Stochastic Stein Discrepancies

Jackson Gorham  
Whisper.ai, Inc  
jackson@whisper.ai  

Anant Raj  
MPI for Intelligent Systems  
Tübingen, Germany  
anant.raj@tuebingen.mpg.de  

Lester Mackey  
Microsoft Research New England  
lmackey@microsoft.com  

Abstract

Stein discrepancies (SDs) monitor convergence and non-convergence in approximate inference when exact integration and sampling are intractable. However, the computation of a Stein discrepancy can be prohibitive if the Stein operator – often a sum over likelihood terms or potentials – is expensive to evaluate. To address this deficiency, we show that stochastic Stein discrepancies (SSDs) based on subsampled approximations of the Stein operator inherit the convergence control properties of standard SDs with probability 1. In our experiments with biased Markov chain Monte Carlo (MCMC) hyperparameter tuning, approximate MCMC sampler selection, and stochastic Stein variational gradient descent, SSDs deliver comparable inferences to standard SDs with orders of magnitude fewer likelihood evaluations.

1 Introduction

Markov chain Monte Carlo (MCMC) methods [7] provide asymptotically correct sample estimates $\frac{1}{n} \sum_{i=1}^{n} h(x_i)$ of the complex integrals $\mathbb{E}_{P}[h(Z)] = \int h(z) dP(z)$ that arise in Bayesian inference, maximum likelihood estimation [20], and probabilistic inference more broadly. However, MCMC methods often require cycling through a large dataset or a large set of factors to produce each new sample point $x_i$. To avoid this computational burden, many have turned to scalable approximate MCMC methods [e.g. 1, 8, 14, 38, 48], which mimic standard MCMC procedures while using only a small subsample of datapoints to generate each new sample point. These techniques reduce Monte Carlo variance by delivering larger sample sizes in less time but sacrifice asymptotic correctness by introducing a persistent bias. This bias creates new difficulties for sampler monitoring, selection, and hyperparameter tuning, as standard MCMC diagnostics, like trace plots and effective sample size, rely upon asymptotic exactness.

To effectively assess the quality of approximate MCMC outputs, a line of work [9, 21–23, 27, 34] developed computable Stein discrepancies (SDs) that quantify the maximum discrepancy between sample and target expectations and provably track sample convergence to the target $P$, even when explicit integration and direct sampling from $P$ are intractable. SDs have since been used to compare approximate MCMC procedures [2], test goodness of fit [11, 27, 28, 33], train generative models [39, 47], generate particle approximations [9, 10, 19], improve particle approximations [25, 31, 32], compress samples [41], conduct variational inference [40], and estimate parameters in intractable models [5].

However, the computation of the Stein discrepancy itself can be prohibitive if the Stein operator applied at each datapoint – often a sum over datapoint likelihoods or factors – is expensive to evaluate.
This expense has led some users to heuristically approximate Stein discrepancies by subsampling data points \([2, 32, 40]\). In this paper, we formally justify this practice by proving that stochastic Stein discrepancies (SSDs) based on subsampling inherit the desirable convergence-tracking properties of standard SDs with probability 1. We then apply our techniques to analyze a scalable stochastic variant of the popular Stein variational gradient descent (SVGD) algorithm \([32]\) for particle-based variational inference. Specifically, we generalize the compact-domain convergence results of Liu \([30]\) to show, first, that SVGD converges on unbounded domains and, second, that stochastic SVGD (SSSVGD) converges to the same limit as SVGD with probability 1. We complement these results with a series of experiments illustrating the application of SSDs to biased MCMC hyperparameter tuning, approximate MCMC sampler selection, and particle-based variational inference. In each case, we find that SSDs deliver inferences equivalent to or more accurate than standard SDs with orders of magnitude fewer datapoint accesses.

The remainder of the paper is organized as follows. In Section 2, we review standard desiderata and past approaches for measuring the quality of a sample approximation. In Section 3, we provide a formal definition of stochastic Stein discrepancies for scalable sample quality measurement and present a stochastic SVGD algorithm for scalable particle-based variational inference. We provide probability 1 convergence guarantees for SSDs and SSVGD in Section 4 and demonstrate their practical value in Section 5. We discuss our findings and posit directions for future work in Section 6.

### Notation

For vector-valued \(g\) on \(\mathbb{R}^d\), we define the expectation \(\mu(g) \triangleq \int g(x)d\mu(x)\) for each probability measure \(\mu\), the divergence \(\langle \nabla, g(x) \rangle \triangleq \sum_{j=1}^d \frac{\partial}{\partial x_j} g_j(x)\), and the \(\|\cdot\|_2\) boundedness and Lipschitzness parameters \(\|g\|_\infty \triangleq \sup_{x \in \mathbb{R}^d} \|g(x)\|_2\) and \(\text{Lip}(g) \triangleq \sup_{x \neq y \in \mathbb{R}^d} \frac{\|g(x) - g(y)\|_2}{\|x - y\|_2}\). For any \(L \in \mathbb{N}\), we write \([L]\) for \(\{1, \ldots, L\}\). We write \(\Rightarrow\) for the weak convergence and \(\overset{a.s.}{\to}\) for almost sure convergence of probability measures. We denote the set of continuous functions on \(\mathbb{R}^d\) by \(C\) or \(C(\mathbb{R}^d)\) and the set of continuously differentiable in both arguments \(k(x, y)\) by \(C^{(1, 1)}\).

### 2 Measuring Sample Quality

Consider any continuous or discrete target distribution \(P\) on \(\mathbb{R}^d\). We will assume that exact expectations under \(P\) are unavailable for many functions of interest, so we will employ a discrete measure \(Q_n \triangleq \frac{1}{n} \sum_{i=1}^n \delta_{x_i}\) based on a sample \((x_i)_{i=1}^n\) to approximate expectations under \(P\). Importantly, we will make no assumptions about the origins or nature of the sample points \(x_i\); they may be the output of i.i.d. sampling, drawn from an arbitrary Markov chain, or even generated by a deterministic quadrature rule.

To assess the usefulness of a given sample, we seek a quality measure that quantifies how well expectations under \(Q_n\) match those under \(P\). At the very least, this quality measure should (i) determine when \(Q_n\) converges to the target \(P\), (ii) determine when \(Q_n\) does not converge to \(P\), and (iii) be computationally tractable. Integral probability metrics (IPMs) \([36]\) are natural candidates, as they measure the maximum absolute difference in expectation between probability measures \(\mu\) and \(\nu\) over a set of test functions \(\mathcal{H}\):

\[
d_{\mathcal{H}}(\mu, \nu) \triangleq \sup_{h \in \mathcal{H}} |\mathbb{E}_\mu[h(X)] - \mathbb{E}_\nu[h(Z)]|.
\]

Moreover, for many IPMs, like the Wasserstein distance \((\mathcal{H} = \{h : \mathbb{R}^d \to \mathbb{R} \mid \text{Lip}(h) \leq 1\})\) and the Dudley metric \((\mathcal{H} = \{h : \mathbb{R}^d \to \mathbb{R} \mid \|h\|_\infty + \text{Lip}(h) \leq 1\})\), convergence of \(d_{\mathcal{H}}(Q_n, P) \to 0\) implies that \(Q_n \Rightarrow P\), in satisfaction of Desideratum (ii). Unfortunately, these same IPMs typically cannot be computed without exact integration under \(P\). Gorham and Mackey \([21]\) circumvented this issue by constructing a new family of IPMs – Stein discrepancies – from test functions known a priori to be mean zero under \(P\). Their construction was inspired by Charles Stein’s three-step method for proving central limit theorems \([44]\):

1. Identify an operator \(T\) that generates mean-zero functions on its domain \(\mathcal{G}\):
   \[
   \mathbb{E}_P[(Tg)(Z)] = 0 \text{ for any } g \in \mathcal{G}.
   \]

2. (Continued...)
The chosen Stein operator \( \mathcal{T} \) and Stein set \( \mathcal{G} \) together yield an IPM-type measure which eschews explicit integration under \( P \):

\[
S(\mu, \mathcal{T}, \mathcal{G}) \triangleq d_{\mathcal{G}}(\mu, P) = \sup_{g \in \mathcal{G}} |E_{\mu}[(\mathcal{T}g)(X)] - E_{P}[(\mathcal{T}g)(Z)]| = \sup_{g \in \mathcal{G}} |E_{\mu}[(\mathcal{T}g)(X)]|.  \tag{1}
\]

Gorham and Mackey [21] named this measure the Stein discrepancy.

2. Lower bound the Stein discrepancy by an IPM known to dominate convergence in distribution. This is typically done for a large class of targets once and thus ensures that \( S(Q_n, \mathcal{T}, \mathcal{G}) \to 0 \) implies \( Q_n \Rightarrow P \) (Desideratum (ii)).

3. Upper bound the Stein discrepancy to ensure that the Stein discrepancy \( S(Q_n, \mathcal{T}, \mathcal{G}) \to 0 \) when \( Q_n \) converges suitably to \( P \) (Desideratum (i)).

Prior work has instantiated a variety of Stein operators \( \mathcal{T} \) and Stein sets \( \mathcal{G} \) satisfying Desiderata (i)-(iii) for large classes of target distributions [9, 18, 21–23, 27, 34, 44, 45, 49]. We will focus on decomposable operators: \( \mathcal{T} = \sum_{l=1}^{L} \mathcal{T}_l \) that decompose as a sum of \( L \) base operators \( \mathcal{T}_l \) that are less expensive to evaluate than \( \mathcal{T} \). A prime example is the Langevin Stein operator derived in [21],

\[
(T_P g)(x) = \langle \nabla \log p(x), g(x) \rangle + \langle \nabla, g(x) \rangle, \tag{2}
\]

applied to a posterior density, \( p(x) \propto \pi_0(x) \prod_{i=1}^{n} \pi(y_i|x) \) for \( \pi_0 \) a prior density, \( \pi(\cdot|x) \) a likelihood function, and \( (y_i)_{i=1}^{n} \) a sequence of observed datapoints. In this case, the Langevin operator \( T_P = \sum_{l=1}^{L} \mathcal{T}_l \) for \( (T_l g)(x) = \langle \nabla \log p_l(x), g(x) \rangle + \frac{1}{2} \langle \nabla, g(x) \rangle \) and \( p_l(x) \triangleq \pi_0(x)^{1/L} \pi(y_l|x) \), so that each base operator involves accessing only a single datapoint.

