Controlling Moments with Kernel Stein Discrepancies

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Abstract

Quantifying the deviation of a probability distribution is challenging when the target distribution is defined by a density with an intractable normalizing constant. The kernel Stein discrepancy (KSD) was proposed to address this problem and has been applied to various tasks including diagnosing approximate MCMC samplers and goodness-of-fit testing for unnormalized statistical models. This article investigates a convergence control property of the diffusion kernel Stein discrepancy (DKSD), an instance of the KSD proposed by Barp et al. (2019). We extend the result of Gorham and Mackey (2017), which showed that the KSD controls the bounded-Lipschitz metric, to functions of polynomial growth. Specifically, we prove that the DKSD controls the integral probability metric defined by a class of pseudo-Lipschitz functions, a polynomial generalization of Lipschitz functions. We also provide practical sufficient conditions on the reproducing kernel for the stated property to hold. In particular, we show that the DKSD detects non-convergence in moments with an appropriate kernel.

1 Introduction

Consider two probability distributions $P$ and $Q$ over $\mathbb{R}^D$, where $P$ is defined by a density function $p$ and $Q$ is arbitrary. We assume that the density $p$ may contain an unknown normalizing constant. Suppose we are interested in comparing the expectations of a test function $f_0$ under these two distributions. As a test function is usually only known up to certain properties (e.g., differentiability or growth conditions), a natural measure to consider is the worst case error, or an integral probability metric [Müller, 1997],

$$\sup_{f \in \mathcal{F}} |E_{X \sim P}[f(X)] - E_{Y \sim Q}[f(Y)]|$$

over a function class $\mathcal{F}$ containing $f_0$. This setting may be interpreted as either evaluating the goodness of fit of a statistical model $P$ against the data distribution $Q$, or assessing an approximation $Q$ to a posterior distribution $P$ in Bayesian inference. Our particular focus in this article is on continuous functions of polynomial growth. In this case, the IPM above implies disagreement in terms of moments, since they are defined by monomials of coordinates.

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As the expectations are rarely analytically tractable, one might compare empirical estimates using samples from both distributions. In some scenarios, however, assuming access to samples from $P$ may be problematic; e.g., correct samples from $P$ are unavailable if the goal is to assess the quality of a Markov chain Monte Carlo sampler $Q$ targeting intractable $P$. One possible way to sidestep the intractable integral is using a Stein discrepancy \cite{Gorham2015},

$$\sup_{g \in \mathcal{G}} \left| \mathbb{E}_{Y \sim Q} \left[ T_P g(Y) \right] \right|,$$

where $T_P$ and $\mathcal{G}$ are a Stein operator and a Stein set (a function class in the domain of $T_P$) inducing functions $T_P g$ whose expectations under $P$ are zero \cite[see Anastasiou et al., 2021, for a review]. Different choices of the operator and the function class yield distinct Stein discrepancies. Two major classes are the graph Stein discrepancies \cite{Gorham2015, Gorham2019} and the kernel Stein discrepancy (KSD) \cite{Chwialkowski2016, Liu2016, Oates2017, Gorham2017}. Notably, it is possible to compute these discrepancies: The KSD circumvents the supremum in the definition and admits a closed-form expression involving kernel evaluations on samples, whereas the graph Stein discrepancy involves solving a linear program.

While successfully avoiding the intractable expectation, a drawback of Stein discrepancies is that they lack interpretability: the test functions $T_P g$ in a Stein discrepancy are not immediately interpretable in terms of a given class $\mathcal{F}$ of interest. Following the spirit of Stein’s method, this problem has been addressed by lower bounding a Stein discrepancy by a known IPM – convergence in the Stein discrepancy then implies the IPM convergence. \cite{Gorham2015} showed that the Langevin graph Stein discrepancy controls the $L^1$-Wasserstein distance (the IPM defined by 1-Lipschitz functions) for distantly dissipative target distributions; \cite{Gorham2019} later generalized this result to heavy-tailed targets with diffusion graph Stein discrepancies. \cite{Gorham2017} proved that the Langevin KSD with the inverse multi-quadratic kernel (IMQ) controls the bounded-Lipschitz metric; \cite{Chen2018} offer other kernel choices. Random feature Stein discrepancies by \cite{Huggins2018} controls the bounded-Lipschitz metric with appropriate features while computable in linear time.

Despite its computational appeal, the KSD is limited in that it need not control convergence in unbounded functions, particularly functions of polynomial growth. This issue has been in part addressed by the aforementioned works on the graph Stein discrepancies. However, their analyses are limited to linearly growing functions – it is unclear how these results extend to functions of faster growth. Polynomially growing functions are of practical interest since they are related to fundamental statistical quantities, such as mean and variance (the latter corresponds to a quadratically growing function). Our objective is thus to extend the reach of the KSD to functions of arbitrary polynomial growth.

In this article, we investigate conditions under which the KSD controls the convergence of expectations of polynomially growing functions. Specifically, we prove that the KSD controls the IPM defined by a class of pseudo-Lipschitz functions, a polynomial generalization of Lipschitz functions. Our KSD bound builds on the finite Stein factor results of \cite{Erdogdu2018}. Our specific contributions are twofold. First, our analysis considers the diffusion kernel Stein discrepancy (DKSD) \cite{Barp2019}, a generalization of the Langevin KSD \cite{Chwialkowski2016, Liu2016, Oates2017, Gorham2017}; this extension allows us to consider heavy-tailed targets. Second, we, for the first time, identify specific practical reproducing kernels that provide polynomial convergence control.

## 2 Background

We begin with background material required to present our main results.
2.1 Notation and definitions

**Pseudo-Lipschitz functions.** A function \( h : \mathbb{R}^D \rightarrow \mathbb{R} \) is called pseudo-Lipschitz continuous (or simply \( C \)-pseudo-Lipschitz) of order \( q \) if it satisfies, for some constant \( C > 0 \),

\[
|h(x) - h(y)| \leq C(1 + \|x\|_2^q + \|y\|_2^q)\|x - y\|_2 \quad \text{for all } x, y \in \mathbb{R}^D,
\]

(1)

where \( \| \cdot \|_2 \) denotes the Euclidean norm. We denote the smallest constant \( C \) satisfying (1) by \( \tilde{\mu}_{\text{pLip}}(h)_{1,q} \). We denote by \( \mathcal{P}_{1,q} \) the set of pseudo-Lipschitz functions of order \( q \) with \( \tilde{\mu}_{\text{pLip}}(h)_{1,q} \leq 1 \). The pseudo-Lipschitz continuity generalizes the Lipschitz continuity (corresponding to the case \( q = 0 \)) and allows us to describe functions of polynomial growth.

**Vectors, matrices, and tensors.** For a real vector \( v \), \( \|v\|_{\text{op}} = \|v\|_2 \). We identify an order \( L \) tensor \( T \in \mathbb{R}^{D_1 \times \cdots \times D_L} \) as a multilinear map from \( \mathbb{R}^{D_1} \times \cdots \times \mathbb{R}^{D_L} \) to \( \mathbb{R} \) via the natural inner product

\[
T : (u_1, \ldots, u_L) \in \mathbb{R}^{D_1} \times \cdots \times \mathbb{R}^{D_L} \rightarrow \mathbb{R}, \quad \left( T, u_1^{(1)} \otimes \cdots \otimes u_1^{(L)} \right) = \sum_{i_1, \ldots, i_L} T_{i_1, \ldots, i_L} u_1^{(1)} \cdots u_1^{(L)},
\]

and define the operator norm \( \|T\|_{\text{op}} \) by

\[
\|T\|_{\text{op}} = \sup_{\|u\|_2 = 1} \left| \left( T, u^{(1)} \otimes \cdots \otimes u^{(L)} \right) \right|.
\]

**Derivatives.** The symbol \( \nabla = (\partial_1, \ldots, \partial_D)^\top \) denotes the gradient operator with \( \partial_d \) denoting the partial derivative with respect to the \( d \)-th coordinate. The symbol \( \nabla^m \) denotes the operator that outputs all the \( m \)-th order partial derivatives, defined as \( (\nabla^m g(x))_{i_1,\ldots,i_m} = \partial_{i_1} \cdots \partial_{i_m} g(x) \). For a vector-valued function \( g : \mathbb{R}^D \rightarrow \mathbb{R}^D \), we define \( \nabla^i g : \mathbb{R}^D \rightarrow \mathbb{R}^{D \times D} \) by \( (\nabla^i g(x))_{k_1,\ldots,k_{i-1},d} = (\nabla^i g_d(x))_{k_1,\ldots,k_{i-1},d} \); i.e., \( \nabla^i \) is applied to \( g \) element-wise. For a matrix valued function \( f \), we define its column-wise divergence by \( (\nabla, f(x)) ; \text{i.e., } (\nabla, f(x))_i = \sum_j \partial_j f_{ji}(x) \).

**Generalized Fourier transform.** Our main result (Proposition 3.4) requires an analogue of the Fourier transform of a function that is not an element of \( L^1 \) or \( L^2 \), where \( L', r \in \{1, 2\} \), denotes the Banach space of \( r \)-integrable functions with respect to the Lebesgue measure. For our purpose, we use the following generalized Fourier transform.

**Definition 2.1** (Generalized Fourier transform [Wendland, 2004, Definition 8.9]). Let \( \Phi \) be a continuous complex-valued function on \( \mathbb{R}^D \) such that for some a constant \( q \geq 0 \), \( \Phi(x) = O(\|x\|_2^q) \) in the limit of \( \|x\|_2 \rightarrow \infty \). A measurable function \( \hat{\Phi} \) is called the generalized Fourier transform of \( \Phi \) if it satisfies the following conditions: (a) the restriction of \( \hat{\Phi} \) on every compact set \( K \subset \mathbb{R}^D \setminus \{0\} \) is square-integrable, and (b) there exists an nonnegative integer \( m \) such that

\[
\int \Phi(x)\gamma(x)dx = \int \hat{\Phi}(\omega)\gamma(\omega)d\omega
\]

is true for all Schwartz functions \( \gamma \) satisfying \( \gamma(\omega) = O(\|\omega\|_2^m) \) for \( \|\omega\|_2 \rightarrow 0 \). The integer \( m \) is called the order of \( \Phi \).

The Fourier transform of \( \Phi \) coincides with the generalized Fourier transform, if it exists. In the following, we limit ourselves to generalized Fourier transforms of order zero.
2.2 Primer of Stein’s method

Stein’s method is a technique to compare distributions, introduced in the seminal paper by Stein [1972]. Stein’s method serves two purposes: it provides a characterization of probability distributions and enables us to upper bound an integral probability metric (IPM) [Müller, 1997]. This section provides a brief introduction to the subject. We refer the reader to the expository papers by Ross [2011] and Anastasiou et al. [2021] for more detailed descriptions of the technique; the latter reference also provides an overview of applications in computational statistics.

A starting point of Stein’s method is identifying an operator characterizing a probability distribution. Formally, for a distribution \( P \) on a set \( \mathcal{X} \), let \( T \) be a linear operator that acts on a set \( \mathcal{G}(T) \) of functions on \( \mathcal{X} \) such that

\[
\mathbb{E}_{X \sim P}[T g(X)] = 0 \quad \text{for each } g \in \mathcal{G}(T),
\]

where we assume that each \( T g \) is a real-valued function. Such an operator \( T \) and a set \( \mathcal{G}(T) \) are respectively called a Stein operator and a Stein set; the identity of the form (2) is known as Stein’s identity.

One can measure the dissimilarity between \( Q \) and \( P \) by examining the magnitude of the expectation \( \mathbb{E}_{X \sim Q}[T g(X)] \) for some \( g \in \mathcal{G}(T) \), since a non-zero expectation indicates \( Q \neq P \). Following this idea, for any subset \( \mathcal{G} \subset \mathcal{G}(T) \), one can construct a discrepancy summary

\[
S(Q, T, \mathcal{G}) = \sup_{g \in \mathcal{G}} \left| \mathbb{E}_{Y \sim Q}[T g(Y)] \right|.
\]

This worst-case discrepancy measure is called a Stein discrepancy, introduced by Gorham and Mackey [2015]. Remarkably, by choosing an appropriate Stein operator and a Stein set, one can construct a computable Stein discrepancy [Gorham and Mackey, 2015, Chwialkowski et al., 2016, Liu et al., 2016, Oates et al., 2017, Gorham et al., 2019, Gorham and Mackey, 2017].

A Stein operator is linked to an IPM via a Stein equation:

\[
T g_f = f - \mathbb{E}_{X \sim P}[f(X)],
\]

where \( f \) is a function of interest, and \( g_f \in \mathcal{G}(T) \) is a solution to the Stein equation (4). The existence of a solution depends on the properties of the test function \( f \), the target distribution \( P \), and the operator \( T \). Assuming that we can take expectations, we obtain

\[
\mathbb{E}_{Y \sim Q}[f(Y)] - \mathbb{E}_{X \sim P}[f(X)] = \mathbb{E}_{Y \sim Q}[T g_f(Y)].
\]

For a function class \( \mathcal{F} \), this relation yields

\[
d_F(P, Q) := \sup_{f \in \mathcal{F}} \left| \mathbb{E}_{Y \sim Q}[f(Y)] - \mathbb{E}_{X \sim P}[f(X)] \right| = \sup_{g \in \mathcal{G}_F} \left| \mathbb{E}_{Y \sim Q}[T g(Y)] \right|,
\]

where \( \mathcal{G}_F = \{ g_f : f \in \mathcal{F} \} \subset \mathcal{G}(T) \) is the set of solutions to the Stein equation. The core of Stein’s method is that the study of the IPM \( d_F(P, Q) \) can be reduced to the evaluation of the Stein discrepancy in (5). The evaluation is typically performed by upper bounding the Stein discrepancy, as a solution \( g_f \) to the Stein equation is often not explicit and only known up to some regularity properties. In Section 3.1, we obtain an upper bound on the IPM defined by a class of pseudo-Lipschitz functions; the upper bound is expressed by a kernel Stein discrepancy, introduced in Section 2.4.
2.3 Generators of Itô diffusions and their Stein equations

In the previous section, the Stein operator was unspecified. Here, we consider the generator of an Itô diffusion as a Stein operator and introduce the result of Erdogdu et al. [2018] characterizing a solution to the Stein equation. This object is related to the diffusion Stein operator considered in the next Section; the diffusion Stein operator is a first-order differential operator, whereas generators considered in this section are of the second order.

For a function \( f \) pseudo-Lipschitz of order \( q \), consider the Stein equation
\[
\mathcal{A}_P u_f = f - \mathbb{E}_{X \sim P}[f(X)],
\] defined by the generator \( \mathcal{A}_P \) of an Itô diffusion with invariant distribution \( P \), where \( u_h : \mathbb{R}^D \to \mathbb{R} \) is a solution to the equation. The diffusion is defined by the following stochastic differential equation:
\[
dZ_t^x = b(Z_t^x)dt + \sigma(Z_t^x)dB_t \text{ with } Z_0^x = x.
\] Here, \( (B_t)_{t \geq 0} \) is a \( D' \)-dimensional Wiener process; \( b : \mathbb{R}^D \to \mathbb{R}^D \) and \( \sigma : \mathbb{R}^D \to \mathbb{R}^{D \times D'} \) represent the drift and the diffusion coefficients. In the following, we assume that \( b \) and \( \sigma \) are locally Lipschitz. The drift coefficient \( b \) is chosen so that the diffusion has \( P \) as an invariant measure:
\[
b(x) = \frac{1}{2p(x)} \langle \nabla, p(x) \{a(x) + c(x)\} \rangle,
\] where \( a(x) = \sigma(x)\sigma(x)^\top \) is the covariance coefficient, \( c(x) = -c(x)^\top \in \mathbb{R}^{D \times D} \) is the skew-symmetric stream coefficient. Then, the generator \( \mathcal{A}_P \) is an operator defined by
\[
\mathcal{A}_P u_f(x) := \langle b(x), \nabla u_f(x) \rangle + \frac{1}{2} \langle \sigma(x)\sigma(x)^\top, \nabla^2 u_f(x) \rangle.
\] Characterizing the regularity of a solution \( u_f \) to (6) requires additional assumptions on the diffusion. Erdogdu et al. [2018] revealed that a solution is a pseudo-Lipschitz function for a fast-converging diffusion. To introduce their result, we first detail required assumptions.

Condition 2.2 (Polynomial growth of coefficients). For some \( q_0 \in \{0, 1\} \) and any \( x \in \mathbb{R}^D \), the drift and the diffusion coefficients of (7) satisfy the growth condition
\[
\|b(x)\|_2 \leq \frac{\lambda_b}{4}(1 + \|x\|_2), \|\sigma(x)\|_F \leq \frac{\lambda_\sigma}{4}(1 + \|x\|_2), \text{ and } \|\sigma(x)\sigma(x)^\top\|_{op} \leq \frac{\lambda_\alpha}{4}(1 + \|x\|_2^{q_0+1}),
\] with \( \lambda_b, \lambda_\sigma, \lambda_\alpha > 0 \).

Condition 2.3 (Dissipativity). For \( \alpha, \beta > 0 \), the diffusion (7) satisfies the dissipativity condition
\[
\mathcal{A}_P \|x\|^2 \leq -\alpha \|x\|^2 + \beta.
\] The operator \( \mathcal{A}_P \) is the generator of an Itô diffusion with coefficients \( b \) and \( \sigma \), and \( \mathcal{A}_P \|x\|_2^2 = 2 \langle b(x), x \rangle + \|\sigma(x)\|_2^2 \).

Condition 2.4 (Wasserstein rate). For \( q \geq 1 \), the diffusion \( Z_t^x \) has \( L^q \)-Wasserstein rate \( \rho_q : [0, \infty) \to \mathbb{R} \) if
\[
\inf_{\text{couplings}(Z_t^x, Z_t^y)} \mathbb{E}[\|Z_t^x - Z_t^y\|_2^{q/1/q}] \leq \rho_q(t) \|x - y\|_2 \text{ for } x, y \in \mathbb{R}^D \text{ and } t \geq 0,
\] where the infimum is taken over all couplings between \( Z_t^x \) and \( Z_t^y \). We further define the relative rates
\[
\tilde{\rho}_1(t) = \log(\rho_2(t)/\rho_1(t)) \text{ and } \tilde{\rho}_2(t) = \log[\rho_1(t)/\{\rho_2(t)\rho_1(0)\}] / \log[\rho_1(t)/\rho_1(0)].
\]
Erdogdu et al. [2018] shows that the solution $u_f$ to the Stein equation (6) satisfies the following property:

**Theorem 2.5** (Finite Stein factors from Wasserstein decay, Erdogdu et al. [2018], Theorem 3.2). Assume that Conditions 2.2, 2.3 and 2.4 for the $L^1$-Wasserstein distance hold and that $f$ is pseudo-Lipschitz of order $q$ with at most degree-$q$ polynomial growth of its $i$-th derivatives for $i = 2, 3, 4$. Then, the solution $u_f$ to the equation (6) is pseudo-Lipschitz of order $q$ with constant $\zeta_i$, and has $i$-th order derivative with degree-$q$ polynomial growth for $i = 2, 3, 4$:

$$\|\nabla^i u_f(x)\|_{op} \leq \zeta_i (1 + \|x\|^q)$$

for $i \in \{2, 3, 4\}$, and $x \in \mathbb{R}^D$.

The constants $\zeta_i$ (called Stein factors) are given as follows:

$$\zeta_i = \tau_i + \xi_i \int_0^\infty \rho_1(t)\omega_{q, i+1}(t + i - 2)dt$$

for $i = 1, 2, 3, 4$.

where

$$\omega_{q, i+1}(t) = 1 + 4\rho_1(t)^{1/(q-i+1)}\rho_1(0)^{1/2} \left[ 1 + \frac{1}{\bar{\alpha}_{q, i+1}} \{(1 \vee \tilde{p}_{q, i+1}(t))2\lambda q + 3(q_a + 1)^{q/2} \} \right],$$

with $\bar{\alpha}_1 = \alpha, \bar{\alpha}_2 = \inf_{t \geq 0} [\alpha - q\lambda_a(1 \vee \tilde{p}_2(t)) + \bar{q}(t)]$, $\tau_1 = 0$, $\tau_i = \mu_{p, L, p}(f)_1, q\bar{\pi}(\hat{f})_{2, q, a, p}\tilde{\nu}_{q, i-1}(\sigma)\kappa_{q, i}(6q)$ for $i = 2, 3, 4$, $\xi_i = \mu_{p, L, p}(f)_1, q\bar{\pi}(\hat{f})_{1, q, i-1}(b)\tilde{\nu}_{q, i-2}(\sigma^{-1})\rho_1(0)\omega_{q, i+1}(1)\kappa_{q, i}(6q)^{i-1}$ for $i = 2, 3, 4$, and

where $\bar{\pi}(f)_{i, q} = \sup_{x \in \mathbb{R}^D} \|\nabla^i f(x)\|_{op}/(1 + \|x\|^q)$, $\bar{\pi}(f)_{a, b, q} = \max_{i=a, \ldots, b} \bar{\pi}(f)_{i, q}$, $\nu_{a, b, q}(g)$ is a constant whose precise form is given in the proof of Erdogdu et al. [2018] Theorem 3.2, and

$$\kappa_{q, i}(q) = 2 + \frac{2\beta}{\alpha} + \frac{q\lambda_a + 6(q_a + 1)^{q/2}}{2\tau q_{q, i+1}}.$$

There are two known sufficient conditions for establishing exponential Wasserstein decay (Condition 2.4). The first is uniform dissipativity, which is a simple (but more restrictive) condition leading to exponential $L^1$- or $L^2$- exponential decay rates.

**Proposition 2.6** (Wasserstein decay from uniform dissipativity, Wang [2020], Theorem 2.5). A diffusion with drift and diffusion coefficients $b$ and $\sigma$ has $L^p$-Wasserstein rate $\rho_q(t) = e^{-rt/2}$, if for all $x, y \in \mathbb{R}^D$,

$$2(b(x) - b(y), x - y) + \|\sigma(x) - \sigma(y)\|^q_{op} - (q - 2)\|\sigma(x) - \sigma(y)\|_{op}^2 \leq -r\|x - y\|^2.$$

The second and more general condition is distant dissipativity. Explicit $L^1$-Wasserstein decay rates from distant dissipativity are obtained by the following result of Gorham et al. [2019] which builds upon the analyses of Eberle [2015] and Wang [2020].

