Generalised Kernel Stein Discrepancy (GKSD): A Unifying Approach for Non-parametric Goodness-of-fit Testing

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Abstract

Non-parametric goodness-of-fit testing procedures based on kernel Stein discrepancies (KSD) are promising approaches to validate general unnormalised distributions in various scenarios. Existing works have focused on studying optimal kernel choices to boost test performances. However, the Stein operators are generally non-unique, while different choices of Stein operators can also have considerable effect on the test performances. In this work, we propose a unifying framework, the generalised kernel Stein discrepancy (GKSD), to theoretically compare and interpret different Stein operators in performing the KSD-based goodness-of-fit tests. We derive explicitly that how the proposed GKSD framework generalises existing Stein operators and their corresponding tests. In addition, we show that GKSD framework can be used as a guide to develop kernel-based non-parametric goodness-of-fit tests for complex new data scenarios, e.g. truncated distributions or compositional data. Experimental results demonstrate that the proposed tests control type-I error well and achieve higher test power than existing approaches, including the test based on maximum-mean-discrepancy (MMD).

1 Introduction

Stein’s method [5] provides an elegant probabilistic tool for comparing distributions based on Stein operators acting on a broad class of test functions, which has been used to tackle various problems in statistical inference, random graph theory, and computational biology. Modern machine learning tasks, such as density estimations [29, 47, 57], model criticisms [34, 48, 55], or generative modellings [20, 40], may extensively involve the modelling and learning with intractable densities, where the normalisation constant (or partition function) is unable to be obtained in closed form. Stein operators may only require access to the distributions through the differential (or difference) of the log density functions (or mass functions), which avoids the knowledge of the normalisation constant. It is particularly useful to study those unnormalised models [29]. As such, Stein’s method has recently caught the attention of the machine learning community and various practical applications have been developed, including variational methods [45], implicit model learning [41], approximate inference [28], non-convex optimisations [16, 54], and sampling techniques [11, 12, 52].

The goodness-of-fit testing procedure aims to check the null hypothesis \( H_0 : q = p \), where \( q \) is the known target distribution and \( p \) is the unknown data distribution only accessible from a set of
samples, $x_1, \ldots, x_n \sim p$. The non-parametric goodness-of-fit testing refers to the scenario where the assumptions made on the distributions $p$ and $q$ are minimal, i.e. the distributions in non-parametric testings are not assumed to be in any parametric families. By contrast, parametric tests (e.g. student t-test or normality test) assume pre-defined parametric family to be tested against and usually deal with summary statistics such as means or standard deviations that can be more restrictive in terms of comparing the full distributions. Kernel-based methods have been applied to compares distributions via rich-enough reproducing kernel Hilbert spaces (RKHS) [8] and achieved state-of-the-art results for non-parametric two-sample test [24] or independence test [23]. Combined with well-defined Stein operators, kernel Stein discrepancy (KSD) [21, 39] has been developed for non-parametric goodness-of-fit testing procedures for unnormalised models, and demonstrate superior test performances in various scenarios including Euclidean data in $\mathbb{R}^d$ [13, 46], discrete data [60], point processes [61], latent variable models [33], conditional densities [32], censored-data [18], directional data [58] as well as data on Riemannian manifold [59]. It is worth to note that for the above-mentioned works on goodness-of-fit tests, specific Stein operators are required to be developed independently to address the statistical inference problem for data scenarios and the Stein operators can have diverse forms and seem to be unconnected. Beyond goodness-of-fit testing, KSD have recently been studied in the context of numerical integration [6], Bayesian inferences [43], density estimations [7, 37] and measure transport [19].

To improve the performances for the goodness-of-fit testing procedures, existing works have focused on selecting [36, 42] and learning [25, 55, 44] an optimal kernel functions, which is adaptive to the finite sample observations. In addition, using the techniques related to kernel mean embedding [51], KSD-based tests also enable the extraction of distributional features to perform computationally efficient tests and model criticisms [30, 59]. Nonetheless, the choice of Stein operators can also have a considerable effect for test performances but this dimension of the research has so far been ignored mostly. Previous works have only demonstrated the non-uniqueness of valid Stein operators, e.g. [60] pointed out (in their Section 3.2) that for random graph models the Stein operator can be build from indicator function or normalised Laplacian. Moreover, [18] has derived three different Stein operators for censored data based on various properties from survival analysis and empirically illustrated their different test performances.

The main contribution of this paper is threefold.

1) Our first contribution is to propose a unifying framework for KSD-based tests, called generalised kernel Stein discrepancy (GKSD). Under this unifying framework, we are able to make connections between the existing KSD-based methods for different data scenarios (introduced in Section 2), via an auxiliary function that we define and discuss in Section 3. With the appropriate choice of auxiliary functions, we then discuss the generalisation power of GKSD by incorporating the designated aspect of different testing scenarios, such as censoring information [18], geometric structures of data [6, 58, 59], and latent variables in the model [33].

2) Our second contribution is to provide comparisons and interpretations for different KSD-based tests with the aid from the auxiliary functions. For example, [18] has empirically shown the different test performances for censored data using the survival-KSD (sKSD) and the martingale-KSD (mKSD). With the GKSD framework, we are able to compare sKSD and mKSD from the perspective of different choices of auxiliary functions, which impose different treatments on the censored part and the uncensored part of the data. Such analysis and interpretation is helpful for explaining the reported empirical test performances.

3) Our third contribution applies GKSD for developing novel Stein goodness-of-fit tests. Understanding the role of auxiliary functions in different KSD methods, we provide a systematic approach to derive valid KSD-based tests on novel testing scenarios. In Section 4, we study the goodness-of-fit testing procedures for distributions with domain constraint. We derive the bounded-domain KSD (bd-KSD) and its corresponding statistical properties. Then we present case studies on testing truncated distributions and compositional data, i.e. data defined on a simplex/hypersimplex. We also compare the test performances with various choices of Stein operators in each case. Then we discuss the optimal choice of Stein operators.

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1 As only one set of samples are observed, the goodness-of-fit testing sometimes is also referred to as the one-sample test or one-sample problem. This is opposed to the two-sample problem where the distribution $q$ is also unknown and appeared in the sample form.
2 Preliminaries

We first review Stein’s method and a set of existing Stein operators developed for testing various data scenarios, followed by a brief reminder on KSD-based goodness-of-fit testing procedure.

2.1 Stein’s method and Stein operators

Stein’s method is usually refer to the Stein characterisation for distributions. Given distribution \( q \), an operators \( T_q \) is called a Stein operator w.r.t. \( q \) if the following Stein’s identity holds for some test function \( f : \mathbb{E}_q [T_q f] = 0 \). The class of such test function \( f \) is called the Stein class for \( q \). We start by introducing the Stein operator and the variations of Stein characterisations in various data scenarios.

**Euclidean Stein operator**

We first review the Stein operator for continuous densities in Euclidean space \( \mathbb{R}^d \) with Cartesian coordinate [21, 39], which is also referred to as the Langevin-diffusion Stein operator [7]. Let \( \mathcal{X} = \mathbb{R}^d \) and \( f_i : \mathcal{X} \to \mathbb{R} \) for \( i = 1, \ldots, d \) be scalar-valued functions on \( \mathcal{X} \). \( f(x) = (f_1(x), \ldots, f_d(x))^\top \in \mathbb{R}^d \) defines a vector-valued function \( f \). Let \( q \) be a smooth probability density on \( \mathcal{X} \) which vanishes at infinity. For a bounded smooth function \( f : \mathbb{R}^d \to \mathbb{R}^d \), the Stein operator \( T_q \) is defined by

\[
T_q f(x) = f(x)^\top \nabla \log q(x) + \nabla \cdot f(x).
\]

The Stein’s identity holds for \( T_q \) in Eq. (1) due to the integration by parts on \( \mathbb{R}^d \):

\[
\mathbb{E}_q [T_q f] = \int_{\mathbb{R}^d} T_q f(x) dq(x) = \int_{\mathbb{R}^d} \sum_{i} \frac{\partial}{\partial x_i} (f_i(x) q(x)) dx = 0,
\]

where the last equality holds since \( f_i(x) q(x) \) vanishes at infinity. Since the Stein operator \( T_q \) depends on the density \( q \) only through the derivatives of \( \log q \), it does not involve the normalisation constant of \( q \), which is a useful property for dealing with unnormalised models [29].

**Censored-data Stein operator**

In practical data scenarios such as medical trials or e-commerce, we encounter data with censoring where the actual event time of interest (or survival times) is not accessible but, instead, a bound or interval, in which the event time is known to belong, is observed. [18] has proposed a set of Stein operators for right-censored data, where the lower bound of the event time is observed. The right-censored data is observed in the form of \( (x, \delta) \) where for the survival time \( x_i \) and censoring time \( c_i \), the observation time is \( t_i = \min\{x_i, c_i\} \) and \( \delta_i = \mathbb{I}_{[x_i < c_i]} \) indicates if we are observing \( x_i \). Denote \( \mu_0 \) as the density of event time \( x \); \( S_{C} \) as the survival function\(^3\) of the censoring time \( C \); the test function \( \omega : \mathbb{R}_+ \to \mathbb{R} \) assumed to vanish at origin, i.e. \( \omega(0) = 0 \); \( \Omega \) the set of functions \( \mathbb{R}_+ \times \{0, 1\} \to \mathbb{R} \), and the operator \( T_{0,\omega} \in \Omega \). The censored-data Stein operator is defined as

\[
(T_{0,\omega})(x, \delta) = \delta \frac{\omega(x) S_{C}(x) \mu_0(x))}{S_{C}(x) \mu_0(x)}.
\]

Denote \( \mathbb{E}_0 \) as taking expectation w.r.t. the observation pair \( (x, \delta) \) where \( x \sim \mu_0 \), which needs to distinguish from \( \mathbb{E}_{\mu_0} \) that takes expectation over \( x \sim \mu_0 \). Note that the censoring distribution, e.g. \( S_{C} \) remains unknown. By Eq. (17) in Appendix, we have the Stein’s identity \( \mathbb{E}_0 [(T_{0,\omega})(x, \delta)] = 0 \).