3 Stochastic Stein Discrepancies

Whenever the Stein operator decomposes as \( \mathcal{T} = \sum_{l=1}^{L} \mathcal{T}_l \), the standard Stein discrepancy objective (1) demands that every base operator \( \mathcal{T}_l \) be evaluated at every sample point \( x_i \); this cost can quickly become prohibitive if \( L \) and \( n \) are large. To alleviate this burden, we will consider a new class of discrepancy measures based on subsampling base operators. To this end, we fix a batch size \( m \) and, for each \( i \in [n] \), independently select a uniformly random subset \( \sigma_i \) of size \( m \) from \([L]\). Then for any \( \mathcal{G} \), we define the stochastic Stein discrepancy (SSD) as the random quantity

\[
SS(Q_n, \mathcal{T}, \mathcal{G}) \triangleq \sup_{g \in \mathcal{G}} \left| \frac{1}{n} \sum_{i=1}^{n} \frac{1}{m} \langle \mathcal{T}_{\sigma_i} g(x_i) \rangle \right|, \tag{3}
\]

where \( \mathcal{T}_{\sigma} \triangleq \sum_{\sigma_i \in \sigma} \mathcal{T}_i \) for each \( \sigma \subseteq [L] \). By construction, the SSD reduces the number of base operator evaluations by a factor of \( m/L \). Nevertheless, we will see in the Section 4 that SSDs inherit the convergence-determining properties of standard SDs with probability 1.

3.1 Stochastic kernel Stein discrepancies

Before turning to the convergence theory we pause to highlight a second property of practical import: when the Stein set is a unit ball of a reproducing kernel Hilbert space (RKHS), the SSD (8) admits a closed-form solution. We illustrate this for the Langevin operator (2) and the kernel Stein set [22]

\[
\mathcal{G}_{k, \| \cdot \|} \triangleq \{ g = (g_1, \ldots, g_d) \mid \| v \|^* \leq 1 \text{ for } v_j \triangleq \| g_j \|_{K_k} \} \tag{4}
\]

with arbitrary vector norm \( \| \cdot \| \) and \( \| \cdot \|_{K_k} \) the RKHS norm of a reproducing kernel \( k \).

**Proposition 1** (SKSD closed form). *If \( k \in C^{(1,1)} \), then \( SS(Q_n, T_P, \mathcal{G}_{k, \| \cdot \|}) = \| w \| \) where, \( \forall j \in [d] \),

\[
w_j^2 \triangleq \frac{1}{m^2} \sum_{i=1}^{n} \sum_{i'=1}^{n} \left( \frac{L}{m} \nabla_{x_{ij}} \log p_{\sigma_j}(x_i) + \nabla_{x_{ij'}} \log p_{\sigma_j}(x_{i'}) + \nabla_{x_{ij'}} \right) k(x_i, x_{i'}).
\]

We call such discrepancies stochastic kernel Stein discrepancies (SKSDs) in homage to the standard kernel Stein discrepancies (KSDs) introduced in [11, 22, 33]. See App. A for the proof of Prop. 1.
We say that an SSD detects convergence if $SS(Q_n, T, \mathcal{G}_n) \to 0$ when $Q_n$ converges to $P$ in a standard probability metric, like the Wasserstein distance, $W_2(Q_n, P) \triangleq \inf_{X \sim Q_n, Z \sim P} \mathbb{E}[\|X - Z\|^2]^{1/2}$ for $a \geq 1$. Our first result, proved in App. B, shows that an SSD detects Wasserstein convergence with probability 1 if its base operators $\mathcal{T}_\sigma$ generate continuous functions that grow no more quickly than a polynomial. Theorem 2 is broad enough to cover all of the Stein operator-set pairings with SD convergence-detection results in [21–23].
Theorem 2 (SSDs detect convergence). Suppose that for some \(a, c > 0\) and each \(\sigma \in \binom{[L]}{m}\) and \(n \geq 1\), \(\tau_n \sigma \in C[\mathbb{R}^d]\), \(\sup_{g \in \mathcal{G}_n} |(\tau_n g)(x)| \leq c(1 + \|x\|^2_2)\), and \(P(\tau_n g) = 0\) for all \(g \in \mathcal{G}_n\). If \(W_a(Q_n, P) \triangleq \inf_{X \sim Q_n, Z \sim P} \mathbb{E}[\|X - Z\|^{a/2}_{[2]}] \to 0\), then \(SS(Q_n, \mathcal{T}, \mathcal{G}_n) \overset{a}{\Rightarrow} 0\).

4.2 Detecting non-convergence with SSDs

We say that an SSD detects non-convergence if \(SS(Q_n, \mathcal{T}, \mathcal{G}_n) \not\Rightarrow 0\) when \(Q_n \not\Rightarrow P\). We will build up to this result in a series of steps. First, we will associate with every SSD, \(SS(Q_n, \mathcal{T}, \mathcal{G}_n)\), a bounded SD with Stein set

\[
\mathcal{G}_{b,n} \triangleq \{ g \in \mathcal{G}_n : \| \tau_n g \| \leq 1, \forall \sigma \in \binom{[L]}{m} \}
\]

in which each Stein function is constrained to be bounded under each base operator \(\tau_n\). We prove in App. C that every SSD detects the non-convergence of its bounded SD.

Theorem 3 (SSDs detect bounded SD non-convergence). If \(S(Q_n, \mathcal{T}, \mathcal{G}_{b,n}) \not\Rightarrow 0\), then, with probability 1, \(SS(Q_n, \mathcal{T}, \mathcal{G}_n) \not\Rightarrow 0\).

Next, we show that for the popular Langevin operator (2) and each Stein set analyzes in [9, 21–23], bounded SDs detect tight non-convergence. That is, if \(Q_n \not\Rightarrow P\), then either \(S(Q_n, \mathcal{T}, \mathcal{G}_n) \not\Rightarrow 0\) or some mass in the sequence \((Q_n)_{n=1}^\infty\) escapes to infinity. The proof is in App. D.

Theorem 4 (Bounded SDs detect tight non-convergence). Consider the Langevin Stein operator \(\mathcal{T}_P(2)\) with Lipschitz \(\nabla \log p\) satisfying distant dissipativity [16, 23] for some \(\kappa > 0\) and \(r \geq 0\):

\[
(\nabla \log p(x) - \nabla \log p(y), x - y) \leq -\kappa \|x - y\|^2 + r, \quad \text{for all} \quad x, y \in \mathbb{R}^d.
\]

Suppose \(\sup_{x \in \mathbb{R}^d} \| \nabla \log p(x) \|^2 / (1 + \|x\|_2) < \infty\) for each \(\sigma \in \binom{[L]}{m}\), and consider the bounded Stein set \(\mathcal{G}_{b,n}(5)\) for any of the following Stein sets \(\mathcal{G}_n\):

(A.1) \(\mathcal{G}_n = \mathcal{G}_k \|\cdot\|_{(4)}\), the kernel Stein set of [22] with \(k(x, y) = \Phi(x - y)\) for \(\Phi \in C^2\) with non-vanishing Fourier transform.

(A.2) \(\mathcal{G}_n = \mathcal{G}_\|\cdot\|_{(5)}\), the classical Stein set of [21] with arbitrary vector norm \(\|\cdot\|\).

(A.3) \(\mathcal{G}_n = \mathcal{G}_\|\cdot\|_{(6)}\), the graph Stein set of [21] with arbitrary vector norm \(\|\cdot\|\) and a finite graph \(G = (V, E)\) with vertices \(V \subset \mathbb{R}^d\).

If \((Q_n)_{n=1}^\infty\) is a tight sequence of probability measures and \(S(Q_n, \mathcal{T}_P, \mathcal{G}_{b,n}) \to 0\) then \(Q_n \Rightarrow P\).

Finally, we prove in App. E that SSDs with coercive test functions enforce tightness, that is, remain bounded away from 0 whenever \((Q_n)_{n=1}^\infty\) is not tight.

Proposition 5 (Coercive SSDs enforce tightness). If \((Q_n)_{n=1}^\infty\) is not tight and \(\tau_n g\) is coercive and bounded below for some \(g \in \bigcap_{n=1}^\infty \mathcal{G}_n\) and \(\forall \sigma \in \binom{[L]}{m}\), then surely \(SS(Q_n, \mathcal{T}, \mathcal{G}_n) \not\Rightarrow 0\).

Taken together, these results imply that SSDs equipped with the Langevin operator and any of the convergence-determining Stein sets of [21–23] detect non-convergence with probability 1, under standard dissipativity and growth conditions on the subsampled operator.

Theorem 6 (Coercive SSDs detect non-convergence). Under the notation of Theorem 4, suppose \(\nabla \log p\) is Lipschitz, \(\sup_{x \in \mathbb{R}^d} \| \nabla \log p(x) \|^2 / (1 + \|x\|_2) < \infty\) for all \(\sigma \in \binom{[L]}{m}\), and, for some \(\kappa > 0\) and \(r \geq 0\),

\[
(\nabla \log p(x) - \nabla \log p(y), x - y) \leq -\kappa \|x - y\|^2 + r, \quad \forall x, y \in \mathbb{R}^d \text{ and } \forall \sigma \in \binom{[L]}{m}.
\]

For each \(n \geq 1\), suppose also that \(\mathcal{G}_n\) satisfies (A.3), (A.2), or (A.1) with \(k(x, y) = (c^2 + \|x - y\|^2_2)\beta\) for \(c > 0\) and \(\beta \in (-1, 0)\). If \(Q_n \not\Rightarrow P\), then, with probability 1, \(SS(Q_n, \mathcal{T}_P, \mathcal{G}_n) \not\Rightarrow 0\).