**Proposition 2.7** (Wasserstein decay from distant dissipativity, Gorham et al. [2019], Corollary 12). A diffusion with drift and diffusion coefficients $b$ and $\sigma$ is called distant dissipative if for the truncated diffusion coefficient

$$\tilde{\sigma}(x) := (\sigma(x)\sigma(x)^T - s^2 I_d)^{1/2}$$

with $M_0(\sigma^{-1}) = \sup_{x \in \mathbb{R}^d} \|\sigma^{-1}(x)\|_{op}$, it satisfies

$$2\frac{\langle b(x) - b(y), x - y \rangle}{s^2\|x - y\|^2_{op}} + \frac{\|\tilde{\sigma}(x) - \tilde{\sigma}(y)\|_{op}^2}{s^2\|x - y\|^2_{op}} - \frac{\|\tilde{\sigma}(x) - \tilde{\sigma}(y)\|_{op}^2}{s^2\|x - y\|^2_{op}} \leq \begin{cases} -K & \|x - y\|_{op} > R \\ L & \|x - y\|_{op} \leq R \end{cases}$$

with $M_0(\sigma^{-1}) = \sup_{x \in \mathbb{R}^d} \|\sigma^{-1}(x)\|_{op}$, it satisfies

$$2\frac{\langle b(x) - b(y), x - y \rangle}{s^2\|x - y\|^2_{op}} + \frac{\|\tilde{\sigma}(x) - \tilde{\sigma}(y)\|_{op}^2}{s^2\|x - y\|^2_{op}} - \frac{\|\tilde{\sigma}(x) - \tilde{\sigma}(y)\|_{op}^2}{s^2\|x - y\|^2_{op}} \leq \begin{cases} -K & \|x - y\|_{op} > R \\ L & \|x - y\|_{op} \leq R \end{cases}$$

with $M_0(\sigma^{-1}) = \sup_{x \in \mathbb{R}^d} \|\sigma^{-1}(x)\|_{op}$, it satisfies

$$2\frac{\langle b(x) - b(y), x - y \rangle}{s^2\|x - y\|^2_{op}} + \frac{\|\tilde{\sigma}(x) - \tilde{\sigma}(y)\|_{op}^2}{s^2\|x - y\|^2_{op}} - \frac{\|\tilde{\sigma}(x) - \tilde{\sigma}(y)\|_{op}^2}{s^2\|x - y\|^2_{op}} \leq \begin{cases} -K & \|x - y\|_{op} > R \\ L & \|x - y\|_{op} \leq R \end{cases}$$
for some $K > 0$ and $R, L \geq 0$. If the distant dissipativity holds, then the diffusion has Wasserstein rate $\rho_1(t) = 2e^{LR^2/8}e^{-rt/2}$ for

$$s^2 r^{-1} \leq \begin{cases} \frac{e}{2} R^2 + e\sqrt{8K^{-1}}R + 4K^{-1} & \text{if } LR^2 \leq 8, \\ 8\sqrt{2\pi} R^{-1} L^{-1/2}(L^{-1} + K^{-1}) \exp\left(\frac{LR^2}{8}\right) + 32R^{-2}K^{-2} & \text{otherwise.} \end{cases}$$

These two conditions also conveniently lead to the dissipativity condition (Condition 2.3) defined above. Therefore, we assume that the diffusion satisfies either of these conditions in the following.

### 2.4 Diffusion Stein operator and the diffusion kernel Stein discrepancy

We next recall the diffusion Stein operator of Gorham et al. [2019], which will be the basis of the Stein discrepancy considered in this paper. For a diffusion process defined in (7), the diffusion Stein operator is defined as an operator that takes as input a vector-valued differentiable function $g : \mathbb{R}^D \to \mathbb{R}^D$ and outputs a real-valued function as follows:

$$T_P g(x) = \frac{1}{p(x)} \langle \nabla, p(x)m(x)g(x) \rangle = 2\langle b(x), g(x) \rangle + \langle m(x), \nabla g(x) \rangle$$

where $b(x) = (\nabla, p(x)m(x))/(2p(x))$ and $m(x) = a(x) + c(x)$. Note that we can recover the Langevin Stein operator [Gorham and Mackey, 2015] by taking $a \equiv I$ and $c \equiv 0$.

Recall the Stein equation for the second-order Stein operator $A_P u_f = f - \mathbb{E}_{X \sim P}[f(X)]$. By relating the definition of $A_P$ to $T_P$, we have that the function $g_f = \nabla u_f/2$ solves the Stein equation $T_PG = f - \mathbb{E}_{X \sim P}[f(X)]$ [Gorham et al., 2019, Section 2]. As a result of Theorem 2.5, we have the following corollary:

**Corollary 2.8.** Let $q \geq 0$. Let $f \in C^3$ be a pseudo-Lipschitz function of order $q$ with derivatives satisfying the polynomial decay condition in Theorem 2.5. The solution $g_f = \nabla u_f/2$ to the Stein equation $T_P g = f - \mathbb{E}_{X \sim P}[f(X)]$ belongs to the set

$$G = \{g : \mathbb{R}^D \to \mathbb{R}^D : \|g(x)\|_2 \leq \sqrt{D}\zeta_1(1 + \|x\|_2^q) \text{,} \quad \|\nabla^i g(x)\|_{op} \leq \zeta_{i+1}(1 + \|x\|_2^q) \text{ for } i \in \{1, 2\}, x \in \mathbb{R}^D \},$$

where $\zeta_1$, $\zeta_2$, and $\zeta_3$ are the Stein factors from Theorem 2.5.

**Proof.** The derivative norm bounds follow directly from Theorem 2.5. Note that the bound on $\|g(x)\|_2$ follows from the pseudo-Lipschitzness of $u_f$ as

$$|\partial_j u_f(x)| = \lim_{h \to 0} \frac{|u_f(x + he_j) - u_f(x)|}{h} \leq \lim_{h \to 0} \zeta_1(1 + \|x + he_j\|_2^{-1} + \|x\|_2^{-1}) \frac{\|he_j\|_2}{|h|} = \zeta_1(1 + 2\|x\|_2^{-1}) \leq 2\zeta_1(1 + \|x\|_2^{-1}),$$

where $\{e_1, \ldots, e_D\}$ is the standard basis of $\mathbb{R}^D$. \qed

The following proposition shows that the diffusion Stein operator induces zero-mean functions (see Appendix 6.5 for a proof).
Proposition 2.9 (The diffusion Stein operator generates zero-mean functions). Let \( q_a \in \{0, 1\} \) be the additional growth exponent of \( \|a(x)\|_{\text{op}} \) from Condition \( 2.2 \). If \( q_a = 0 \), assume \( P \) has a finite \( q \)-th moment; if \( q_a = 1 \), a finite \( (q + 1) \)-th moment. Let \( g \in C^1 \) be a function with the following growth conditions:

\[
\|g(x)\|_2 \leq C_0 (1 + \|x\|_2^{q-1}),
\|\nabla g(x)\|_{\text{op}} \leq C_1 (1 + \|x\|_2^{q-1}),
\]

for each \( x \in \mathbb{R}^D \), and some positive constants \( C_0 \) and \( C_1 \). Then, we have \( \mathbb{E}_{X \sim P}[T_P g(X)] = 0 \).

We can construct a computable Stein discrepancy by combining the diffusion Stein operator with a reproducing kernel Hilbert space (RKHS) \[ \text{Aronszajn, 1950} \]. Here, we recall the definition of the diffusion kernel Stein discrepancy (DKSD) proposed by \[ \text{Barp et al., 2019} \]. For a distribution \( Q \) on \( \mathbb{R}^D \), the DKSD is defined by

\[
S(Q, T_P, B_1(\mathcal{G}_\kappa)) = \sup_{g \in B_1(\mathcal{G}_\kappa)} \mathbb{E}_{Y \sim Q}[T_P g(Y)],
\]

where \( B_1(\mathcal{G}_\kappa) \) is the unit ball of a vector-valued RKHS \( \mathcal{G}_\kappa \) determined by a matrix-valued kernel \( \kappa : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}^{D \times D} \) \[ \text{Carmeli et al., 2006} \]. In the following, by abuse of notation, we use \( S(Q, T_P, \mathcal{G}_\kappa) \) to denote the DKSD \( S(Q, T_P, B_1(\mathcal{G}_\kappa)) \). Note that the Langevin KSD \[ \text{Chwialkowski et al., 2016; Liu et al., 2016; Gorham and Mackey, 2017} \] is obtained as a specific instance of the DKSD by choosing \( a(x) \equiv \text{Id}, \ c \equiv 0 \), and \( \kappa = \kappa \text{Id} \) for a scalar-valued kernel \( \kappa \) and the \( D \)-dimensional identity matrix \( \text{Id} \). Note that in this case, the vector-valued RKHS \( \mathcal{G}_\kappa \) corresponds to the Cartesian product \( \prod_{k=1}^D \mathcal{H}_k \) of \( D \)-copies of a scalar-valued RKHS \( \mathcal{H}_k \) with inner product \( (g, g') = \sum_{d=1}^D \langle g_d, g'_d \rangle \). Also, we obtain the Langevin KSD with a reweighted kernel \( w(x)\kappa(x, y)w(y) \) by choosing \( a(x) = w(x)\text{Id} \) with \( w \) a scalar-valued positive function. The use of an RKHS leads to a closed-form expression for the DKSD,

\[
S(Q, T_P, \mathcal{G}_\kappa)^2 = \mathbb{E}_{X, X' \sim Q \otimes Q}[h_p(X, X')],
\]

where

\[
h_p(x, y) = \frac{1}{p(x)p(y)} \left\langle \nabla_y, \nabla_x, (p(x)m(x)\kappa(x, y)m(y)^\top p(y)) \right\rangle,
\]

provided that \( x \mapsto \|T_P \kappa(x, \cdot)\|_{\mathcal{G}_\kappa} \) is integrable with respect to \( Q \) \[ \text{Barp et al., 2019; Theorem 1} \]. In particular, we can compute the DKSD exactly if the distribution \( Q \) is given by a finitely-supported distribution \( Q_N = \sum_{i \leq N} w_i \delta_{x_i} \), with \( \{x_1, \ldots, x_N\} \subset \mathbb{R}^D \), \( \delta_{x_i} \) being the Dirac measure having all mass at \( x_i \), and nonnegative weights \( w_i \) such that \( \sum_{i \leq N} w_i = 1 \); in this case, the expression \( 8 \) yields

\[
S(Q_N, T_P, \mathcal{G}_\kappa)^2 = \sum_{i,j=1}^N w_i w_j h_p(x_i, x_j).
\]

Although the majority of the following analyses focus on the simple RKHS \( \kappa = \kappa \text{Id} \), we present results using a general vector-valued RKHS where possible.

An appropriate choice of the RKHS enables the DKSD to distinguish distributions. Proposition 1 of \[ \text{Barp et al., 2019} \] states that \( S(Q, T_P, \mathcal{G}_\kappa)^2 = 0 \) if and only if \( P = Q \) under the following conditions: (a) \( Q \) admits a differentiable density \( q \) such that \( \nabla \log q - \nabla \log p \) is integrable with respect to \( Q \); (b) \( \kappa \) is integrally strictly positive definite, i.e., \( \int \mu(dx)^\top \kappa(x, y)\mu(dy) > 0 \) for any vector Borel measure \( \mu \); and (c) the RKHS of \( \kappa \) is contained in the Stein class with respect to \( T_Q \). In the next section, we show that the DKSD separates arbitrary Borel measures from \( P \), lifting the density requirement for \( Q \). Our result is proved by lower bounding the DKSD with a separating IPM.
3 Main results

We formalize our objective in this article, as outlined in the introduction. Let $P$ be a distribution over $\mathbb{R}^D$ defined by a continuously differentiable density function $p$. For a distribution $Q$, we are interested in the maximum discrepancy over a function class $\mathcal{F}$: $\sup_{f \in \mathcal{F}} |\mathbb{E}_{Y \sim P}[f(X)] - \mathbb{E}_{Y \sim Q}[f(Y)]|$. Our focus is on functions with polynomial growth order of $q \geq 1$. Therefore, we specify the function class $\mathcal{F}$ to be a subset of pseudo-Lipschitz functions of order $q - 1$

$$\mathcal{F}_q := \{ f : \mathbb{R}^D \to \mathbb{R} : f \in C^3 \text{ with } \mu_{p\text{Lip}}(f)_{1,q-1} \leq 1 $$

and $$\sup_x \|\nabla^i f(x)\|_{\text{op}}/(1 + \|x\|_{q-1}^{2}) \leq 1 \text{ for } i \in \{2, 3\} \}.$$ We define an IPM corresponding to the class $\mathcal{F}_q$ by

$$d_{\mathcal{F}_q}(P, Q) = \sup_{f \in \mathcal{F}_q} |\mathbb{E}_{Y \sim P}[f(X)] - \mathbb{E}_{Y \sim Q}[f(Y)]|.$$

(10)

Appendix 7.5 shows that $\mathcal{F}_q$ contains degree-$q$ polynomial functions of $(x_1, \ldots, x_D) \in \mathbb{R}^D$, if scaled appropriately. Note that for this class, we can take the Stein factors $\{\zeta_1, \zeta_2, \zeta_3\}$ that are independent of test functions and only depend on the diffusion through $b(x)$ and $\sigma(x)$. Unfortunately, the IPM $d_{\mathcal{F}_q}$ is not computable as it involves an intractable integral. Thus, we aim to relate the IPM $d_{\mathcal{F}_q}$ to the DKSD, a computable discrepancy measure.

Before presenting results concerning the DKSD, we first show a convergence property of $d_{\mathcal{F}_q}$. In the following, we denote the set of probability measures with finite $q$-th moments by $\mathcal{P}_q := \{ \text{probability measure } \mu : \int \|x\|^q d\mu(x) < \infty \}$.

**Proposition 3.1.** Let $P \in \mathcal{P}_q$ be a probability measure on $\mathbb{R}^D$ with a finite $q$-th moment with $q \geq 1$. For a sequence of probability measures $\{Q_1, Q_2, \ldots, \} \subset \mathcal{P}_q$, the following conditions are equivalent:

(a) $d_{\mathcal{F}_q}(Q_n, P) \to 0$ as $n \to \infty$, and (b) as $n \to \infty$, the sequence $Q_n$ converges weakly to $P$, and $\mathbb{E}_{X \sim Q_n}[\|X\|_2^q] \to \mathbb{E}_{X \sim P}[\|X\|_2^q]$.

**Proof.** We relate the metric $d_{\mathcal{F}_q}$ to the bounded-Lipschitz metric [see, e.g., Dudley 2002 Section 11.2] and make use of uniform integrability. See Appendix 6.1 for a complete proof.

The above result shows that the distance $d_{\mathcal{F}_q}$ characterizes both weak convergence (convergence in distribution) and convergence with respect to the $q$-th moment. For sequences in $\mathcal{P}_q$, another example of a metric characterizing this topology is $L^q$-Wasserstein distance defined by the Euclidean distance [see, e.g., Villani 2009 Theorem 6.9].

In the following, we make an additional assumption on the growth of the stream coefficient in the DKSD.

**Condition 3.2** (Polynomial growth of the stream coefficient). For any $x \in \mathbb{R}^D$, the stream coefficient of (7) satisfies the growth condition

$$\|c(x)\|_{\text{op}} \leq \lambda_c/4 (1 + \|x\|_2)^{q_a+1}$$

with $\lambda_c > 0$ and $q_a$ as in Condition 2.2.

Note that under Conditions 2.2 3.2 we have

$$\|m(x)\|_F \leq \sqrt{D}\|m(x)\|_{\text{op}} \leq \sqrt{D}\lambda_m (1 + \|x\|_2)^{q_a+1} \text{ with } \lambda_m = \frac{\lambda_a \vee \lambda_c}{4}.$$
3.1 Uniform integrability and DKSD bounds

To prove our main result, we make use of a standard notion of uniformly integrable $q$-th moments, defined as follows:

**Definition 3.3** (Uniform integrability with respect to $q$-th moments [Ambrosio et al., 2005, Eq. 5.1.19]). Let $q > 0$. A sequence of probability measures $\mathcal{Q} = \{Q_1, Q_2, \ldots\} \subset \mathcal{P}_q$ is said to have uniformly integrable $q$-th moments if

$$\lim_{r \to \infty} \limsup_{n \to \infty} \int \{\|x\|_2 > r\} \|x\|^q_dQ_n(x) = 0.$$ 

It is known that for weakly converging sequences, convergence of a moment is equivalent to the uniform integrability of the moment [Ambrosio et al., 2005, Lemma 5.1.7] (see also Lemma 7.3 in Appendix 7.2). Intuitively, uniform integrability is a condition enforcing that the probability mass does not diverge too fast along the sequence. If $q = 0$, the above definition is reduced to uniform tightness [see, e.g., Dudley, 2002, Chapter 9]. The uniform integrability is a stricter condition in that it requires the decay rate of the tail probability to stay faster than a degree-$q$ polynomial.

Our first result shows that for sequences with a uniformly integrable moment, the DKSD implies convergence in $d_{\mathcal{F}_q}$. In fact, the complete proof of this result in Appendix 6.2 provides an explicit upper bound on $d_{\mathcal{F}_q}$ in terms of the DKSD.

**Proposition 3.4.** Let $\Phi \in C^2$ be a positive definite function with non-vanishing generalized Fourier transform $\Phi$. Let $w(x) = (v^2 + \|x\|^2)^{q_w}$ with real numbers $v \geq 1$ and $q_w \geq 0$. Let $\mathcal{G}_{k,\text{id}}$ be the RKHS defined by kernel $k_{\text{id}}$ with $k(x, y) = \Phi_w(x, x') + \ell(x, x')$, where $\Phi_w(x, x') = w(x)w(x')\Phi(x - x')$ and $\ell$ is an optional positive definite kernel. Then, for a sequence of measures $\mathcal{Q} = \{Q_1, Q_2, \ldots\} \subset \mathcal{P}_{q + q_a}$ with uniformly integrable $(q + q_a)$-th moments, we have $\mathcal{S}(Q_n, T_P, \mathcal{G}_{k,\text{id}}) \to 0$ only if $d_{\mathcal{F}_q}(P, Q_n) \to 0$.

**Proof.** We only provide a proof sketch here and refer the reader to Appendix 6.2 (see Proposition 6.7 for the precise statement) for the full proof. Our strategy is to bound the IPM $d_{\mathcal{F}_q}$ explicitly by the DKSD. Consider the Stein equation $T_PG_f = f - \mathbb{E}_{X \sim P}[f(X)]$ for $f \in \mathcal{F}_q$. We approximate $T_PG_f$ by mollification. Specifically, we decompose the function $T_PG_f$ into three parts:

$$\mathcal{T}_F P G_f = \mathcal{T}_F P G_{f_{\text{trunc}}} + \mathcal{T}_F P G_{\text{RKHS}} + \frac{\|G_{\text{RKHS}}\|_{\mathcal{G}_{k,\text{id}}}}{\mathcal{T}_F P G_{\text{RKHS}} + \|\Phi\|_{\mathcal{G}_{k,\text{id}}}}.$$ 

In the first step, we truncate $T_PG_f$ to make it bounded and ignore the tail expectation. In the second step, we approximate the truncated function with a smooth function. In the last step, we show that the smooth function is an RKHS function if the kernel $\Phi$ is chosen appropriately. The expectations of truncation and approximation errors are evaluated using the characterization of $g_f$ derived in Corollary 2.8; the expectation of the third term can be bounded by the DKSD. Thus, we obtain a bound on $d_{\mathcal{F}_q}$ in terms of the DKSD. If the DKSD term vanishes, the rest of the error terms can be made arbitrarily small. \qed

When $q_a = 1$, i.e., we have a quadratic growth of the operator norm of the covariance coefficient, we need approximating distributions $\{Q_1, Q_2, \ldots\}$ to have an extra moment. This requirement is placed in order to make the Stein discrepancy upper bound well-defined; otherwise, the upper bound is vacuous. This being said, if one is willing to make the assumption $Q \neq P$, it is appropriate to assume a higher-order moment. For example, any numerical quadrature method is represented by a discrete measure with a finite support, thereby guaranteeing a finite moment of any order. Note that in proving the uniform
integrability of a sequence of measures \( Q = \{Q_1, Q_2, \ldots \} \), it is not sufficient to assume that each \( Q \in Q \) has a finite moment of a higher order (a sufficient condition is having their moments of that order uniformly bounded).

### 3.2 The DKSD detects non-uniform integrability

In the previous section, we assumed that the approximating distributions \( \{Q_1, Q_2, \ldots \} \) had uniformly integrable \( q \)-th moments if \( \|a(x)\|_{op} \) grows linearly, or \( (q + 1) \)-th moments if quadratically. Proposition [3.4] indicates that we can use any kernel formed by a positive definite function for diagnosing non-convergence. However, such a kernel alone is not enough when the uniform integrability is violated. Indeed, in the case of weak convergence, Gorham and Mackey [2017] demonstrated that an inadequate choice of the kernel yields a discrepancy that converges to zero even when the sequence is not uniformly tight and hence non-convergent; the IMQ kernel suggested by Gorham and Mackey [2017] ensures that vanishing KSD implies the tightness of the sequence. Analogously, we explore conditions that allow us to check the uniform integrability using the DKSD.

The following two lemmas characterize uniform integrability using the DKSD:

**Lemma 3.5.** Let \( Q = \{Q_1, Q_2, \ldots \} \subset P_q \) be a sequence of probability measures for \( q > 0 \). Let \( G_\kappa \) be the RKHS of \( \mathbb{R}^D \)-valued functions defined by a matrix-valued kernel \( \kappa : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}^{D \times D} \). Suppose that for any \( \varepsilon > 0 \), there exists \( r_\varepsilon > 0 \) and a function \( g \in G_\kappa \) such that \( T_P g(x) \geq \|x\|_2^2 1\{\|x\|_2 > r_\varepsilon \} - \varepsilon \) for any \( x \in \mathbb{R}^D \). Then, \( Q \) has uniformly integrable \( q \)-th moments if \( S(Q_n, T_P, G_\kappa) \to 0 \) as \( n \to \infty \).