The key challenge for this Stein operator is that the survival function for censoring time \( S_{C} \) is unknown and not included in the null hypothesis. Hence, [18] applied tricks in survival analysis to derive a computationally feasible feasible operator: the survival Stein operator. This operator has an unbiased estimation from the empirical observations. For the hazard function \( \lambda_0 \) associated with \( \mu_0 \), the Survival Stein operator \( T_{0,\omega}^{(s)} \) is defined as

\[
(T_{0,\omega}^{(s)})(x, \delta) = \delta (\omega(x) + \frac{\lambda_0(x)}{\lambda_0(x)} \omega(x)) - \lambda_0(x) \omega(x).
\]

By the martingale identities, [18] also proposed the martingale Stein operator,

\[
(T_{0,\omega}^{(m)})(x, \delta) = \delta \frac{\omega(x)}{\lambda_0(x)} - \omega(x).
\]

Details for known identities regarding survival analysis and martingales can be found in Appendix A.

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\(^3\)Another important approach to develop Stein operator is via Barbour’s generator approach [4].

\(^3\)Survival function is defined as \( S(x) = 1 - F(x) \) where \( F(x) = \int_0^x \mu(s) ds \) is the c.d.f. of the event time.
Latent-variable Stein operator  Latent variable models are powerful tools in generative modelling and statistical inference. However, such models generally do not have closed form density expressions due to the integral operator w.r.t. latent spaces. The latent Stein operator was constructed via samples of the latent variables and the corresponding conditional densities [33]. Let \( q(x) \propto \int q(x|z)\pi(z)dz \) be the target distribution which is not accessible in closed form, even its unnormalised version. Sample \( z_1, \ldots, z_m \sim q(z|x) \). The latent variable Stein operator is defined as

\[
T_{q,z}f(x) = \frac{1}{m} \sum_{j=1}^{m} T_{q(x|z_j)}f(x)
\]

A closely related construction is the Stochastic Stein Operator [22], which has been developed for computationally efficient posterior sampling procedures. Additional details and comparisons with latent variable Stein operator are included in Appendix F.

Second-order Stein operator  To address distributions defined on Riemannian manifolds, Stein operators involving second-order differential operators have been studied [6, 37]. For smooth Riemannian manifold \( M \) and scalar-valued function \( f : M \to \mathbb{R} \), the second-order Stein operator for density \( q \) on \( M \) is defined as

\[
T^{(2)}_q f(x) = \nabla \tilde{f}(x)^\top \nabla \log q + \Delta \tilde{f}(x),
\]

where \( \Delta \tilde{f} = \nabla \cdot \nabla \tilde{f} \) denotes the corresponding Laplace-Beltrami operator\(^4\). We note that the second-order operator is also applicable for Euclidean manifold, i.e. when the test function class is chosen in the particular form: \( f = \nabla \tilde{f} \). Stein operator in Eq. (6) replicates that in Eq. (1).

Coordinate-dependent Stein operator  Consider coordinate system \((\theta^1, \ldots, \theta^d)\) that is almost everywhere in \( M \). For a density \( q \) on \( M \), the Stein operator with the chosen coordinate is defined as

\[
T^{(1)}_q f = \sum_{i=1}^{d} \left( \frac{\partial f}{\partial \theta^i} + f \frac{\partial}{\partial \theta^i} \log(qJ) \right),
\]

where \( J = (\det G)^{1/2} \) is the volume element. \( T^{(1)}_q \) can be shown as a Stein operator via differential forms and relevant Stoke’s theorem [58].

2.2 Kernel Stein discrepancies (KSD)

With any well-defined Stein operator, we can choose an appropriate RKHS w.r.t. the data scenario to construct its corresponding KSD. Let \( p, q \) be distributions satisfying regularity conditions for the relevant testing scenarios and the test function class to be the unit ball RKHS, \( B_1(\mathcal{H}) \), KSD between distributions \( p \) and \( q \) is defined as

\[
\text{KSD}(p||q; \mathcal{H}) = \sup_{f \in B_1(\mathcal{H})} \mathbb{E}_p[|T_q f|].
\]

It is known from Stein’s identity that for any test functions in the Stein class, \( p = q \) implies \( \text{KSD}(p||q) = 0 \). In the testing procedure, a desirable property of the discrepancy measure is that \( \text{KSD}(q||p) = 0 \) if and only if \( p = q \). As such, we require our RKHS to be sufficiently large to capture any possible discrepancies between \( p \) and \( q \), which requires mild regularity conditions [13, Theorem 2.2] for KSD to be a proper discrepancy measure. Algebraic manipulations produce the following quadratic form:

\[
\text{KSD}^2(p||q) = \mathbb{E}_{x,\tilde{x} \sim p} [h_q(x, \tilde{x})],
\]

where \( h_q(x, \tilde{x}) = \langle T_q k(x, \cdot), T_q k(\tilde{x}, \cdot) \rangle_{\mathcal{H}} \) does not involve distribution \( p \) and \( k(x, \cdot) \) denotes the kernel associated with RKHS \( \mathcal{H} \).

\(^4\)Specifically, consider \( \partial x^i \) as the basis vector on Tangent space of \( x \), \( T_x M \). \( \nabla \tilde{f} = \sum_{i,j} (G^{-1})_{ij} \frac{\partial}{\partial x^j} \partial x^i \), denotes the (Riemannian) gradient operator, where \( G \in \mathbb{R}^{d \times d} \) denotes the metric tensor matrix; the divergence operator is \( \nabla \cdot s = \sum_i s_i \frac{\partial}{\partial x^i} + s_t \frac{\partial}{\partial s} \log \sqrt{\det(G)} \) for \( s = s_1 \partial x^1, \ldots, s_d \partial x^d \). In the Euclidean case, \( G \equiv I \), the identity matrix, which is independent of \( x \).
2.3 Goodness-of-fit tests with KSD

Now, suppose we have relevant samples \( x_1, \ldots, x_n \) from the unknown distribution \( p \). To test the null hypothesis \( H_0 : p = q \) against the (broad class of) alternative hypothesis \( H_1 : p \neq q \), KSD can be empirically estimated via Eq. (9) using U-statistics or V-statistics [56]; given the significance level of the test, the critical value can be determined by wild-bootstrap procedures [14] or spectral estimation [31] based on the Stein kernel matrix \( H_{rs} = h_q(x_r, x_s) \); the rejection decision is then made by comparing empirical test statistics with the critical value. In this way, the systematic procedure for non-parametric goodness-of-fit testing is obtained, which is applicable to unnormalised models.

3 Generalised Kernel Stein Discrepancy (GKSD)

In this section, we generalise the Stein operator in a particular way studied in this paper that is simple enough to interpret but powerful enough to cover all the Stein operators discussed in Section 2.1.

3.1 Generalised Stein operator

Let \( f \) be appropriately bounded test function as defined in Section 2.1. We consider a new operator for density \( q \), the generalised Stein operator \( T_{q,g} \) that also depends on the auxiliary function \( g : \mathbb{R}^d \to \mathbb{R}^d \),

\[
(T_{q,g}f)(x) = T_q f \circ g(x) = \sum_{i=1}^{d} g_i(x) f_i(x) \frac{\partial}{\partial x_i} \log q(x) + g_i(x) \frac{\partial}{\partial x_i} f_i(x) + f_i(x) \frac{\partial}{\partial x_i} g_i(x),
\]

(10)

where \( \circ \) denotes the element-wise product. The Stein’s identity \( E_q[\partial_q f \circ g(x)] = 0 \) holds for all bounded function \( g \), due the similar argument of integration by parts as derived for Eq. (1).

With Stein operator \( T_{q,g} \), we may want to define the generalised kernel Stein discrepancy (GKSD):

\[
\text{GKSD}_g(p||q; \mathcal{H}) = \sup_{\|f\|_H \leq 1} \mathbb{E}_p[\langle T_{q,g} f \circ g(x) \rangle] = 0.
\]

(11)

We note that \( \text{GKSD}_g^2 \) also admits the following quadratic form similar to Eq. (9).

**Proposition 1.** Let \( f \in \mathcal{H} \), the RKHS associated with kernel \( K \). For fixed choice of bounded \( g \),

\[
\text{GKSD}_g^2(p||q; \mathcal{H}) = \mathbb{E}_{x,\tilde{x} \sim p}[h_{q,g}(x, \tilde{x})],
\]

(12)

where \( h_{q,g}(x, \tilde{x}) = \langle T_{q,g} K(x, \cdot), T_{q,g} K(\tilde{x}, \cdot) \rangle_{\mathcal{H}} \).