We prove this claim in App. F.
4.3 Convergence of SVGD and SSVGD

Discussing the convergence of SVGD and SSVGD will require some additional notation. For each step size $\epsilon > 0$ and suitable probability measure $\mu$, define the SVGD update rule

$$T_{\mu,\epsilon}(x) = x + \epsilon \mathbb{E}_{X \sim \mu}[\nabla \log p(X')k(X', x) + \nabla k(X', x)],$$

and let $\Phi_{\epsilon}(\mu)$ denote the distribution of $T_{\mu,\epsilon}(X)$ when $X \sim \mu$. If SVGD is initialized with the point set $(x_i^0)_{i=1}^n$, then the output of SVGD after each round $r$ is described by the recursion

$$Q_{n,r} = \Phi_{\epsilon_{r-1}}(Q_{n,r-1})$$

for each round $r > 0$ with $Q_{n,0} \triangleq \frac{1}{n} \sum_{i=1}^n \delta_{x_i^0}$.

Liu [30] used this recursion to analyze the convergence of non-stochastic SVGD in three steps. First, Thm. 3.2 of [30] showed that, if the SVGD initialization $Q_{n,0}$ converges weakly to a probability measure $Q_{\infty,0}$ as $n \to \infty$, then, on each round $r > 0$, the $n$-point output $Q_{n,r}$ converges weakly to $Q_{\infty,r} \triangleq \Phi_{\epsilon_{r-1}}(Q_{\infty,r-1})$. Next, Thm. 3.3 of [30] showed that the Langevin KSD $S(Q_{\infty,r}, T_P, G_k) \to 0$ as $r \to \infty$ for a suitable sequence of step sizes $\epsilon_{r}$. Finally, Thm. 8 of [22] implied that $Q_{\infty,r} \Rightarrow P$ for suitable kernels and targets $P$.

A gap in this analysis lies in the stringent assumptions of the first step: Thm. 3.2 of [30] only applies when $f(x,z) = \nabla \log p(x)k(x,z) + \nabla_x k(x,z)$ is both bounded and Lipschitz, but the growth of $\nabla \log p(x)k(x,z)$ typically invalidates both assumptions (consider, for example, the standard Gaussian $\nabla \log p(x) = -x$ with any translation invariant kernel $k$). Our next theorem, proved in App. G, fills this gap by showing that, on round $r$, both the SVGD output $Q_{n,r}$ and the SSVGD output $Q_{n,r}^m$ converge to $Q_{\infty,r}$ with probability 1 under assumptions commonly satisfied by $p$ and $k$.

**Theorem 7** (Wasserstein convergence of SVGD and SSVGD). Suppose SVGD and SSVGD are initialized with $Q_{n,0} = \frac{1}{n} \sum_{i=1}^n \delta_{x_i^0}$ satisfying $W_1(Q_{n,0}, Q_{\infty,0}) \to 0$. If for some $c_1, c_2 > 0$,

$$\left\{ \begin{array}{l}
\text{Lip}(\nabla \log p(x)k(x,\cdot) + \nabla_x k(x,\cdot)) \leq c_1(1 + ||x||_2) \\
\text{Lip}(\nabla \log p(\cdot)k(\cdot,z) + \nabla_z k(\cdot,z)) \leq c_2(1 + ||z||_2)
\end{array} \right. \quad (6)$$

then $W_1(Q_{n,r}, Q_{\infty,r}) \to 0$ as $n \to \infty$ for each round $r$. If, in addition, for some $c_0 > 0$,

$$\max_{\sigma \in \Sigma_m} \sup_{z \in \mathbb{R}^d} ||\nabla \log p_\sigma(x)k(x,z)||_2 \leq c_0(1 + ||x||_2), \quad (7)$$

then, for each round $r$, $W_1(Q_{n,r}^m, Q_{n,r}) \overset{a.s.}{\to} 0$ as $n \to \infty$.

As an illustration of the applicability, we highlight that the growth assumptions (6) and (7) all hold for standard bounded radial kernels like the Gaussian, Matérn, inverse multiquadric, and inverse log [9] kernels paired with Lipschitz $\nabla \log p$ and linear-growth $\nabla \log p_\sigma$.

5 Experiments

In this section, we demonstrate the practical benefits of using SSDs as drop in replacements for standard SDs. In each of our experiments, the target is a posterior distribution of the form $p(x) \propto \prod_{i=1}^L p_i(x)$ where $p_i(x) \propto \pi_0(x)^{1/2} \pi(y|x)$ for $\pi_0$ a prior density, $\pi(\cdot|x)$ a likelihood function, and $(y_i)_{i=1}^L$ a sequence of observed datapoints. The SKSDs in Sections 5.1 and 5.2 use an inverse multiquadric base kernel $k(x,y) = (1 + ||x - y||_2^2)^\beta$ with $\beta = -\frac{1}{2}$ as in [22]. Julia [6] code recreating the experiments in Sections 5.1 and 5.2 and Python code recreating the experiments in Section 5.3 is available at https://github.com/jgorham/stochastic_stein_discrepancy.

5.1 Hyperparameter selection for approximate MCMC

Stochastic gradient Langevin dynamics (SGLD) [48] with constant step size $\epsilon$ is an approximate MCMC method introduced as a scalable alternative to the popular Metropolis-adjusted Langevin algorithm [42]. A first step in using SGLD is selecting an appropriate step size $\epsilon$, as overly large values lead to severe distributional biases (see the right panel of the Fig. 1 triptych), while overly small values yield slow mixing (as in the left panel of the Fig. 1 triptych). In [48, Section 5.1], the posterior over the means of a Gaussian mixture model (GMM) was used to illustrate the utility of SGLD, and in [21, Section 5.3], the spanner graph Stein discrepancy was employed to select an
appropriate $\epsilon > 0$ for a fixed computational budget. We recreate the experimental setup of [21, Section 5.3] to assess the ability of a stochastic KSD to effectively tune SGLD.

We used the same model parameterization as Welling and Teh [48], which was a posterior distribution with $L = 100$ likelihood terms contributing to the posterior density. We adopted the same experimental methodology as [21, Section 5.3]: for a range of $\epsilon$ values, we generated 50 independent SGLD pilot chains of length $n = 1000$. For each sample of size $n$, we computed the IMQ KSD without any subsampling and the SKSD with batch sizes $m = 1$ and $m = 10$. In Figure 1, we see that both SKSDs behave in step with the standard KSD: the choice of $\epsilon = 5 \times 10^{-3}$ minimizes the KSD over the average of the 50 trials for all variants of KSD. Moreover, the fastest SKSD required one hundredth the number of likelihood evaluations of the standard KSD. Hence, subsampling can lead to significant speed-ups with little degradation in inferential quality even when the total number of likelihood terms is moderate.

### 5.2 Selecting biased MCMC samplers

Gorham and Mackey [22, Sec. 4.4] used the KSD to choose between two biased sampling procedures. Namely, they compared two variants of the approximate MCMC algorithm stochastic gradient Fisher scoring (SGFS) [1]. The full variant of this sampler—called SGFS-f—requires inverting a $d \times d$ matrix to produce each sample iterate. A more computationally expedient variant—called SGFS-d—instead inverts a $d \times d$ matrix but first zeroes out all off-diagonal entries. Both MCMC samplers are uncorrected discretizations of a continuous-time process, and their invariant measures are asymptotically biased away from the target $P$. Accordingly, the SSD can be employed to assess whether the greater number of sample iterates generated by SGFS-d under a fixed computational budget outweighs the additional cost from asymptotic bias.

In both [22, Sec 4.4] and [1, Sec 5.1], the chosen target $P$ was a Bayesian logistic regression with a flat prior. The training set was constructed by selecting a subset of 10,000 images from the MNIST dataset that had a 7 or 9 label, and then reducing each covariate vector of 784 pixel values to a dimension 50 vector via random projections. After including an intercept term, Ahn et al. [1] generated a posterior sample of 50,000 sample iterates (each in $\mathbb{R}^{51}$) for both samplers. In [22, Sec 4.4], the authors showed the KSD preferred the sample iterates generated from SGFS-f for any number of sample iterates, while in [1, Sec 5.1], the authors showed even the best bivariate marginals generated by SGFS-d were inferior to SGFS-f at matching the target posterior $P$.

In Figure 2, we compare the exact KSDs with the stochastic KSDs obtained from sampling 100 and 1,000 of the 10,000 likelihood terms i.i.d. for each posterior sample iterate. Notice that the stochastic KSD prefers SGFS-f over SGFS-d for each subsampling parameter as well, in accordance
with the exact KSD. However, the most aggressively subsampled stochastic KSD requires 100 times fewer likelihood evaluations than its standard analogue.

5.3 Particle-based variational inference with SSVGD

SSGD was developed to iteratively improve a $n$-point particle approximation $Q_n$ to a given target distribution. To illustrate the practical benefit of the stochastic SVGD algorithm analyzed in Section 4.3 over standard SVGD, we reproduce the Bayesian neural network experiment from [32, Section 5] on three datasets used in their experiment. We adopt the exact experimental setup of [32] and adapt their code to compare SSVGD (Algorithm 1) with minibatch sizes $m = 0.1L$ and $m = 0.25L$ with standard SVGD ($m = L$). The procedure was run 20 times for each configuration, and each time we started with an independently sampled train-test split. The training sets for the boston, yacht, and naval datasets had 409, 209, and 10, 241 datapoints and $d = 13, 6$, and 17 covariates, respectively. The boston dataset was first published in [24] while the latter two are available on the UCI repository [13]. The root mean-squared error (RMSE) and log likelihood were computed on the test set, and a summary is presented in Fig. 3. SSVGD yields more accurate approximations for all likelihood computation budgets considered, even for the modestly sized datasets, and this effect is magnified in the larger naval dataset.
6 Discussion and Future Work

To reduce the cost of assessing and improving sample quality, we introduced stochastic Stein discrepancies which inherit the convergence-determining properties of standard SDs with probability 1 while requiring orders of magnitude fewer likelihood evaluations. While our work was focused on measuring sample quality, we believe that other inferential tasks based on decomposable Stein operators can benefit from these developments. Prime candidates include SD-based goodness-of-fit testing [11, 27, 28, 33], KSD-based sampling [9, 10, 19], improving Monte Carlo estimation with control variates [3, 35, 37], improving sample quality through reweighting [25, 31] or thinning [41], and parameter estimation in intractable models [5]. Integrating variance reduction techniques [e.g., 12, 43] into the SSD computation is another promising direction, as the result could more closely mimic standard SDs while offering comparable computational savings. Finally, while the Langevin operator received special attention in our analysis, our results also extend to other popular Stein operators like the diffusion operators of [23] and the discrete operators of [49].