**Proof.** For any \( \varepsilon > 0 \), we have

\[
\int_{\{\|x\|_2 > r_\varepsilon \}} \|x\|_2^2 dQ_n(x) \leq \int T_P g(x) dQ_n(x) \leq \|g\|_2 S(Q_n, T_P, G_\kappa) + \varepsilon.
\]

Letting \( n \to \infty \) concludes the proof. \( \square \)

**Lemma 3.6** (KSD upper-bounds the integrability rate). Let \( G_\kappa \) be the RKHS of \( \mathbb{R}^D \)-valued functions defined by a matrix-valued kernel \( \kappa : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}^{D \times D} \). Suppose there exists a function \( g \in G_\kappa \) such that \( T_P g(x) \geq \nu \) for any \( x \in \mathbb{R}^D \) with some constant \( \nu \in \mathbb{R} \), and \( \lim \inf \|x\|_2^{-(q + \theta)} T_P g(x) \geq \eta \) for some \( q \geq 0, \eta > 0, \) and \( \theta > 0 \) as \( \|x\|_2 \to \infty \). Then, for sufficiently small \( \varepsilon > 0 \), we have

\[
R_q(Q, \varepsilon) := \inf \left\{ r \geq 1 : \int_{\{\|x\|_2 > r\}} \|x\|_2^2 dQ(x) \leq \varepsilon \right\}
\]

\[
\leq \left\{ 2 \left( 1 + \frac{q}{\theta} \right) \left( \frac{S(Q, T_P, G_\kappa) - \nu}{\eta \varepsilon} \right) \right\}^{\frac{q + \theta}{2}}.
\]

where \( S(Q, T_P, G_\kappa) = \infty \) if \( Q \notin P_{q + \theta} \). Thus, for a sequence of measures \( \{Q_1, Q_2, \ldots \} \subset P_q \) we have

\[
\limsup_{n \to \infty} S(Q_n, T_P, G_\kappa) < \infty \Rightarrow \limsup_{n \to \infty} R_q(Q_n, \varepsilon) < \infty.
\]

In particular, if the sequence \( \{Q_1, Q_2, \ldots \} \) does not have uniformly integrable \( q \)-th moments, then Stein discrepancy \( S(Q_n, T_P, G_\kappa) \) diverges.

**Proof.** The proof is in Appendix [7.4.1] \( \square \)
The quantity $R_q(Q, \varepsilon)$ (termed an integrability rate) in Lemma 3.6 represents the radius of a ball, outside of which the tail moment integral becomes negligible. Note that $Q \in P_q$ is equivalent to having $R_q(Q, \varepsilon) < \infty$ for each $\varepsilon > 0$. In particular, if a sequence $\{Q_n\}_{n \geq 1}$ does not have uniformly integrable $q$-th moments, the integrability rate $R_q(Q_n, \varepsilon)$ diverges.

The above two lemmas require the Stein-modified RKHS to have a function growing at a certain rate. The first lemma requires a stronger condition in that it requires a function that approximates the power function $\|x\|^q$ arbitrarily well. The existence proof for the first lemma is left as future work, and we focus on the second lemma. Note that the second lemma in contrast relies on the existence of a function that behaves as $\|x\|^q$ outside a ball; we can create an RKHS that satisfy this requirement using a linear kernel and the diffusion Stein operator, provided that the diffusion satisfies the dissipativity condition (Condition 2.3).

**Lemma 3.7** (Tilted linear kernels have the lower bound properties). Suppose the diffusion targeting $P$ satisfies the dissipativity condition (Condition 2.3) with $\alpha, \beta > 0$ and the coefficient condition (Condition 2.2) with $\lambda_0 > 0$ and $q_a \in \{0, 1\}$. Let $w(x) = (v^2 + \|x\|^\frac{q_u - u}{2})^q_u$ with $q_u \geq 0$, $u \geq 0$, and $v > 0$. Assume $(q_u - u) < 2\alpha/\lambda_0$ if $q_a = 1$. Let

$$k(x, x') = w(x)w(x')(x, x').$$

There exists a function $g \in G_{cld}$ such that $\|g\|_{G_{cld}} = \sqrt{D}$ and the corresponding diffusion Stein operator $T_P$ satisfies

$$T_Pg(x) \geq \nu \text{ for any } x \in \mathbb{R}^D, \text{ and } \liminf_{\|x\|_2 \to \infty} \|x\|^{-2(q_u - u - 1)}T_Pg(x) \geq \eta$$

for some $\nu \in \mathbb{R}$ and $\eta > 0$.

**Proof.** The proof can be found in Appendix 7.4.2. 

The next result is an immediate consequence of Lemma 3.7.

**Corollary 3.8.** Define symbols as in Lemma 3.7. For the RKHS $G_{cld}$ of a kernel $k = k_1 + k_2$ with $k_1$ an arbitrary positive definite kernel and $k_2$ the kernel from Lemma 3.7 there exists a function $g \in G_{cld}$ such that the corresponding diffusion Stein operator $T_P$ satisfies

$$T_Pg(x) \geq \nu \text{ for any } x \in \mathbb{R}^D, \text{ and } \liminf_{\|x\|_2 \to \infty} \|x\|^{-2(q_u - u - 1)}T_Pg(x) \geq \eta$$

for some $\nu \in \mathbb{R}$ and $\eta > 0$. In particular, if the RKHSs of kernels $k_1$ and $k_2$ do not overlap, $\|g\|_{G_{cld}} = \sqrt{D}$.

### 3.3 Recommended kernel choice

We have established the conditions required for the DKSD to control the pseudo-Lipschitz metric $d_{F_q}$. In the following, we present our recommended settings.

**Linear growth case** When $q_a = 0$, we need the uniform integrability with respect to the $q$-th moment. We recommend the following kernel function

$$k_{\Phi, q, \theta}(x, x') = w_{q, \theta}(x; v)w_{q, \theta}(x'; v)\left(\Phi(x - x') + \tilde{k}_{lin}(x, x'; v)\right),$$

(11)
where the weight $w_{q, \theta}$ is given by

$$w_{q, \theta}(x; v) = (v^2 + \|x\|_2^2)^{\frac{q+\theta}{2}}$$

with $v \geq 1$, and $\tilde{k}_{\text{lin}}$ denotes the normalized linear kernel:

$$\tilde{k}_{\text{lin}}(x, x') = \frac{v^2 + \langle x, x' \rangle}{\sqrt{v^2 + \|x\|_2^2} \sqrt{v^2 + \|x'\|_2^2}}.$$ 

This choice ensures that the two kernels in the sum (11) have the same growth rate. The kernel $\Phi(x - x')$ can be any function with a non-vanishing (generalized) Fourier transform. Examples are the exponentiated quadratic (EQ) kernel, the IMQ kernel, and the Matérn class kernels [Matérn 1986, Stein 1999]. Note that the normalized linear kernel enables us to use light-tailed kernels (e.g., the EQ or the Matérn kernels) that are recommended against by Gorham and Mackey [2017]. In particular, one benefit of the Matérn class is that we can use rougher functions: the RKHS of an IMQ kernel consists of infinitely differentiable functions, whereas a Matérn kernel can specify an RKHS of finitely differentiable functions. The increased complexity would render the DKSD more sensitive to the difference between distributions (see Section 4.3).

**Quadratic growth case** When $q_a = 1$, we need the uniform integrability with respect to the $(q + 1)$-th moment. Therefore, we recommend to use the same form of the kernel as in (11) except that $w_{q, \theta}$ is replaced with

$$w_{q+1, \theta}(x) = (v^2 + \|x\|_2^2)^{\frac{q+\theta}{2}}.$$  

(12)

### 3.4 The DKSD detects convergence

We have shown that vanishing DKSD implies convergence in $d_{F_q}$. Here, we clarify conditions on which the DKSD converges to zero.

**Proposition 3.9.** Let $\mathcal{G}_\kappa$ be the RKHS defined by a matrix-valued kernel $\kappa : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}^{D \times D}$. Let $q \geq 1$. Assume that any function $g$ in the unit ball $\mathcal{B}_1(\mathcal{G}_\kappa)$ satisfies the following: there exist some constants $C_0, C_1,$ and $C_2$ such that

$$\|\nabla^i g(x)\|_{op} \leq C_i(1 + \|x\|_2^{q-1}) \text{ for any } x \in \mathbb{R}^D \text{ and } i \in \{0, 1, 2\}.$$ 

Assume a linear growth condition on $m$ (Conditions 2.2, 3.2 with $q_a = 0$). Assume that $b$ is $\phi_1(b)$-Lipschitz in the Euclidean norm, and $m$ is $\phi_1(m)$-Lipschitz in the Frobenius norm. Suppose $P \in \mathcal{P}_q$. Then,

$$S(Q, T_P, \mathcal{G}_\kappa) \leq C_{b,m}d_{p,\text{Lip}_1,q}(Q, P),$$

where

$$C_{b,m} = \frac{\lambda_{b,m}C_1(5 + 2^q - 1)}{4} + 4C_0\phi_1(b) + \lambda_mC_2D(5 + 2^q - 1) + 2\sqrt{D}C_1\phi_1(m).$$

In particular, we have $S(Q_n, T_P, \mathcal{G}_\kappa) \to 0$ if $d_{F_q}(P, Q_n) \to 0$.

**Proof.** The claim follows from showing that a Stein-modified RKHS function $T_P g$ is pseudo-Lipschitz of order $q$. The full proof is available in Appendix 6.4.
Proposition 3.10. Let \( G_\kappa \) be the RKHS of \( \mathbb{R}^D \)-valued functions defined by a matrix-valued kernel \( \kappa : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}^{D \times D} \), \( q \geq 1 \). Assume that any function \( g \) in the unit ball \( B_1(\mathcal{G}_\kappa) \) satisfies the following: there exist some constants \( C_0, C_1, C_2 \) such that
\[
\| \nabla_i g(x) \|_{\text{op}} \leq C_i (1 + \| x \|^{q - 1/2}) \text{ for any } x \in \mathbb{R}^D \text{ and } i \in \{0, 1, 2\}.
\]
Assume a quadratic growth condition on \( m \) (Conditions 2.2, 3.2 with \( q_{\text{a}} = 1 \)). Assume that \( b \) is \( \phi_1(b) \)-Lipschitz, and \( m \) is pseudo-Lipschitz of order 1 in the operator norm with constant \( \tilde{\mu}_{\text{pLip}}(m)_{1,1} \). Suppose \( P \in \mathcal{P}_{q+1} \). Then,
\[
S(Q, T_P, \mathcal{G}_\kappa) \leq C_{b,m} d_{\text{pLip}_{1,q+1}}(Q, P),
\]
where
\[
C_{b,m} = (5 + 2^q) \left( \frac{\lambda_b C_1}{4} + \frac{\lambda_m C_2 D}{2} + C_1 D \tilde{\mu}_{\text{pLip}}(m)_{1,1} \right) + 4 \phi_1(b) C_0.
\]
In particular, we have \( S(Q_n, T_P, \mathcal{G}_\kappa) \to 0 \) if \( d_{\mathcal{F}_q}(P, Q_n) \to 0 \).

Proof. The proof proceeds as in the previous proposition and can be found in Appendix 6.4.

Note that the two propositions above require stronger convergence requirements than that of \( d_{\mathcal{F}_q} \).

4 Experiments

We conduct numerical experiments to examine the theory developed above. In the first two experiments, we investigate how a kernel choice affects the KSD’s ability to detect the non-convergence in \( d_{\mathcal{F}_q} \) using simple light-tailed and heavy-tailed target distributions. Then, we present a cautionary case study, in which, even though the KSD will asymptotically detect moment discrepancies by Proposition 3.4, a large sample size is needed for the KSD to detect discrepancies arising from isolated modes.

4.1 The Langevin KSD

Our first problem studies the behavior of Langevin KSD corresponding to the choice \( a \equiv \text{Id}, c \equiv 0 \). This setting allows us to contrast with the IMQ kernel previously recommended by Gorham and Mackey [2017], which is known to control the bounded-Lipschitz metric.

4.1.1 Non-convergence in mean

We first consider a problem where a sequence does not converge in mean to their target and therefore not in \( d_{\mathcal{F}_q} (q = 1) \). In this case, the function class \( \mathcal{F}_q \) includes linearly growing functions and therefore characterizes mean non-convergence. We choose a target \( P \) and an approximating sequence \( \{Q_1, Q_2, \ldots\} \) as follows:
\[
P = \mathcal{N}(-\mathbf{1}, \text{Id}), \ Q_n = \left( 1 - \frac{1}{n+1} \right) P + \frac{1}{n+1} \mathcal{N}((n+1)\mathbf{1}, \text{Id}), \ n \geq 1,
\]
where \( \mathbf{1} = 1/\sqrt{D} \) and \( \mathcal{N}(\mu, \Sigma) \) denotes the multivariate Gaussian distribution over \( \mathbb{R}^D \) with mean \( \mu \) and covariance \( \Sigma \). We take \( D = 5 \). While the sequence \( \{Q_1, Q_2, \ldots\} \) converges weakly to \( P \), it does not
converge in mean. Indeed, by construction, the approximating sequence has the following biased limit:

\[
\lim_{n \to \infty} \mathbb{E}_{Y \sim Q_n}[Y] = \lim_{n \to \infty} \left(1 - \frac{1}{n + 1}\right) \mathbb{E}_{X \sim P}[X] + \frac{1}{n + 1} \mathbb{E}_{Z \sim \mathcal{N}(n + 1, 1, \text{Id})}[Z] = \mathbb{E}_{X \sim P}[X] + 1.
\]

We examine the kernel choice $\theta = 0.5$. For the weight function $w_{1,\theta}$, we take $\theta = 0.5$. We use $v = 1$ for the linear kernel and the weight function. For the translation-invariant kernel $\Phi$, we use the IMQ kernel $k_{\text{IMQ}}(x, x') = (1 + \|x - x'\|^2_2)^{-1/2}$. We also consider the case $\theta = 0$. We compare these two choices against using $k_{\text{IMQ}}$ alone.

For the above set of kernels, we investigate how the KSD between $P$ and $Q_n$ changes along the sequence. The KSD requires estimation as the expectation with respect to $k$ we use the IMQ kernel $φ$ and define a sample approximation to $Q_n$:

\[
Q_{n,N} = \left(1 - \frac{1}{n + 1}\right) \frac{1}{N} \sum_{i=1}^{N} \delta_{X_i} + \frac{1}{n + 1} \frac{1}{N} \sum_{i=1}^{N} \delta_{\tilde{X}_i}.
\]

As an estimate of the KSD, we compute the KSD between $P$ and $Q_{n,N}$; this estimate can be exactly computed using (9). In the following, we set $N = 500$. One might instead generate an i.i.d. sample from $Q_n$ directly. This approach might result in underestimating the KSD, since the mixture weight of the perturbation distribution $\mathcal{N}(n + 1, \text{Id})$ decreases as $n$ grows and thus we may not observe samples from this distribution if the sample size is relatively small.

Figure 1: Comparisons of KSD with different kernels. Settings: (a) IMQ; the IMQ kernel $k_{\text{IMQ}}$ (solid line), (b) IMQ sum (lin.) $\theta = 0$; the sum of the IMQ kernel and the normalized linear kernel (dashed line), (c) IMQ sum (lin.) $\theta = 0.1$; the sum of the IMQ kernel and the normalized linear kernel with tilting $\theta = 0.1$ (dash-dotted line).

Figure 1a shows the change of the KSD along the sequence for the three kernels. It can be seen that both the IMQ kernel and the sum kernel with $\theta = 0$ decay to non-zero constant values. To investigate the effect of bias due to the finite-sample approximation, we also vary the sample size $N$ for a large value of $n$; Figure 1b shows the result with $n = 10^6$. We can see that the KSD increases for all kernels for off-target samples, indicating that their population KSDs are underestimated in Figure 1a. For comparison, we also plot the KSD between $P$ and $P_N = \sum_{i \leq N} \delta_{X_i}$ with $X_i \overset{i.i.d.}{\sim} P$ in Figure 1c where all the KSDs decrease.
to zero. These observations imply that the IMQ kernel alone might be sufficient for detecting mean non-convergence. In contrast, the kernel with the additional tilting \( \theta = 0.1 \) diverges as \( n \) increases. By design, this kernel choice induces a function growing super-linearly, and its KSD can therefore capture the non-convergence of the mean. Remarkably, although the case \( \theta = 0 \) is not guaranteed by our theory, the KSD does not decay to zero, implying possibility to relax the growth condition in Lemma 3.6.

4.1.2 Non-convergence in variance

As in the previous section, we consider a case where a sequence does not converge in variance to their target and therefore not in \( d_{F_q}(q = 2) \). We use the following target and approximating sequence:

\[
P = \mathcal{N}(0, \text{Id}), \quad Q_n = \left(1 - \frac{1}{n+1}\right)P + \frac{1}{n+1}\mathcal{N}(0, 2(n+1)\text{Id}), \quad n \geq 1.
\]

As with the mean shift problem above, this example is constructed so that the sequence converges in distribution but not in variance, since the Gaussian in the second term always adds diagonal covariance \( 2\text{Id} \).

![Figure 2](image)

(a) Off-target sequence with non-converging variances with \( N \) fixed at 500.

(b) Effect of sample size \( N \). Sequence index \( n \) fixed at \( n = 10^6 \).

(c) On-target sequence formed by i.i.d samples from the target.

Figure 2: Comparisons of KSD with different kernels in the variance perturbation problem. Settings: (a) IMQ; the IMQ kernel \( k_{\text{IMQ}} \) (solid line), (b) IMQ sum (lin.) \( \theta = 0 \); the sum of the IMQ kernel and the normalized linear kernel \( q = 1 \) (dashed line), (c) IMQ sum (quad.) \( \theta = 0 \); the sum of the IMQ kernel and the normalized linear kernel with quadratic tilting \( q = 2 \) (dotted line), (d) IMQ sum (quad.) \( \theta = 0.1 \); The sum of the IMQ kernel and the normalized linear kernel with quadratic tilting \( q = 2 \) and additional reweighting \( \theta = 0.1 \) (dash-dotted line).

Figure 2a shows the KSD’s transition along the approximating sequence for our four kernel choices. Again, the IMQ and the IMQ sum (lin.) kernels have a similar trend. In this case, however, their KSDs decay to zero as the sample size \( N \) increases (Figure 2b), confirming that having a function of linear growth is not sufficient to detect the non-convergence. For the two kernels yielding quadratically growing Stein-KRKHS functions, we see that their KSDs indeed detect the non-convergence; in particular, the behavior of the KSD with \( \theta = 0 \) closely follows that of \( \theta = 0.1 \).
4.2 The DKSD and heavy-tailed distributions

In this section, we turn to heavy-tailed distribution to investigate the performance of the DKSD. Heavy-tailed distributions such as Student’s $t$-distributions have bounded score functions, and it is known that the Langevin KSD fail to detect non-convergence for this target class [Gorham and Mackey, 2017, Theorem 10].

As our target $P$, we use the standard multivariate $t$-distribution with the degrees of freedom $\nu > 1$ defined by the density

$$p(x) = \frac{\Gamma\left(\frac{\nu + D}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right)\nu^{\frac{D}{2}}\pi^{\frac{D}{2}}} \left(1 + \frac{\|x\|_2^2}{\nu}\right)^{-\frac{\nu + D}{2}}.$$  

The $t$-distribution is uniformly dissipative with $\sigma(x) = \sqrt{1 + \frac{\nu - 1}{\nu - \|x\|^2_2}}\Id$ and $\lambda_a = 4$. If $\nu > 2$, the diffusion is dissipative (Condition 2.3) with $\alpha = 1 - \frac{2}{\nu}$ (see Lemma 7.9). According to Lemma 3.7, the allowed power of the weight is $q_w < \left(\alpha + 1\right)/2 < 1$. As Proposition 3.4 requires uniform integrability of the higher moment, this bound on $q_w$ implies that the DKSD can only be used for examining mean convergence. In the following, we take $\nu = 4$ and consider the same perturbation as in the previous section:

$$Q_n = \left(1 - \frac{1}{n + 1}\right)P + \frac{1}{n + 1}\mathcal{N}\left((n + 1)\bar{1}, \Id\right), \ n \geq 1.$$  

The DKSD is estimated as in the previous section.

We consider the quadratic growth case in Section 3.3 (the tilting function is defined by Eq. 12). We compare the following two kernels: (a) $q = 0$ (uniform integrability of the first moment), (b) $q = 1$ (the second moment). The case $q = 1$ conforms to the requirement of Proposition 3.4 whereas the case $q = 0$ violates it. We also include the IMQ kernel as a baseline.

Figure 3: Comparisons of DKSD with different kernels with the target the standard $t$-distribution. Settings: (a) IMQ sum (lin.) $\theta = 0.1$; the sum of the IMQ kernel and the normalized linear kernel $q = 0$ (dashed line), (b) IMQ sum (quad.) $\theta = 0.1$; The sum of the IMQ kernel and the normalized linear kernel with quadratic tilting $q = 1$ and additional reweighting $\theta = 0.1$ (dash-dotted line).

Figure 3 demonstrates the result. While our theory requires the uniform integrability of the second moment, the linear-growth DKSD detects non-convergence; the same trend is observed for the quadratic-growth counterpart as expected. Recall that as the linear-growth DKSD characterizes the uniform integrability of the first moment, weak convergence control is sufficient for determining convergence in mean.
The success of the linear-growth DKSD may therefore be attributed to its ability to control weak convergence; this feature should be proved without the extra uniform integrability condition, and we leave this task as future work. Finally, the stricter requirement may be considered as an artifact of the strong claim of Proposition 3.4 which deals with the uniform convergence under a class of pseudo-Lipschitz functions.

We also examine a sequence formed by samples from the target, as in Section 4.1.1 (Figure 3c). Unlike the Gaussian case, three kernels show different rates of DKSD convergence. The DKSD with growing functions are more sensitive to discrepancies in the tail of the distribution and therefore are slower to converge; this observation is more relevant to heavy-tailed distributions than lighter-tailed ones.

4.3 Cautionary tale: distribution mixtures with isolated components

Our final experiment concerns the following distributions:

\[ P = \frac{1}{2} \mathcal{N}(\mu_1, \text{Id}) + \frac{1}{2} \mathcal{N}(\mu_2, \text{Id}), \quad \tilde{Q}_\pi = \pi \mathcal{N}(\mu_1, \text{Id}) + (1 - \pi) \mathcal{N}(\mu_2, \text{Id}), \]

where \(0 \leq \pi \leq 1\). The target \(P\) is supported by our theory, since Gaussian mixtures are known to be distantly dissipative [Gorham et al., 2019, Example 3]. However, when the distance \(\|\mu_1 - \mu_2\|_2\) between the two modes is large, the KSD is unable to capture the discrepancy of the mixture ratio \(\pi\) unless a very large sample size is observed. Indeed, the Wasserstein rate \(\rho_1(t) = 2e^{LR^2/8}e^{-rt/2}\) in Proposition 2.7 has an exponent depending on \(R = \|\mu_1 - \mu_2\|_2\), and the diffusion therefore suffers from the slow convergence when \(R\) is large, rendering the KSD insensitive to this difference for smaller sample sizes; Figure 4 illustrates this point. This issue has been noted by [Gorham et al., 2019, Section 5.1] and [Wenliang and Kanagawa, 2021].