For different choice of auxiliary functions \( g \), GKSD exhibits distinct diffusion pattern induced by \( g \). We note that, by choosing \( g_i(x) \equiv 1 \), \( \forall i \in [d] \), GKSD recovers the KSD with Stein operator in \( \mathbb{R}^d \) in Eq. (1). Some related ideas have been discussed using interpretations on Fisher information metric [50, Section 7.2]; as well as the form of invertible matrix for diffusion kernel Stein discrepancy (DKSD) [7, Theorem 1]. Even though those formulations can have implicit connections to GKSD in Eq. (12), previous works did not study the relationship with existing KSDs proposed for various goodness-of-fit testing scenarios, which we now proceed to show.

3.2 Generalising existing Stein operators

The specific choice of \( g \) and its interplay with \( f \) can be helpful to understand the conditions in various testing scenarios. In this section, we show that, with appropriate choice of the auxiliary function \( g \), GKSD is capable of generalising the KSDs derived from Stein operators introduced in Section 2.1. To specify the equivalence notion, we denote \( \cong \) as identical formulations beyond the equality between evaluation values. All proofs and detailed derivations are included in the Appendix B.

**Theorem 1** (Censored-data Stein operator). Let dimension of the data \( d = 1 \) and w.l.o.g., the test function \( \omega \) is assumed to vanishes at 0. For \( g : \mathbb{R}^+ \to \mathbb{R} \), choosing \( g(x) = S_C(x) \), GKSD with \( T_{\mu_0,g} \) recovers the censored-data KSD with Stein operator defined in Eq. (2).

\[
\mathbb{E}_{\mu_0}[T_{\mu_0,S_C} \omega] \cong \mathbb{E}_0[(T_0 \omega)(x, \delta)] = 0.
\]

(13)
It is not difficult to see that the result holds from directly applying identity in Eq. (17) (explained in Appendix A). However, it is worth noting that during the testing procedure, \( S_C \) is \textit{unknown} so we do not have direct access to \( g \) here. Moreover, the expectation on l.h.s. of Eq. (13) is w.r.t. the density of survival time \( \mu_0 \) for GKSD, where the expectation on the r.h.s. is \( E_0 \), w.r.t. the paired observation incorporating censoring information. Theorem 1 serves the purpose of explicitly demonstrating how a particular choice of auxiliary function can bridge the gap between censored-data Stein operator with the Stein operator on distributions without the presence censoring information. Moving on, it will also be interesting to understand how the auxiliary function may explain the Stein operators in Eq. (3) and Eq. (4) when \( E_0 \) applies to GKSD, where the expectation is taken over the paired variable \((x, \delta)\).

**Theorem 2** (Martingale Stein operator). Assume the same setting as in Theorem 1. Further assume that the positive definite test function \( \omega : \mathbb{R}_+ \to \mathbb{R} \) is integrable such that \( \int_0^x \omega(s)ds < \infty, \forall x; \mu_0(t) > 0 \) for the survival times so the inverse of its corresponding hazard function \( \lambda_0(x) = \frac{\mu_0(x)}{S_0(x)} \) is then well-defined on \( \mathbb{R}_+ \). For \( g : \mathbb{R}_+ \to \mathbb{R} \), choosing

\[
g(x) = \delta \lambda_0(x)^{-1} + (1 - \delta) \int_0^x \frac{\mu_0(s)\omega(s)ds}{\mu_0(x)\omega(x)},
\]

GKSD with \( T_{\mu_0, g} \) recovers the martingale KSD with Stein operator defined in Eq. (4).

\[
E_0[ T_{\mu_0, g} \omega ] \triangleq E_0[ (T_0^{(m)} \omega)(x, \delta) ] = 0. \tag{14}
\]

The \( \delta \)-dependent decomposition of \( g \) above, reveals the relationship between how censoring is incorporated in the martingale Stein operator, i.e. through the hazard function for uncensored data while through an interaction between the density \( \mu_0 \) and the test function \( \omega \) in the censored part. Similarly, choosing \( \delta \)-dependent auxiliary function \( g \) can recover Survival Stein operator in Eq. (3).

**Corollary 1** (Survival Stein operator). Assume the conditions in Theorem 2 hold. For \( g : \mathbb{R}_+ \to \mathbb{R} \), choosing

\[
g(x) = \delta + (1 - \delta) \int_0^x \frac{\mu_0(s)\omega(s)\lambda_0(s)ds}{\mu_0(x)\omega(x)},
\]

GKSD with \( T_{\mu_0, g} \) recovers the survival KSD with Stein operator defined in Eq. (3).

\[
E_0[ T_{\mu_0, g} \omega ] \triangleq E_0[ (T_0^{(s)} \omega)(x, \delta) ] = 0.
\]

**Comparisons between \( T_0^{(m)} \) and \( T_0^{(s)} \)** From Theorem 2 and Corollary 1, we now explicitly see:

1) \textit{in the uncensored part}: the diffusion for martingale Stein operator \( T_0^{(m)} \) is through the inverse of hazard function while the survival Stein operator \( T_0^{(s)} \) has constant auxiliary function, replicating diffusion in the form of Eq. (1) in 1 dimension;

2) \textit{in the censored part}: both Stein operators rely on the integral form where density \( \mu_0 \) and test function \( \omega \) interacts, while survival Stein operator \( T_0^{(s)} \) involves the hazard function \( \lambda_0 \) within the integral, making it much harder to estimate empirically.

Our results show that for \( T_0^{(s)} \), the censoring information is only extracted from the censored part of data \((\delta = 0)\) while the uncensored part of data \((\delta = 1)\) are treated exactly the same as Eq. (1). However for \( T_0^{(m)} \), the censoring information is re-calibrated via both censored part and uncensored part of data, which results in more accurate empirical estimation compared to that of \( T_0^{(s)} \). The theoretical interpretations corroborate the empirical findings reported in [18].

**Theorem 3** (Latent-variable Stein operator). Assume \( q(x|z) \) vanishes at infinity \( \forall z \). Given sample \( z = \{z_j\}_{j \in [m]} \sim q(z|x) \), the sample-based \( z \)-dependent auxiliary function \( g : \mathcal{Z} \to \mathbb{R}^d \) is chosen to be \( g_t(z) = \frac{1}{m} \sum_j \delta_{z_j}(z), \forall t \in [d] \). GKSD recovers the latent Stein operator in Eq. (5).

\[
E_q[ T_{q, g} \mathbf{f} ] \triangleq \sum_j E_q(x|z_j) [ T_{q(x|z_j)} \mathbf{f} ] = 0.
\]

By choosing the auxiliary function as the finite sum of delta measures on the latent variable locations, the auxiliary function is effectively performing the sampling procedure to construct the random kernel for the latent Stein operator proposed in [33], to surpass the intractability rising from integral operation over the latent variables.
Theorem 4 (Second-order Stein operator). Choosing \( g(x) = \frac{\partial}{\partial x} \log f(x) \), GKSD recovers the second-order Stein operator defined in Eq. (6), \( \mathcal{T}_{q, \log f} f = \mathcal{T}_{q}^{(2)} f \).

Using the fact that \( g \cdot f = (\log f)' f = f' \), choosing \( g = (\log f)' \) produces the extra order on the differential operator. For the more general formulation, which can be chosen based on the linear operator \( \mathcal{L} \) are discussed in Appendix G. By choosing the linear operator itself to be the differential operator will automatically recover such second-order Stein operator. The multivariate version and the Riemannian manifold version are also applicable. Details are included in the Appendix.

Theorem 5 (Coordinate-dependent Stein operator). Choosing \( g_i(x) = \log J, \forall i \), GKSD recovers the Stein operator defined in Eq. (7).\( \sum_i \int_X \mathcal{T}_q (f_i \log J) dqJ = \sum_i \int_X \frac{\partial}{\partial x_i} (f_i qJ) = 0. \)

Proof. The result follows from separating the last term in Eq. (7): \( \log(qJ) = \log q + \log J. \)

With the particular choice of coordinate system, choosing the auxiliary function \( g \) to be the log of Jacobian can be interpreted as changing the diffusion pattern to incorporate coercive expectation w.r.t. taking expectation over the density. This can be explicitly shown via Stoke’s theorem in differential form [58]. In addition, the idea of using auxiliary function to incorporate domain properties or constraints can be very useful for problems where the data has a complicated and irregular domain. We provide detailed study on this for goodness-of-fit testing below in Section 4.

Remarks. Beyond generalising KSDs in various testing scenarios, GKSD can also recover learning objectives for unnormalised models such as score matching [29] i.e. score matching can be derived in terms of GKSD with specific choice of kernel and auxiliary function.

Theorem 6. Let \( f, q \) be scalar functions. Choosing \( g(x) = 1/\sqrt{p(x)} \), and kernel \( k(x, x') = \delta_{x=x'} \), GKSD in the form of Eq. (10) recovers the score matching objective.

Detailed reviews on score matching and additional discussions are provided in Appendix D.

4 GKSD Application: Testing Data with Domain Constraints

We show that different choices of auxiliary functions in the generalised Stein operator are able to produce appropriate Stein operators for testings in various data scenarios. GKSD can then be useful to develop a systematic approach for new kernel Stein tests when appropriately auxiliary functions are used. In this section, we apply GKSD for testing data with general domain constraint.

Let \( q \) be a probability distribution defined on a compact domain\(^5\) \( V \) with boundary \( \partial V \). Denote the unnormalised density \( \tilde{q}(x) \propto q(x), x \in V \). Common examples include the truncated Gaussian distribution on interval \([a, b]\) or compositional data that defined on a simplex/hyper-simplex. Complex boundaries such as polygon \([47, 63]\) or non-negative constraint for graphical models \([62]\) have been studied. Such a problem setting is commonly observed when the observed data is only a subset of the domain or consists of structural constraint such as compositional data. For instance, if a local government would like to study the spread of the disease during the pandemic, while the infectious information is not accessible from other countries, one may need to validate model assumptions with the domain truncated by the designated border.