Broader Impact

This work provides both producers and consumers of approximate inference techniques with a valid diagnostic for assessing those approximations at scale. It also analyzes a scalable algorithm (SSSVGD) for improving approximate inference. We expect that many existing users of Stein discrepancies will want to employ stochastic Stein discrepancies to reduce their overall computational costs. In addition, the ready availability of a scalable diagnostic may stimulate the more widespread use of approximate MCMC methods. However, any inferential tool combined with the wrong data or inappropriate model can lead to incorrect and harmful conclusions, so care must be taken in interpreting the results of any downstream analysis.

References

[1] S. Ahn, A. Korattikara, and M. Welling. Bayesian posterior sampling via stochastic gradient Fisher scoring. In Proc. 29th ICML, ICML’12, 2012.
[2] C. Aicher, S. Putcha, C. Nemeth, P. Fearnhead, and E. Fox. Stochastic gradient mcmc for nonlinear state space models. arXiv preprint arXiv:1901.10568, 2019.
[3] R. Assaraf and M. Caffarel. Zero-variance principle for monte carlo algorithms. Phys. Rev. Lett., 83:4682–4685, Dec 1999. doi: 10.1103/PhysRevLett.83.4682. URL https://link.aps.org/doi/10.1103/PhysRevLett.83.4682.
[4] G. Bachman and L. Narici. Functional Analysis. Academic Press textbooks in mathematics. Dover Publications, 1966. ISBN 9780486402512.
[5] A. Barp, F. Briol, A. Duncan, M. Girolami, and L. Mackey. Minimum stein discrepancy estimators. In Advances in Neural Information Processing Systems, pages 12964–12976, 2019.
[6] J. Bezanson, A. Edelman, S. Karpinski, and V. Shah. Julia: A fresh approach to numerical computing. arXiv preprint arXiv:1411.1607, 2014.
[7] S. Brooks, A. Gelman, G. Jones, and X.-L. Meng. Handbook of Markov chain Monte Carlo. CRC press, 2011.
[8] T. Chen, E. Fox, and C. Guestrin. Stochastic Gradient Hamiltonian Monte Carlo. In Proc. 31st ICML, ICML’14, 2014.
[9] W. Chen, L. Mackey, J. Gorham, F. Briol, and C. Oates. Stein points. In International Conference on Machine Learning, pages 844–853, 2018.
[10] W. Y. Chen, A. Barp, F. Briol, J. Gorham, M. Girolami, L. Mackey, and C. Oates. Stein point markov chain monte carlo. In International Conference on Machine Learning, pages 1011–1021, 2019.
[11] K. Chwialkowski, H. Strathmann, and A. Gretton. A kernel test of goodness of fit. In Proc. 33rd ICML, ICML, 2016.
[12] A. Defazio, F. Bach, and S. Lacoste-Julien. Saga: A fast incremental gradient method with support for non-strongly convex composite objectives. In Advances in neural information processing systems, pages 1646–1654, 2014.

[13] D. Dua and C. Graff. UCI machine learning repository, 2017. URL http://archive.ics.uci.edu/ml.

[14] C. DuBois, A. Korattikara, M. Welling, and P. Smyth. Approximate slice sampling for Bayesian posterior inference. In Proc. 17th AISTATS, pages 185–193, 2014.

[15] R. M. Dudley. Real analysis and probability. Chapman and Hall/CRC, 2018.

[16] A. Eberle. Reflection couplings and contraction rates for diffusions. Probab. Theory Related Fields, pages 1–36, 2015. doi: 10.1007/s00440-015-0673-1.

[17] S. Eklisheva and C. Houdré. Transportation distance and the central limit theorem. arXiv preprint math/0607089, 2006.

[18] M. A. Erdogdu, L. Mackey, and O. Shamir. Global non-convex optimization with discretized diffusions. In Advances in Neural Information Processing Systems, pages 9671–9680, 2018.

[19] F. Futami, Z. Cui, I. Sato, and M. Sugiyama. Bayesian posterior approximation via greedy particle optimization. In Proceedings of the AAAI Conference on Artificial Intelligence, volume 33, pages 3606–3613, 2019.

[20] C. J. Geyer. Markov chain Monte Carlo maximum likelihood. Computer Science and Statistics: Proc. 23rd Symp. Interface, pages 156–163, 1991.

[21] J. Gorham and L. Mackey. Measuring sample quality with Stein’s method. In C. Cortes, N. D. Lawrence, D. D. Lee, M. Sugiyama, and R. Garnett, editors, Adv. NIPS 28, pages 226–234. Curran Associates, Inc., 2015.

[22] J. Gorham and L. Mackey. Measuring sample quality with kernels. In Proceedings of the 34th International Conference on Machine Learning-Volume 70, pages 1292–1301. JMLR. org, 2017.

[23] J. Gorham, A. Duncan, S. Vollmer, and L. Mackey. Measuring sample quality with diffusions. The Annals of Applied Probability, 29(5):2884–2928, 2019.

[24] D. Harrison Jr and D. Rubinfeld. Hedonic housing prices and the demand for clean air. 1978.

[25] L. Hodgkinson, R. Salomone, and F. Roosta. The reproducing stein kernel approach for post-hoc corrected sampling. arXiv preprint arXiv:2001.09266, 2020.

[26] W. Hoeffding. Probability inequalities for sums of bounded random variables. In The Collected Works of Wassily Hoeffding, pages 409–426. Springer, 1994.

[27] J. Huggins and L. Mackey. Random feature stein discrepancies. In Advances in Neural Information Processing Systems, pages 1899–1909, 2018.

[28] W. Jitkrittum, W. Xu, Z. Szabó, K. Fukumizu, and A. Gretton. A linear-time kernel goodness-of-fit test. In Advances in Neural Information Processing Systems, pages 262–271, 2017.

[29] L. Li, Y. Li, J.-G. Liu, Z. Liu, and J. Lu. A stochastic version of stein variational gradient descent for efficient sampling. arXiv preprint arXiv:1902.03394, 2019.

[30] Q. Liu. Stein variational gradient descent as gradient flow. In Advances in neural information processing systems, pages 3115–3123, 2017.

[31] Q. Liu and J. Lee. Black-box importance sampling. In Artificial Intelligence and Statistics, pages 952–961, 2017.

[32] Q. Liu and D. Wang. Stein variational gradient descent: A general purpose Bayesian inference algorithm. In Advances in neural information processing systems, pages 2378–2386, 2016.
[33] Q. Liu, J. Lee, and M. Jordan. A kernelized Stein discrepancy for goodness-of-fit tests. In Proc. of 33rd ICML, volume 48 of ICML, pages 276–284, 2016.

[34] L. Mackey and J. Gorham. Multivariate Stein factors for a class of strongly log-concave distributions. Electron. Commun. Probab., 21:14 pp., 2016. doi: 10.1214/16-ECP15.

[35] A. Mira, R. Solgi, and D. Imparato. Zero variance markov chain monte carlo for bayesian estimators. Statistics and Computing, 23(5):653–662, 2013.

[36] A. Müller. Integral probability metrics and their generating classes of functions. Ann. Appl. Probab., 29(2):pp. 429–443, 1997.

[37] C. J. Oates, M. Girolami, and N. Chopin. Control functionals for Monte Carlo integration. Journal of the Royal Statistical Society: Series B (Statistical Methodology), pages n/a–n/a, 2016. ISSN 1467-9868. doi: 10.1111/rssb.12185.

[38] S. Patterson and Y. Teh. Stochastic gradient Riemannian langevin dynamics on the probability simplex. In Adv. NIPS 26, pages 3102–3110, 2013.

[39] Y. Pu, Z. Gan, R. Henao, C. Li, S. Han, and L. Carin. Vae learning via stein variational gradient descent. In Advances in Neural Information Processing Systems, pages 4237–4246, 2017.

[40] R. Ranganath, D. Tran, J. Altosaar, and D. Blei. Operator variational inference. In Advances in Neural Information Processing Systems, pages 496–504, 2016.

[41] M. Riabiz, W. Chen, J. Cockayne, P. Swietach, S. Niederer, L. Mackey, and C. Oates. Optimal thinning of mcmc output. arXiv preprint arXiv:2005.03952, 2020.

[42] G. Roberts and R. Tweedie. Exponential convergence of Langevin distributions and their discrete approximations. Bernoulli, 2(4):341–363, 1996. ISSN 1350-7265. doi: 10.2307/3318418.

[43] M. Schmidt, N. Le Roux, and F. Bach. Minimizing finite sums with the stochastic average gradient. Mathematical Programming, 162(1-2):83–112, 2017.

[44] C. Stein. A bound for the error in the normal approximation to the distribution of a sum of dependent random variables. In Proc. 6th Berkeley Symposium on Mathematical Statistics and Probability (Univ. California, Berkeley, Calif., 1970/1971), Vol. II: Probability theory, pages 583–602. Univ. California Press, Berkeley, Calif., 1972.

[45] C. Stein, P. Diaconis, S. Holmes, and G. Reinert. Use of exchangeable pairs in the analysis of simulations. In Stein’s method: expository lectures and applications, volume 46 of IMS Lecture Notes Monogr. Ser., pages 1–26. Inst. Math. Statist., Beachwood, OH, 2004.

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

[47] D. Wang and Q. Liu. Learning to Draw Samples: With Application to Amortized MLE for Generative Adversarial Learning. arXiv:1611.01722, Nov. 2016.

[48] M. Welling and Y. Teh. Bayesian learning via stochastic gradient Langevin dynamics. In ICML, 2011.