![Figure 4: KSDs for Gaussian mixture target P, where mode separation parameter \(\|\mu_1 - \mu_2\|_2\) is chosen from \(\{3, 5\}\) with \(D = 5\). The IMQ sum kernel with \(\theta = 0\) is used. The dashed line indicates the KSD between \(P\) and empirical measures \(Q_{\pi,N}\) formed by i.i.d. samples of size \(N\) from \(\tilde{Q}_\pi\) with \(\pi = 0.1\). The dash-dotted line shows the KSD of empirical measures \(P_N\) given by i.i.d. samples of size \(N\) from the target \(P\). The larger the mode separation \(\|\mu_1 - \mu_2\|_2\), the large number of sample points is required to distinguish from the target.](image-url)

We detail our experimental procedure. In this setting, we use an i.i.d. sample \(\{X_i\}_{i=1}^N\) from \(\tilde{Q}_\pi\) to form a sequence of empirical distributions \(Q_{\pi,N} = N^{-1} \sum_{i \leq N} \delta_{X_i}\), and again exactly compute the KSD.
between $P$ and $Q_{\pi,N}$. In the following, we set $\mu_1 = -30 \cdot 1$, $\mu_2 = -10 \cdot 1$ and $D = 5$. With $N$ fixed at 500, we vary the mixture ratio $\pi$ from 0 to 1/2 using a regular grid of size 30. We noticed that the KSD’s trajectory has different trends depending on the drawn samples. We therefore repeat this procedure 100 times and provide a summary.

Our main question is whether the KSD can detect mean discrepancies due to isolated components based on a sample of size $N$. It is clear that the mean of $Q_{\pi,N}$ changes significantly as $\pi$ increases to 1/2. To this end, we consider the sum kernel in (11) with $q = 1$, ensuring that the Stein-modified RKHS has a function of linear growth. As the sequence has uniformly integrable first moments, we simply do not apply the additional tilting (i.e., $\theta = 0$). We examine two choices of the translation invariant kernel $\Phi$: the IMQ kernel $k_{\text{IMQ}}(x, x') = \left(1 + \|x - x'\|^2/\sigma^2\right)^{-1/2}$ and the following Matérn kernel

$$k_{\text{Mat}}(x, x') = \left(1 + \frac{\sqrt{3}\|x - x'\|}{\sigma}\right) \exp\left(-\frac{\sqrt{3}}{\sigma}\|x - x'\|\right).$$

First, we fix the bandwidth $\sigma$ to 1 for both kernels. Figure 5 plots the KSD value against the mixture ratio, along with the KSD’s density estimate computed from different sample draws. We observe that for both kernels, their KSDs do not change along the sequence.

![Figure 5: Comparison between the IMQ and the Matérn kernels in the mixture problem. Without bandwidth optimization. A dot represents the average of KSDs computed with different sample draws.](image)

This observation implies that the bandwidth choice may be suboptimal, making the KSD too weak to detect the change in the mixing proportion. Therefore, we next consider optimizing the bandwidth $\sigma$ for each $Q_{\pi,N}$ to improve the sensitivity. Following the approaches in nonparametric hypothesis testing [Gretton et al. 2012, Sutherland et al. 2016, Jitkrittum et al. 2016, 2017], we choose a bandwidth by optimizing the power of a test using the objective $S(Q_{\pi,N}, T_P, g_{\text{KRD}})^2/\sqrt{v_{H_1}}$, where $v_{H_1} = \text{Var}_{X \sim Q_{\pi,N}, X' \sim Q_{\pi,N}}[h_P(X, X')]$. This objective is a proxy of the power of the KSD goodness-of-fit tests [Chwialkowski et al. 2016, Liu et al. 2016] and can be computed exactly. The optimization procedure may be interpreted as seeking a bandwidth that allows us to conclude $P \neq Q_{\pi,N}$ using as few sample points as possible, without using the whole of $Q_{\pi,N}$. We choose a bandwidth that maximizes the objective from a regular grid between $10^{-3}$ and $10^3$ (in the logarithmic scale with base 10); the grid size 20.
Figure 6: Comparison between the IMQ and the Matérn kernels in the mixture problem. With optimized bandwidth for each kernel. A dot represents the average of KSDs computed with different sample draws.

Figure 6 shows the result. Both kernels manifest decreasing trends. The IMQ kernel tends to take larger values near $\pi = 0$, but stays at the same value past the point $\pi = 0.3$. In contrast, the Matérn kernel keeps the decreasing trend and captures the discrepancy. The Matérn kernel may therefore be thought of as more stable and inducing a stringent discrepancy measure.

We can attribute the KSD’s weak dependence on the mixture ratio to the score function [Wenliang and Kanagawa, 2021]. To see this, consider a density

$$r_\pi(x) = \pi p_1(x) + (1 - \pi)p_2(x), \ 0 < \pi < 1.$$  

The score function of $r_\pi$ is given by

$$s_{r,\pi}(x) = \tilde{\pi}(x)s_{p_1}(x) + (1 - \tilde{\pi}(x))s_{p_2}(x),$$

where $\tilde{\pi}(x) = \frac{\pi p_1(x)}{\pi p_1(x) + (1 - \pi)p_2(x)}$, and $s_p(x)$ denotes $\nabla \log p(x)$ for a density $p$. The function $\tilde{\pi}(x)$ represents the posterior probability of an observation $x$ arising from the mixture component $p_1$. We claim that for any two $\pi \neq \pi'$, the difference between $s_{r,\pi}$ and $s_{r,\pi'}$ is virtually absent. Our reasoning is as follows: $s_{r,\pi}(x)$ becomes $s_{p_1}$ (or $s_{p_2}$) in the high-probability region of $p_1$ (or $p_2$); thus, the difference between two score functions is negligible under $r_{x'}$ for any other configuration $\pi'$ so long as two components are concentrated in separate regions as in the Gaussian mixture example. This pathology is due to the following behavior of the posterior density $\tilde{\pi}(x)$: it becomes effectively a binary-valued function that outputs 1 in the high-density region of $p_1$ and 0 in the counterpart of $p_2(x)$. Indeed, if $p_1(x) \gg p_2(x)$, the posterior $\tilde{\pi}(x) \approx 1$ and is effectively independent of $\pi$. Figure 7 illustrates this situation for a Gaussian mixture in $D = 1$. Hence, in this case, varying the mixing proportion $\pi$ does not modify the score function $s_{r,\pi}$ significantly. Thus, as the KSD between two densities depends on the difference of their score functions [Liu et al., 2016, Definition 3.2], the KSD can be insensitive to mismatches of the mixture ratios.
Figure 7: A two component Gaussian mixture and its posterior probability \( \tilde{\pi}(x) \) of component assignment.

5 Conclusion

In this article, we have shown that the diffusion kernel Stein discrepancy controls the pseudo-Lipschitz metric \( d_{F_q} \), the worst-case expectation error over a class of polynomially growing function. A particular consequence of this result is that we may interpret the KSD in terms of convergence of moments. Our experiments confirm that the kernel Stein discrepancy with our proposed kernel choices indeed detects non-convergence in \( d_{F_q} \).

A theoretical shortcoming of our result is that we need a coercive function to characterize the uniform integrability (Lemma 3.6). Lemma 3.5 shows that we only need a function dominating a function of the form \( x \mapsto \|x\|^q 1_{\{\|x\|>r\}} \). A related question to address is whether we can remove the uniform integrability of a higher order moment in Proposition 3.4. As heavy-tailed distributions have finitely many moments, assuming a higher-order moment can be restrictive.

References

Milton Abramowitz and I.A. Stegun. *Handbook of Mathematical Functions: With Formulas, Graphs, and Mathematical Tables*. DOVER PUBN INC, June 1965. ISBN 0486612724. URL https://www.ebook.de/de/product/1675514/handbook_of_mathematical_functions_with_formulas_graphs_and_mathematical_tables.html.

Luigi Ambrosio, Nicola Gigli, and Giuseppe Savaré. *Gradient flows in metric spaces and in the space of probability measures*. Lectures in Mathematics ETH Zürich. Birkhäuser Verlag, Basel, 2005. ISBN 978-3-7643-2428-5; 3-7643-2428-7.

Andreas Anastasiou, Alessandro Barp, FranÃ§ois-Xavier Briol, Bruno Ebner, Robert E. Gaunt, Fatemeh...
Ghaderinezhad, Jackson Gorham, Arthur Gretton, Christophe Ley, Qiang Liu, Lester Mackey, Chris. J. Oates, Gesine Reinert, and Yvik Swan. Stein’s method meets computational statistics: A review of some recent developments. To appear in Statistical Science, May 2021.

N. Aronszajn. Theory of reproducing kernels. *Transactions of the American Mathematical Society*, 68 (3):337–337, March 1950.

Alessandro Barp, Francois-Xavier Briol, Andrew Duncan, Mark Girolami, and Lester Mackey. Minimum Stein discrepancy estimators. In *Advances in Neural Information Processing Systems*, volume 32, 2019.

Claudio Carmeli, Ernesto De Vito, and Alessandro Toigo. Vector valued reproducing kernel Hilbert spaces of integrable functions and Mercer theorem. *Analysis and Applications*, 4(4):377–408, 2006. ISSN 0219-5305. doi: 10.1142/S0219530506000838.

Wilson Ye Chen, Lester Mackey, Jackson Gorham, Francois-Xavier Briol, and Chris Oates. Stein points. In *Proceedings of the 35th International Conference on Machine Learning*, pages 844–853, 2018. URL https://proceedings.mlr.press/v80/chen18f.html.

Kacper Chwialkowski, Heiko Strathmann, and Arthur Gretton. A kernel test of goodness of fit. In *Proceedings of The 33rd International Conference on Machine Learning*, pages 2606–2615, 2016.

R. M. Dudley. *Real Analysis and Probability*. Cambridge University Press, oct 2002. doi: 10.1017/cbo9780511755347.

Andreas Eberle. Reflection couplings and contraction rates for diffusions. *Probability Theory and Related Fields*, 166(3-4):851–886, oct 2015. doi: 10.1007/s00440-015-0673-1.

Murat A. Erdogdu, Lester Mackey, and Ohad Shamir. Global non-convex optimization with discretized diffusions. In Samy Bengio, Hanna M. Wallach, Hugo Larochelle, Kristen Grauman, Nicolo Cesa-Bianchi, and Roman Garnett, editors, *Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, December 3-8, 2018, Montréal, Canada*, pages 9694–9703, 2018. URL https://proceedings.neurips.cc/paper/2018/hash/3ffebeb08d23c609875d7177ee769a3e9-Abstract.html.

Jackson Gorham and Lester Mackey. Measuring sample quality with Stein’s method. In *Advances in Neural Information Processing Systems*, volume 28, pages 226–234, 2015.

Jackson Gorham and Lester Mackey. Measuring sample quality with kernels. In *Proceedings of The 34th International Conference on Machine Learning*, pages 1292–1301, 2017.

Jackson Gorham, Andrew B Duncan, Sebastian J Vollmer, and Lester Mackey. Measuring sample quality with diffusions. *Annals of Applied Probability*, 2019.

Arthur Gretton, Dino Sejdinovic, Heiko Strathmann, Sivaraman Balakrishnan, Massimiliano Pontil, Kenji Fukumizu, and Bharath K Sriperumbudur. Optimal kernel choice for large-scale two-sample tests. In *Advances in Neural Information Processing Systems*, volume 25, pages 1205–1213, 2012.

Jonathan Huggins and Lester Mackey. Random feature Stein discrepancies. In *Advances in Neural Information Processing Systems*, volume 31, pages 1899–1909, 2018.

Wittawat Jitkrittum, Zoltán Szabó, Kacper P Chwialkowski, and Arthur Gretton. Interpretable distribution features with maximum testing power. In *Advances in Neural Information Processing Systems*, volume 29, pages 181–189, 2016.
Wittawat Jitkrittum, Wenkai Xu, Zoltan Szabo, Kenji Fukumizu, and Arthur Gretton. A linear-time kernel goodness-of-fit test. In Advances in Neural Information Processing Systems, volume 30, 2017.

Olav Kallenberg. Foundations of Modern Probability, volume 99 of Probability Theory and Stochastic Modelling. Springer International Publishing, third edition, 2021. ISBN 978-3-030-61871-1; 978-3-030-61870-4. doi: 10.1007/978-3-030-61871-1.

Qiang Liu, Jason Lee, and Michael Jordan. A kernelized Stein discrepancy for goodness-of-fit tests. In Proceedings of The 33rd International Conference on Machine Learning, pages 276–284, 2016.

Bertil Matérn. Spatial variation, volume 36 of Lecture Notes in Statistics. Springer-Verlag, Berlin, second edition, 1986. ISBN 3-540-96365-0. doi: 10.1007/978-1-4615-7892-5. With a Swedish summary.

Alfred Müller. Integral probability metrics and their generating classes of functions. Advances in Applied Probability, 29(2):429–443, 1997. ISSN 0001-8678. doi: 10.2307/1428011.

Chris J Oates, Mark Girolami, and Nicolas Chopin. Control functionals for Monte Carlo integration. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 79(3):695–718, 2017.

Nathan Ross. Fundamentals of Stein’s method. Probability Surveys, 8:210–293, 2011.

Charles Stein. A bound for the error in the normal approximation to the distribution of a sum of dependent random variables. In Proceedings of the Sixth Berkeley Symposium on Mathematical Statistics and Probability (Univ. California, Berkeley, Calif., 1970/1971), Vol. II: Probability theory, pages 583–602, 1972.

Michael L. Stein. Interpolation of spatial data. Springer Series in Statistics. Springer-Verlag, New York, 1999. ISBN 0-387-98629-4. doi: 10.1007/978-1-4612-1494-6. Some theory for Kriging.

Danica J. Sutherland, Hsiao-Yu Tung, Heiko Strathmann, Soumyajit De, Aaditya Ramdas, Alex Smola, and Arthur Gretton. Generative models and model criticism via optimized maximum mean discrepancy. In 4th International Conference on Learning Representations, ICLR 2016, San Juan, Puerto Rico, May 2-4, 2016, Conference Track Proceedings. 2016.

Cédric Villani. Optimal transport: old and new. Springer Berlin Heidelberg, 2009. doi: 10.1007/978-3-540-71050-9.

Feng-Yu Wang. Exponential contraction in Wasserstein distances for diffusion semigroups with negative curvature. Potential Analysis, 53(3):1123–1144, feb 2020. doi: 10.1007/s11118-019-09800-z.

Holger Wendland. Scattered Data Approximation. Cambridge University Press, dec 2004. doi: 10.1017/cbo9780511617539.

Li K. Wenliang and Heishiro Kanagawa. Blindness of score-based methods to isolated components and mixing proportions. In NeurIPS Workshop "Your Model is Wrong: Robustness and misspecification in probabilistic modeling", December 2021.
6 Proofs of main results

6.1 Characterization of pseudo-Lipschitz metrics

**Proposition 6.1.** Let $P \in \mathcal{P}_q$ be a probability measure on $\mathbb{R}^D$ with a finite $q$-th moment with $q \geq 1$. For a sequence of probability measures $\{Q_1, Q_2, \ldots, \} \subset \mathcal{P}_q$, the following conditions are equivalent:
(a) $d_{F_q}(Q_n, P) \rightarrow 0$ as $n \rightarrow \infty$, and (b) as $n \rightarrow \infty$, the sequence $Q_n$ converges weakly to $P$, and $\mathbb{E}_{X \sim Q_n} [\|X\|^q] \rightarrow \mathbb{E}_{X \sim P} [\|X\|^q]$.

**Proof.** (a) $\Leftarrow$ (b) Our goal is to show that the following quantity can be made arbitrarily small by taking sufficiently large $n$:

$$
\sup_{f \in \mathcal{F}_q} \left| \int f \, dQ_n - \int f \, dP \right| = \sup_{f \in \mathcal{F}_q} \left| \int (f - f(0)) \, d(Q_n - P) + \int f(0) \, d(Q_n - P) \right|_{n \to \infty} = \sup_{f \in \mathcal{F}_q} \left| \int \bar{f} \, d(Q_n - P) \right|,
$$

where $\bar{f}$ denotes $f - f(0)$. To this end, we smoothly truncate a function $\bar{f}$ using the bump function $1_{R,1}$ of Lemma 7.8 with $r = R$ and $\delta = 1$ for some $R \geq 1$ (the function $1_{R,1}(x)$ vanishes if $\|x\|_2 > R + 1$). Specifically, we break up the integral on the RHS as

$$
\sup_{f \in \mathcal{F}_q} \left| \int \bar{f} \, d(Q_n - P) \right| = \sup_{f \in \mathcal{F}_q} \left| \int \bar{f} 1_{R,1} \, d(Q_n - P) + \int \bar{f} (1 - 1_{R,1}) \, d(Q_n - P) \right|
$$

and evaluate each term below.

As a preparatory step, we clarify some properties of $\bar{f}$. Note that for any $f \in \mathcal{F}_q$, we have $|\bar{f}(x)| = |f(x) - f(0)| \leq (1 + \|x\|^{q-1})\|x\|_2$ for $x \in \mathbb{R}^D$. This implies that we have

$$
\|\bar{1}_{R,1}\|_\infty = \sup_{x \in \mathbb{R}} |\bar{f}(x)| 1_{R,1}(x) < (R + 1) + (R + 1)^q =: C_{1,R}
$$

and as $\bar{1}_{R,1}(x)$ is everywhere differentiable,

$$
\|\bar{1}_{R,1}\|_L = \sup_{x,y \in \mathbb{R}^D, x \neq y} \frac{|\bar{1}_{R,1}(x) - \bar{1}_{R,1}(y)|}{\|x - y\|_2} \leq \sup_{x \in \mathbb{R}^D} 1_{R,1}(x) \|\nabla \bar{f}(x)\|_2 + \bar{f}(x) \|\nabla 1_{R,1}(x)\|_2 \leq \sqrt{D} \{1 + 2(R + 1)^{q-1}\} + 8e^{-1} \{1 + R + (R + 1)^q\} =: C_{2,R}
$$

Let $C_R = 2(C_{1,R} \vee C_{2,R})$ Then, $\bar{1}_{R,1}/C_R$ belongs to the set of bounded Lipschitz functions $BL_1 = \{f : \mathbb{R}^D \to \mathbb{R} : \|f\|_\infty + \|f\|_L \leq 1\}$.

We are ready to bound the quantity of interest. For $\varepsilon > 0$, using the weak convergence assumption, take $n$ large enough so that

$$
d_{BL_1}(P, Q_n) := \sup_{f \in BL_1} \left| \int f \, dQ_n - \int f \, dP \right| < \frac{\varepsilon}{2C_R},
$$
which is possible as the bounded Lipschitz metric $d_{BL_1}$ metrizes weak convergence [Dudley, 2002, Section 11.3]. The definition of $R$ has been left unspecified; here, we take $R$ such that

$$\int_{\{\|x\|_2 > R\}} \|x\|^2_2 dP(x) \vee \sup_{n \geq 1} \int_{\{\|x\|_2 > R\}} \|x\|^2_2 dQ_n(x) < \varepsilon.$$  

The existence of $R$ is guaranteed by Lemma [7,3] for a weakly converging sequence of probability measures $\{Q_1, Q_2, \ldots \}$, the convergence in the $q$-th moment is equivalent to the $q$-th moment uniform integrability. Then,

$$\sup_{f \in F_q} \left| \int \tilde{f} d(Q_n - P) \right| \leq \sup_{f \in F_q} C_R \left| \int C^{-1}_R \cdot f_{1,R,1} d(Q_n - P) \right| + \sup_{f \in F_q} \left| \int (1 - f_{1,R,1}) d(Q_n - P) \right| \leq C_R \sup_{f \in BL_1} \left| \int f d(Q_n - P) \right| + \sup_{f \in F_q} \left| \int f_{1,R,1} dQ_n \right| + \sup_{f \in F_q} \left| \int (1 - f_{1,R,1}) dP \right| \leq C_R \epsilon + \epsilon + \epsilon = \epsilon.$$

The third line follows from the bounded Lipschitzness of $f_{1,R,1}/C_R$ and the triangle inequality; the fourth line is another application of the triangle inequality and $1 - f_{1,R,1}(x) \leq 1 \{\|x\|_2 > R\}$; the fifth line is true because $|\tilde{f}(x)| = |f(x) - f(0)| \leq (1 + \|x\|^{q-1}_2)\|x\|_2$ for any $x \in \mathbb{R}^D$, and because of the definition of $R$.

(a) $\Rightarrow$ (b) We first prove that convergence in $d_{F_q}$ implies weak convergence. For any $\varepsilon > 0$ and $f \in BL_1$, define the Gaussian convolution $f_\varepsilon(x) = \mathbb{E}_G[f(x - \varepsilon G)]$ with $G$ is a standard Gaussian random vector. The function is infinitely differentiable and satisfies, by the Lipschitzness of $f$,

$$\sup_{x \in \mathbb{R}^D} |f(x) - f_\varepsilon(x)| \leq \varepsilon \mathbb{E}[\|G\|_2].$$

By Lemma [7,1] we have constant bounds on the operator norms of the derivatives up to the third order; the bounding constants depend on $\varepsilon$. With $C_\varepsilon$ the maximum of the bounding constants, we $C_\varepsilon^{-1}f_\varepsilon \in F_q$. Then,

$$d_{BL_1}(Q_n, P) = \sup_{f \in BL_1} \left| \int f dQ_n - \int f dP \right| \leq \sup_{f \in BL_1} \left| \int f - f_\varepsilon dQ_n + \int f - f_\varepsilon dP + C_\varepsilon \left| \int C^{-1}_\varepsilon f_\varepsilon d(Q_n - P) \right| \right| \leq 2\varepsilon \mathbb{E}[\|G\|_2] + C_\varepsilon d_{F_q}(P, Q_n).$$

Taking the successive limits of $n, \varepsilon$ shows that $d_{BL_1}(Q_n, P) \rightarrow 0$, implying the weak convergence of the sequence.