4.1 Stein operators on compact domains

To create the KSD-type test for data on domain \( V \), we first consider the Stein operators for densities on \( V \). We develop such a Stein operator guided by the generalised Stein operator in Eq. (10). Unlike densities on unbounded domain that is commonly assumed to vanish at infinity, densities on compact domain may not usually vanish at the boundary. Hence, direct application of Stein operator on \( \mathbb{R}^d \) may require the knowledge of normalised density at the boundary, which defeat the purpose of KSD testing for unnormalised models. To address this issue, we utilise the auxiliary function in GKSD.

Consider a bounded smooth function \( g : \mathbb{R}^d \rightarrow \mathbb{R}^d \) such that \( q_i(\partial V) = 0, \forall i \in [d] \) and for unnormalised \( \tilde{q} \) on \( V \), the bounded-domain Stein operator is defined as \( \mathcal{T}_{\tilde{q}, g} f(x) = \left( q \sum_i \frac{\partial}{\partial x_i} (q g_i f_i) \right) (x) \). With the aid from auxiliary function \( g \), it is not hard to check the Stein’s identity holds w.r.t. \( q \).

\(^5\)It is common that \( V \) is embedded in some non-compact domain \( \Omega \), e.g. truncated distribution from \( \mathbb{R}^d \).
4.2 Bounded-domain kernel Stein discrepancy (bd-KSD)

With the Stein operator $\tilde{T}_{\bar{g}, \bar{g}}$, we proceed to define the bounded-domain Kernel Stein Discrepancy (bd-KSD) for goodness-of-fit testing, similar to the Section 2.2. We consider the unit ball RKHS function $f \in B_1(\mathcal{H})$ as the test function class and we find the “best” function to distinguish densities $\bar{p}$ and $\bar{q}$ on $\mathcal{V}$ by taking supremum over $B_1(\mathcal{H})$: bd-KSD$_{\bar{g}}(\bar{q}||\bar{p}) = \sup_{f \in B_1(\mathcal{H})} \mathbb{E}_{\bar{p}}[\tilde{T}_{\bar{g}, \bar{g}}f(x)]$. Standard reproducing property gives the quadratic form bd-KSD$_{\bar{g}}(\bar{q}||\bar{p})^2 = \mathbb{E}_{x,x' \sim \bar{q}}[h_{\bar{q}, \bar{g}}(x, x')]$, where $h_{\bar{q}, \bar{g}}(x, x') = \langle \tilde{T}_{\bar{g}, \bar{g}}k(x, \cdot), \tilde{T}_{\bar{g}, \bar{g}}k(x', \cdot) \rangle_{\mathcal{H}}$.

Let $L(x) = (L_1(x), \ldots, L_d(x))^\top \in \mathbb{R}^d$ with $L_i(x) = \frac{\partial}{\partial x^i} \log \frac{\bar{q}(x)}{\bar{p}(x)}$, we show that under mild regularity conditions, bd-KSD is a property discrepancy measure on $\mathcal{V}$.

**Theorem 7** (Characterisation of bd-KSD). Let $\bar{p}, \bar{q}$ be smooth densities defined on $\mathcal{V}$. Assume: 1) kernel $k$ is compact universal [9, Definition 2(ii)]; 2) $\mathbb{E}_{x, x' \sim \bar{q}}[h_{\bar{q}, \bar{g}}(x, x')] < \infty$; 3) $\mathbb{E}_q \|L(x)\|^2 < \infty$; 4) $g_i(x) > 0$ whenever $q(x) > 0$. Then, bd-KSD$_{\bar{g}}(\bar{q}||\bar{p}) \geq 0$ and bd-KSD$_{\bar{g}}(\bar{q}||\bar{p}) = 0$ if and only if $\bar{p} = \bar{q}$.

**Goodness-of-fit test with bd-KSD** Similar procedure as introduced in Section 2.2 applies to test the null hypothesis $H_0 : \bar{p} = \bar{q}$ against the alternative $H_1 : \bar{p} \neq \bar{q}$. Observed samples $x'_1, \ldots, x'_n \sim \bar{p}$ on $\mathcal{V}$, the empirical U-statistic [38] can be computed, bd-KSD$_{\bar{g}}(\bar{q}||\bar{p}) = \frac{1}{n(n-1)} \sum_{i \neq j} h_{\bar{q}, \bar{g}}(x'_i, x'_j)$.

The asymptotic distribution is obtained via U-statistics theory [38, 56] as follows. We denote the convergence in distribution by $\overset{d}{\rightarrow}$.

**Theorem 8.** Assume the conditions in Theorem 7 holds. 1) Under $H_0 : \bar{p} = \bar{q}$,

$$n \cdot \text{bd-KSD}_{\bar{g}}(\bar{q}||\bar{p})^2 \overset{d}{\rightarrow} \sum_{j=1}^{\infty} w_j (Z_j^2 - 1),$$

where $Z_j$ are i.i.d. standard Gaussian random variables and $w_j$ are the eigenvalues of the Stein kernel $h_{\bar{q}, \bar{g}}(x, x')$ under $\bar{p}(x')$: $\int_{\mathcal{V}} h_{\bar{q}, \bar{g}}(x, x') \phi_j(x') \bar{q}(x') \mathrm{d}x' = w_j \phi_j(x)$, where $\phi_j(x) \neq 0$ is the non-trivial eigen-function for Stein kernel operator $h_{\bar{q}, \bar{g}}$. 2) Under $H_1 : \bar{p} \neq \bar{q}$,

$$\sqrt{n} \cdot (\text{bd-KSD}_{\bar{g}}(\bar{q}||\bar{p})^2 - \text{bd-KSD}_{\bar{g}}(\bar{q}||\bar{p})^2) \overset{d}{\rightarrow} \mathcal{N}(0, \sigma^2),$$

where $\sigma^2 = \text{Var}_{x \sim \bar{p}}[\mathbb{E}_{z \sim \bar{q}}[h_{\bar{q}, \bar{g}}(x, z)]] > 0$ produces the non-degenerate $U$-statistics.

The goodness-of-fit testing then follows the standard procedures in Section 2.3 by applying bd-KSD.

4.3 Case studies: truncated distributions and compositional data

We first consider the distributions with truncated boundaries. In Fig. 1 (left), an example of two-component Gaussian mixture truncated in a unit ball is plotted in $B_1(\mathbb{R}^2)$. It is obvious that the density $q(x)$ does not necessarily vanish at the truncation boundary. Truncated distributions, including truncated Gaussian distributions [26, 27], truncated Pareto distributions [2], or truncated power-law distributions [15] have been studied. In particular, left-truncated distributions are of special interest in survival analysis [35]. To the best of our knowledge, goodness-of-fit testing procedures for general truncated distributions has not yet been established.

We also consider the compositional data where the distribution is defined on a simplex, $S^{d-1} = \{x^d \in [0,1], \sum_{i=1}^d x^i = 1\}$, which is a compact domain. A common example for compositional distribution is the Dirichlet distribution, with unnormalised density of the form $\tilde{q}(x) \propto \prod_{i=1}^d (x^i)^{\alpha_i - 1}, \forall x \in S^{d-1}$, where $\alpha_i > 0$ are the concentration parameters. An example Dirichlet distribution
We include additional simulation results and insights on effect of different $p$ which relates to the Euclidean distance from the boundary raising to chosen power where samples are generated from the null model and a two-sample test is then performed. Such strategy to test goodness-of-fit has been considered previously \cite{31, 58}.

**Truncated Distribution in Unit Ball**

Requiring to vanish at the boundary and take into account the rotational invariance of the unit ball, the auxiliary functions can be chosen as $g_i^{(1)}(x) = 1 - ||x||^p$, which relates to the Euclidean distance from the boundary raising to chosen power $p$. Similar form of auxiliary function, with $p = 1$, was discussed for density estimation on truncated domains\cite{47}. For larger $p$, more weights are concentrated to the center of the ball. We present the case where the null is 2-component mixture of Gaussian with identity variance and the alternative with correlation coefficient perturbed by $\nu$. In this case, the difference between the null and alternative distributions are concentrated towards the center, making $g^{(1)}$ based bd-KSD a better test as shown in Table. 1.

**Compositional Distributions:** With boundary definition $D_i = \{x| x^i = 0\}$, a natural choice of auxiliary function $g$ is more sensitive on the boundary where distributions are more different, bd-KSD based on $g^{(1)}$ produces higher power as shown in Table. 1.

Moreover, results in Table. 1 also show that bd-KSD based tests outperforms the MMD based tests. We include additional simulation results and insights on effect of different $g$ choice in Appendix C.

**Real data experiments**

We illustrate real-data testing scenarios for the presented case studies.