[49] J. Yang, Q. Liu, V. Rao, and J. Neville. Goodness-of-fit testing for discrete distributions via stein discrepancy. In International Conference on Machine Learning, pages 5561–5570, 2018.
A Proof of Prop. 1: SKSD closed form

Our proof will parallel that of Gorham and Mackey [22, Prop. 2] for non-stochastic KSDs. For each \( j \in [d] \) and each \( \sigma_i \), we define the coordinate operators

\[
\frac{1}{m} (T_j \varphi)(x) = \left( \frac{1}{m} \nabla x_j \log p_{\sigma_i}(x) + \nabla x_j \right) f(x)
\]

for \( f : \mathbb{R}^d \to \mathbb{R} \). For each \( g = (g_1, \ldots, g_d) \in G_k, |||| \) and \( x \in \mathbb{R}^d \), our \( C^{(1,1)} \) assumption on \( k \) and the proof of [46, Cor. 4.36] imply that

\[
(T_{\sigma_i} g)(x) = \sum_{j=1}^d (T_j \varphi) g_j(x) = \sum_{j=1}^d T_j \varphi g_j(x, \cdot) = \sum_{j=1}^d \left( g_j, T_j k(x, \cdot) \right)_{\mathcal{K}_k}.
\]

Meanwhile, the result [46, Lem. 4.34] yields

\[
\left( \frac{1}{m} T_j k(x, \cdot), \frac{1}{m} T_j k(x', \cdot) \right) = \left( \frac{1}{m} \nabla x_j \log p_{\sigma_i}(x) + \nabla x_j \right) \left( \frac{1}{m} \nabla x_{i'} \log p_{\sigma_{i'}}(x') + \nabla x_{i'} \right) k(x, x')
\]

for all \( i, i' \in [n] \) and \( j \in [d] \). Therefore, the advertised

\[
w_j^2 = \frac{1}{m} \sum_{i=1}^n \sum_{i'=1}^n \left( \frac{1}{m} T_j \varphi g, \frac{1}{m} T_j \varphi g' \right)_{\mathcal{K}_k} = \| \frac{1}{m} \sum_{i=1}^n \frac{1}{m} T_j \varphi \|_{\mathcal{K}_k}^2.
\]

Finally, our assembled results and norm duality give

\[
SS(Q_n, T_P, G_k, ||||) = \sup_{g \in G_k} \left\{ \frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{\sigma \in (\mathcal{U}_m)} B_{i\sigma} (T_{\sigma} g)(x_i) \right\} \quad \text{for} \quad B_{i\sigma} \triangleq \mathbf{1}[\sigma = \sigma_i]
\]

\[
= \sup_{g \in G_k} \left\{ \left( \frac{1}{m} \right)^{-1} \sum_{\sigma \in (\mathcal{U}_m)} \mu_{\mu_{\sigma}}(T_{\sigma} g) \right\} \quad \text{for} \quad \mu_{\mu_{\sigma}} \triangleq \left( \frac{1}{m} \right)^{-1} \frac{1}{n} \sum_{i=1}^n B_{i\sigma} b_{\sigma}.
\]

B Proof of Theorem 2: SSDs detect convergence

We will find it useful to write

\[
SS(Q_n, T, G) = \sup_{g \in G} \left\{ \frac{1}{n} \sum_{i=1}^n \frac{1}{m} \sum_{\sigma \in (\mathcal{U}_m)} B_{i\sigma} (T_{\sigma} g)(x_i) \right\} \quad \text{for} \quad B_{i\sigma} \triangleq \mathbf{1}[\sigma = \sigma_i]
\]

\[
= \sup_{g \in G} \left\{ \left( \frac{1}{m} \right)^{-1} \sum_{\sigma \in (\mathcal{U}_m)} \mu_{\mu_{\sigma}}(T_{\sigma} g) \right\} \quad \text{for} \quad \mu_{\mu_{\sigma}} \triangleq \left( \frac{1}{m} \right)^{-1} \frac{1}{n} \sum_{i=1}^n B_{i\sigma} b_{\sigma}.
\]

For any set \( K \), let \( I_K(x) = \mathbf{1}[x \in K] \). Our proof relies on a lemma, proved in App. B.1, that, given a uniformly integrable function \( f \), boosts almost sure convergence in distribution into almost sure uniform convergence for the expectations of all continuous functions dominated by \( |f| \).

Lemma 8 (Convergence of random measures). Consider two sequences of random measures \( (\nu_n)_{n=1}^\infty \) and \( (\tilde{\nu}_n)_{n=1}^\infty \) on \( \mathbb{R}^d \) satisfying \( \nu_n(h) \rightarrow \tilde{\nu}_n(h) \) \( a.s. \) 0 for each bounded and continuous \( h \). For each compact set \( K \subset \mathbb{R}^d \),

\[
\sup_{h \in C(\mathbb{R}^d)} |\nu_n(h I_K) - \tilde{\nu}_n(h I_K)| \xrightarrow{a.s.} 0.
\]

If, in addition, \( f \) is almost surely uniformly \( \nu_n \)-integrable and uniformly \( \tilde{\nu}_n \)-integrable, then

\[
\sup_{h \in C(\mathbb{R}^d); |h| \leq |f|} |\nu_n(h) - \tilde{\nu}_n(h)| \xrightarrow{a.s.} 0.
\]

Since \( W_n(Q_n, P) \rightarrow 0 \), [17, Proof of Cor. 1] implies that \( Q_n(h) \rightarrow P(h) \) for all bounded continuous \( h \) and \( f(x) = c(1 + ||x||^2) \) is uniformly \( Q_n \)-integrable and \( P \)-integrable. Moreover, for each \( \sigma \in (\mathcal{U}_m) \), \( \mu_{\nu_n}(h) \xrightarrow{a.s.} \frac{1}{m} Q_n(h) \) for all bounded \( h \) by Lemma 9, and since, for any compact set \( K \), \( \mu_{\nu_n}(f I_K) \leq \left( \frac{1}{m} \right)^{-1} \frac{1}{n} \sum_{i=1}^n B_{i\sigma} b_{\sigma} \cdot \mu_{\mu_{\sigma}}(f I_K) \cdot f \) is also uniformly \( \mu_{\nu_n} \)-integrable. The assumption \( P(T g) = 0 \) for all \( g \in G_n \), the triangle inequality, the continuity and polynomial growth of each function in \( T_{\sigma} G_n \), and Lemma 8 now imply

\[
SS(Q_n, T, G_n) = \sup_{g \in G_n} \left\{ \left( \frac{1}{m} \right)^{-1} \sum_{\sigma \in (\mathcal{U}_m)} \mu_{\mu_{\sigma}}(T_{\sigma} g) - \frac{1}{m} Q_n(T g) + \frac{1}{m} Q_n(T g) - \frac{1}{m} P(T g) \right\}
\]

\[
\leq \left( \frac{1}{m} \right)^{-1} \sum_{\sigma \in (\mathcal{U}_m)} \sup_{h \in C(\mathbb{R}^d); |h| \leq |f|} |\mu_{\nu_n}(h) - \frac{1}{m} Q_n(h)| + \frac{1}{m} |Q_n(h) - P(h)| \xrightarrow{a.s.} 0.
\]
B.1 Proof of Lemma 8: Convergence of random measures

Fix any $\epsilon > 0$. By [15, Cor. 11.2.5], the set of continuous functions on the compact set $K$ is separable in the supremum norm. Since any bounded continuous function on $K$ can be extended to a bounded continuous function on $\mathbb{R}^d$, there therefore exists a sequence of bounded continuous functions $(h_k)_{k=1}^{\infty}$ on $\mathbb{R}^d$ such that

$$P(\sup_{h \in C(\mathbb{R}^d)} |\nu_n(hI_K) - \tilde{\nu}_n(hI_K)| > \epsilon \text{ i.o.}) \leq P(\max_{k \geq 1} |\nu_n(h_k) - \tilde{\nu}_n(h_k)| > \epsilon/2 \text{ i.o.})$$

$$\leq \sum_{k=1}^{\infty} P(|\nu_n(h_k) - \tilde{\nu}_n(h_k)| > \epsilon/2 \text{ i.o.}) = 0,$$

where we have used the union bound and our almost sure convergence assumption for bounded continuous functions. The first result (9) now follows since $\epsilon$ was arbitrary.

We next assume that the event $E$ on which $f$ is uniformly $\nu_n$ and $\tilde{\nu}_n$-integrable occurs with probability 1, and fix any $\epsilon > 0$. On $E$ there exists $K_\epsilon$ such that $\sup_n \max(\nu_n(|f|I_{K_\epsilon}^c)), \tilde{\nu}_n(|f|I_{K_\epsilon}^c)) \leq \epsilon/2$. Furthermore, on $E$

$$\sup_{h \in C(\mathbb{R}^d)} |\nu_n(h) - \nu_n(hI_K)| + |\tilde{\nu}_n(h) - \tilde{\nu}_n(hI_K)| \leq \sup_{h \in C(\mathbb{R}^d)} \nu_n(h|I_{K_\epsilon}^c) + \tilde{\nu}_n(h|I_{K_\epsilon}^c)$$

$$\leq \nu_n(|f|I_{K_\epsilon}^c) + \tilde{\nu}_n(|f|I_{K_\epsilon}^c) \leq \epsilon.$$

Therefore, the triangle inequality and our first result (9) give

$$P(\sup_{h \in C(\mathbb{R}^d)} |\nu_n(h) - \tilde{\nu}_n(h)| > 2\epsilon \text{ i.o.})$$

$$\leq P(E^c) + P(\sup_{h \in C(\mathbb{R}^d)} |\nu_n(hI_K) - \tilde{\nu}_n(hI_K)| > \epsilon \text{ i.o.}) = 0.$$

The second result now follows since $\epsilon$ was arbitrary.