Next, we show that convergence in $d_{F_q}$ implies $\mathbb{E}_{X \sim Q_n}\|X\|_2^q \rightarrow \mathbb{E}_{X \sim P}\|X\|_2^q$. As the weak convergence has been established above, we only need to show that the sequence $\{Q_1, Q_2, \ldots \}$ has uniformly integrable $q$-th moments. As $P \in \mathcal{P}_q$, we can take $R$ satisfying

$$\int_{\|x\|_2 > R} \|x\|_2^q dP(x) \leq \varepsilon.$$
Consider the function \( f_{q,R}(x) = \|x\|_2^q (1 - R_1(x)) \) with the smooth bump function \( 1_{R_1} \) of Lemma 7.8. This function has derivatives, up to the third order, growing in the order of \( \|x\|_2^{q-1} \), and therefore with a proper scaling \( C_R > 0 \) (depending on \( R \)), we have \( f_{q,R} \in \mathcal{F}_q \). By the convergence in \( d_{\mathcal{F}_q} \), for any \( \varepsilon > 0 \) we can take \( N \) such that for any \( n > N \),

\[
\int f_{q,R} dQ_n \leq \int f_{q,R} dP + C_R \varepsilon.
\]

These choices yield,

\[
\int_{\|x\|_2 > R + 1} \|x\|^2 dQ_n(x) \leq \int f_{q,R} dQ_n
\]

\[
\leq C_R^{-1} \left( \int f_{q,R} dP + C_R \varepsilon \right)
\]

\[
\leq \int_{\|x\|_2 > R + 1} \|x\|^2 dP + \varepsilon \leq 2 \varepsilon.
\]

Thus, we have arrived at the desired conclusion \( \lim_{r \to \infty} \limsup_{n \to \infty} \int_{\|x\|_2 > r} \|x\|^2 dQ_n(x) = 0 \).

**Corollary 6.2.** For \( q \geq 1 \), let \( d_{\operatorname{pLip},q-1}(P,Q) \) be the IPM defined by \( \operatorname{pLip}_{q-1} \), the set of functions that are pseudo-Lipschitz of order \( q - 1 \) with its pseudo-Lipschitz constant bounded by 1. For a sequence of probability measures \( \{Q_1,Q_2,\ldots\} \subset \mathcal{P}_q \), the following conditions are equivalent: (a) \( d_{\operatorname{pLip},q-1}(Q_n,P) \to 0 \) as \( n \to \infty \), and (b) as \( n \to \infty \), the sequence \( Q_n \) converges weakly to \( P \), and \( \mathbb{E}_{X \sim Q_n} \|X\|_2^q \to \mathbb{E}_{X \sim P} \|X\|_2^q \).

**Proof.** The direction (a) \( \Rightarrow \) (b) results from Proposition 3.1, as \( d_{\mathcal{F}_q}(P,Q) \leq d_{\operatorname{pLip},q-1}(P,Q) \). The other direction (b) \( \Rightarrow \) (a) can be shown as in the proof of Proposition 3.1.

### 6.2 Uniform integrability and a DKSD lower bound

Our goal is to show a KSD bound on the IPM \( d_{\mathcal{F}_q}(P,Q) \).

Let \( g \) be a solution to the Stein equation \( T_P g = f - \mathbb{E}_{X \sim P}[f(X)] \) for \( f \in \mathcal{F}_q \). We approximate \( T_P g \) by mollification. Specifically, we decompose the function \( T_P g \) into three parts:

\[
T_P g = T_P g_{\text{trunc}} + T_P g_{\text{trunc}} - T_P g_{\text{RKHS}} + \frac{\|g_{\text{RKHS}}\|_{\text{RKHS}}}{\|g_{\text{RKHS}}\|} T_P g_{\text{RKHS}}.
\]

We elaborate on each step as follows.

**Step 1: Smoothly truncating \( g \).** Let us start with the following notion.

**Definition 6.3** (Integrability rate of order \( q \)). For any probability measure \( Q \) and \( \varepsilon > 0 \), the integrability rate \( R_q(Q,\varepsilon) \) of order \( q \) is defined as

\[
R_q(Q,\varepsilon) := \inf \left\{ r \geq 1 : \int_{\{\|x\|_2 > r\}} \|x\|_2^q dQ(x) \leq \varepsilon \right\},
\]

where we use the convention \( \inf \emptyset = \infty \).
Note that $Q \in P_q$ is equivalent to having $R_q(Q, \varepsilon) < \infty$ for each $\varepsilon > 0$. In the following, for each $\varepsilon > 0$ and a probability measure $Q$, we consider the integrability rate $R = R_{q+q_a}(Q, \varepsilon)$. Let where $1_{R,1}$ be a smooth bump function from Lemma 7.8, which vanishes outside the centered Euclidean ball of radius $R + 1$. For a function $g \in G$, we consider a truncated version $g_{R,1} := 1_{R,1} \cdot g$. The truncation results yields the following error estimate:

**Lemma 6.4.** Let $Q \in P_{q+q_a}$ a probability measure and $R = R_{q+q_a}(Q, \varepsilon)$. For each $\varepsilon > 0$, we have

$$\left| \int T_P g dQ - \int T_P g_{R,1} dQ \right| \leq c_{P,D} \cdot \varepsilon$$

with $c_{P,D} = 2\sqrt{D} \zeta \left( \lambda_b + 8\varepsilon^{-1} \right) + D\lambda_m \zeta_2$.

**Proof.** Observe that for each $x \in \mathbb{R}^D$,

$$|T_P g(x) - T_P g_{R,1}(x)| \leq \left| (2b(x), g(x)(1 - 1_{R,1}))(x) \right| + \left| (m(x), \nabla g(1 - 1_{R,1}))(x) \right|$$

$$\leq 2\|b(x)\|_2\|g(x)\|_2\|1 - 1_{R,1}(x)\|_2 + D\|1 - 1_{R,1}(x)\| \|m(x)\|_{op}\|\nabla g(x)\|_{op}$$

$$+ \|\nabla 1_{R,1}(x)\|_2\|g(x)\|_2$$

$$\leq 1\{\|x\|_2 > R\} \left\{ \left\{ \frac{\lambda_b}{2} (1 + \|x\|_2) + 8\varepsilon^{-1} \right\} \cdot D\zeta_1 + D\zeta_2\lambda_m (1 + \|x\|_2^{q + 1}) \right\} (1 + \|y\|_2^{-1}).$$

By the definition of $R$, we have

$$\int_{\{\|x\|_2 > R\}} \|x\|_2^q dQ \leq \int_{\{\|x\|_2 > R\}} \|x\|_2^{q + q_a} dQ \leq \varepsilon.$$

for any $0 \leq q' < q + q_a$. Thus,

$$\left| \int T_P g dQ - \int T_P g_{R,1} dQ \right| \leq \int_{\|x\|_2 > R} \left\{ \left\{ \frac{\lambda_b}{2} (1 + \|x\|_2) + 8\varepsilon^{-1} \right\} \cdot D\zeta_1 (1 + \|x\|_2^{q + 1}) + D\zeta_2\lambda_m (1 + \|x\|_2^{q + 1}) \right\} dQ(x)$$

$$\leq \left\{ 2\sqrt{D} \zeta \left( \lambda_b + 8\varepsilon^{-1} \right) + D\lambda_m \zeta_2 \right\} \varepsilon.$$

\[\square\]

**Step 2: Constructing a smooth approximation to $g_{R,1}$**. We consider approximating the function $g_{R,1}$ with an RKHS function. For later use, we consider factorizing $g_{R,1}$ using a differentiable positive function $w(x) : \mathbb{R}^D \to [1, \infty)$; i.e.,

$$g_{R,1}(x) = w(x)g_{R,1}^w,$$

where $g_{R,1}^w := g_{R,1}/w$. We assume that $\sup_{x \in \mathbb{R}^D} \|\nabla \log w(x)\|_2 =: M_w < \infty$. We also define a helper function

$$B_w(z) := \sup_{x \in \mathbb{R}^D, u \in [0, 1]} \frac{w(x)}{w(x - uz)}.$$
The form of \( w \) will be specified below, which will be of the form \( w(x) = (v^2 + \|x\|_2^2)^q_w \); for this \( w \), we have \( B_w(z) = O(\|z\|_2^p) \). Note that \( 0 < p \leq 1 \), \( B_w(\rho z) \leq B_w(z) \).

For fixed \( \rho > 0 \), we define a smooth approximation \( g_{\rho}^w \) to by convolution,

\[
g_{\rho}^w(x) := \mathbb{E}_Z \left[ g_{R,1}^w(x - \rho Z) \right],
\]

where \( Z \) is a \( \mathbb{R}^D \)-valued random variable with \( \mathbb{E}[\|Z\|_2^2 B_w(Z)] < \infty \) (its law will be specified in the sequel). The following result quantifies the approximation error and mirrors the proof of Lemma 12 of [Gorham and Mackey [2017]]; here, we do not assume the Lipschitzness of the drift \( b \) (assuming the Lipschitzness will improve the \( D \)-dependency of the bound).

**Lemma 6.5.** Let \( g_{R,1}^w := g_{R,1}/w \) and \( g_{\rho}^w(x) := \mathbb{E}_Z \left[ g_{R,1}^w(x - \rho Z) \right] \). For each fixed \( \rho \in (0,1] \), the approximation \( g_{\rho}^w \) satisfies the following:

\[
\left| \int T_P(wg_{\rho}^w)\,dQ - \int T_Pg_{R,1}^w\,dQ \right|
\leq \rho \cdot U_{P,D,w} \cdot \left( 1 + R + 2\varepsilon \right) \cdot \left\{ 1 + (R + 1)^q - 1 \right\}
\]

where \( U_{P,D,w} = \left\{ 2\lambda_b + M_w\lambda_m \right\} \cdot \tilde{u}_{P,D,w}^{(1)} \cdot \tilde{u}_{P,D,w}^{(2)} \). Let \( \tilde{u}_{P,D,w}^{(1)} \) and \( \tilde{u}_{P,D,w}^{(2)} \) are constants given respectively in Lemmas 7.10 and 7.11 with \( \delta = 1 \).

**Proof.** By Lemmas 7.10 and 7.11, for each \( x \in \mathbb{R}^D \), we have

\[
\left| T_P(wg_{\rho}^w)(x) - T_Pwg_{R,1}^w(x) \right|
\leq \left| 2w(x)\langle b(x), g_{\rho}^w(x) - g_{R,1}^w(x) \rangle \right| + |w(x)|m(x)\langle \nabla g_{\rho}^w(x) - \nabla g_{R,1}^w(x) \rangle|
\leq w(x)\left\{ 2\|b(x)\|_2 + \|m(x)\|_{\text{op}} \| \nabla \log w(x) \|_2 \right\} \| g_{\rho}^w(x) - g_{R,1}^w(x) \|_2 + Dw(x)\|m(x)\|_{\text{op}} \| \nabla g_{\rho}^w(x) - \nabla g_{R,1}^w(x) \|_{\text{op}}
\leq \rho \cdot \left\{ 1 + (R + 1)^q - 1 \right\} \left\{ \frac{\lambda_b}{2} \left( 1 + \|x\|_2 \right) + M_w\lambda_m \left( 1 + \|x\|_2^q + 1 \right) \right\} \tilde{u}_{P,D,w}^{(1)} + D\lambda_m \cdot \left( 1 + \|x\|_2^q + 1 \right) \tilde{u}_{P,D,w}^{(2)}
\]

Note that

\[
\int (1 + \|x\|_2^q + 1)^q_{\frac{1}{2}} \,dQ(x) \leq 1 + R^{q_{\rho} + 1} + \int_{\{\|x\|_2^q + 1\}} \left( 1 + \|x\|_2^q + 1 \right) \,dQ(x)
\leq 1 + R^{q_{\rho} + 1} + 2\varepsilon.
\]

As a consequence,

\[
\left| \int T_Pwg_{\rho}^w\,dQ - \int T_Pg_{R,1}^w\,dQ \right|
\leq \rho (1 + R^{q_{\rho} + 1} + 2\varepsilon) \left\{ \frac{\lambda_b}{2} + M_w\lambda_m \right\} \tilde{u}_{P,D,w}^{(1)} + D\lambda_m \tilde{u}_{P,D,w}^{(2)} \left( 1 + (R + 1)^q - 1 \right).
\]
\[\blacksquare\]
Step 3: Measuring the RKHS norm of $w g^w_p$. The RKHS norm of $w g^w_p$ is derived once we specify the convolution distribution and the RKHS kernel function. The former will be specified below; for the latter, we assume that the scalar kernel is given by a weighted kernel

$$k(x, x') = w(x)w(x')\tilde{k}(x, x'),$$

where $\tilde{k}(x, x')$ is another positive definite kernel. This choice yields

$$\| wg^w_p \|_{G_{k1d}} = \sqrt{\sum_{d=1}^{D} \| w(g^w_p)_d \|^2_{G_k}} = \sqrt{\sum_{d=1}^{D} \| (g^w_p)_d \|^2_{G_k}},$$

where $(g^w_p)_d$ is the $d$th component of $g^w_p$. Thus, we only need to check the $G_k$ norm of each coordinate function of $g^w_p$.

We consider the tilting function $w(x) = (v^2 + \|x\|_2^2)^{q_w}$ with $v \geq 1$ and $q_w \in [0, \infty)$. We specify the law of the convolution variable $Z$ in (6.2) (i.e., the convolution kernel) with the sinc density from Lemma 7.5

$$s_{\tilde{q}_w}(x) = \prod_{d=1}^{D} \frac{\sin(4\tilde{q}_w(x_d))}{S_{\tilde{q}_w}},$$

where $S_{\tilde{q}_w} = \int_{-\infty}^{\infty} \sin(4\tilde{q}_w(x))dx$, $\tilde{q}_w = [q_w] + 1$ with the symbol $[x]$ denoting the smallest integer greater than or equal to $x$. Lemma 7.5 guarantees that $s_{\tilde{q}_w}$ is well-defined and has a finite $\tilde{q}_w$-th moment. Note that by the convolution theorem and $\| s_{\tilde{q}_w} \|_{L_1} = 1$, the Fourier transform $\hat{s}_{\tilde{q}_w}$ of $s_{\tilde{q}_w}$ satisfies

$$|\hat{s}_{\tilde{q}_w}(\omega)|^2 \leq (2\pi)^{-D/4} \{ \| \omega \|_\infty \leq 4\tilde{q}_w \} \text{ for } \omega \in \mathbb{R}^D,$$

where $\| \omega \|_\infty = \max_{d=1,\ldots,D} |\omega_d|$.  

**Lemma 6.6.** Let $g_{R,1} = g \cdot 1_{R,1}$ with $1_{R,1}$ a smooth bump function from Lemma 7.8. Let $w(x) = (v^2 + \|x\|_2^2)^{q_w}$ with $v \geq 1$ and $q_w > 0$. Let $\Phi_w(x, x') = w(x)w(x')\tilde{\Phi}(x - x')$ where $\tilde{\Phi} \in C^2$ is a positive definite function with non-vanishing generalized Fourier transform $\tilde{\Phi}$. Define the convolution $g^w_p$ of $g_{R,1}$ by

$$g^w_p(x) := \mathbb{E}_Z \left[ g_{R,1}(x - \rho Z) \right],$$

where $Z$ has the law with density $s_{\tilde{q}_w}$ from Lemma 7.5 with $\tilde{q}_w = [q_w] + 1$. Let $k = \Phi_w$. Then, the RKHS norm $\| w g^w_p \|_{G_{k1d}}$ is evaluated as

$$\| w g^w_p \|_{G_{k1d}} \leq (2\pi)^{-D/4} D\zeta_1 \sup_{\| \omega \|_\infty \leq \tilde{q}_w} \Phi(\omega)^{-1} \cdot \sqrt{\text{Vol}(\mathcal{B}_{R+1})} \cdot \left( 1 + (R + 1)^{q_w - 1} \right),$$

where $\text{Vol}(\mathcal{B}_{R+1})$ is the volume of the Euclidean ball of radius $R + 1$. In particular, the same conclusion holds if the kernel $k$ is given by $k = \Phi_w + \ell$, where $\ell$ is another positive definite kernel.

**Proof.** We first address the case $k(x, x') = \Phi_w(x, x')$. As $(g^w_p)_d$ is given by the convolution with $s(x) = \rho^{-D} s_{\tilde{q}_w}(x/\rho)$, by the convolution theorem (Wendland 2004, Theorem 5.16), its Fourier transform of is expressed by the product

$$(2\pi)^{D/2} (\hat{g}^w_R)_{d}(\omega) \hat{s}(\omega) = (2\pi)^{D/2} (\hat{g}^w_R)_{d}(\omega) \hat{\tilde{s}}_{\tilde{q}_w}(\rho \omega),$$

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The rest of the proof follows from the definition of the vector-valued RKHS $\Phi$. As we have shown that each component of

$$\Phi(k) = \Phi_{\phi_w}(k),$$

where $\Phi_{\phi_w}(k)$ denotes the volume of the unit ball in the Euclidean space $\mathbb{R}^D$, $F_P(t) = \sup_{\|\omega\| \leq t} \Phi(\omega)^{-1}$, and $\bar{q}_w = \lceil q_w \rceil + 1$. Therefore, for a sequence of measures $\{Q_1, Q_2, \ldots\}$ in $\mathcal{P}_{q+q_w}$ with uniformly integrable $(q + q_w)$-th moments, we have $S(Q_n, T_P, G_{k1d}) \to 0$ only if $d_{Fr}(P, Q_n) \to 0$. 

\[\text{Proposition 6.7. Let } \varepsilon > 0 \text{ be an arbitrary fixed positive real number. Let } \rho \in (0, 1) \text{ be a fixed number. Let } \Phi \in C^2 \text{ be a positive definite function with non-vanishing generalized Fourier transform } \Phi. \text{ Let } w(x) = (v^2 + \|x\|^2)^{q_w} \text{ with real numbers } v \geq 1 \text{ and } q_w \geq 0. \text{ Let } G_{k1d} \text{ be the RKHS defined by kernel } k_{1d} \text{ with } K(x, y) = \Phi_{w}(x, x') + \ell(x, x') \text{ where } \Phi_{w}(x, x') = w(x)w(x')\Phi(x-x'). \text{ Let } Q \text{ be a probability measure in } \mathcal{P}_{q+q_w} \text{ and } R := R_{q+q_w}(Q, \varepsilon/\epsilon_{P,D}). \text{ Then, we have}

\[d_{Fr}(P, Q) \leq \varepsilon + \rho U_{P,D,\omega} \cdot (1 + R^{q_w+1} + 2\varepsilon) \cdot \{1 + (R + 1)^{q_w-1}\}
\]

\[(2\pi)^{-D/4} D\zeta_1 \sqrt{\text{Vol}(B_1(\mathbb{R}^D)) (R + 1)^D} \cdot (1 + (R + 1)^{q_w-1}) F_{\Phi}(4\bar{q}_w \rho^{-1}) S(Q, T_P, G_{k1d}),\]

where $\text{Vol}(B_1(\mathbb{R}^D))$ denotes the volume of the unit ball in the Euclidean space $\mathbb{R}^D$, $F_{\Phi}(t) = \sup_{\|\omega\| \leq t} \Phi(\omega)^{-1}$, and $\bar{q}_w = \lceil q_w \rceil + 1$. Therefore, for a sequence of measures $\{Q_1, Q_2, \ldots\}$ in $\mathcal{P}_{q+q_w}$ with uniformly integrable $(q + q_w)$-th moments, we have $S(Q_n, T_P, G_{k1d}) \to 0$ only if $d_{Fr}(P, Q_n) \to 0$.\]
Proof. Using the results obtained so far, we have for a function \( f \in \mathcal{F}_q \),
\[
|E_{Y \sim Q} f(Y) - E_{X \sim P} [f(X)]| = |E_{Y \sim Q} T_P g(Y) |
\leq |E_{Y \sim Q} [T_P g(Y) - T_P g_{R,1}(Y)]|
+ |E_{Y \sim Q} [T_P g_{R,1}(Y) - T_P w g^w_{\rho}(Y)]| + |E_{Y \sim Q} T_P w g^w_{\rho}(Y)|
\leq |E_{Y \sim Q} [T_P g(Y) - T_P g_{R,1}(Y)]|
+ |E_{Y \sim Q} [T_P g_{R,1}(Y) - T_P w g^w_{\rho}(Y)]| + \|w g^w_{\rho}\|_{G_{kl}} S(Q, T_P, G_{kl})
\leq \varepsilon + \rho U_{P,D,w}(1 + R^2 + 2\varepsilon) \cdot \{1 + (R + 1)^{q-1}\}
+ (2\pi)^{-D/4} D\zeta_1 F_\Phi(4\tilde{\sigma}_w \rho^{-1}) \sqrt{\text{Vol}(B_1(\mathbb{R}^D))} (R + 1)^D S(Q, T_P, G_k).
\]

Taking the supremum over \( \mathcal{F}_q \) completes the proof of the first claim.

For the second claim, if the sequence has uniformly integrable \( q \)-th moments, we can take finite \( r \geq 1 \) such that \( R_{q+n}(Q_n, \varepsilon) \leq r \) for all \( n \geq 1 \). Thus, if \( S(Q, T_P, G_{k1d}) \to 0 \), taking successive limits of \( n, \rho, \varepsilon \) shows \( d_{\mathcal{F}_q}(P, Q_n) \to 0 \).

\[ \square \]

6.3 The diffusion Stein operator and zero-mean functions

Proposition 6.8 (The diffusion Stein operator generates zero-mean functions). Let \( q_a \in \{0, 1\} \) be the additional growth exponent of \( \|a(x)\|_{op} \) from Condition 2.2. If \( q_a = 0 \), assume \( P \) has a finite \( q \)-th moment; if \( q_a = 1 \), a finite \((q + 1)\)-th moment. Let \( g \in C^1 \) be a function with the following growth conditions:
\[
\|g(x)\|_2 \leq C_0 (1 + \|x\|_2^{\frac{q}{2}-1}),
\|\nabla g(x)\|_{op} \leq C_1 (1 + \|x\|_2^{\frac{q}{2}-1}),
\]
for each \( x \in \mathbb{R}^D \), and some positive constants \( C_0 \) and \( C_1 \). Then, we have \( E_{X \sim P} [T_P g(X)] = 0 \).