1) **Chicago Crime Dataset**\cite{7} We consider the relevant score-matching based objective, TruncSM \cite{47}, to fit the Gaussian mixture model, using half of the data and test on the other half. We set $\alpha = 0.01$; repeat 200 trials. Bold number indicates the best power performance.

| Test Powers  | Truncated in $B_1(\mathbb{R}^d)$ | Compositional Data on $S^2$ |
|--------------|---------------------------------|-----------------------------|
| $\nu = 0.1$  | 0.235                           | 0.430                        |
| $\nu = 0.3$  | 0.760                           | 0.715                        |
| $\nu = 1.0$  | 1.000                           | 0.905                        |
| bd-KSD($g^{(1)}$) | 0.235 | 0.430 |
| MMD          | 0.045                           | 0.090                        |


2) **Three-composition AFM of 23 aphyric Skye lavas data**\cite{3} The variables A, F and M represent the relative proportions of $Na_2 + K_2O$, $Fe_2O_3$ and $MgO$, respectively. We fit the Gaussian kernel density estimation \cite{10}, using half of the data and test on the other half. We choose the auxiliary function $g^{(2)}$, the min distance to the closest boundary. The bd-KSD gives p-value 0.004 which rejects the null hypothesis, indicating the fit is not good enough.

**Conclusion and discussions**

The present work proposes a general framework to unify and compare the existing KSD-based tests; as well as to design new KSD-based tests. Our empirical results for testing data with domain constraint validate our claim that Stein operators can have considerable effect on the test performances of KSD-based tests. Beyond, more rigorous treatment on choice of $g$ can be an interesting future direction.

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\footnote{Specifically, $q(x) = 0$ at boundary $D_i = \{x | x^i = 0\}$ for $\alpha > 1$; while $q(x) > 0$ on $D_i$ for $\alpha \in (0, 1)$.}

\footnote{Data can be found at \url{https://data.cityofchicago.org}.}
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A Known Identities

Expectations in Survival Analysis

We know the following identities in survival analysis, which will be useful for discussions in the main text: for any measurable function $\phi$,

$$
\mathbb{E}_0[\Delta \phi(T)] = \int_0^\infty \phi(s) \mu_0(s) S_C(s) \, ds,
$$

(16)

$$
\mathbb{E}_0[(1 - \Delta) \phi(T)] = \int_0^\infty \phi(s) \mu_C(s) S_0(s) \, ds.
$$

(17)

where $\mu_C$ here denotes the p.d.f. of the censoring distribution and $S_0$ denotes the survival function w.r.t. $\mu_0$.

Martingales in Survival Analysis

The following identity is useful to understand the martingale Stein operator in [18]

$$
\mathbb{E}_0 \left[ \Delta \phi(T) - \int_0^T \phi(t) \lambda_0(t) \, dt \right] = 0,
$$

(18)

which holds under the null hypothesis, where $\lambda_0$ is the hazard function under the null $\mu_0$. Let $N_i(x)$ and $Y_i(x)$ be the individual counting and risk processes, defined by $N_i(x) = \delta_i \mathbb{1}_{\{T_i \leq x\}}$ and $Y_i(x) = \mathbb{1}_{\{T_i \geq x\}}$, respectively. Then, the individual zero-mean martingale for the $i$-th individual corresponds to

$$
M_i(x) = N_i(x) - \int_0^x Y_i(y) \lambda_0(y) \, dy,
$$

where $\mathbb{E}_0[M_i(x)] = 0$ for all $x$.

Additionally, let $\phi : \mathbb{R}_+ \to \mathbb{R}$ such that $\mathbb{E}_0 \left| \int_0^x \phi(y) \, dM_i(y) \right| < \infty$ for all $x$, then $\int_0^x \phi(y) \, dM_i(y)$ is a zero-mean $(\mathcal{F}_x)$-martingale (see Chapter 2 of [1]). Then, taking expectation, we have

$$
\mathbb{E}_0 \left[ \int_0^\infty \phi(x) \, dM_i(x) \right] = \mathbb{E}_0 \left[ \int_0^\infty \phi(x) (dN_i(x) - Y_i(x) \lambda_0(x) \, dx) \right]
$$

$$
= \mathbb{E}_0 \left[ \Delta \phi(T) - \int_0^T \phi(x) \lambda_0(x) \, dx \right] = 0,
$$

as stated above. The martingale property is useful to derive the martingale Stein operator in Eq. (4). For more details, see [18].

B Proofs and Derivations

Proof of Proposition 1

Proof. Standard reproducing properties and taking the supremum over unit ball RKHS apply,

$$
\text{GKSD}_g(p\|q; \mathcal{H}) = \sup_{\|f\|_{\mathcal{H}} \leq 1} \mathbb{E}_p[\langle T_{q,g} K(x, \cdot), f \rangle_{\mathcal{H}}] = \|\mathbb{E}_p[T_{q,g} K(x, \cdot)]\|_{\mathcal{H}}.
$$

Specifically, assume $f_i(x) = (k(x, \cdot), f_i)$, the setting in [13, 46],

$$
T_{q,g} K(x, \cdot) = \sum_{i=1}^d g_i(x) \left( \frac{\partial \log q(x)}{\partial x^i} k(x, \cdot) + \frac{\partial k(x, \cdot)}{\partial x^i} \right) + \frac{\partial g_i(x)}{\partial x^i} k(x, \cdot).
$$
We can write \( h_{q,g}(x, \tilde{x}) \) explicitly as
\[
\begin{align*}
    h_{q,g}(x, \tilde{x}) = & \sum_{i=1}^{d} \left( \frac{\partial^2 k(x, \tilde{x})}{\partial x^i \partial \tilde{x}^i} + \frac{\partial \log q(x)}{\partial x^i} \frac{\partial k(x, \tilde{x})}{\partial \tilde{x}^i} + \frac{\partial \log g(\tilde{x})}{\partial \tilde{x}^i} \frac{\partial k(x, \tilde{x})}{\partial x^i} + \frac{\partial \log q(x)}{\partial x^i} \frac{\partial \log q(\tilde{x})}{\partial \tilde{x}^i} k(x, \tilde{x}) \right) \\
    & \cdot g_i(x) g_i(\tilde{x}) + \frac{\partial g_i(x)}{\partial x^i} \frac{\partial g_i(\tilde{x})}{\partial \tilde{x}^i} k(x, \tilde{x}).
\end{align*}
\]
which recovers the quadratic form, which only depends on density \( q \) but not \( p \).

Proof of Theorem 2

Proof. Note that the expectation on l.h.s. of Eq. (13) is integrating over the density of survival time \( \mu_0 \) where the expectation on the r.h.s., having the multiplication of \( \delta \) in \( T_{0}\omega \) in Eq. (2), is taken over the paired observation incorporating censoring information. Using the identity in Eq. (17), we have
\[
    \mathbb{E}_{\mu_0}[T_{\mu_0, \delta}\omega] = \int_{\mathbb{R}^+} T_{\mu_0, \delta}\omega(s) \mu_0(s) ds
\]
\[
    = \int_{\mathbb{R}^+} \left( \omega'(s) + \omega(s) \frac{g'(s)}{g(s)} + (\log \mu_0(s))' \right) g(s) \mu_0(s) ds
\]
\[
    = \int_{\mathbb{R}^+} \left( \omega'(s) + \omega(s) \frac{S_C(s)}{S_C(s)} + \omega(s) \mu_0(x)' \right) \mu_0(s) S_C(s) ds
\]
\[
    = \int_{\mathbb{R}^+} \omega'(s) S_C(s) \mu_0(s) + \omega(s) S_C'(s) \mu_0(s) + \omega(s) S_C(s) \mu_0(x)'
\]
\[
    = \int_{\mathbb{R}^+} S_C(s) \mu_0(s) = (T_0\omega)(x, \delta) \mu_0(x) S_C(x) ds = \mathbb{E}_{0}[T_0\omega](x, \delta) = 0.
\]
We also note that \( S_C(0) = 1, S_C(\infty) = 0 \) by definition of survival functions. As such, \( g(x) \) is bounded almost everywhere in \( \mathbb{R}^+ \) which satisfy the conditions for testing.

Proof of Theorem 2

Proof. To show the equivalence relation in the sense of Eq. (14), we need to consider the presence of indicator variable \( \delta \). This is essentially different from the proof of Theorem 1. Recall the following identity between hazard function and density: \( \log \mu_0(s) = \frac{\mu_0'(x)}{\mu_0(x)} = \frac{\lambda_0'(x)}{\lambda_0(x)} - \lambda_0(x) \) since
\[
    \frac{\lambda_0'(x)}{\lambda_0(x)} = \frac{\mu_0'(x)}{S_0(x) \lambda_0(x)} + \frac{\mu_0(x)}{S_0(x) \lambda_0(x)} = \frac{\mu_0'(x)}{\mu_0(x)} + \lambda_0(x).
\]
Denote \( \zeta(x) = \frac{\int_0^t \mu_0(s) \omega(s) ds}{\mu_0(x) \omega(x)} \), such that we can write \( g = \delta \lambda_0^{-1} + (1 - \delta) \zeta \). Decompose the Stein operator \( T_{\mu_0, \delta} \) w.r.t. \( \delta \), we have
\[
    T_{\mu_0, \delta}\omega = \delta T_{\mu_0, \lambda_0^{-1}}\omega + (1 - \delta) T_{\mu_0, \zeta}\omega
\]
as \( T_{\mu_0} \) is also linear operator w.r.t \( g \). We now decompose the above two components \( T_{\mu_0, \lambda_0^{-1}} \) and \( T_{\mu_0, \zeta} \) using the form of Eq. (10),
\[
    T_{\mu_0, \lambda_0^{-1}}\omega = \lambda_0^{-1} \left( \omega' + \omega \log \mu_0' \right) + \lambda_0^{-1} \omega
\]
\[
    = \lambda_0^{-1} \left( \omega' + \omega \frac{\lambda_0'(x)}{\lambda_0(x)} - \lambda_0(x) \right) + \lambda_0 \lambda_0^{-1} \omega
\]
\[
    = \lambda_0^{-1} \left( \omega' + \omega \lambda_0 - \lambda_0 \right)
\]
\[
    = \lambda_0^{-1} \omega' - \omega
\]
the second line equality follows from Eq. (19) while the third line follows from $\lambda_0^{-1'} = -\frac{\lambda_0'}{\lambda_0}$. The derivation is interesting that it reveals that the uncensored data in the martingale Stein operator is connected to the Langevin-diffusion via the inverse of hazard function, i.e. when $\delta \equiv 1$ (or absence of censoring), $T_{\mu_0, \lambda_0^{-1}} \omega = T_0^{(m)} \omega$.

