (x) \leq \|f\|_{\mathcal{H}(k)} \|\partial^a k \circ \phi^{-1}\|_{\mathcal{H}(k_\phi^{-1})} \), and

\[
f \circ \phi^{-1}(x) = (f \circ \phi^{-1}_b, k \circ \phi^{-1})_{\mathcal{H}(k_\phi^{-1})} \leq \|f\|_{\mathcal{H}(k)} \|k \circ \phi^{-1}\|_{\mathcal{H}(k_\phi^{-1})},
\]

This shows that

\[
\|f\|_{W^2_2(M)}^2 \leq \|f\|_{\mathcal{H}}^2 \sum_b \sum_a \int \left( D^2 + D \|k \circ \phi^{-1}\|_{\mathcal{H}(k_\phi^{-1})} \|\partial^a k \circ \phi^{-1}\|_{\mathcal{H}(k_\phi^{-1})} \right) \text{d}x
\]

Since \( k \in C^{2\nu}(M \times M) \), \( \phi^{-1} \) is smooth, and \( |a| \leq \nu \), then \( k \circ \phi^{-1}_x \) and \( \partial^a k \circ \phi^{-1}_x \) are continuous. From this it follows that the right hand side of Eqn. 21 is finite because the domain of integration is compact. \( \square \)

Lemma 6 demonstrates that the space \( \mathcal{H}(k_2) \) reproduced by the kernel \( k_2 \) in Eqn. 12 is continuously embedded in \( W^2_2 \) for all \( D < \nu < \alpha \).

## B Alternative Differential Operators

The application of a differential operator to a kernel, in order to induce certain constraints, is similar in spirit to that of [Scheuerer and Schlather (2012)] where divergence-free and curl-free vector fields were modelled. In this appendix some possible alternatives to the differential operator \( \tau \) used in the main text are presented. Recall that our aim is to introduce an “integrates to zero” constraint. To this end, recall vector fields \( s = s_1 \partial_{q_1} + \cdots + s_m \partial_{q_m} \) are differential operators, so that we can consider the directional derivative of a function \( f : M \to \mathbb{R} \) in the direction \( s \), denoted \( s(f) = s_1 \partial_{q_1} f + \cdots + s_m \partial_{q_m} f \). Now, note that \( \nabla \cdot (fs) = s(f) + f \nabla \cdot s \). In particular, if \( s = \nabla h \), then \( \nabla \cdot (f \nabla h) = f \Delta h + (\nabla h)(f) \).

From the above identities we have that, for a closed manifold \( M \), vector field \( s \) and function \( f \),

\[
\int_M s(f) + f \nabla \cdot s \text{ d}V = 0.
\]
The operator $\tau$ in the main text is thus the special case with $s = p \nabla h$ and $f = 1$. Another possibility is $f = p$ and $s = \nabla h$:

$$\int_M (\nabla h)(p) + p \Delta h \, dV = 0.$$  

Similarly, we also have Green’s identity

$$\int_M f \Delta g - g \Delta f \, dV = 0$$

In particular, if $f$ satisfies the Poisson equation $\Delta f = \rho$, then

$$\int_M f \Delta g - g \rho \, dV = 0$$

and if $f$ is harmonic ($\Delta f = 0$), then

$$\int_M f \Delta g \, dV = 0.$$  \hspace{1cm} (21)

This suggests other possible differential operators, for example if we take $g := ph$ in Eqn. 21 we obtain a differential operator $\tau(h) = \frac{f \Delta (ph)}{p}$ for any harmonic $f$. Of course, any linear combination of the above operators integrates to zero as well. Moreover, one may obtain further operators by using transformations. Under a conformal transformation of the Riemannian metric, $\tilde{g} := e^{f} g$ for some smooth function $f$, then $\Delta_{\tilde{g}} = e^{-f} \Delta_{g} + (1 - n/2) e^{-2f} \nabla g f$. In particular when $n = 2$ we find $\Delta_{\tilde{g}} = e^{-f} \Delta_{g}$. Under an isometry $\Phi : (M, g_M) \rightarrow (N, g_N)$ we have $\Phi^* \Delta_{g_N} = \Delta_{g_M} \Phi^*$, where $\Phi^* f := f \circ \Phi$ is the pullback. It follows that if $\Phi$ is a diffeomorphism $\Phi^* \Delta_{g_N} = \Delta_{\Phi^* g_N} \Phi^*$.

Several of the operators just described contain degrees of freedom that could themselves be cast within the optimisation problem in Eqn. 2 However, a basic computational preference is afforded to differential operators that do not have additional degrees of freedom and are of low differential order; this was one reason for our choice of $\tau$ in the main text, as no degrees of freedom are involved and only first order derivatives of $p$ are required.