Proof. The proof is essentially that of [Gorham et al. 2019 Proposition 3]. Note that by the moment assumption on \( P \), we have \( E_{X \sim P} \left[(1 + \|X\|_2^{q+1})(1 + \|X\|_2^{\frac{q}{2}-1})\right] < \infty \) and thus
\[
E_{X \sim P} [T_P g(X)] \leq 2E_{X \sim P} [\|b(X)\|_2 \|g(X)\|_2 + D E_{X \sim P} [\|m(x)\|_{op} \|\nabla g(X)\|_{op} ] < \infty.
\]

Thus, we may apply the dominated convergence theorem and then the divergence theorem to obtain
\[
E_{X \sim P} [T_P g(X)] = \lim_{r \to \infty} \int_{B_r} \langle \nabla, p(x) \{a(x) + c(x)\} g(x) \rangle dx
= \lim_{r \to \infty} \int_{\partial B_r} \langle n_r(z), \{a(x) + c(x)\} g(z) \rangle p(z) dz,
\]
where \( dz \) denotes the \((D - 1)\)-dimensional Hausdorff measure, \( B_r = \{ x \in \mathbb{R}^D : \|x\|_2 \leq r \} \), and \( \partial B_r = \{ x \in \mathbb{R}^D : \|x\|_2 = r \} \). Let
\[
f(r) = \int_{\partial B_r} \|a(z) + c(z)\|_{op} \|g(z)\|_2 p(z) dz
\]
Then we have
\[
\int_{\partial B_r} \langle n_r(z), g(z) \rangle p(z) dz \leq f(r).
\]

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By the coarea formula (and integration with polar coordinates), we have
\[
\int_0^\infty f(r)dr = \int_0^\infty \left\{ \int_{\partial B_r} \|a(x) + c(x)\|_{\text{op}}\|g(z)\|_2 p(z)dz \right\} dr \\
\leq 2\lambda_m C_0 \int_0^\infty \left\{ \int_{\partial B_r} (1 + \|z\|_2^{q_a+1})(1 + \|z\|_2^{q_b-1})p(z)dz \right\} dr \\
= 2\lambda_m C_0 \int (1 + \|x\|_2^{q_a+1})(1 + \|x\|_2^{q_b-1})p(x)dx < \infty.
\]
Thus, we have \( \lim \inf_{r \to \infty} f(r) = 0 \) and therefore \( \mathbb{E}_{X \sim P}[T_P g(X)] = 0. \)

6.4 DKSD upper bounds

**Proposition 6.9.** Let \( G_k \) be the RKHS defined by a matrix-valued kernel \( \kappa : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}^{D \times D} \). Let \( q \geq 1 \). Assume that any function \( g \) in the unit ball \( B_1(G_k) \) satisfies the following: there exist some constants \( C_0, C_1, \) and \( C_2 \) such that
\[
\|\nabla^i g(x)\|_{\text{op}} \leq C_i(1 + \|x\|_2^{q_i-1}) \text{ for any } x \in \mathbb{R}^D \text{ and } i \in \{0, 1, 2\}.
\]
Assume a linear growth condition on \( m \) (Conditions 2.2, 3.2 with \( q_a = 0 \)). Assume that \( b \) is \( \phi_1(b) \)-Lipschitz in the Euclidean norm, and \( m \) is \( \phi_1(m) \)-Lipschitz in the Frobenius norm. Suppose \( P \in \mathcal{P}_q \).

Then,
\[
S(Q, T_P, G_k) \leq C_{b,m} d_{\text{plip}_1,q}(Q, P),
\]
where
\[
C_{b,m} = \frac{\lambda_b C_1(5 + 2q_1-1)}{4} + 4C_0 \phi_1(b) + \lambda_m C_2 D(5 + 2q_1-1) + 2\sqrt{D}C_1 \phi_1(m)
\]
In particular, we have \( S(Q_n, T_P, G_k) \to 0 \) if \( d_{F_q}(P, Q_n) \to 0 \).

**Proof.** For any \( g \in B_1(G_k) \), we show that \( T_P g \) is a pseudo-Lipschitz function of order \( q \). By the derivative assumptions, we have
\[
\|g(x) - g(y)\|_2 \leq C_1 \frac{1}{2} (1 + \|x\|_2^{q_1-1} + \|y\|_2^{q_1-1})\|x - y\|_2,
\]
and
\[
\|\nabla g(x) - \nabla g(y)\|_2 \leq C_2 \frac{1}{2} (1 + \|x\|_2^{q_1-1} + \|y\|_2^{q_1-1})\|x - y\|_2.
\]
Also,
\[
\frac{(1 + \|x\|_2)(1 + \|x\|_2^{q_1-1} + \|y\|_2^{q_1-1})}{(1 + \|x\|_2^{q_1} + \|y\|_2^{q_1})} (1 + \|x\|_2 + \|y\|_2^{q_1}) \leq 5 + 2q_1-1
\]
Using these estimates, we obtain
\[
|T_P g(x) - T_P g(y)| \leq 2|b(x)|_2\|g(x) - g(y)\|_2 + 2|b(x) - b(y)|_2\|g(y)\|_2 \\
+ D\|m(x)\|_{\text{op}}\|\nabla g(x) - \nabla g(y)\|_{\text{op}} + \sqrt{D}\|m(x) - m(y)\|_F\|\nabla g(y)\|_{\text{op}} \\
\leq C_{b,m} (1 + \|x\|_2^{q_1} + \|y\|_2^{q_1})\|x - y\|_2,
\]
where
\[
C_{b,m} = \frac{\lambda_b C_1(5 + 2q_1-1)}{4} + 4C_0 \phi_1(b) + \frac{\lambda_m C_2 D(5 + 2q_1-1)}{2} + 2\sqrt{D}C_1 \phi_1(m).
\]

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As a result, for any $g \in B_1(G_\kappa)$,
\[
\|E_{X \sim Q} T_P g(X) \| = C_{b,m} \| E_{X \sim Q} T_P g(X) - E_{Y \sim P} T_P g(Y) \| \\
\leq C_{b,m} d_{f_q}(Q_n, P),
\]
where the equality holds since $E_{Y \sim P} T_P g(Y) = 0$ by Proposition 2.9. Taking the supremum over $B_1(G_\kappa)$ provides the required relation $S(Q, T_P, G_\kappa) \leq C_{b,m} d_{f_q}(Q_n, P)$.

**Proposition 6.10.** Let $G_\kappa$ be the RKHS of $\mathbb{R}^D$-valued functions defined by a matrix-valued kernel $\kappa : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}^{D \times D}$. Let $q \geq 1$. Assume that any function $g$ in the unit ball $B_1(G_\kappa)$ satisfies the following: there exist some constants $C_0, C_1, C_2$ such that
\[
\| \nabla^i g(x) \|_{op} \leq C_i (1 + \| x \|_{2^q}^{q-1}) \text{ for any } x \in \mathbb{R}^D \text{ and } i \in \{0, 1, 2\}.
\]
Assume a quadratic growth condition on $m$ (Conditions 2.2, 3.2 with $q_a = 1$). Assume that $b$ is $\phi_1(b)$-Lipschitz, and $m$ is pseudo-Lipschitz of order 1 in the operator norm with constant $\tilde{\mu}_{p\text{Lip}}(m)_{1,1}$. Suppose $P \in \mathcal{P}_{q+1}$. Then,
\[
S(Q, T_P, G_\kappa) \leq C_{b,m} d_{p\text{Lip}_{1,q+1}}(Q, P),
\]
where
\[
C_{b,m} = (5 + 2^q) \left( \frac{\lambda_b C_1}{4} + \frac{\lambda_m C_2 D}{2} + C_1 D \tilde{\mu}_{p\text{Lip}}(m)_{1,1} \right) + 4\phi_1(b) C_0.
\]
In particular, we have $S(Q_n, T_P, G_\kappa) \to 0$ if $d_{\mathcal{P}_{q+1}}(P, Q_n) \to 0$.

**Proof.** The proof proceeds as in Proposition 3.9. For any $g \in B_1(G_\kappa)$, we have
\[
\| T_P g(x) - T_P g(y) \|
\leq 2 \| b(x) \|_2 \| g(x) - g(y) \|_2 + 2 \| b(x) - b(y) \|_2 \| g(y) \|_2 \\
+ D \| m(x) \|_{op} \| \nabla g(x) - \nabla g(y) \|_{op} + \sqrt{D} \| m(x) - m(y) \|_F \| \nabla g(y) \|_{op}
\leq \frac{\lambda_b C_1}{4} (1 + \| x \|_2) (1 + \| x \|_2^{q-1} + \| y \|_2^{q-1}) \| x - y \|_2 + 2\phi_1(b) C_0 (1 + \| x \|_2^{q-1}) \| x - y \|_2 \\
+ \frac{\lambda_m C_2 D}{8} (1 + \| x \|_2^2) (1 + \| x \|_2^{q-1} + \| y \|_2^{q-1}) \| x - y \|_2 \\
+ C_1 D \tilde{\mu}_{p\text{Lip}}(m)_{1,1} (1 + \| x \|_2^{q-1} + \| y \|_2^{q-1}) \| x - y \|_2
\leq C_{b,m} (1 + \| x \|_2^{q+1} + \| y \|_2^{q+1}) \| x - y \|_2,
\]
where
\[
C_{b,m} = (5 + 2^q) \left( \frac{\lambda_b C_1}{4} + \frac{\lambda_m C_2 D}{2} + C_1 D \tilde{\mu}_{p\text{Lip}}(m)_{1,1} \right) + 4\phi_1(b) C_0.
\]

\[\square\]

7 Auxiliary results

7.1 Results from previous work

**Lemma 7.1** (An extended version of Gorham et al. (2019) Lemma 17). Let $G$ be a $D$-dimensional standard normal random vector, and fix $s > 0$. If $f : \mathbb{R}^D \to \mathbb{R}$ bounded and measurable, and $f_s(x) =$
$\mathbb{E}[f(x + sG)]$, then
\[
M_0(f_s) \leq M_0(f), \quad M_1(f_s) \leq \sqrt{\frac{2}{\pi}} M_0(f), \quad M_2(f_s) \leq \sqrt{\frac{2}{s^2}} M_0(f), \quad \text{and} \quad M_3(f_s) \leq \frac{3M_0(f)}{s^3},
\]
where $M_0(f_s) = \sup_{x \in \mathbb{R}^D} |f_s(x)|$, and $M_i(f_s) = \sup_{x \in \mathbb{R}^D} \|\nabla^i f_s(x)\|_{op}$ for $i \in \{1, 2, 3\}$.

Proof. We prove the bound on $M_3(f_s)$, as the other bounds are given in [Gorham et al. 2019, Lemma 17]. Let $\phi_s \in C^\infty$ be the density of $sG$ and $*$ be the convolution operator. By Leibniz’s rule,
\[
\langle \nabla^3 f_s, u_1 \otimes u_2 \otimes u_3 \rangle = \langle (f * \nabla^3 \phi_s)(x), u_1 \otimes u_2 \otimes u_3 \rangle.
\]
The RHS can be evaluated as
\[
\left| \langle (f * \nabla^3 \phi_s)(x), u_1 \otimes u_2 \otimes u_3 \rangle \right| = \left| \int f(x - y) \langle \nabla^3 \phi_s(y), u_1 \otimes u_2 \otimes u_3 \rangle \, dy \right| \\
\leq \frac{M_0(f)}{s^6} \int \left\{ \prod_{i=1}^3 \langle y, u_i \rangle - s^2 \sum_{ijk} \langle u_i, y \rangle \langle u_j, u_k \rangle \right\} \phi_s(y) \, dy \\
\leq \frac{M_0(f)}{s^6} \sqrt{\int \left\{ \prod_{i=1}^3 \langle y, u_i \rangle - s^2 \sum_{ijk} \langle u_i, y \rangle \langle u_j, u_k \rangle \right\}^2 \phi_s(y) \, dy} \\
= \frac{M_0(f)}{s^6} \sqrt{s^6 \mathbb{E} \left[ \sum_{ijk} \langle u_i, G \rangle \langle u_j, u_k \rangle \right]^2} \\
\leq \frac{3M_0(f)}{s^3} \cdot \|u_1\|_2 \|u_2\|_2 \|u_3\|_2.
\]
where $\sum_{ijk}$ denotes the sum over the choices of $(i, j, k)$ from $\{(1, 2, 3), (2, 1, 3), (3, 1, 2)\}$, the equality holds by Isserlis’ theorem, and the last inequality follows from the Cauchy-Schwarz inequality after expanding the square. \(\square\)

7.2 Miscellaneous results

Definition 7.2 ($f$-uniform integrability). Let $Q$ be a set of probability measures on $\mathbb{R}^D$, and $f : \mathbb{R}^D \to [0, \infty)$ be a nonnegative function that is integrable for each $Q \in Q$. The function $f$ is called uniformly integrable with respect to $Q$, or the set $Q$ is called $f$-uniformly integrable if
\[
\lim_{r \to \infty} \sup_{Q \in Q} \int_{\{f(x) > r\}} f \, dQ = 0.
\]
Note that for a sequence $Q = \{Q_1, Q_2, \ldots\}$, the $f$-uniform integrability is equivalent to having
\[
\lim_{r \to \infty} \limsup_{n \to \infty} \int_{\{f(x) > r\}} f \, dQ_n = 0.
\]
The following lemma is an analogue of [Kallenberg 2021, Lemma 5.11]:

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Lemma 7.3. Let \( Q_1, Q_2, \ldots \) be a sequence of probability measures on a separable metric space \( X \) weakly converging to \( Q \). Then, for a nonnegative continuous function \( f \), we have

1. \( \int f \, dQ \leq \liminf_{n \to \infty} \int f \, dQ_n \),
2. \( \lim_{n \to \infty} \int f \, dQ_n \to \int f \, dQ < \infty \iff Q = \{ Q_1, Q_2, \ldots \} \) is \( f \)-uniformly integrable.

Proof. The proof follows [Kallenberg 2021, Lemma 5.11]. Below, we use the notation \( \mu(f) = \int f \, d\mu \) for a measure \( \mu \).

For any \( r > 0, x \mapsto f(x) \wedge r \) is a bounded continuous function. Thus, by the weak convergence assumption,

\[
\liminf_{n \to \infty} Q_n(f) \geq \liminf_{n \to \infty} Q_n(f \wedge r) = Q(f \wedge r).
\]

The first claim follows as we let \( r \to \infty \).

For the second claim, let us assume that \( Q \) is \( f \)-uniformly integrable. For any \( r > 0 \), we have

\[
|Q_n(f) - Q(f)| \\
\leq |Q_n(f) - Q_n(f \wedge r)| + |Q_n(f \wedge r) - Q_n(f \wedge r)| + |Q(f \wedge r) - Q(f)|.
\]

The first term on the RHS satisfies

\[
|Q_n(f) - Q_n(f \wedge r)| = Q_n((f - r)1_{\{f > r\}}) \\
\leq 2Q_n(f1_{\{f > r\}}) \\
\leq 2 \sup_n Q_n(f1_{\{f > r\}}).
\]

Note that \( Q(f) \leq \liminf_{n \to \infty} Q_n(f) < \infty \). Thus, letting \( n \to \infty \) and then \( r \to \infty \) proves the claim. For the other direction, assume \( Q_n(f) \to Q(f) < \infty \). With a fixed \( r > 0 \), as \( n \to \infty \),

\[
Q_n(f1_{\{f > r\}}) \leq Q_n(f - f \wedge (r - f)_+) \\
\to Q(f - f \wedge (r - f)_+),
\]

where we denote \((a)_+ = \max(a, 0)\). Since \( x \mapsto f(x) \wedge (r - f(x))_+ \) converges to \( f \) point-wise as \( r \to \infty \), by the dominated convergence theorem we have \( Q(f - f \wedge (r - f)_+) \to 0 \). \( \square \)

Lemma 7.4. Let \( w(x) = (a + b\|x\|^2)^q \) with \( a \geq 1, b > 0, \) and \( q > 0 \). Then,

\[
B_w(z) := \sup_{x \in \mathbb{R}^D, u \in [0, 1]} \frac{w(x)}{w(x - uz)} \\
\leq \left( 1 + 2 \left( 1 + \frac{b\|z\|^2}{a} \right) \right)^q \]

and

\[
M_w := \sup_{x \in \mathbb{R}^D} \|\nabla \log w(x)\|_2 = \sup_{x \in \mathbb{R}^D} \frac{2bq\|x\|_2}{a + b\|x\|^2} \leq q\sqrt{\frac{b}{a}}.
\]
Proof. We have
\[ w(x + uz) \leq \left( \frac{a + b\|x + uz\|^2}{a + b\|x\|^2} \right)^q \leq \left( 1 + \frac{\|x + uz\|^2}{\|x\|^2} \right)^q \]
\[ \leq \left( 1 + 2 \frac{\|x\|^2 + \|z\|^2}{a/b + \|x\|^2} \right)^q \]
\[ \leq \left( 1 + 2 \left( 1 + \frac{\|z\|^2}{a} \right)^q \right). \]

The first claim follows by observing
\[ \sup_{x \in \mathbb{R}^D, u \in [0,1]} \frac{w(x)}{w(x - u)} \leq \sup_{u \in [0,1]} \frac{w(x + uz)}{w(x)}. \]

The second claim can be checked easily. \( \square \)

Lemma 7.5 (A sinc function density and its moments). For an integer \( q \geq 1 \), let \( s_q : \mathbb{R}^D \to (0, \infty) \) be a probability density function defined by
\[ s_q(x) = \left( \frac{1}{I_{q, \infty}} \right)^D \prod_{d=1}^{D} (\text{sinc}(x_d))^{4q}, \]
where
\[ \text{sinc} : \mathbb{R} \to \mathbb{R}, \text{sinc}(x) = \begin{cases} \frac{\sin(x)}{x} & x \neq 0, \\ 1 & x = 0. \end{cases} \]
and \( I_{q,t} = 2 \int_{0}^{t} \text{sinc}^{4q}(x)dx \) for \( t \in (0, \infty) \). Let \( Z \) be a random variable with the law specified by \( s_{4q} \). Then, the \( q \)-th moment \( \mathbb{E}[\|Z\|^q_2] \) is finite. Specifically, it has the following upper bound:
\[ \mathbb{E}[\|Z\|^q_2] \leq \begin{cases} \frac{3D\log 2}{\pi} \left( \frac{I_{q,1}}{I_{q, \infty}} + \frac{1}{2q - q'/q'} \frac{1}{I_{q, \infty}} \right)^D, & q = 1, \\ q' \text{ is an integer such that } 1 \leq q' \leq q. \end{cases} \]

Proof. The density \( s_q \) is nonnegative due to the even power. We have
\[ I_{q, \infty} = \int_{0}^{\infty} \text{sinc}^{4q}(x)dx \leq \int_{0}^{\infty} \text{sinc}^2(x)dx = \frac{\pi}{2}, \]
where inequality holds as \( |\text{sinc}^2(x)| \leq 1 \) everywhere, and the upper integral value is obtained by integration by parts and using \( \int_{0}^{\infty} \text{sinc}(x) = \pi/2 \) [see, e.g., Abramowitz and Stegun 1965 Chapter 5]. Thus, \( I_{q, \infty} < \infty \), and the existence of the density \( s_q \) is guaranteed.

Assume \( q > 1 \), the moment estimates are derived as follows:
\[ I_{q, \infty}^D \mathbb{E}[\|Z\|^{q'}_2] \]
\[ = \int \|z\|^{q'}_2 s_q(z)dz \leq \int \|z\|^{q'}_2 s_q(z)dz \]
\[ = \sum_{i_1+\ldots+i_D=q'} \left( \frac{q'}{i_1!i_2!\ldots i_D!} \right) \prod_{d=1}^{D} 2 \int_{0}^{\infty} \frac{\sin^{2q}(z_d)}{|z_d|^{2q-1}} \left( \frac{\sin(z_d)}{z_d} \right)^{2q} dz_d. \]
The inequality holds because $\|\cdot\|_1$ upper bounds $\|\cdot\|_2$. By noting that $\text{sinc}(x) \leq 1$ for all $x \in \mathbb{R}$, we can further evaluate the integral:

$$
\int_0^\infty \sin^{2q}(zd) \left( \frac{\sin(zd)}{zd} \right)^{2q} \frac{dzd}{|zd|^{2q-1}} 
\leq \int_0^1 \left( \frac{\sin(zd)}{zd} \right)^{2q} dzd + \int_1^\infty \frac{1}{|zd|^{2q-i_d}} dzd 
= \frac{I_{4q,1}}{2} + \frac{1}{(2q-i_d)-1} \leq \frac{I_{4q,1}}{2} + \frac{1}{(2q-q')-1}.
$$

Thus, we have

$$
\mathbb{E}[\|Z\|_{q'}^q] \leq D_q\left( \frac{I_{4q,1}}{I_{4q,\infty}} + \frac{2}{(2q-q')-1} \frac{1}{I_{4q,\infty}} \right)^D.
$$

When $q = 1$, a similar computation shows

$$
\mathbb{E}[\|Z\|_2] \leq \frac{2D}{I_{4q,\infty}} \int_0^\infty \frac{\sin^4(zd)}{z_d^3} dzd \cdot \prod_{d' \neq d}^D \int \frac{\sin^4(zd)}{z_d^3} dzd' 
= \frac{2D \log 2}{I_{4,\infty}} = \frac{3D \log 2}{\pi}.
$$

Remark 7.6. The tedious expectation estimate is derived to ensure that the inside of the power function is small (typically less than $1$).