On the other hand, we rewrite the martingale Stein operator in Eq. (4) as $(T_0^{(m)} \omega)(x, \delta) = \delta \frac{\omega'(x)}{\lambda_0(x)} - \omega(x) = \delta \left( \frac{\omega'(x)}{\lambda_0(x)} - \omega(x) \right) - (1 - \delta) \omega(x)$. For GKSD to match this operator, we need to find $\zeta$ such that $T_{\mu_0, \zeta} \omega = \omega$. $T_{\mu_0, \zeta} \omega = \omega (\zeta' + \zeta \log \mu_0) + \omega' \zeta = \omega (\zeta' + \zeta \log \mu_0' + \zeta (\log \omega)' = -\omega.$ \hspace{1cm} (21)

As $\omega(x) > 0$ for $\mu_0(x) > 0$ for $x > 0$, Eq. (21) gives the following autonomous differential equation form
\[ \zeta' = -\zeta (\log \mu_0' + \log \omega') - 1, \] \hspace{1cm} (22)
solving which yields
\[ \zeta(x) e^{\log \mu_0(x)} + \log \omega(x) = \int_0^x e^{\log \mu_0(s)} + \log \omega(s) ds \]
\[ \zeta(x) \mu_0(x) \omega(x) = \int_0^x \mu_0(s) \omega(s) ds \]
as $\omega(0) = 0$ by assumption. $\zeta(x) = \int_0^x \frac{\mu_0(s) \omega(s) ds}{\mu_0(x) \omega(x)}$ as proposed. Putting together, we have
\[ T_{\mu_0, g\omega} = \delta T_{\mu_0, \lambda_0^{-1}} \omega + (1 - \delta) T_{\mu_0, \zeta} \omega = \delta \left( \frac{\omega'(x)}{\lambda_0(x)} - \omega(x) \right) - (1 - \delta) \omega = T_0^{(m)} \omega \]
and the Stein’s identity result follows by taking the expectation of the same form, $E_0[T_{\mu_0, g\omega}] = E_0[T_0^{(m)} \omega] = 0$. \qed

Proof of Corollary 1

**Proof.** The proof follows from decomposing the survival Stein operator $T_0^{(s)} \omega$ in to the uncensored part and censored part, similar to Eq. (20).

\[ (T_0^{(s)} \omega)(x, \delta) = \delta \omega'(x) + \delta \omega(x) - \omega(x) \lambda_0(x) = \delta \omega'(x) + \delta \omega(x) - \omega(x) \lambda_0(x) \]
\[ = \delta \omega'(x) + \delta \omega(x) - \omega(x) \left( \frac{\lambda_0'(x)}{\lambda_0(x)} - \lambda_0(x) \right) - (1 - \delta) \omega(x) \lambda_0(x) \]
\[ = \delta \omega'(x) + \delta \omega(x) \frac{\mu_0'(x)}{\mu_0(x)} - (1 - \delta) \omega(x) \lambda_0(x) \]
\[ = \delta \left( \omega'(x) + \omega(x) \log \mu_0(x)' \right) - (1 - \delta) \omega(x) \lambda_0(x). \]

where the term involving $\delta$, the uncensored part, is just the Langevin-diffusion Stein operator in 1d. Similar to Eq. (21), we solve the following autonomous differential equation for the censored part,
\[ T_{\mu_0, \zeta} \omega = \omega (\zeta' + \zeta \log \mu_0' + \zeta (\log \omega)' = -\omega \lambda_0. \] \hspace{1cm} (23)
which simplifies to
\[ \zeta' = -\zeta (\log \mu_0' + \log \omega') - \lambda_0. \hspace{1cm} (24) \]
Solving the differential equation with boundary condition $\omega(0) = 0$, we get $\zeta(x) = \int_0^x \frac{\mu_0(s) \omega(s) \lambda_0(s) ds}{\mu_0(x) \omega(x)}$. As such, using $g = \delta + (1 - \delta) \zeta$, the result follows
\[ T_{\mu_0, g\omega} = \delta T_{\mu_0} \omega + (1 - \delta) T_{\mu_0, \zeta} \omega = (T_0^{(s)} \omega)(x, \delta). \] \qed
which is the second-order operator in 1d.

where equality (a) uses the marginalisation and equality (b) utilises the fact that differential form defined in the main text. Similar derivation as Eq. (25) above, we have

For the multivariate case, choosing $g: \mathbb{R}^d \to \mathbb{R}^d$ such that $g_i(x) = \frac{\partial}{\partial x^i} f_i(x) \partial x^i$, where $\partial x^i$ is the differential form defined in the main text. Similar derivation as Eq. (25) above, we have

Remarks In the main text, we discussed the advantages and disadvantages of KSD-based test with $T_0^{(m)}$ and $T_0^{(s)}$, which corroborate the empirical findings in [18]. Moreover, [18] studied the testing procedure via c.d.f. transformation followed by testing the uniform null density, which they call model-free implementation. This procedure has been shown to achieve higher test power. Similar testing strategy via c.d.f. transformation has been studied in [17] using MMD-based test. Notice that since $F_0$ is monotone and $u_i = F_0(t_i) = \min \{ F_0(x_i), F_0(c_i) \}$, thus $\delta_i$ remains consistent. Under this transformation, the null hypothesis is equivalent to test whether $F_0(x_i)$ is distributed as a uniform random variable. In this setting, the observations for the test is based on $\{ (u_i, \delta_i) \} \in \mathbb{N}$, where the Stein operator used is independent of density of $x \sim f_0$. Instead, $\mu_0(u) = 1$ and $\lambda_0 = \lambda_\mu = \frac{1}{1-x}$ are used to construct the Stein operator and

$$\left(T_0^{(m)} \omega\right)(u, \delta) = \delta \omega'(u)(1 - u) - \omega(u)$$

for $u = F_0(x)$ (notice that $F_0(0) = 0$). From our result, we see that with the particular choice of the uniform null, there is no more interaction between test function and density in the censored part, e.g.

$$\zeta(x) = \int_0^x \frac{\omega(s)/(1-x)ds}{\omega(x)}$$

resulting a better estimation accuracy from the samples, thus higher test power.

Similarly, [18] exploited another monotone transformation via the cumulative hazard function from the null $\Lambda_0$, such that $\Lambda_0(X) \sim \text{Exp}(1)$. In this case, $\mu_0(x) = \exp(-x)$ which still require interaction between $\mu_0$ and $\lambda_0$ in $\zeta$, resulting in decrease in estimation accuracy. Our results explain the empirical finding in [18] that the test power from the model-free implementation of the test using cumulative hazard transformation is not higher than using the c.d.f. transformation.

Proof of Theorem 3

Proof. As $g_i$ consists of finite sum of delta measures on locations $z_j$ sampled from $q(z|x)$, it’s derivative is 0 everywhere excluding a finite number of points which is a set of measure zero. Recall that the marginalisation of the density $q(x) = \int q(x, z)dz$, $E_q[T_{q,z}f] = \int \sum_i T_q(g_i(x)f_i(x))q(x, z)dx dz$

$$\overset{(a)}{=} \int_x \sum_i \left[ \int \left( \log q(x)^g(x_i, f_i(x)) + (g_i^g(x) f_i(x))^\prime \right) q(x|z)dx \right] \pi(z)dz$$

$$\overset{(b)}{=} \frac{1}{m} \sum_i \int_x \sum_j \left[ \log q(x|z_j)^g f_i(x) + f_i(x)^\prime \right] q(x|z_j)dx$$

$$= \frac{1}{m} \sum_j E_q[q(z_j)]t_q[z_j] = E_q[T_{q,z}f]$$

where equality (a) uses the marginalisation and equality (b) utilises the fact that $z_j$ are samples from $q(z|x) \propto \pi(z)q(x|z)$.

It is also worth to note that, the average on taking expectations over Stein operators for conditional operator does not involve a notion of auxiliary function $g$. This corresponds to the fact that $z$-dependent auxiliary function $g$ here is independent of $x$ and the derivative w.r.t. $x$ vanishes.

Proof of Theorem 4

Proof. It is not difficult to see that

$$T_q(fg) = T_q(f\log f)^\prime = T_q(f^\prime) = f^\prime + \log q f^\prime$$

which is the second-order operator in 1d.

For the multivariate case, choosing $g: \mathbb{R}^d \to \mathbb{R}^d$ such that $g_i(x) = \frac{\partial}{\partial x^i} f_i(x) \partial x^i$, where $\partial x^i$ is the differential form defined in the main text. Similar derivation as Eq. (25) above, we have

$$T_{q,g}(\mathbf{f}) = \sum_i T_q(\frac{\partial}{\partial x^i} \log f_i) f_i = \sum_i \frac{\partial^2}{\partial x^i} f_i \partial x^i + \log q \frac{\partial}{\partial x^i} f_i \partial x^i = T_q \nabla \cdot \mathbf{f}.$$
Proof of Theorem 7

Proof. The Theorem extends from [13, Theorem 2.2] with additional assumptions \( q_i(x) > 0 \) if \( q(x) > 0 \), together with appropriate compact universality condition for the kernel. For more general settings, having a proper notion of universal kernel would extend Theorem 7 to show that GKSD is a proper discrepancy in desired testing scenarios.