C Proof of Theorem 3: SSDs detect bounded SD non-convergence

Since $S(Q_n, T, \mathcal{G}_b) \neq 0$, there exists $\epsilon > 0$ such that $S(Q_n, T, \mathcal{G}_b) > \epsilon$ infinitely often (i.o.). Fix any $\epsilon$. For each $n$, choose $h_n = T_f g_n$ for $g_n \in \mathcal{G}_b$ satisfying $Q_n(h_n) \geq S(Q_n, T, \mathcal{G}_b) - \epsilon/2$. Then since $T = (L_m)^{-1} \sum_{\sigma \in (L_m)^{\infty}} T_\sigma$,

$$S(Q_n, T, \mathcal{G}_b) - \epsilon/2 \leq Q_n(h_n) - (L_m)^{-1} \sum_{\sigma \in (L_m)^{\infty}} \mu_{n\sigma}(T_\sigma g_n) + (L_m)^{-1} \sum_{\sigma \in (L_m)^{\infty}} \mu_{n\sigma}(T_\sigma g_n)$$

$$\leq (L_m)^{-1} \sum_{\sigma \in (L_m)^{\infty}} (L_m Q_n(T_\sigma g_n) - \mu_{n\sigma}(T_\sigma g_n)) + SS(Q_n, T, \mathcal{G}).$$

Moreover, since $\|T_\sigma g_n\|_{\infty} \leq 1$ for all $\sigma \in (L_m)^{\infty}$ and $n$, Lemma 9, proved in App. C.1, implies that $L_m Q_n(T_\sigma g_n) - \mu_{n\sigma}(T_\sigma g_n) \overset{a.s.}{\to} 0$ for each $\sigma$.

**Lemma 9 (Bounded function convergence).** Fix any triangular array of points $(x_i^n)_{i \in [n], n \geq 1}$ in $\mathbb{R}^d$, and, for each $n \geq 1$, define the measures

$$\nu_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i^n} \quad \text{and} \quad \tilde{\nu}_n = \frac{1}{n} \sum_{i=1}^{n} \frac{B_i}{\tau} \delta_{x_i^n},$$

where $B_i \overset{i.i.d.}{\sim} \text{Ber}(\tau)$ are independent Bernoulli random variables with $P(B_i = 1) = \tau$. If $\|h_n\|_{\infty} \leq 1$ for each $n$, then, with probability 1,

$$|\tilde{\nu}_n(h_n) - \nu_n(h_n)| \leq \tau^{-1} \sqrt{\frac{\log(n) + 2\log(\log(n))}{2n}}$$

for all $n$ sufficiently large. Hence, $\tilde{\nu}_n(h_n) - \nu_n(h_n) \overset{a.s.}{\to} 0$.

Hence

$$P(SS(Q_n, T, \mathcal{G}_b) \neq 0) \geq P(SS(Q_n, T, \mathcal{G}_b) \leq \epsilon/2 \text{ i.o.})$$

$$\geq P(Q_n(T_\sigma g_n) - \mu_{n\sigma}(T_\sigma g_n) < \frac{\epsilon}{2} \text{ eventually, } \forall \sigma = 1.$$
C.1 Proof of Lemma 9: Bounded function convergence

The result will follow from the following lemma which establishes rates of convergence for subsampled measure expectations to their non-subsampled counterparts.

**Lemma 10.** Under the notation of Lemma 9, for any \(a \in [1, 2]\), \(\delta \in (0, 1)\), and \(h : \mathbb{R}^d \rightarrow \mathbb{R}\),

\[
\nu_n(h) - \nu(h) \leq \frac{\tau^{-1} \sqrt{2 \log(1/\delta)}}{n} (\nu_n(|h|^a))^{1/a} \quad \text{with probability at least} \quad 1 - \delta \quad \text{and}
\]

\[
\nu_n(h) - \tilde{\nu}_n(h) \leq \frac{\tau^{-1} \sqrt{2 \log(1/\delta)}}{n} (\nu_n(|h|^a))^{1/a} \quad \text{with probability at least} \quad 1 - \delta.
\]

**Proof** Fix any \(a \in [1, 2], \delta \in (0, 1)\), and \(h : \mathbb{R}^d \rightarrow \mathbb{R}\). Since

\[
\tilde{\nu}_n(h) = \frac{1}{n} \sum_{i=1}^n B_{h} h(x_i^n)
\]

is an average of independent variables \(\tau^{-1} B_{h} h(x_i^n) \in [0, \tau^{-1} h(x_i^n)]\) with \(\mathbb{E}[\tilde{\nu}_n(h)] = \nu(h)\), Hoeffding’s inequality [26, Thm. 2] implies

\[
\tilde{\nu}_n(h) - \nu(h) \leq \frac{\tau^{-1} \sqrt{2 \log(1/\delta)}}{n} \sum_{i=1}^n h(x_i^n) \quad \text{with probability at least} \quad 1 - \delta \quad \text{and}
\]

\[
\nu_n(h) - \tilde{\nu}_n(h) \leq \frac{\tau^{-1} \sqrt{2 \log(1/\delta)}}{n} \sum_{i=1}^n h(x_i^n) \quad \text{with probability at least} \quad 1 - \delta.
\]

Moreover, since \(\|\|_2 \leq \|\|_a\), we have \(\sqrt{\sum_{i=1}^n h(x_i^n)^2 / n^2} \leq (\sum_{i=1}^n |h(x_i^n)|^a / n^a)^{1/a}\), and the advertised result follows. \(\Box\)

By Lemma 10 with \(a = 2\),

\[
\sum_{n=1}^\infty \mathbb{P}(\|\nu_n(h) - \tilde{\nu}_n(h)\| \geq \tau^{-1} \sqrt{\frac{\log(1/\delta_n)}{2n}}) \leq \sum_{n=1}^\infty \delta_n < \infty
\]

for \(\delta_n = 1/(n \log^2(n))\). The result now follows from the Borel-Cantelli lemma.

D Proof of Theorem 4: Bounded SDs detect tight non-convergence

We consider each Stein set candidate in turn.

**Kernel Stein set** Suppose \(G_n\) satisfies (A.1). Since, for any vector norm \(\|\|\) on \(\mathbb{R}^d\), there exists \(c_d\) such that \(\{g \in G_{k,\|\|} : \max_{\sigma \in \{L_i\}_m} \|T_{\sigma} g\|_\infty \leq 1 \} \subseteq c_d \{g \in G_{k,\|\|} : \max_{\sigma \in \{L_i\}_m} \|T_{\sigma} g\|_\infty \leq 1\}\) [4], it suffices to assume \(\|\| = \|\|_2\).

Let us define \(\Xi(x) = (1 + \|x\|_2)^{1/2}\). From the argument in [22, Sec. E.1, Proof of Thm. 5], there is a set of test functions \(\mathcal{H}\) such that \(\|h\|_\infty \leq 1\) and \(\text{Lip}(h) \leq 1 + \sqrt{d-1}\) uniformly for all \(h \in \mathcal{H}, d_{\mathcal{H}}(Q_n, P) \rightarrow 0\) only if \(Q_n \Rightarrow P\), and also for each \(h \in \mathcal{H}\) there exists an accompanying function \(g_h\) such that \(T_p g_h = h - P(h)\) and \(\|\Xi g_h\|_\infty \leq M_P\) for some constant \(M_P > 0\) independent of \(h\).

Fix an \(\epsilon > 0\) and, since \((Q_n)_{n=1}^\infty\) is tight, select a compact set \(K_{\epsilon}\) satisfying \(\sup_{\nu} Q_n(K_{\epsilon}) \leq \epsilon\). Let \(K_{\epsilon}^1 = \{x \in K_{\epsilon} : d(x, y) \leq 1\text{ for some } y \in K_{\epsilon}\}\). The argument in [22, Proof of Thm. 13] constructs a truncation \(g_0)\) such that \(g_h(x) = g_0(x)\) for all \(x \in K_{\epsilon}, g_0(x) = 0\) for all \(x \notin K_{\epsilon}^1\), \(\|\Xi g_0 - T_{\rho} g_0\|_\infty \leq C_0\) for a constant \(C_0 > 0\) not depending on \(h\) or \(\epsilon\), and \(\|g_0(x)\|_2 \leq \|g_h(x)\|_2\) for all \(x\). From the final property, we can thus conclude \(\|\Xi g_0\|_\infty \leq \|\Xi g_h\|_\infty \leq M_P\).

By assumption, for all \(\sigma \in \{L_i\}_m\), there is a constant \(\beta > 0\) such that \(\|\nabla \log p_\sigma(x)\|_2 \leq \beta(1 + \|x\|_2)\) for all \(x\). Let us define \(A(x) = \frac{\Xi(x)}{\beta(1 + \|x\|_2)}\), and we note since \(\nabla \log p = \frac{L}{m} \sum_{\sigma \in \{L_i\}_m} \nabla \log p_\sigma\), an application of the triangle inequality yields \(\|\nabla \log p(x)\|_2 \leq A(x)\) for all \(x\). Moreover, since \(L/m \geq 1\) we have \(\|\nabla \log p_\sigma(x)\|_2 \leq A(x)\) for all \(x\) and \(\sigma\).

From the construction in [22, Proof of Lemma 12], there is a random variable \(Y\) with finite first moment such that the function \(g_{\epsilon}(x) = \mathbb{E}[g_0(x + \epsilon Y)]\) satisfies \(\|\Xi g_{\epsilon} - T_{\rho} g_{\epsilon}\|_\infty \leq C_1 \epsilon\) and \(g_{\epsilon} \in C_{\epsilon} G_n\) for constants \(C_1 > 0\) independent of \(\epsilon\) and \(h\) and \(C_\epsilon > 0\) independent of \(h\). By use of the
Another use of the triangle inequality yields

\[ \| A g_r \| \leq \sup_{x, u \in (0,1]} A(x) E[A(x)][g_0(x + eY)] = \sup_{x, u \in (0,1]} E\left[ \frac{A(x)}{A(x + uy)} \Xi(x + uy) \right] \leq M_P E[B(Y)], \]

where \( B(y) \triangleq \sup_{x, u \in (0,1]} A(x)/\Xi(x + uy) \). Moreover, \( E[B(Y)] \) is finite, since \( \Xi(z) \geq 2^{-1/2}(1 + |z|) \) for all \( z \) implies that, for any \( y \),

\[
B(y) = \sup_{x, u \in (0,1]} A(x) \Xi(x + uy) \leq \sup_{x, u \in (0,1]} \sqrt{2} \frac{A(x)}{1 + |uy|} = \sup_{x, u \in (0,1]} \sqrt{2} A(z - uy)
\]

\[
\leq \sup_{z, u \in (0,1]} \sqrt{2} A(z) \sup_{u \in (0,1]} \frac{\beta \|y\|}{1 + |z|} = \sqrt{2} A(y),
\]

where we used the triangle inequality in the penultimate inequality. Thus for any \( \sigma \), by Cauchy-Schwarz, (10), the triangle inequality and fact both \( \| A^{-1} \nabla \log p_\sigma \| \leq 1 \) and \( \| A^{-1} \nabla \log p \| \leq 1 \), we have

\[
\frac{1}{m} T_\sigma g_e - T_\sigma g_r \| = \| (\frac{1}{m} \nabla \log p_\sigma - \nabla \log p, g_e) \| \leq \| A^{-1} (\frac{1}{m} \nabla \log p_\sigma - \nabla \log p) \| \| A g_r \| \leq M_P E[B(Y)] \| A g_r \| \leq (1 + \gamma) M_P E[B(Y)] + \frac{\gamma}{m} \| T_\sigma g_r \|.
\]

