Kernel Thinning

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Abstract
We introduce kernel thinning, a new procedure for compressing a distribution \( P \) more effectively than i.i.d. sampling or standard thinning. Given a suitable reproducing kernel \( k \) and \( \mathcal{O}(n^2) \) time, kernel thinning compresses an \( n \)-point approximation to \( P \) into a \( \sqrt{n} \)-point approximation with comparable worst-case integration error across the associated reproducing kernel Hilbert space. With high probability, the maximum discrepancy in integration error is \( \mathcal{O}_d(n^{-1/2} \sqrt{\log n}) \) for compactly supported \( P \) and \( \mathcal{O}_d(n^{-1/2} (\log n)^{(d+1)/2} \sqrt{\log \log n}) \) for sub-exponential \( P \) on \( \mathbb{R}^d \). In contrast, an equal-sized i.i.d. sample from \( P \) suffers \( \Omega(n^{-1/4}) \) integration error. Our sub-exponential guarantees resemble the classical quasi-Monte Carlo error rates for uniform \( P \) on \([0,1]^d\) but apply to general distributions on \( \mathbb{R}^d \) and a wide range of common kernels. We use our results to derive explicit non-asymptotic maximum mean discrepancy bounds for Gaussian, Matérn, and B-spline kernels and present two vignettes illustrating the practical benefits of kernel thinning over i.i.d. sampling and standard Markov chain Monte Carlo thinning, in dimensions \( d = 2 \) through 100.

Keywords: coresets, distribution compression, Markov chain Monte Carlo, maximum mean discrepancy, reproducing kernel Hilbert space, thinning

1. Introduction

Monte Carlo and Markov chain Monte Carlo (MCMC) methods (Brooks et al., 2011) are commonly used to approximate intractable target expectations \( \mathbb{E}_{X \sim P}[f(X)] \) with asymptotically exact averages \( \mathbb{P}_n f \triangleq \frac{1}{n} \sum_{i=1}^{n} f(x_i) \) based on points \( (x_i)_{i=1}^{n} \) generated from a Markov chain. A standard practice, to minimize the expense of downstream function evaluation, is to thin the Markov chain output by discarding every \( t \)-th sample point (Owen, 2017). Such sample compression is critical in fields like computational cardiology in which each function evaluation triggers an organ or tissue simulation consuming thousands of CPU hours (Niederer et al., 2011; Augustin et al., 2016; Strocchi et al., 2020). Unfortunately, standard thinning also leads to a significant reduction in accuracy: thinning one’s chain to \( n^{\frac{1}{2}} \) sample points, for example, increases integration error from \( \Theta(n^{-1/2}) \) to \( \Theta(n^{-1/4}) \). In this work, we introduce a more effective thinning strategy, providing \( o(n^{-\frac{1}{4}}) \) integration error when \( n^{\frac{1}{2}} \) points are returned.

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We call our strategy kernel thinning as we focus on integration in a reproducing kernel Hilbert space (RKHS, Berlinet and Thomas-Agnan, 2011) with a kernel \( k \) and norm \( \| \cdot \|_k \). The worst-case error between sample and target expectations over the RKHS unit ball is given by the kernel maximum mean discrepancy (MMD, Gretton et al., 2012),

\[
\text{MMD}_k(P, P_n) \triangleq \sup_{\|f\|_k \leq 1} \|Pf - P_n f\|,
\]

and we call a sequence of points \((x_i)_{i=1}^n\) an \((n, \varepsilon)\)-MMD coreset for \((k, P)\) if \(\text{MMD}_k(P, P_n) \leq \varepsilon\). For a bounded kernel \( k \), \( n^{\frac{1}{2}} \) i.i.d. draws from \( P \) yield a \( \left(n^{\frac{1}{2}}, n^{-\frac{1}{4}}\right)\)-MMD coreset with high probability, and comparable guarantees hold for a thinned geometrically ergodic Markov chain (see Prop. 1). A benchmark for improvement is provided by the online Haar strategy of Dwivedi et al. (2019), which generates an \( \left(n^{\frac{1}{2}}, \mathcal{O}(n^{-\frac{1}{2}} \log^{2d} n)\right)\)-MMD coreset from \( 2n^{\frac{1}{2}} \) i.i.d. sample points when \( P \) is specifically the uniform distribution on the unit cube \([0, 1]^d\).