Denote \( s_{q,g}(\cdot) = \mathbb{E}_{x \sim p}[T_{q,g}k(x, \cdot)] \in \mathcal{H} \) and we can write the quadratic form bd-KSD as bd-KSD\(_g(q||p)\) = \( ||s_{q,g}(\cdot)||^2 \geq 0 \). If \( p = q \), then bd-KSD\(_g(q||p)\) = 0 from the Stein’s identity.

Conversely, if bd-KSD\(_g(q||p)\) = 0, then \( s_{q,g}(x) = 0 \), \( \forall x \), s.t. \( p(x) > 0 \). Then, from \( \log(q/p) = \log(\tilde{q}) - \log(\tilde{p}) \), we obtain,

\[
\mathbb{E}_{x' \sim \tilde{p}} [L_i(x')k(x', x)] = (s_{q,g})_i(x) - \mathbb{E}_{x' \sim \tilde{p}} \left[ T_{q,g}k(x', x) \right] = 0,
\]

for every \( x \) with positive densities. As \( g_i(x) > 0 \) for \( q(x) > 0 \), and \( k \) is compact-universal at \( V \), the injectivity result in [9, Theorem 4(b)] implies that \( L_i = 0 \), \( \forall i \in [d] \). Therefore, \( \log(q/p) \) is constant on \( V \). Since both \( \tilde{p} \) and \( \tilde{q} \) are both densities on \( V \) that integrate to one, we conclude \( \tilde{p} = \tilde{q} \).

C Additional Simulation Results

We investigate the test performances on various problems, comparing different choice of \( g \). In the following problems, we apply the Gaussian kernel with median distance as bandwidth [24].

1. Truncated Gaussian distribution in \( B_1(\mathbb{R}^3) \)

\[
\tilde{q}_\nu(x) \propto \mathcal{N}(x|0, \Sigma_\nu), \forall x \in B_1(\mathbb{R}^3), \Sigma_\nu = \begin{pmatrix} 1 + \nu & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}
\]

where \( \nu > -1 \). We test the null model \( \tilde{q}_0 \) against the alternative \( \tilde{q}_1 \) with perturbation of variance parameter \( \nu = 1.0 \). The test power of bd-KSD, with different choice of \( g^{(p)} \), is shown in Fig. 2(a).

All tests have increasing test powers as the simple size increases, which is what we expect. As the alternative is having variance difference in the first direction \( x^1 \), the test captures such difference better when more weights are put on near the origin (refer Fig. 2(d) for \( g(x) \) values). Hence, the test power increases with the increase of parameter \( (p) \) for auxiliary function \( g^{(p)} \). For \( p > 1 \), the bd-KSD tests outperforms the MMD test\(^8\).

|      | n=100  | n=400  | n=700  | n=1000 |
|------|--------|--------|--------|--------|
| bd-KSD(p=4) | 0.004  | 0.010  | 0.030  | 0.018  |
| bd-KSD(p=2) | 0.008  | 0.018  | 0.022  | 0.012  |
| bd-KSD(p=1) | 0.010  | 0.016  | 0.020  | 0.028  |
| bd-KSD(p=0.5) | 0.006  | 0.008  | 0.010  | 0.030  |
| MMD      | 0.022  | 0.014  | 0.018  | 0.032  |
| KSD\(_g(x) \equiv 1\) | 1.00   | 1.00   | 1.00   | 1.00   |

Table 2: Rejection rate under the null; \( \alpha = 0.01 \); 500 trials.

The rejection rate under the null is reported in Table 2. The bd-KSD tests, with appropriately choice of \( q \) incorporating the boundary conditions, achieve well-controlled Type-I errors. MMD-based tests also achieves the well-controlled Type-I errors. However, applying the KSD tests in Eq. (9) are unable to have controlled test level due to the violation of Stein’s identity, which is what we expect.

2. Truncated Gaussian mixture in \( B_1(\mathbb{R}^3) \)

\[
\tilde{q}_\nu(x) \propto \frac{1}{2} \mathcal{N}(x|\mu_1, \Sigma_\nu) + \frac{1}{2} \mathcal{N}(x|\mu_2, \Sigma_\nu), \forall x \in B_1(\mathbb{R}^3),
\]

\(^8\)For all MMD-based tests, we draw \( n \) samples from the null samples when the sample size of observed data is \( n \).
where \( \mu_1 = (-1, 0, 0), \mu_2 = (1, 0, 0) \) and \( \Sigma_\nu \) (as defined above) is shared between two components. We test the null model \( q_0 \) against the alternative \( \tilde{q} - \frac{1}{2} \). The test power with increasing sample size is shown in Fig. 2(b). Similar as the previous case, the bd-KSD of \( g(p) \) with larger parameter value \( p \) achieves better test power. MMD-based tests perform slightly better that bd-KSD with \( g^{(1)} \). However, MMD suffers from slow computational time due to the sampling procedure in a bounded domain, as shown in Fig. 2(c).

We test the null model \( q_0 \) against the alternative \( q_{1,0.3} \) with perturbation of the concentration parameter in the first dimension \((x^1)\). The test power of bd-KSD, with the choice of geometric mean function \( g^{(1)} \) and the minimum distance-to-boundary function \( g^{(2)} \), and the MMD-based test are shown in Fig. 3. From the result, we see that the bd-KSD tests have higher test power compared to MMD-based test power. The test power increases as sample size increases (Fig. 3 left) and decreases as the dimension of the problem increases (Fig. 3 right), which is what would we expect. We also see that geometric mean function \( g^{(1)} \) induces a better Stein operator for bd-KSD testing on compositional data compared to the minimum distance-to-boundary function \( g^{(2)} \).

### 3. Dirichlet distributions in \( S^{d-1} \)

\[
\tilde{q}_\nu(x) \propto (x^1)^\nu \cdot \Pi_{i=1}^{d-2} (x^i)^{(-0.5)}, \forall x \in S^{d-1}
\]

We test the null model \( \tilde{q}_0 \) against the alternative \( q_{0,0.3} \) with perturbation of the concentration parameter in the first dimension \((x^1)\). The test power of bd-KSD, with the choice of geometric mean function \( g^{(1)} \) and the minimum distance-to-boundary function \( g^{(2)} \), and the MMD-based test are shown in Fig. 3. From the result, we see that the bd-KSD tests have higher test power compared to MMD-based test power. The test power increases as sample size increases (Fig. 3 left) and decreases as the dimension of the problem increases (Fig. 3 right), which is what would we expect. We also see that geometric mean function \( g^{(1)} \) induces a better Stein operator for bd-KSD testing on compositional data compared to the minimum distance-to-boundary function \( g^{(2)} \).

### D Generalising Learning Objective for Unnormalised Models

Beyond generalising existing Stein operators, GKSD with the generalised Stein operator in the form of Eq. (10) can also help us to understand learning objectives for unnormalised models such as score matching, when appropriate choice of auxiliary function and kernel function are chosen.

Recall the score matching objective [29],

\[
J(p||q) = \mathbb{E}_p \left[ (\log p(x)' - \log q(x)')^2 \right].
\]

(26)

\( J(p||q) \geq 0 \) and the equality holds if and only if \( p = q \) under mild regularity conditions [29].

#### GKSD Recovers Score Matching

The discrepancy measure in score matching objective is constructed via the squared difference between derivative of log densities, without the presence of test function as opposed in the KSD-type of discrepancy measure. Hence, instead of just specifying the auxiliary function \( g \) to recover various
We note that the choice of auxiliary function $g$ in the previous results, we need specific kernel function here to recover the score matching objective.

Proof of Theorem 6

Proof. We rewrite $g$ in the form involving density ratio between $q$ and $p$, such that

$$g = \frac{q}{p} \cdot \frac{\sqrt{p}}{\xi}.$$ 

Then we can write the GKSD of the following form,

$$\text{GKSD}_{q}(q||p) = \mathbb{E}_{p}[(\log q(x))'((f\xi)(x) + (f\xi)'(x)) \frac{q}{p}(x)] + \mathbb{E}_{p}[(f\xi)(x)\frac{q}{p}'(x)]$$ 

$$= \mathbb{E}_{q}[(\log q(x))'((f\xi)(x) + (f\xi)'(x)) \frac{q}{p}(x)] + \mathbb{E}_{p}[(f\xi)(x)\frac{q}{p}'(x)]$$ 

$$= \mathbb{E}_{p}[\frac{f(x)}{\sqrt{p(x)}}((\log q(x))' - (\log p(x))')]$$ 

The first expectation is 0 under Stein’s identity of operator in Eq. (10) and the second expectation follows from

$$\left(\frac{q(x)}{p(x)}\right)' = \frac{q'}{p}(x) - \frac{qp'}{p^2}(x) = \frac{q}{p}((\log q(x))' - (\log p(x))')$$