Another use of the triangle inequality yields \( \| T_\sigma g_r \| \leq \| h - P(h) - T_\sigma g_r \| + \| h - P(h) \| \), and so combining this with the above results, again using the triangle inequality, establishes

\[
| h - P(h) - T_\sigma g_r | \leq C_1 \epsilon + C_0 K_\epsilon^r, \quad \| T_\sigma g_r \| \leq (1 + \gamma) M_P E[B(Y)] + \frac{\gamma}{m} (C_1 \epsilon + C_0 + 2), \quad \text{and} \quad g_e \in C_1 G_n.
\]

One final application of the triangle inequality ensures for any \( \epsilon \in (0,1) \),

\[
d_\mathcal{H}(Q_n, P) \triangleq \sup_{h \in \mathcal{H}} |Q_n(h) - P(h)| \leq \sup_{h \in \mathcal{H}} |Q_n(T_\sigma g_h) + C_1 \epsilon + C_0 Q_n(K_\epsilon^r) \mid \leq \max(C_1, (1 + \gamma) M_P E[B(Y)] + \frac{\gamma}{m} (C_1 \epsilon + C_0 + 2)) S(Q_n, T_\sigma G_{\epsilon, n}) + (C_0 + C_1) \epsilon.
\]

Since \( \epsilon \) was arbitrary, whenever \( S(Q_n, T_\sigma G_{\epsilon, n}) \rightarrow 0 \), we have \( d_\mathcal{H}(Q_n, P) \rightarrow 0 \) and hence \( Q_n \Rightarrow P \).

**Classical Stein set** Suppose \( G_n \) satisfies (A.2), and consider \( G_\epsilon, \| g \|_2 \) for \( k(x, y) = \rho(x - y) \triangleq (\epsilon^2 + |x - y|_2^2)^\beta \) with \( \beta < 0 \) and \( c > 0 \). Since \( \nabla^3 \rho(0) \) is bounded for \( s \in \{0, 2, 4\} \), [46, Cor. 4.36] implies that \( G_{k, \|g\|_2} \subseteq c_0 G_n \) for some \( c_0 \). The result now follows since \( G_{k, \|g\|_2} \) also satisfies (A.1).

**Graph Stein set** If \( G_n \) satisfies (A.3), the result follows as \( G_n \) contains the classical Stein set \( G_{\|g\|_2} \).

**E Proof of Prop. 5: Coercive SSDs enforce tightness**

Let \( f(x) = \min_{\sigma \in (1, m)} (T_\sigma g)(x) \). Since \( f \) is bounded below, \( C = \inf_{x \in \mathbb{R}^d} f(x) \) is finite. Define

\[
\gamma(r) \triangleq \inf \{ f(x) - C : \| x \|_2 \geq r \},
\]

so that \( \gamma \) is nonnegative, coercive, and non-decreasing, as \( f \) is coercive. Since \( (Q_n)_{n=1}^\infty \) is not tight, there exist \( \epsilon > 0 \) and \( R > 0 \) such that \( \limsup_n Q_n(\| X \|_2 > R) \geq \epsilon \) and \( \gamma(R) \epsilon + C > 0 \). Moreover, since \( \gamma \) is non-decreasing and nonnegative, Markov’s inequality gives

\[
Q_n(\| X \|_2 > R) \leq Q_n(\gamma(\| X \|_2) > \gamma(R)) \leq \mathbb{E}_{Q_n}[\gamma(\| X \|_2)] / \gamma(R) \leq (Q_n(f) - C) / \gamma(R).
\]

Meanwhile, our assumption on \( g \) and the SSD subset representation (3) imply that, surely,

\[
Q_n(f) = \frac{1}{n} \sum_{i=1}^n f(x_i) \leq \frac{1}{n} \sum_{i=1}^n (T_\sigma g)(x_i) \leq \frac{\gamma}{\mathcal{P}} SS(Q_n, T, G_n).
\]

Hence, \( SS(Q_n, T, G_n) \) surely does not converge to zero, as

\[
\limsup_n \frac{\gamma}{\mathcal{P}} SS(Q_n, T, G_n) \geq \gamma(R) \limsup_n Q_n(\| X \|_2 > R) + C \geq \gamma(R) \epsilon + C > 0.
\]
F  Proof of Theorem 6: Coercive SSDs detect non-convergence

We consider each Stein set candidate in turn.

Kernel Stein set  Suppose \( G_n \) satisfies (A.1) with \( k(x, y) = (c^2 + \|x - y\|^2)^\beta \) for \( c > 0 \) and \( \beta \in (-1, 0) \). If \( Q_n \neq P \), then, by Theorem 4, either \( \mathcal{S}(Q_n, T_P, G_{b,n}) \neq 0 \) for \( b,n = \{ g \in \mathcal{G} : \max_{\sigma \in \{ |\tau_{\gamma}g|\}_{\infty} \leq 1 \} \text{ or } \mathcal{G}(n) \}_{\gamma=1} \) is not tight.

If \( \mathcal{S}(Q_n, T_P, G_{b,n}) \neq 0 \), then, with probability 1, \( \mathcal{S}(Q_n, T_P, G_n) \neq 0 \) by Theorem 3.

Now suppose \( (\mathcal{G}(n))_{\gamma=1} \) is not tight, and consider any \( \sigma \in \{ |\tau_{\gamma}g|\}_{\infty} \). Since \( \nabla \log p_\sigma \) has at most linear growth and satisfies distant dissipativity, the proof of [22, Lem. 16] constructs a function \( g \in \mathcal{G} \) that is independent of the choice of \( \sigma \) and satisfies \( \tau_{\gamma}g \geq f_\sigma \) for some coercive bounded-below \( f_\sigma \). Since \( \{ |\tau_{\gamma}g|\}_{\infty} \) has finite cardinality we have \( \tau_{\gamma}g \geq f \) for a common coercive bounded-below function \( f(x) = \min_{\sigma \in \{ |\tau_{\gamma}g|\}_{\infty}} f_\sigma(x) \). Therefore, surely, \( \mathcal{S}(Q_n, T_P, G_n) \neq 0 \) by Prop. 5.

Classical Stein Set  Suppose \( G_n = G_{\|\cdot\|} \) satisfies (A.2). By the proof of Theorem 4, for any \( c > 0 \) and \( \beta \in (-1, 0) \), there is a constant \( c_0 > 0 \) such that \( G_{k,\|\cdot\|} \leq c_0 G_n \). Hence \( \mathcal{S}(Q_n, T_P, G_{k,\|\|}) \leq c_0 \mathcal{S}(Q_n, T_P, G_n) \) for all \( n \) and the result follows.

Graph Set  Suppose \( G_n \) satisfies (A.3). Then \( G_n \) contains \( G_{\|\cdot\|} \) and the result follows.

G  Proof of Theorem 7: Wasserstein convergence of SVGD and SSVGD

G.1  Additional notation

For each \( \epsilon > 0 \) and collection of \( n \) points \( (x^n_i)_{i=1}^n \) with associated discrete measure \( \nu_n = \frac{1}{n} \sum_{i=1}^n \delta_{x^n_i} \), we define the random one-step SVGD mapping

\[
T^{m}_{\nu_n,\epsilon,n}(x) = x + \epsilon \frac{1}{n} \sum_{j=1}^n \frac{\mathbf{E}}{m} \nabla \log p_\sigma_j(x^n_j) k(x^n_j, x) + \nabla x_j k(x^n_j, x)
\]

for \( (\sigma_j)_{j=1}^n \) independent uniformly random size-\( m \) subsets of \([L]\). We also let \( \Phi_{\epsilon,n}^m(\mu) \) denote the random distribution of \( T^{m}_{\nu_n,\epsilon,n}(X) \) when \( X \sim \mu \).

G.2  Proof of Theorem 7

We will prove the desired result by induction. For our base case we have, \( W_1(Q_{n,0}^m, Q_{n,0}) = 0 \) and \( W_1(Q_{n,0}, Q_{\infty,0}) \rightarrow 0 \) by assumption, and hence \( c_0(1 + \|\cdot\|_2) \) is \( Q_{\infty,0} \)-integrable and uniformly \( Q_{n,0} \)-integrable by [17, Proof of Cor. 1].