Our contributions After describing our problem setup in Sec. 2, we introduce in Sec. 3 a practical procedure, kernel thinning, for compressing an input point sequence into a provably high-quality coreset. Kernel thinning uses non-uniform randomness and a less smooth square-root kernel \( k_{\text{rt}} \) (see Def. 1) to partition the input into subsets of comparable quality and then refines the best of these subsets. Given \( n \) input points sampled i.i.d. or from a fast-mixing Markov chain, the result is, with high probability, an \( \left(n^{\frac{1}{2}}, \mathcal{O}(n^{-\frac{1}{2}} \sqrt{\log n})\right)\)-MMD coreset for \( P \) and \( k_{\text{rt}} \) with bounded support, an \( \left(n^{\frac{1}{2}}, \mathcal{O}(n^{-\frac{1}{2}} \sqrt{\log n} \log n)\right)\)-MMD coreset for \( P \) and \( k_{\text{rt}} \) with light tails, and an \( \left(n^{\frac{1}{2}}, \mathcal{O}(n^{-\frac{1}{2}} + \frac{d}{2} \log n \log \log n)\right)\)-MMD coreset for \( P \) and \( k_{\text{rt}}^2 \), \( \rho > 2d \) moments. For compactly supported or light-tailed \( P \) and \( k_{\text{rt}} \), these results compare favorably with the \( \Omega(n^{-\frac{1}{2}}) \) lower bounds of Sec. 1.1. Our guarantees extend more generally to any predetermined input point sequence, even deterministic ones based on quadrature or kernel herding (Chen et al., 2010), and give rise to explicit, non-asymptotic error bounds for a wide variety of popular kernels including Gaussian, Matérn, and B-spline kernels. Moreover, our algorithm runs in \( \mathcal{O}(n^2) \) time given \( \mathcal{O}(n \min(d, n)) \) space.

While \( \left(n^{\frac{1}{2}}, \mathcal{O}(n^{-\frac{1}{2}} \log^d n)\right)\)-MMD coresets have been developed for specific \((k, P)\) pairings like the uniform distribution \( P \) on the unit cube paired with a Sobolev kernel \( k \) (see Sec. 1.1), to the best of our knowledge, no prior \( \left(n^{\frac{1}{2}}, o(n^{-\frac{1}{2}})\right)\)-MMD coreset constructions were known for the range of \( P \) and \( k \) studied in this work. Our results rely on three principal contributions. First, we establish an important link between MMD coresets for \( k \) and \( L^\infty \) coresets for \( k_{\text{rt}} \). We say a sequence of points \((x_i)_{i=1}^n\) is a \((n, \varepsilon)\)-\( L^\infty \) coreset for \((k_{\text{rt}}, P)\) if

\[
\sup_{x \in \mathbb{R}^d} |(P - P_n)k_{\text{rt}}(x)| \leq \varepsilon \quad \text{for} \quad P k_{\text{rt}} \triangleq \mathbb{E}_{X \sim P} [k_{\text{rt}}(X, \cdot)] \quad \text{and} \quad P_n k_{\text{rt}} \triangleq \frac{1}{n} \sum_{i=1}^n k_{\text{rt}}(x_i, \cdot).
\]

In Sec. 3.2, we show that any \( L^\infty \) coreset for \((k_{\text{rt}}, P)\) is also an MMD coreset for \((k, P)\) with quality depending on the tail decay of \( k_{\text{rt}} \) and \( P \).

Second, we prove in Sec. 5.2 that, with high probability and for a wide range of kernels, kernel thinning compresses any input \((n, \varepsilon)\)-\( L^\infty \) coreset into an order \( \left(n^{\frac{1}{2}}, \varepsilon + n^{-\frac{1}{2}} \sqrt{d \log n}\right)\)-\( L^\infty \) coreset with even tighter guarantees for lighter-tailed targets. Third, as a building

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2. Dwivedi et al. (2019) specifically control the star discrepancy, a quantity which in turn upper bounds a Sobolev space MMD called the \( L^2 \) discrepancy (Hickernell, 1998; Novak and Woźniakowski, 2010).
block for kernel thinning, we introduce and analyze a Hilbert space generalization of the self-balancing walk of Alweiss et al. (2021) to partition a sequence of functions (like \( K_t(x, \cdot) \)) into nearly equal halves. Our analysis of this self-balancing Hilbert walk in Sec. 4 may be of independent interest for solving the online vector balancing problem (Spencer, 1977) in Hilbert spaces. In Sec. 6, two vignettes illustrate the practical benefits of kernel thinning over (a) i.i.d. sampling in dimensions \( d = 2 \) through 100 and (b) standard MCMC thinning when targeting challenging differential equation posteriors. We conclude with a discussion in Sec. 7 and proofs in the appendices.