For the RKHS $\mathcal{H}$ equipped with $\delta$-type kernel\(^9\), $k(x, \tilde{x}) = \delta_{x=\tilde{x}}$, we recover the original score-matching objective in [29] since

$$\sup_{f \in \mathcal{H}} \mathbb{E}_{p}[\frac{f(x)}{\sqrt{p(x)}}((\log p(x))' - (\log q(x))')] = \mathbb{E}_{p}[k(x, \cdot)((\log p(x))' - (\log q(x))')]$$

$$= \mathbb{E}_{x, \tilde{x} \sim p}\left[\frac{k(x, \tilde{x})}{\sqrt{p(x)p(\tilde{x})}}((\log p(x))' - (\log q(x))')(\log p(\tilde{x}))' - (\log q(\tilde{x}))')\right]$$

$$= \int \int \frac{\delta_{x=\tilde{x}}}{\sqrt{p(x)p(\tilde{x})}}((\log p(x))' - (\log q(x))')(\log p(\tilde{x}))' - (\log q(\tilde{x}))')p(x)p(\tilde{x})dxd\tilde{x}$$

$$= \int \int \frac{1}{p(x)}((\log p(x))' - (\log q(x))')^2p(x)^2dxdx = \mathbb{E}_{p}[(\log p(x))' - (\log q(x))']^2].$$

We note that the choice of auxiliary function $g$ here depends on the data density $p$, which is unknown in practice. Score matching relied on the following result for estimating the empirical version of the objective [29],

$$J(p||q) = \mathbb{E}_{p}[(\log p(x) - \log q(x))']^2 = \mathbb{E}_{p}\left[\log q(x)' + \frac{1}{2} \log q(x)''\right].$$

E Kernel Discrete Stein Discrepancy

In this section, we briefly review the kernel discrete Stein discrepancy (KDSD) introduced in [60]. First we need some definitions.

\(^9\)We note that this kernel is not bounded but integrally bounded by probability density. Note that, this particular formulation echos [7, Theorem 10], where the $\delta$ measure is treated as limit of vanishing bandwidth.
Definition 1. [Definition 1 [60]] (Cyclic permutation). For a set X of finite cardinality, a cyclic permutation \( \pi : X \rightarrow X \) is a bijective function such that for some ordering \( x[1], x[2], \ldots, x|X| \) of the elements in X, \( \pi(x[i]) = x[(i + 1) \mod |X|], \forall i = 1, 2, \ldots, |X| \).

Definition 2. [Definition 2 [60]] Given a cyclic permutation \( \pi \) on X, for any d-dimensional vector \( x = (x_1, \ldots, x_d) \top \in X^d \), write \( \pi \circ x := (x_\pi(1), x_\pi(2), \ldots, x_\pi(d)) \top \). For any function \( f : X^d \rightarrow \mathbb{R} \), denote the (partial) difference operator as

\[
\Delta_x f(x) := f(x) - f(\pi(x)), \quad i = 1, \ldots, d
\]

and introduce the difference operator:

\[
\Delta_\pi f(x) := (\Delta_{x_1} f(x), \ldots, \Delta_{x_d} f(x))\top.
\]

Here we use the notation \( \Delta_\pi \) to distinguish it from the notation in the main text, where we used \( \Delta_s \) to denote the (partial) difference operator as

\[
\Delta_s f(x) := f(x) - f(\pi s(x)) = f(x) - f(x_{\pi s(0)}) = f(x) - f(x_{\pi s(1)}).
\]

For discrete distributions \( q, [60] \) propose the following discrete Stein operator, which is based on the difference operator \( \Delta_\pi \) constructed from a cyclic permutation:

\[
\mathcal{A}_q^D f(x) = f(x) \frac{\Delta_q(x)}{|q(x)|} - \Delta_\pi^* f(x),
\]

where \( \Delta_\pi^* \) denotes the adjoint operator of \( \Delta_\pi \).

In [60], the generalisation that better characterises the density \( q \) is stated in the following form,

\[
\mathcal{A}_{q, \mathcal{L}} f(x) = f(x) \frac{\mathcal{L} q(x)}{|q(x)|} - \mathcal{L}^* f(x),
\]

where \( \mathcal{L}^* \) is the adjoint operator of \( \mathcal{L} \).

F Stochastic Stein Discrepancy

[22] proposed stochastic Stein discrepancy (SSD) via the following subset operators.

Given prior \( \pi_0 \), likelihood \( \pi(\cdot|x) \) and samples \( y_1, \ldots, y_L \), the posterior density \( q(x) \propto \pi_0(x)^{1/L} \prod_{l=1}^{L} \pi(y_l|x) \). With uniformly sampled index set \( \sigma \subset [L] \) with \( |\sigma| = m \), the stochastic Stein operator is defined as

\[
T_\sigma f(x) = \frac{L}{m} f(x)\top \nabla \log q_\sigma(x) + \nabla \cdot f(x)
\]

for test function \( f \) and \( q_\sigma(x) := \pi_0(x)^{m/L} \prod_{l \in \sigma} \pi(y_l|x) \). The stochastic Stein variational gradient descent (SSVGD) is then developed for sampling procedures and nice convergence properties has been shown in [22].

where the latent samples \( z_j \) are functionally analogous to the observations \( y_l \) in SSD. The key difference is that for every single \( x \) in SSD, multiple \( y_l \) acts on it; while for latent Stein operator, only one \( z_j \) acts on it at a time.

G Additional Generalisation

The choice of the Langevin-diffusion type of Stein operator in Section 2.1 is not unique and many other Stein operators can characterise the same distribution. A particular method to generalise the Stein operator in Eq. (1), is via an appropriate linear operator \( \mathcal{L} \) acting on the test function \( f \), i.e.

\[
T_{q, \mathcal{L}} f = T_q(\mathcal{L} f) = \mathcal{L} f\top \nabla \log q + \nabla \cdot \mathcal{L} f.
\]

Some related ideas involving \( \mathcal{L} \) to generalise learning objectives for unnormalised model have been discussed in the context of score matching [49]. [60] suggests similar formulation for characterising discrete KSD, while not yet investigated.

\(10\) In [49], \( \mathcal{L} \) acts on density \( q \) instead of the test function \( f \) here, where a common choice of \( \mathcal{L} \) is marginalization operator.

\(11\) In [60], \( \mathcal{L} f(x) = \sum_{x'} l(x, x') f(x') \), for discrete variable \( x \) and bivariate function \( l \). Different from [49], \( \mathcal{L} \) may act on both the probability mass function or the test function. For the particular form of discrete KSD studied in [60] \( \mathcal{L} \) is chosen as the partial difference operator, which is essentially different from the diffusion based generalisation in Eq. (34) for continuous variables. More details are included in Appendix E.
In the presented work, we focus on a class of new Stein operators derived from Eq. (34) where the linear operator $L$ is chosen as the element-wise product using a vector-valued function $g$ that we call the auxiliary function. Even though this is a subclass of Stein operators in Eq. (34), we show that, with specific choice of $g$, the class of Stein operators in this particular form is just enough to generalise the set of Stein operators introduced in Section 2.1.

Such formulation can be more general than the element-wise product cases developed in the main text. However, the elementwise product formulation is the simplest case to generalise existing Stein operators for goodness-of-fit test.

To see the interplay between Eq. (34) and Eq. (10). We use the generalisation of second order operator in Theorem 4 as an example. Multivariate notion utilises the $\nabla$ notation as defined in the main text. In the $\mathbb{R}^d$ case, the metric tensor terms $[\mathbf{G}^{-1}]_{ij} = \delta_{ij}$ so that the We show here the more interesting scenario for the Riemannian manifold case, where the choice of generalised Stein operator correspond to the second-order operator incorporating the Riemannian metric.

As $[\mathbf{G}^{-1}]_{ij}$ may not vanish when $i \neq j$ in the Riemannian manifold scenario, it is not possible to generalise the second-order Stein operator for Riemannian manifold with the form of Eq. (10) using elementwise product between vector-valued functions; however, with the more general formulation in Eq. (34), we are able to show this.

**Corollary 2.** For scalar test function $\tilde{f} : \mathcal{M} \to \mathbb{R}$, choosing $\mathcal{L}\tilde{f}(x) = \sum_{i,j} [\mathbf{G}^{-1}]_{ij} \frac{\partial}{\partial x^i} \tilde{f}(x) \frac{\partial}{\partial x^j}$, the Stein operator in the form of Eq. (34) recovers the second-order differential operator defined in Eq. (6) for Riemannian manifold, $\mathcal{T}_q, \mathcal{L}\tilde{f} = \mathcal{T}_q^{(2)} \tilde{f}$.

**Proof.** By definition, we know that $\mathcal{L}\tilde{f} = \nabla \tilde{f}$ incorporating the Riemannian metric $G$. Thus,

$$\mathcal{T}_q, \mathcal{L}\tilde{f} = \mathcal{T}_q \nabla \tilde{f} = \nabla \tilde{f}^T \nabla \log q(x) + \nabla \cdot \nabla \tilde{f} = \mathcal{T}_q^{(2)} \tilde{f}$$

by construction. And the $\nabla$ and $\Delta$ notation is also w.r.t. the Riemannian manifold $\mathcal{M}$ given metric tensor $G$.

We note from the Corollary 2 that, for each vector direction $\partial x^i$, it is summed over all possible differential operator, $\frac{\partial}{\partial x^i}$, acting on scalar test function $\tilde{f}$, instead of just using $\frac{\partial}{\partial x^i}$. Hence, the element-wise operation over vector-valued test function $f$ in Eq. (10) does not generalise this form. An additional note to combine the element-wise product form of Eq. (10) and the second-order Stein operator on Riemannian manifold can be the following.