Now, fix any \( r \geq 0 \) and assume \( W_1(Q_{n,r}, Q_{\infty,r}) \rightarrow 0 \), so that \( c_0(1 + \|\cdot\|_2) \) is uniformly \( Q_{n,r} \)-integrable by [17, Proof of Cor. 1]. Therefore, there exists a constant \( C' > 0 \) such that

\[
\sup_{n \geq 1} c_0(1 + Q_{\infty,0}(\|\cdot\|_2)) + c_2(1 + Q_{n,0}(\|\cdot\|_2)) \leq C'.
\]

In addition, let \( \mathcal{E} \) be the event on which \( W_1(Q_{n,r}, Q_{n,r}) \rightarrow 0 \) as \( n \rightarrow \infty \), and assume \( \mathbb{P}(\mathcal{E}) = 1 \). On \( \mathcal{E} \) we find that \( c_0(1 + \|\cdot\|_2) \) is also uniformly \( Q_{n,r} \)-integrable by [17, Proof of Cor. 1]. Therefore, on \( \mathcal{E} \), there exists a constant \( C' \) such that

\[
\sup_{n \geq 1} c_0(1 + Q_{n,r}(\|\cdot\|_2)) + Q_{\infty,0}(\|\cdot\|_2)) + c_2(1 + Q_{n,r}(\|\cdot\|_2)) \leq C.
\]

By the triangle inequality,

\[
W_1(Q_{n,r+1}, Q_{n,r+1}) = W_1(\Phi_{\epsilon,n}^m(Q_{n,r}), \Phi_{\epsilon,r}(Q_{n,r})) \\
\leq W_1(\Phi_{\epsilon,n}^m(Q_{n,r}), \Phi_{\epsilon,r}(Q_{n,r})) + W_1(\Phi_{\epsilon,r}(Q_{n,r}), \Phi_{\epsilon,r}(Q_{n,r})).
\]

(11)

On \( \mathcal{E} \), our linear growth assumption (7), the uniformly \( Q_{n,r} \)-integrability of \( c_0(1 + \|\cdot\|_2) \), and the following lemma establish that the Wasserstein distance \( W_1(\Phi_{\epsilon,n}^m(Q_{n,r}), \Phi_{\epsilon,r}(Q_{n,r})) \) between one step of SSVGD and one step of SVGD from a common starting point converges to 0 almost surely as \( n \) grows. The proof of Lemma 11 can be found in App. G.3.
Lemma 11 (One-step convergence of SSVGD to SVGD). Fix any triangular array of points \((x^n_i)_{i \in [n], n \geq 1}\) in \(\mathbb{R}^d\), and define the discrete probability measures \(\nu_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{x^n_i}\). If \(\nabla \log p_\sigma(\cdot)k(\cdot, z)\) is continuous for each \(z \in \mathbb{R}^d\) and \(\sigma \in \begin{pmatrix} L \cr m \end{pmatrix}\) and

\[
 f(x) \triangleq \sup_{z \in \mathbb{R}^d, \sigma \in \begin{pmatrix} L \cr m \end{pmatrix}} \|\nabla \log p_\sigma(x)\|_\infty |k(x, z)|
\]

is \(\nu_n\)-uniformly integrable, then, for any \(\epsilon > 0\), \(W_1(\Phi_{\epsilon_n}^n(\nu_n), \Phi_\epsilon(\nu_n)) \xrightarrow{a.s.} 0\) as \(n \to \infty\).

To control the second term in the bound (11), we provide a second lemma, proved in App. G.4, which establishes the pseudo-Lipschitzness of the one-step SVGD mapping \(\Phi_\epsilon\).

Lemma 12 (Wasserstein pseudo-Lipschitzness of SVGD). Suppose that, for some \(c_1, c_2 > 0\),

\[
 \sup_{x \in \mathbb{R}^d} \|\nabla_x (\nabla \log p(x)k(x, z) + \nabla_x k(x, z))\|_{op} \leq c_1 (1 + \|x\|_2) \quad \text{and} \quad \sup_{x \in \mathbb{R}^d} \|\nabla_x (\nabla \log p(x)k(x, z) + \nabla_x k(x, z))\|_{op} \leq c_2 (1 + \|z\|_2).
\]

Then, for any \(\epsilon > 0\) and probability measures \(\mu, \nu\),

\[
 W_1(\Phi_\epsilon(\mu), \Phi_\epsilon(\nu)) \leq W_1(\mu, \nu)(1 + \epsilon c_1 (1 + \mu(\|\cdot\|_2) + \epsilon c_2 (1 + \nu(\|\cdot\|_2)).
\]

On \(\mathcal{E}\), our pseudo-Lipschitz assumptions (6) and Lemma 12 imply

\[
 W_1(\Phi_\epsilon(Q_{n,r}^m, \Phi_\epsilon(Q_{n,r}) \leq W_1(Q_{n,r}^m, Q_{n,r})(1 + \epsilon c_1 (1 + Q_{n<r}(\|\cdot\|_2) + \epsilon c_2 (1 + Q_{n,r}(\|\cdot\|_2)))
\]

\[
 \leq CW_1(Q_{n,r}^m, Q_{n,r}) \to 0.
\]

Hence, on \(\mathcal{E}\), \(W_1(Q_{n,r+1}^m, Q_{n,r+1}) \xrightarrow{a.s.} 0\). Identical reasoning yields \(W_1(Q_{\infty,r+1}, Q_{\infty,r+1}) \to 0\), completing our induction.

G.3 Proof of Lemma 11: One-step convergence of SSVGD to SVGD

Note that the random one-step SSVGD mapping takes the form

\[
 T_{\nu_n, \epsilon_n}(x) = x + \epsilon \nu_n(\nabla \sigma_j k(\cdot, x)) + \epsilon \begin{pmatrix} L \cr m \end{pmatrix}^{-1} \sum_{\sigma \in \begin{pmatrix} L \cr m \end{pmatrix}} \nu_\sigma(\nabla \log p_\sigma(\cdot)k(\cdot, x))
\]

for \(\nu_\sigma = \begin{pmatrix} L \cr m \end{pmatrix} \frac{1}{m} \frac{1}{n} \sum_{i=1}^{n} B_{j\sigma} \delta_{x^n_i}\) and \(B_{j\sigma} = I[\sigma = \sigma_j]\). Moreover, by Kantorovich-Rubinstein duality, we may write the \(1\)-Wasserstein distance as

\[
 W_1(\Phi_{\epsilon_n}^m(\nu_n), \Phi_\epsilon(\nu_n)) = \sup_{f \in M_1(f)} \Phi_{\epsilon_n}^m(\nu_n)(f) - \Phi_\epsilon(\nu_n)(f)
\]

\[
 = \sup_{f \in M_1(f)} f(T_{\nu_n, \epsilon_n}(x^n_i)) - f(T_{\nu_n, \epsilon_n}(x^n_i))
\]

\[
 \leq \frac{1}{n} \sum_{i=1}^{n} \left\|T_{\nu_n, \epsilon_n}(x^n_i) - T_{\nu_n, \epsilon_n}(x^n_i)\right\|_2
\]

\[
 = \left(\frac{L}{m}\right)^{-1} \frac{1}{n} \sum_{i=1}^{n} \left\|\nabla \log p_\sigma(\cdot)k(\cdot, x^n_i)\right\|_2 - \nu_\sigma(\nabla \log p_\sigma(\cdot)k(\cdot, x^n_i))
\]

\[
 \leq \left(\frac{L}{m}\right)^{-1} \sum_{\sigma} \frac{\epsilon \sqrt{d}}{\sqrt{n}} \left\|\nabla \log p_\sigma(\cdot)k(\cdot, x^n_i)\right\|_\infty - \nu_\sigma(\nabla \log p_\sigma(\cdot)k(\cdot, x^n_i))
\]

\[
 \leq \epsilon \sqrt{d} \left(\frac{L}{m}\right)^{-1} \sum_{\sigma} \sup_{h \in C(\mathbb{R}^d)} \left|\nabla \sigma(\cdot)k(\cdot, x^n_i)\right| \nu_\sigma(h) - \frac{L}{m} \nu_\sigma(h).
\]

where we have used the triangle inequality and norm relation \(\|\cdot\|_2 \leq \sqrt{d}\|\cdot\|_\infty\) in the penultimate display.

For each \(\sigma \in \begin{pmatrix} L \cr m \end{pmatrix}\), since \(|f|\) is uniformly \(\nu_n\)-integrable, and \(\nu_\sigma(\|f\|_{I_K}) \leq \left(\frac{L}{m}\right)^{\frac{1}{m}} \nu_\sigma(\|f\|_{I_K})\) for every compact set \(K\), we find that \(|f|\) is uniformly \(\nu_n\)-integrable for each \(\sigma\). In addition, for each \(\sigma\), since \(\nu_\sigma(h) - \frac{L}{m} \nu_\sigma(h) \xrightarrow{a.s.} 0\) for all bounded \(h\) by Lemma 9, we have \(\sup_{h \in C(\mathbb{R}^d)} \left|\nabla \sigma(\cdot)k(\cdot, x^n_i)\right| \nu_\sigma(h) - \frac{L}{m} \nu_\sigma(h) \xrightarrow{a.s.} 0\) by Lemma 8. The result now follows from the bound (12).

G.4 Proof of Lemma 12: Wasserstein pseudo-Lipschitzness of SVGD

Assume that \(\mu\) and \(\nu\) have integrable means (or else the advertised claim is vacuous), and select \((X', Z')\) to be an optimal 1-Wasserstein coupling of \((\mu, \nu)\). The triangle inequality, Jensen’s inequality,
and our pseudo-Lipschitzness assumptions imply that

\[
\|T_{\mu,\epsilon}(x) - T_{\nu,\epsilon}(z)\|_2 \leq \|x - z\|_2 \\
+ \epsilon \|E[\nabla \log p(X')k(X', x) + \nabla_x k(X', x) - (\nabla \log p(X')k(X', z) + \nabla k(X', z))]| \|_2 \\
+ \epsilon \|E[\nabla \log p(X')k(X', z) + \nabla_x k(X', z) - (\nabla \log p(Z')k(Z', z) + \nabla z k(Z', z))]| \|_2 \\
\leq \|x - z\|_2 (1 + \epsilon c_1 (1 + E[|X'|_2])) + \epsilon c_2 E[|X' - Z'|_2] (1 + \|z\|_2) \\
= \|x - z\|_2 (1 + \epsilon c_1 (1 + \mu(\|\cdot\|_2)) + \epsilon c_2 W_1(\mu, \nu)(1 + \|z\|_2).
\]

Since \( T_{\mu,\epsilon}(X') \sim \Phi_\epsilon(\mu) \) and \( T_{\nu,\epsilon}(Z') \sim \Phi_\epsilon(\nu) \), we conclude that

\[
W_1(\Phi_\epsilon(\mu), \Phi_\epsilon(\nu)) \leq E[|T_{\mu,\epsilon}(X') - T_{\nu,\epsilon}(Z')|_2] \\
\leq E[|X' - Z'|_2] (1 + \epsilon c_1 (1 + \mu(\|\cdot\|_2)) + \epsilon c_2 W_1(\mu, \nu)(1 + E[|Z'|_2]) \\
= W_1(\mu, \nu)(1 + \epsilon c_1 (1 + \mu(\|\cdot\|_2)) + \epsilon c_2 (1 + \nu(\|\cdot\|_2)).
\]