**Notation** Throughout, we will make frequent use of the norms \( \| k \|_\infty = \sup_{x, y} |k(x, y)| \) and \( \| f \|_\infty = \sup_x |f(x)| \) and the shorthand \( \mathbb{P}_n \triangleq \frac{1}{n} \sum_{i=1}^n \delta_{x_i}, [n] \triangleq \{1, \ldots, n\}, \mathbb{R}_+ \triangleq \{x \in \mathbb{R} : x \geq 0\}, B(x; R) \triangleq \{y \in \mathbb{R}^d \mid \| x - y \|_2 < R\} \), and \( a \wedge b \triangleq \min(a, b) \). The set \( \mathcal{A}^c \) denotes the complement of a set \( \mathcal{A} \subset \mathbb{R}^d \), and \( 1_A(x) = 1 \) if \( x \in \mathcal{A} \) and 0 otherwise. We say \( a \) is of order \( b \) and write \( a = O(b) \) or \( a \gtrsim b \) to denote that \( a \leq cb \) for some universal constant \( c \). Throughout, we view the success probability \( \delta \) as a fixed constant. We use \( a = \Omega(b) \) or \( a \gtrsim b \) to denote \( a \geq cb \) for some universal constant \( c \). We write \( a = \Theta(b) \) when \( a = \Omega(b) \) and \( a = O(d) \). Moreover, we use \( a = O_d(b), a \gtrsim_d b, a = \Omega_d(b), a \gtrsim_d b \) to indicate dependency of constant on \( d \). We say \( f(n) = o(n) \) if \( \lim_{n \to \infty} f(n)/n = 0 \). We also write order \((n, \epsilon)\)-MMD (or \( L^\infty \) coreset) to mean an \((n, O(\epsilon))\)-MMD (or \( L^\infty \)) coreset. For point sequences \( S, S' \) with empirical distributions \( Q_n, Q'_n \), we overload our MMD notation to write \( \text{MMD}_k(\mathbb{P}, S) \triangleq \text{MMD}_k(\mathbb{P}, Q_n) \) and \( \text{MMD}_k(S, S') \triangleq \text{MMD}_k(Q_n, Q'_n) \).

### 1.1 Related work on MMD coresets

Here we review lower bounds and prior strategies for generating coresets with small MMD and defer discussion of prior \( L^\infty \) coreset constructions to Sec. 5.3. We highlight that while \((n^{\frac{1}{2}}, o(n^{-\frac{1}{2}}))\)-MMD coresets have been developed for specific \((\mathbb{P}, k)\) pairings like the uniform distribution \( \mathbb{P} \) on the unit cube paired with a Sobolev kernel \( k \), to the best of our knowledge, no prior \((n^{\frac{1}{2}}, o(n^{-\frac{1}{2}}))\)-MMD coreset constructions were known for the range of \( \mathbb{P} \) and \( k \) studied in this work.

**Lower bounds** For any bounded and radial (i.e., \( k(x, y) = \kappa(\|x - y\|_2^2) \)) kernel satisfying mild decay and smoothness conditions, Phillips and Tai (2020, Thm. 3.1) showed that any procedure outputting coresets of size \( n^{\frac{1}{2}} \) must suffer \( \Omega(\min(\sqrt{d} n^{-\frac{1}{2}}, n^{-\frac{1}{2}})) \) MMD for some (discrete) target distribution \( \mathbb{P} \). This lower bound applies, for example, to Matérn kernels and to infinitely smooth Gaussian kernels. For any continuous and shift-invariant (i.e., \( k(x, y) = \kappa(x - y) \)) kernel taking on at least two values, Tolstikhin et al. (2017, Thm. 1) showed that any estimator of \( \mathbb{P} \) (even non-corest estimators) based only on \( n \) i.i.d. draws from \( \mathbb{P} \) must suffer \( \Omega(n^{-\frac{1}{2}}) \) MMD with probability at least \( 1/4 \) for some discrete target \( \mathbb{P} \). If, in addition, \( k \) is characteristic (i.e., \( \text{MMD}_k(\mathbb{P}, Q) \neq 0 \) when \( \mathbb{P} \neq Q \), then Tolstikhin et al. (2017, Thm. 6) establish the same lower bound for some continuous target \( \mathbb{P} \) with infinitely differentiable density. These last two lower bounds hold, for example, for Gaussian, Matérn, and B-spline kernels and apply in particular to any thinning algorithm that compresses \( n \) i.i.d. sample points without additional knowledge of \( \mathbb{P} \). For light-tailed \( \mathbb{P} \) and \( k_{rt} \), the kernel thinning guarantees of Thm. 1 will match each of these lower bounds up to factors of \( \sqrt{\log(n)} \) and constants depending on \( d \).
Order \((n^{\frac{1}{2}}, n^{-\frac{1}{2}})\)-MMD coresets for general \(\mathbb{P}\)  By Prop. A.1 of Tolstikhin et al. (2017), an i.i.d. sample from \(\mathbb{P}\) yields an order \((n^{\frac{1}{2}}, n^{-\frac{1}{2}})\)-MMD coreset with high probability. Chen et al. (2010) showed that kernel herding with a finite-dimensional kernel (like the linear \(k(x, y) = \langle x, y \rangle\)) finds an \((n^{\frac{1}{2}}, (C_{\mathbb{P}, k, d}n)^{-\frac{1}{2}})\)-MMD coreset for an implicit parameter \(C_{\mathbb{P}, k, d}\). However, Bach et al. (2012) showed that their analysis does not apply to any infinite-dimensional kernel (like the Gaussian, Matérn, and B-spline kernels studied in this work), as \(C_{\mathbb{P}, k, d}\) would necessarily equal 0. The best known rate for kernel herding with bounded infinite-dimensional kernels (Lacoste-Julien et al., 2015, Thm. G.1) guarantees an order \((n^{\frac{1}{2}}, n^{-\frac{1}{2}})\)-MMD coreset, matching the i.i.d. guarantee. For bounded kernels, the same guarantee is available for Stein Point MCMC (Chen et al., 2019, Thm. 1) which greedily minimizes MMD\(^3\) over random draws from \(\mathbb{P}\) and for a variant of the greedy sign selection algorithm described in Karnin and Liberty (2019, Sec. 3.1).\(^4\) Slightly inferior guarantees were established for Stein points (Chen et al., 2018, Thm. 1) and Stein thinning (Riabiz et al., 2021, Thm. 1), both of which accommodate unbounded kernels as well.