Lemma 7.7. Let $f(t) = e^{-1/t}1_{(0,\infty)}(t)$. Let

$$
h(t) = \frac{f(r + \delta - t)}{f(r + \delta - t) + f(t - r)}.
$$

Then, $h(t) = 0$ for $t \geq r + \delta$, $h(t) = 1$ for $t \leq r$, and $0 < h(t) < 1$ otherwise. Moreover, the first two derivatives of $h$ satisfies the following: for any $t \geq 0$,

$$
\left| \frac{dh}{dt} \right| (t) \leq \begin{cases} 
\frac{2}{\delta^2} & \delta \leq 1/2, \\
8e^{1/\delta - 2} & \delta > 1/2
\end{cases},
$$

$$
\left| \frac{d^2h}{dt^2} \right| (t) \leq \begin{cases} 
2 \left( 1 - 2\delta \right) + \frac{2}{\delta^2} \left( 1 + 4e^{-1/\delta} \right) & 0 \leq \delta \leq 1/2 - \sqrt{1/12}, \\
\frac{96\sqrt{3}}{(\sqrt{3}-1)^2} e^{-2\sqrt{3} - 1} e^{1/\delta} + \frac{2}{\delta} \left( 1 + 4e^{-1/\delta} \right) & 1/2 - \sqrt{1/12} < \delta \leq 1/2, \\
\left( \frac{96\sqrt{3}}{(\sqrt{3}-1)^2} e^{-2\sqrt{3} - 1} + 32e^{-4}(e^{1/\delta} + 4) \right) e^{1/\delta} & \delta > 1/2.
\end{cases}
$$

Proof. The cutoff property of $h$ is well known, and therefore we focus only on the bounds on the derivatives.
As a preparatory step, let us write down the first three derivatives of \( f \), which are given, for \( t > 0 \), as follows:

\[
f'(t) = \frac{1}{t^2}e^{-1/t},
\]

\[
f''(t) = \frac{1}{t^4}e^{-1/t}(-2t + 1), \quad \text{and}
\]

\[
f^{(3)}(t) = \frac{6}{t^6}e^{-1/t}(6t^2 - 6t + 1) = \frac{6}{t^6}e^{-1/t}\left\{ t - \left( \frac{1}{2} + \sqrt{\frac{1}{12}} \right) \right\} \left\{ t - \left( \frac{1}{2} - \sqrt{\frac{1}{12}} \right) \right\}.
\]

The first derivative \( f' \) increases from 0 to 1/2 and then decreases. Thus, \( f'(t) \leq f'(\delta \wedge 1/2) \) for \( \delta > 0 \) and \( 0 < t \leq \delta \). The second derivative \( f'' \) increases from zero to its maximum at \( t = \left( 1/2 - \sqrt{1/12} \right) \), and we have \( f''(t) \leq f''\left\{ \delta \wedge (1/2 - \sqrt{1/12}) \right\} \) for \( \delta > 0 \) and \( 0 < t \leq \delta \). Also, note that we have for \( 0 \leq t - r \leq \delta \),

\[
\frac{1}{f(\delta - (t-r)) + f(t-r)} \leq \frac{1}{f(\delta)}.
\]

Now we evaluate the first derivative of \( h \). We consider the region \( r < t < r + \delta \), as otherwise \( h \) is constant. Using \( h \leq 1 \), we obtain

\[
\left| \frac{dh}{dt} \right| = -\frac{f'(r + \delta - t)f(t-r)}{f(r + \delta - t) + f(t-r)} + \frac{f'(t-r)}{f(r + \delta - t) + f(t-r)} \leq \frac{2f'\left( \delta \wedge 1/2 \right)}{f(\delta)} \begin{cases} 2^{-1/2} & \delta \leq 1/2 \\ 8^{-1/2} & \delta > 1/2 \end{cases}.
\]

The second derivative can be similarly evaluated as follows:

\[
\left| \frac{d^2h}{dt^2} \right| = -\frac{f''(r + \delta - t)f(t-r) - 2f'(r + \delta - t)f'(r-t) + f''(t-r)f(r + \delta - t)}{(f(r + \delta - t) + f(t-r))^2} \leq \left( \frac{f''(r + \delta - t)}{f(r + \delta - t) + f(t-r)} \right) + 2\left( \frac{f'(t-r)}{f(r + \delta - t) + f(t-r)} \right) \left( \frac{f'(r - \delta - t)}{f(r + \delta - t) + f(t-r)} \right)
\]

\[
+ 2\left( \frac{f''(t-r)}{f(r + \delta - t) + f(t-r)} \right) \left( \frac{f'(r - \delta - t)}{f(r + \delta - t) + f(t-r)} \right)
\]

\[
+ 2\left( \frac{f''(r - \delta - t)}{f(r + \delta - t) + f(t-r)} \right) \left( \frac{f'(r - \delta - t)}{f(r + \delta - t) + f(t-r)} \right)
\]

\[
+ \left( \frac{f''(t-r)}{f(r + \delta - t) + f(t-r)} \right) \left( \frac{f'(r - \delta - t)}{f(r + \delta - t) + f(t-r)} \right) \leq \left( \frac{f''(r + \delta - t)}{f(r + \delta - t) + f(t-r)} \right) + 2\left( \frac{f'(r + \delta - t)f'(t-r)}{(f(r + \delta - t) + f(t-r))^2} \right)
\]

\[
+ 2\left( \frac{f''(t-r)}{f(r + \delta - t) + f(t-r)} \right) \left( \frac{f'(r - \delta - t)}{f(r + \delta - t) + f(t-r)} \right) \left( \frac{f'(r - \delta - t)}{f(r + \delta - t) + f(t-r)} \right).
\]
Consequently, we have the constant and has zero derivatives. According to Lemma 7.7, the first derivative satisfies \[ f''(\delta \land 1/2) \leq \frac{2 \left(1 - \frac{2\delta}{\delta^2}\right) + \frac{2}{\delta^3} \left(1 + 4e^{-1/\delta}\right)}{f(\delta)} \] for \( 0 \leq \delta \leq \frac{1}{2} - \frac{1}{\sqrt{12}} \). Then, we have the second derivative can also be evaluated as \[ f''(\delta \land 1/2) \leq \frac{8}{\delta^2} \left(1 - \frac{2\delta}{\delta^2}\right) + \frac{2}{\delta^3} \left(1 + 4e^{-1/\delta}\right) \] for \( \delta > \frac{1}{2} \).

**Lemma 7.8.** Let \( f(t) = e^{-t/1_{(0\infty)}}(t) \). Let \( 1_{r,\delta}(x) = h(\|x\|_2) \) be a smooth bump function defined by
\[
 h(t) = \frac{f(r + \delta - t)}{f(r + \delta - t) + f(t - r)}.
\]

Then, we have \( 1_{r,\delta}(x) \leq 1 \) for \( \|x\|_2 \leq r, \) \( 0 < 1_{r,\delta}(x) \leq 1 \) for \( r < \|x\|_2 < r + \delta, \) and \( \|x\|_2 \geq r + \delta; \) the gradient \( \nabla 1_{r,\delta}(x) \) vanishes outside \( \{x \in \mathbb{R}^D : r < \|x\|_2 < r + \delta\}. \) Furthermore, we can uniformly bound the derivative norms \( \|\nabla x 1_{r,\delta}(x)\|_2 \) and \( \|\nabla x 1_{r,\delta}(x)\|_2 \) by constants depending only on \( \delta. \) Specifically,
\[
\|\nabla x 1_{r,\delta}(x)\|_2 \leq \frac{2}{\delta^2} 1_{(0,1/2)}(\delta) + 8e^{1/\delta - 2} (1_{1/2,\infty})(\delta)
\]
and
\[
\|\nabla^2 x 1_{r,\delta}(x)\|_{op} \leq \frac{d^2 h}{dt^2}(\|x\|_2) + 2 \frac{d h}{dt}(\|x\|_2) \leq \frac{2}{\delta^2} 1_{(0,1/2)}(\delta) + 8e^{1/\delta - 2} (1_{1/2,\infty})(\delta).\]

**Proof.** We restrict the evaluation of the derivatives to the region \( r < \|x\|_2 \leq r + \delta, \) as otherwise \( h \) is constant and has zero derivatives. According to Lemma 7.7, the first derivative satisfies
\[
\|\nabla x h(\|x\|_2)\|_2 = \left| \left| \left| \frac{d h}{dt} \frac{x}{\|x\|_2} \right| \right|_{t=\|x\|_2} \right|_2 \leq \frac{2}{\delta^2} 1_{(0,1/2)}(\delta) + 8e^{1/\delta - 2} (1_{1/2,\infty})(\delta).
\]
The second derivative can be also evaluated as
\[
\nabla^2 x h(\|x\|_2) = \frac{d^2 h}{dt^2} \frac{x \otimes x}{\|x\|_2} + \frac{d h}{dt} \frac{1}{\|x\|} \left( f - \frac{x \otimes x}{\|x\|^2} \right).
\]
Consequently, we have
\[
\|\nabla^2 x h(\|x\|_2)\|_{op} = \sup_{\|u\|_2 = \|v\|_2 = 1} \langle u, \nabla^2 x h(\|x\|_2) v \rangle \leq \frac{d^2 h}{dt^2}(\|x\|_2) + \frac{d h}{dt}(\|x\|_2) \|x\|_2.
\]
The rest of the proof follows from the estimates of Lemma 7.7.
Lemma 7.9. For \( \nu > 2 \), let the standard multivariate t-distribution be

\[
p(x) = \frac{\Gamma \left( \frac{\nu+D}{2} \right)}{\Gamma \left( \frac{\nu}{2} \right) \nu^{\frac{D}{2}} \pi^\frac{D}{2}} \left( 1 + \frac{\|x\|^2}{\nu} \right)^{-\frac{\nu+D}{2}}.
\]

Then, the t-distribution satisfies the dissipativity condition in Proposition 2.6 with \( q = 1 \) and \( \sigma(x) = \sqrt{1 + \nu^{-1}\|x\|^2} \). For this choice, we have \( \lambda_\alpha = 4 \), and the diffusion is dissipative (Condition 2.3) with \( \alpha = 1 - 2\nu^{-1} \).

**Proof.** For this density, we have

\[
\nabla \log p(x) = -\frac{\nu + D}{\nu} \frac{x}{1 + \nu^{-1}\|x\|^2}, \quad a(x) = 1 + \nu^{-1}\|x\|^2, \quad \text{and} \quad 2b(x) = a(x)\nabla \log p(x) + \langle \nabla, a(x) \rangle = -\frac{\nu + D - 2}{\nu} x.
\]

Thus,

\[
2\langle b(x) - b(y), x - y \rangle + \|\sigma(x) - \sigma(y)\|^2 + \|\sigma(x) - \sigma(y)\|_\op^2
\]

\[
= -\frac{\nu + D - 2}{\nu} \|x - y\|^2 + (D - 1) \left( \sqrt{1 + \nu^{-1}\|x\|^2} - \sqrt{1 + \nu^{-1}\|y\|^2} \right)^2
\]

\[
\leq -\frac{\nu + D - 2}{\nu} \|x - y\|^2 + \frac{D-1}{\nu} \|x - y\|^2
\]

\[
= -\left( 1 - \frac{1}{\nu} \right) \|x - y\|^2.
\]

In particular,

\[
\mathcal{A}_P\|x\|^2 = 2\langle b(x), x \rangle + \|\sigma(x)\|_\op^2
\]

\[
= -\frac{\nu + D - 2}{\nu} \|x\|^2 + D(1 + \nu^{-1}\|x\|^2)
\]

\[
= -(1 - 2\nu^{-1}) \|x\|^2 + D.
\]

\(\square\)

### 7.3 Results concerning approximation

**Lemma 7.10.** Let \( B_w(z) = \sup_{x \in \mathbb{R}^D, u \in [0, 1]} w(x)/w(x - uz) \) and \( M_w = \sup_{x \in \mathbb{R}^D} \| \nabla \log w(x) \|_2 \). Let \( Z \) be a random variable with \( \mathbb{E}_Z[\|Z\|_2 B_w(Z)] < \infty \). With fixed \( \rho \in (0, 1] \), define for \( g_{R, \delta}^w := g_{R, \delta}/w \), the convolution

\[
g_{R, \delta}^w(x) = \mathbb{E}_Z \left[ \frac{g_{R, \delta}(x - \rho Z)}{w(x - \rho Z)} \right].
\]

We have

\[
\|g_{R, \delta}^w - g_{\rho}^w\|_2 \leq \rho \frac{\mathbb{E}_w(x)}{w(x)} \cdot \hat{u}_{R, \delta, D, w}^{(1)} \{ 1 + (R + \delta)^{q-1} \}
\]

with a constant

\[
\hat{u}_{R, \delta, D, w}^{(1)} = \left[ \sqrt{D} \zeta_1 M_w \mathbb{E} \left[ \|Z\|_2 B_w(\rho Z) \right] + \{ \zeta_2 + C_\delta \zeta_1 \} \right],
\]

where \( C_\delta \) is a constant bounding \( \| \nabla 1_{R, \delta}(x) \|_2 \) satisfying \( C_\delta = 8e^{-\delta} \) for \( \delta > 1/2 \).
Proof. By the definition of \( g_\rho \), we have

\[
g_\rho^w(x) - g_{R,\delta}^w(x) = \mathbb{E}_Z \left[ g_{R,\delta}(x - \rho Z) \left\{ \frac{1}{w(x - \rho Z)} - \frac{1}{w(x)} \right\} + \frac{g_{R,\delta}(x - \rho Z) - g_{R,\delta}(x)}{w(x)} \right].
\]

To bound each quantity inside the expectation, we derive their norm estimates. For \( g_{R,\delta} \), we have

\[
M_0(g_{R,\delta}) := \sup_{x \in \mathbb{R}^D} \|g_{R,\delta}(x)\|_{op} = \max_{\|x\| \leq R+\delta} \|g(x)\|_2 = \sqrt{D}\zeta_1 \{1 + (R + \delta)^{q-1}\}
\]

and

\[
\tilde{\pi}(g_{R,\delta})_{1,0} := \sup_{x' \in \mathbb{R}^D} \|\nabla g_{R,\delta}(x')\|_{op} \leq \sup_{x' \in \mathbb{R}^D} 1_{R,\delta}(x) \|\nabla g(x)\|_{op} + \sup_{x' \in \mathbb{R}^D} \|\nabla 1_{R,\delta}(x)\|_2 \|g(x)\|_2 \leq (\zeta_2 + C_\delta \zeta_1) \{1 + (R + \delta)^{q-1}\},
\]

where \( C_\delta \) is a universal constant depending on \( \delta \). Further, by the fundamental theorem of calculus,

\[
\|g_{K,\delta}(x - \rho Z) - g_{K,\delta}(x)\|_2 \leq \rho \int_0^1 \|\nabla g_{R,\delta}(x - t\rho Z)\|_2 dt_2 \leq \rho \int_0^1 \|\nabla g_{R,\delta}(x - t\rho Z)\|_{op} \|Z\|_2 dt_2 \leq \rho \|Z\|_2 \tilde{\pi}(g_{R,\delta})_{1,0}.
\]

We also have

\[
\left\| \frac{1}{w(x - \rho Z)} - \frac{1}{w(x)} \right\| = \rho \int_0^1 \left\| \frac{\nabla w}{w^2}(x - t\rho Z), Z \right\| dt \leq \rho \|Z\|_2 \frac{1}{w(x)} \int_0^1 \frac{w(x)}{w(x - t\rho Z)} \left\| \frac{\nabla w}{w}(x - t\rho Z) \right\|_2 dt \leq \rho M_w \frac{\|Z\|_2 B_w(\rho Z)}{w(x)}.
\]

Combining these evaluations yields

\[
\|g_\rho^w(x) - g_{R,\delta}^w(x)\|_2 \leq \mathbb{E}_Z \left[ \|g_{R,\delta}(x - \rho Z)\|_2 \left\| \frac{1}{w(x - \rho Z)} - \frac{1}{w(x)} \right\| \right] + \mathbb{E}_Z \left[ \left\| g_{R,\delta}(x - \rho Z) - g_{R,\delta}(x) \right\| \right] \leq \frac{\rho}{w(x)} \left[ M_w \mathbb{E}[\|Z\|_2 B_w(\rho Z)] M_0(g_{R,\delta}) + \tilde{\pi}(g_{R,\delta})_{1,0} \right] = \sqrt{D}\zeta_1 M_w \mathbb{E}[\|Z\|_2 B_w(\rho Z)] + (\zeta_2 + C_\delta \zeta_1) \cdot \frac{\rho \{1 + (R + \delta)^{q-1}\}}{w(x)}.
\]
Lemma 7.11. Define symbols as in Lemma 7.10. For each fixed $\rho \in (0, 1]$, we have

$$\|\nabla g^w_{\rho}(x) - \nabla g^w_{R,\delta}(x)\|_{\text{op}} \leq \frac{\rho}{w(x)} \tilde{u}_P^{(2)} \cdot \{1 + (R + \delta)^{q-1}\},$$

where

$$\tilde{u}_P^{(2)} = \left\{(1 + M_w)(\zeta_3 + 2C_\delta \zeta_2 + C_{R,\delta} \zeta_1) \mathbb{E} \|Z\|_2 \right\}.$$ 

where $C_\delta$ and $C_{R,\delta}$ are respective uniform bounds on $\|\nabla 1 \|_2$ and $\|\nabla^2 1 \|_{\text{op}}$, satisfying $C_\delta = 8e^{-\delta}$ and

$$C_{R,\delta} = \frac{8}{R} e^{1/\delta - 2} + \left(\frac{96\sqrt{3}}{(\sqrt{3} - 1)^4} + e^{-2/\delta - 1} + 32e^{-1/\delta + 4}\right)e^{1/\delta}.$$

for $\delta > 1/2$.

Proof. Before the proof, we introduce a notation. We denote the $l$-mode (vector) product of a tensor $T \in \mathbb{R}^{D_1 \times \cdots \times D_L}$ with a vector $v \in \mathbb{R}^{D_l}$ by $T \times_l v$. The resulting tensor is of order $L - 1$; its size is $(D_1, \ldots, D_{l-1}, D_{l+1}, \ldots, D_L)$; it is expressed element-wise as

$$(T \times_l v)_{i_1 \cdots i_{l-1}i_{l+1} \cdots i_L} = \sum_{i_l=1}^{D_l} T_{i_1 \cdots i_l \cdots i_{L}} v_{i_l}.$$

First, note that

$$\|\nabla g^w_{\rho}(x) - \nabla g^w_{R,\delta}(x)\|_{\text{op}} \leq \left\|\mathbb{E}_Z \left[\nabla g^w_{R,\delta}(x - \rho Z) - \nabla g^w_{R,\delta}(x)\right]\right\|_{\text{op}}$$

$$+ \left\|\mathbb{E}_Z \left[\frac{\nabla \log w(t - \rho Z)}{w(x - \rho Z)} \otimes \nabla g_{R,\delta}(x - \rho Z) - \frac{\nabla \log w(x)}{w(x)} \otimes \nabla g_{R,\delta}(x)\right]\right\|_{\text{op}}.$$ (16)

In the first line, we have exchanged the gradient and the expectation operation. We evaluate each term below.

The term (a) is evaluated as

$$\left\|\mathbb{E}_Z \left[\frac{\nabla g_{R,\delta}(x - \rho Z)}{w(x - \rho Z)} - \frac{\nabla g_{R,\delta}(x)}{w(x)}\right]\right\|_{\text{op}} \leq \left\|\mathbb{E}_Z \left[\nabla g_{R,\delta}(x - \rho Z) \left(\frac{1}{w(x - \rho Z)} - \frac{1}{w(x)}\right)\right]\right\|_{\text{op}}$$

$$+ \frac{1}{w(x)} \left\|\mathbb{E}_Z \left[\nabla g_{R,\delta}(x - \rho Z) - \nabla g_{R,\delta}(x)\right]\right\|_{\text{op}}.$$ (17)

The term (i) is bounded as

$$(i) \leq \mathbb{E}_Z \left[\left|\frac{1}{w(x - \rho Z)} - \frac{1}{w(x)}\right| \left\|\nabla g_{R,\delta}(x - \rho Z)\right\|_{\text{op}}\right]$$

$$\leq \frac{\rho}{w(x)} M_w \tilde{\pi}(g_{R,\delta})_{1,0} \mathbb{E}_Z \left[\|Z\|_2 B_w(\rho Z)\right].$$

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The term (ii) is evaluated as follows. By the fundamental theorem of calculus,
\[ \nabla g_{R,\delta}(x - \rho Z) - \nabla g_{R,\delta}(x) = -\rho \int_0^1 \nabla^2 g_{R,\delta}(x - t\rho Z) \hat{x}_1 Z \, dt. \]

Note that the operator norm of \( \nabla^2 g_{R,\delta} \) is bounded by
\[
\tilde{\pi}(g_{R,\delta})_{2,0} := \sup_{x \in \mathbb{R}^D} \| \nabla^2 g_{R,\delta}(x) \|_\text{op}
\leq \sup_{x \in \mathbb{R}^D} \left( 1_{R,\delta}(x) \| \nabla^2 g(x) \|_\text{op} + 2 \| \nabla^1 g_{R,\delta}(x) \|_2 \| g_{R,\delta}(x) \|_2 + \| \nabla^2 g_{R,\delta}(x) \|_2 \| g_{R,\delta}(x) \|_2 \right)
\leq \sup_{x \in \mathbb{R}^D} \left( 1_{R,\delta}(x) \zeta_3 + 2 \| \nabla^1 g_{R,\delta}(x) \|_2 \zeta_2 + \| \nabla^2 g_{R,\delta}(x) \|_2 \zeta_1 \right) (1 + \| x \|^q - 1)
\leq (\zeta_3 + 2C_\delta \zeta_2 + C_R,\delta \zeta_1) \{ 1 + (R + \delta)^{q-1} \}. \tag{18}
\]

Thus, the operator norm in the term (ii) is bounded as
\[
\| \mathbb{E}_Z \left[ \nabla g_{R,\delta}(x - \rho Z) - \nabla g_{R,\delta}(x) \right] \|_\text{op}
\leq \mathbb{E}_Z \left[ \| \nabla g_{R,\delta}(x - \rho Z) - \nabla g_{R,\delta}(x) \|_\text{op} \right]
\leq \mathbb{E}_Z \left[ \| Z \|_2 \sup_{\| u^{(i)} \|_2 = 1} \left\{ \left\| \int_0^1 \nabla^2 g_{R,\delta}(x - t\rho Z) \hat{x}_1 Z \|_2 \, dt \right\|_2 \right\} \right]
\leq \rho \mathbb{E}_Z \left[ \| Z \|_2 \int_0^1 \sup_{\| u^{(i)} \|_2 = 1} \left\| \langle \nabla^2 g_{R,\delta}(x - t\rho Z), u^{(1)} \otimes u^{(2)} \otimes u^{(3)} \rangle \right\|_2 \right] \right]
\leq \rho \mathbb{E}_Z \left[ \| \mathbb{E}_Z \left[ \| \nabla^2 g_{R,\delta}(x - t\rho Z) \|_\text{op} \right] dt \right]
\leq \rho \mathbb{E}_Z \left[ \| \mathbb{E}_Z \left[ \| \nabla^2 g_{R,\delta}(x - t\rho Z) \|_\text{op} \right] dt \right]
\leq \rho \tilde{\pi}(g_{R,\delta})_{2,0} \mathbb{E}_Z \| Z \|_2.
\]

Thus, the term (ii) is bounded by
\[
\frac{\rho}{w(x)} \tilde{\pi}(g_{K,\delta})_{2,0} \mathbb{E}_Z \| Z \|_2.
\]
Similarly, we can evaluate the term (b) in (16) for some \( \eta > 0 \) and \( \nu > 0 \):

\[
(b) = \frac{1}{w(x)} \left| \langle \nabla \log w(t - \rho Z), \nabla g_{R,\delta}(x - \rho Z) - \nabla g_R(x) \rangle \right|_{\text{op}}
\]

\[
\leq \frac{1}{w(x)} \left| E_Z \left[ \left| \nabla \log w(t - \rho Z) - \nabla \log w(x) \right| \right| \nabla g_{R,\delta}(x - \rho Z) - \nabla g_R(x) \right|_{\text{op}}
\]

\[
\leq \frac{1}{w(x)} E_Z \left[ \left| \nabla \log w(t - \rho Z) - \nabla \log w(x) \right| \right| \nabla g_{R,\delta}(x - \rho Z) - \nabla g_R(x) \right|_{\text{op}}
\]

\[
\leq \frac{M_w}{w(x)} \left[ \left| \nabla \log w(t - \rho Z) - \nabla \log w(x) \right| \right| \nabla g_{R,\delta}(x - \rho Z) - \nabla g_R(x) \right|_{\text{op}}
\]

\[
+ \frac{2M_w}{w(x)} \pi(g_{R,\delta})_{2,0} E_Z \left[ \left| g_{R,\delta} \right|_{\text{op}} \right] B_w(\rho Z)
\]

\[
\leq \frac{\rho M_w}{w(x)} \left( \left[ \left| \nabla \log w(t - \rho Z) - \nabla \log w(x) \right| \right| \nabla g_{R,\delta}(x - \rho Z) - \nabla g_R(x) \right|_{\text{op}} \right)
\]

\[
\leq \frac{\rho M_w}{w(x)} \left( E_Z \left[ \left| g_{R,\delta} \right| \right|_{\text{op}} \right] B_w(\rho Z)
\]

With \( B(\rho Z) \leq B(Z) \) in mind, combining the results, we obtain

\[
\left| \nabla \log w(x) - \nabla g_{R,\delta}(x) \right|_{\text{op}} \leq \frac{\rho}{w(x)} \hat{u}^{(2)}_{P,\delta,D,w}(x) \{ 1 + (R + \delta)^{q-1} \},
\]

where

\[
\hat{u}^{(2)}_{P,\delta,D,w} = (1 + M_w) E_Z \left[ \left| g_{R,\delta} \right| \right|_{\text{op}} B_w(\rho Z)
\]

\[
+ M_w (1 + 2M_w) E_Z \left[ \left| g_{R,\delta} \right| \right|_{\text{op}} B_w(\rho Z)
\]

\[
= \left\{ (1 + M_w) (\zeta_3 + 2C_{\delta} \zeta_2 + C_{R,\delta} \zeta_1) E_Z \left[ \left| g_{R,\delta} \right| \right|_{\text{op}} B_w(\rho Z)
\right) + M_w (1 + 2M_w) (\zeta_2 + C_{R,\delta} \zeta_1) E_Z \left[ \left| g_{R,\delta} \right| \right|_{\text{op}} B_w(\rho Z) \right\}.
\]

\[
\square
\]

### 7.4 Results for DKSD

#### 7.4.1 DKSD and uniform integrability

**Lemma 7.12 (KSD upper-bounds the integrability rate).** Let \( \mathcal{G}_\kappa \) be the RKHS of \( \mathbb{R}^D \)-valued functions defined by a matrix-valued kernel \( \kappa : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}^{D \times D} \). Suppose there exists a function \( g \in \mathcal{G}_\kappa \) such that \( T_P g(x) \geq \nu \) for any \( x \in \mathbb{R}^D \) with some constant \( \nu \in \mathbb{R} \), and \( \lim \inf \| x \|_2^{-(q+\theta)} T_P g(x) \geq \eta \) for some \( q \geq 0, \eta > 0, \) and \( \theta > 0 \) as \( \| x \|_2 \to \infty \). Then, for sufficiently small \( \varepsilon > 0 \), we have

\[
R_q(Q, \varepsilon) := \min \left\{ r, \inf \left\{ \| Q \|_2 \geq r \left\| x \|_2^q \left\| dQ(x) \right\| \leq \varepsilon \right\} \right\}
\]

\[
\leq 2 \left( 1 + \frac{q}{\theta} \right) \left( \frac{S(Q, T_P, \mathcal{G}_\kappa) - \nu}{\eta \varepsilon} \right)^{\frac{1}{q+\theta}}.
\]
where \(S(Q, T_P, G_n) = \infty\) if \(Q \notin \mathcal{P}_{q+\theta}\). Thus, for a sequence of measures \(\{Q_1, Q_2 \ldots\} \subset \mathcal{P}_q\) we have
\[
\limsup_{n \to \infty} S(Q_n, T_P, G_n) < \infty \Rightarrow \limsup_{n \to \infty} R_q(Q_n, \varepsilon) < \infty.
\]

In particular, if the sequence \(\{Q_1, Q_2 \ldots\}\) does not have uniformly integrable \(q\)-th moments, then Stein discrepancy \(S(Q_n, T_P, G_n)\) diverges.

**Proof.** Let \(g \in G_{kld}\) be a function with the stated properties. Let \(f(x) = \|x\|_2^q(1\{\|x\|_2 > r\})\). We consider the integral
\[
\int_{\|x\|_2 > r} \|x\|_2^q dQ(x) = \int f(x) dQ(x) = \int_0^\infty Q(\{f(x) > t\}) dt.
\]
By dividing the range of the integral, we obtain
\[
\int_0^\infty Q(\{f(x) > t\}) dt = r^q Q(\|x\|_2 > r) + \int_{r^q}^\infty Q(\{f(x) > t\}) dt = r^q Q(\|x\|_2 > r) + \int_r^\infty Q(\|x\|_2 > t^{1/q}) dt,
\]
where we regard the second term as zero when \(q = 0\).

We evaluate the tail probabilities in terms of the Stein discrepancy. Following the proof of [Gorham and Mackey 2017 Lemma 17], we define \(\gamma(r) = \inf \{T_P g(x) - \nu : \|x\|_2 \geq r\}\). By assumption, there exists \(r_\eta > 0\) such that \(T_P g \geq \eta \|x\|_2^{q+\theta}\) for \(\|x\|_2 > r_\eta\). Define \(r_\gamma := r_\eta \vee 2\nu/\gamma\). It is straightforward to check that for \(r \geq r_\gamma\), we have \(\gamma(r) \geq \eta r^{q+\theta}/2\). By Markov’s inequality,
\[
Q(\|x\|_2 > r) \leq \frac{\mathbb{E}_{X \sim Q} \gamma(\|X\|_2)}{\gamma(r)} \leq \frac{\mathbb{E}_{X \sim Q} [T_P g(X) - \nu]}{\gamma(r)} \leq \frac{S(Q, T_P, G_{kld}) - \nu}{\gamma(r)}.
\]

These observations yield the following estimate of the above integral:
\[
\int_{\|x\|_2 > r} \|x\|_2^q dQ(x) = r^q Q(\|x\|_2 > r) + \int_r^\infty Q(\|x\|_2 > t^{1/q}) dt
\leq r^q \frac{S(Q, T_P, G_{kld}) - \nu}{\gamma(r)} + 1_{\{q > 0\}} \int_r^\infty \frac{S(Q, T_P, G_{kld}) - \nu}{\gamma(t)} dt
\leq 2 \frac{S(Q, T_P, G_{kld}) - \nu}{\eta r^{\theta}} + 21_{\{q > 0\}} \int_r^\infty \frac{S(Q, T_P, G_{kld}) - \nu}{\eta t^{1+\theta/q}} dt
\leq 2 \frac{S(Q, T_P, G_{kld}) - \nu}{\eta} \left(1 + \frac{q}{\theta} \frac{1}{r^{\theta/q} 1_{\{q > 0\}}} \right)
\leq 2 \left(1 + \frac{q}{\theta} \right) \frac{S(Q, T_P, G_{kld}) - \nu}{\eta} \frac{1}{r^{\theta/q}}
\]
where we assume \(r \geq r_\gamma \vee 1\). Therefore, for \(\varepsilon > 0\), by taking sufficiently large \(r_\varepsilon \geq 1\) such that
\[
2 \left(1 + \frac{q}{\theta} \right) \frac{S(Q, T_P, G_{kld}) - \nu}{\eta} \frac{1}{r^{\theta/q}} \leq \varepsilon
\]
we have
\[
\int_{\|x\|_2 > r_\varepsilon} \|x\|_2^q dQ \leq \varepsilon.
\]

Therefore, the order-\(q\) integrability rate \(R_q(Q, \varepsilon)\) satisfies
\[
R_q(Q, \varepsilon) \leq \left\{ 2 \left(1 + \frac{q}{\theta} \right) \frac{S(Q, T_P, G_{kld}) - \nu}{\eta \varepsilon} \right\}^{\frac{q}{\theta}} \vee r_\gamma.
\]

For sufficiently small \(\varepsilon\), the Stein discrepancy term dominates \(r_\gamma\). Thus, the claim has been proved. \(\square\)
7.4.2 The DKSD with the tilted linear kernel detects non-uniform integrability

**Lemma 7.13** (Tilted linear kernels have the lower bound properties). Suppose the diffusion targeting $P$ satisfies the dissipativity condition (Condition 2.3) with $\alpha, \beta > 0$ and the coefficient condition (Condition 2.2) with $\lambda_a > 0$ and $q_a \in \{0, 1\}$. Let $w(x) = (v^2 + \|x\|^2)^{q_a - u}$ with $q_a \geq 0$, $u \geq 0$, and $v > 0$. Assume $(q_w - u) < 2\alpha/\lambda_a$ if $q_a = 1$. Let

$$k(x, x') = w(x)w(x')(x, x').$$

There exists a function $g \in \mathcal{G}_{k\text{ld}}$ such that $\|g\|_{\mathcal{G}_{k\text{ld}}} = \sqrt{D}$ and the corresponding diffusion Stein operator $T_P$ satisfies

$$T_P g(x) \geq \nu \text{ for any } x \in \mathbb{R}^D, \text{ and } \liminf_{\|x\|_2 \to \infty} \|x\|_2^{-2(q_w-u+1)}T_P g(x) \geq \eta$$

for some $\nu \in \mathbb{R}$ and $\eta > 0$.

**Proof.** We prove that the function $g(x) = -w(x)x$ satisfies the properties in the statement. Note that the kernel $k$ is the linear kernel tilted by $(v^2 + \|x\|^2)^{q_w-u}$. The function $g$ then belongs to the RKHS $\mathcal{G}_{k\text{ld}}$, since each component is the product of two functions from the RKHSs of the respective kernels. It is straightforward to check $\|g\|_{\mathcal{G}_{k\text{ld}}} = \sqrt{D}$. Applying the diffusion Stein operator yields

$$T_P g(x) = w(x)\left(-2(b(x), x) - (m(x), I_\mathbb{R}) - \frac{2(q_w - u)}{v^2 + \|x\|^2} (m(x), x \otimes x)\right)$$

$$= w(x)\left(-Ap\|x\|^2_2 - \frac{2(q_w - u)}{v^2 + \|x\|^2_2} (\sigma(x)\sigma(x)^\top, x \otimes x)\right).$$

We first address the case $q_w - u \leq 0$. In this case, we have

$$T_P g(x) \geq w(x)(\alpha\|x\|^2_2 - \beta),$$

where the inequality follows from Condition 2.3 and the nonnegative second term inside the parentheses above. From this estimate, the following relation holds for $\|x\|_2 > R = \sqrt{\beta/\alpha + 1}$,

$$T_P g(x) \geq \eta\|x\|_2^{2(q_w-u+1)},$$

where $\eta = (1 + v^2/R^2)^{q_w-u}\alpha\{1 - \beta/(\alpha + \beta)\} > 0$. As $T_P g(x)$ is continuous, it has the minimum in the centered closed ball of radius $R$. Thus,

$$T_P g(x) \geq \nu := 0 \vee \min_{0 \leq \|x\|_2 \leq R} T_P g(x)$$

$$= -\beta w(0).$$

We next show the case $q_w - u > 0$. Using Condition 2.3 and the growth condition (Condition 2.2), we obtain

$$T_P g(x) \geq w(x)\left(\alpha\|x\|^2_2 - \beta - \frac{\lambda_a(q_w - u)}{2} \frac{\|x\|^2_2}{(v^2 + \|x\|^2_2)} (1 + \|x\|_2^{q_a+1})\right)$$

This estimate provides us the lower bound

$$T_P g(x) \geq \eta\|x\|_2^{2(q_w-u+1)}.$$
for \( \|x\|_2 > R_1 = R_0 + 1 \), with \( \eta = (1 + v^2/R^2)^{q_w - u} f(R_1) \) where

\[
f(r) = \left\{ \alpha - \frac{1}{r^2} \left( \beta + \frac{\lambda_a(q_w - u)}{2} \frac{r^2}{v^2 + r^2} \right) \right\},
\]

and \( R_0 \) is chosen such that \( f(R_0) = 0 \). The existence of such \( R_0 \) is guaranteed if \( f \) is increasing and achieves a positive value; the case \( q_a = 0 \) automatically satisfies this requirement, whereas the case \( q_a = 1 \) further requires

\[
\alpha > \frac{\lambda_a(q_w - u)}{2}.
\]

To show a uniform lower bound, note that with \( R_1 \) above, \( T_{Pg}(x) \geq 0 \) for \( \|x\|_2 > R_1 \), and

\[
T_{Pg}(x) \geq -w(R_1) \left\{ \beta + \frac{\lambda_a(q_w - u)}{2} \frac{R_1^2}{v^2 + R_1^2} \right\} (1 + R_1^{q_a + 1})
\]

for \( \|x\|_2 \leq R_1 \).

### 7.4.3 The KSD with the tilted IMQ kernel detects non-uniform integrability

**Lemma 7.14.** Suppose the diffusion targeting \( P \) satisfies the dissipativity condition (Condition 2.3) with \( \alpha, \beta > 0 \) and the coefficient condition (Condition 2.2) with \( \lambda_a > 0 \) and \( q_a \in \{0, 1\} \). Let \( w(x) = (v^2 + \|x\|^2)^{q_w - u} \) with \( q_w \geq 0 \), \( u \geq 0 \), and \( v > 0 \). Assume \( (q_w - u) < 2\alpha/\lambda_a \) if \( q_a = 1 \). Let

\[
k(x, x') = w(x)w(y)(v_0^2 + \|x - x'\|^2)^{-t}
\]

for \( t \in (0, 1) \). Then, there exists a function \( g \in \mathcal{G}_{k_{ld}} \) such that with any fixed \( s \in (0, (t + 1)/2) \),

\[
T_{Pg}(x) \geq \nu \text{ for any } x \in \mathbb{R}^D \text{ and } \liminf_{\|x\|_2 \to \infty} \|x\|_2^{-(q_w - u + s)} T_{Pg}(x) \geq \eta
\]

for some \( \nu \in \mathbb{R} \) and \( \eta > 0 \).

**Proof.** From the proof of Lemma 16 of [Gorham and Mackey, 2017], for any fixed \( 2s \in (0, t + 1) \) and \( w > v_0/2 \), we have that the function

\[
g(x) = -2\alpha \frac{x}{(w^2 + \|x\|^2)^{1-s}}
\]

is an element of \( \mathcal{G}_{k_{ld}} \) with the RKHS norm \( \mathcal{D}(w, v_0, s, t)^{1/2} < \infty \) [see Lemma 16 of [Gorham and Mackey, 2017] for the norm estimate] The rest of the proof proceeds as in Lemma 3.7. 

### 7.5 Polynomial functions are pseudo-Lipschitz functions

We show that the class \( \mathcal{F}_q \) suffices for characterizing convergence in moments.

**Lemma 7.15.** Let \( q \geq 1 \) be an integer. The \( q \)-th power \( \|x\|_2^q \) of the Euclidean norm is a pseudo-Lipschitz function of order \( q - 1 \). Its pseudo-Lipschitz constant is bounded by \( 1 \vee q/2 \).
Proof. The case $q = 1$ follows from the triangle inequality. For $q \geq 2$, the claim follows by observing
\[
\|x\|_2^q - \|y\|_2^q \leq q \int_0^1 \|tx + (1-t)y\|_2^{q-2} (tx + (1-t)y, x-y) \, dt \\
\leq q\|x-y\|_2 \int_0^1 \|tx + (1-t)y\|_2^{q-2} \, dt \\
\leq q\|x-y\|_2 \int_0^1 t\|x\|_2^{q-1} + (1-t)\|y\|_2^{q-1} \, dt \\
= \frac{q}{2}(\|x\|_2^{q-1} + \|y\|_2^{q-1})\|x-y\|_2 \\
\leq \frac{q}{2}(1 + \|x\|_2^{q-1} + \|y\|_2^{q-1})\|x-y\|_2,
\]
where we have applied Jensen’s inequality to derive the third line.

\[\]
Lemma 7.16. Let $q \geq 1$ be an integer. Let $\mathbf{q} = (q_1, \ldots, q_D) \in \{0, \ldots, q\}^D$ be a multi-index such that $\sum_{d=1}^D q_d = q \geq 1$. Then, $\mathbf{x}^\mathbf{q} := \prod_{d=1}^D x_{q_d}^d$ is pseudo-Lipschitz of order $q-1$. Its pseudo-Lipschitz constant $\bar{\mu}_{\text{lip}}(\mathbf{x}^\mathbf{q})_{q-1}$ is bounded by $1 / (2(D-1)+1) \cdot q/2$, and its degree $q-1$ polynomial derivative coefficient $\bar{\pi}(\mathbf{x}^\mathbf{q})_{q-1,i}$ is bounded by $\text{max}_{d=1, \ldots, D} q_d! (i+D-1)$.

Proof. We first prove the following relationship:
\[
|x^\mathbf{q} - y^\mathbf{q}| \leq C_D \frac{q}{2}(\|x\|^{q-1} + \|y\|^{q-1})\|x-y\|_2,
\]
where $C_D = 2(D-1)+1$. From the proof of Lemma 7.15, for $D = 1$, we have
\[
|x^\mathbf{q} - y^\mathbf{q}| \leq \frac{q}{2}(\|x\|^{q-1} + \|y\|^{q-1})|x-y|.
\]
For $D > 1$, suppose that the relation is true for $D-1$. Take a multi-index $\mathbf{q}$ of size $q$. For $q = 1$, the claim is true with Lipschitz constant 1. Without loss of generality, we may assume $\|x\|_2 \geq \|y\|_2$. Then, for $q > 1$,
\[
|x^\mathbf{q} - y^\mathbf{q}| \\
= \prod_{d=1}^{D-1} x_d^q \cdot x_D^d - \prod_{d=1}^{D-1} x_d^q \cdot y_D^d + \prod_{d=1}^{D-1} x_d^q \cdot y_D^d - \prod_{d=1}^{D-1} y_d^q \cdot y_D^d \\
\leq \prod_{d=1}^{D-1} x_d^q \cdot |x_D^d - y_D^d| + |y_D^d| \cdot \prod_{d=1}^{D-1} x_d^q - \prod_{d=1}^{D-1} y_d^q \\
\leq \|x\| \sum_{d=1}^{D-1} q_d \frac{q D}{2}(\|x_D^d\|^{q_d-1} + \|y_D^d\|^{q_d-1})\|x_D - y_D\| \\
+ |y_D| \cdot \sum_{d=1}^{D-1} q_d (\|x\|_2^{q-d} - \|y\|_2^{q-d}) \sum_{d=1}^{D-1} q_d \|x_D - y_D\|_2 \\
\leq \|x-y\|_2 \left\{ \frac{q D}{2}\|x\|_2^{q-1} q_d \cdot (\|x\|_2^{q-1} + \|y\|_2^{q-1}) \\
+ \|y\|_2^{q-1} C_D-1 \frac{q D}{2}\|x_D - y_D\|_2 \sum_{d=1}^{D-1} q_d \right\} \\
\leq \|x-y\|_2 \left\{ \frac{q D}{2}\|x\|_2^{q-1} + C_D-1 \frac{q D}{2}\|x_D - y_D\|_2 \sum_{d=1}^{D-1} q_d \right\} \\
\leq \frac{q}{2}\|x-y\|_2 (C_D-1 + 2)\|x\|_2^{q-1} + C_D-1 \|y\|_2^{q-1} \\
\leq \frac{q}{2}(C_D-1 + 2)\|x-y\|_2 (\|x\|_2^{q-1} + \|y\|_2^{q-1}).
\]
\[\]
Solving \( C_D = C_{D-1} + 2 \) yields \( C_D = 2(D - 1) + 1 \). Therefore,

\[
|x^q - y^q| \leq \frac{q}{2} (2(D - 1) + 1) \cdot (1 + \|x\|_{2}^{q-1} + \|y\|_{2}^{q-1}) \|x - y\|_2.
\]

Next we check the degree \( q \) polynomial coefficient of the \( i \)-th derivatives. We assume \( q \geq i \) below, as the derivatives are zero otherwise. Note that we have

\[
(\nabla^i x^m)_{l_1, \ldots, l_i} = \prod_{d=1}^{D} \frac{n_d!}{(n_d - m_d)!} \cdot x_d^{q_d - m_d} \cdot 1_{\{q_d \geq m_d\}},
\]

where \( m_d := \# \{l_d : l_d = d\} \), and

\[
\|\nabla^i x^m\|_{op} = \sup_{\|u(d)\|_2 = 1} \left| \sum_{m_d=i} \prod_{d=1}^{D} \left( \frac{q_d!}{(q_d - m_d)!} \cdot x_d^{q_d - m_d} \cdot 1_{\{q_d \geq m_d\}} \right) u_{l_d} \right|
\]

\[
\leq \max_d q_d! \sup_{\|u(d)\|_2 = 1} \sum_{m_d=i} \prod_{d=1}^{D} \|x\|_2^{q_d - m_d} |u_{l_d}|
\]

\[
\leq \max_d q_d! \sup_{\|u(d)\|_2 = 1} \sum_{m_d=i} \prod_{d=1}^{D} \|x\|_2^{q_d - m_d} |u_{l_d}| \|x\|_2^{m_d}
\]

\[
\leq \max_d q_d! \left( \frac{i + D - 1}{D - 1} \right) \|x\|_2^{i - m_d}.
\]

Therefore,

\[
\hat{\pi}(x^q)_{q-1,i} = \sup_{x \in \mathbb{R}^D} \|\nabla^i x^m\|_{op} \leq \max_d q_d! \left( \frac{i + D - 1}{D - 1} \right) \sup_{x \in \mathbb{R}^D} \frac{\|x\|_2^{i - m_d}}{1 + \|x\|_2^{m_d - i}}.
\]

Consider the function \( f(r) = r^m / (1 + r^{m+i-1}) \) on \([0, \infty)\) with \( m > 0, i \geq 1 \). If \( i = 1 \), the function is monotonically increasing and its supremum is \( \lim_{r \to \infty} f(r) = 1 \). If \( i > 1 \), the function is nonnegative, and by taking the derivative, it can be shown that the function takes its maximum at \( r^* = \{m/(i - 1)\}^{m/(m+i-1)} \) with its value

\[
f(r^*) = \frac{m^{m-1}/r^{m+i-1}}{1 + m/r^{m+i-1}} \leq \frac{m^{-1}}{1 + m^{-1}} < 1.
\]

Thus, we have

\[
\hat{\pi}(x^q)_{i,q} \leq \max_{d=1, \ldots, D} q_d! \left( \frac{i + D - 1}{D - 1} \right).
\]

The above result indicates that if we divide a given monomial \( x^q := \prod_{d=1}^{D} x_d^{q_d} \) by the maximum of \( 1 \vee (2(D - 1) + 1) \cdot q/2 \) and \( \max_{d=1, \ldots, D} q_d! \left( \frac{3 + D - 1}{D - 1} \right) \), we have \( x^q \in F_q \), where \( F_q \) is the pseudo-Lipschitz class used in \([10]\).