Finite-dimensional kernels Harvey and Samadi (2014) construct \((n^{\frac{1}{2}}, \sqrt{dn^{-\frac{1}{2}} \log 2.5 \, n})\)-MMD coresets for finite-dimensional linear kernels on \(\mathbb{R}^d\) but do not address infinite-dimensional kernels.

Uniform distribution on \([0,1]^d\) Hickernell (1998); Novak and Wozniakowski (2010) show that low discrepancy quasi-Monte Carlo (QMC) methods generate \((n^{\frac{1}{2}}, \mathcal{O}(n^{-\frac{1}{2}} \log^d n))\)-MMD coresets when \(\mathbb{P}\) is the uniform distribution on the unit cube \([0,1]^d\) (see Dick et al., 2013, for a contemporary QMC overview). For the same target, the online Haar strategy of Dwivedi et al. (2019) yields an \((n^{\frac{1}{2}}, \mathcal{O}(n^{-\frac{1}{2}} \log^2 n))\)-MMD coreset. These constructions satisfy our quality criteria but are tailored specifically to the uniform distribution on the unit cube.

Unknown coreset quality On compact manifolds, optimal coresets of size \(n^{\frac{1}{2}}\) minimize the weighted Riesz energy (a form of relative MMD with a weighted Riesz kernel) at known rates (Borodachov et al., 2014); however, practical minimum Riesz energy (Borodachov et al., 2014) and minimum energy design (Joseph et al., 2015, 2019) constructions have not been analyzed. When \(k\) is nonnegative and the kernel matrix \((k(x_i, x_j))_{i,j=1}^n\) satisfies a strong diagonal dominance condition, Kim et al. (2016, Cor. 3, Thm. 6) show that greedy optimization of MMD\(_k\) yields an MMD-critic coreset \(\hat{S}\) of size \(n^{\frac{1}{2}}\) satisfying

\[
\text{MMD}_{k}^2(\hat{S}) \leq (1 - \frac{1}{e}) \text{MMD}_{k}^2 + \frac{1}{e} \mathbb{P}_n \mathbb{P}_n k
\]

for \(\text{MMD}_{k} = \min_{|S| = \sqrt{n}} \text{MMD}_{k}(\mathbb{P}_n, S)\).

However, in the usual case in which \(\mathbb{P}_n \mathbb{P}_n k = \Omega(1)\), this error bound does not decay to 0 with \(n\). Paige et al. (2016) analyze the impact of approximating a kernel in super-sampling with a reservoir but do not analyze the quality of the constructed MMD coreset. For the conditionally positive definite energy distance kernel, Mak and Joseph (2018) establish that an optimal coreset of size \(n^{\frac{1}{2}}\) has \(o(n^{-\frac{1}{2}})\) MMD but do not provide a construction; in addition, Mak and Joseph (2018) propose two support points convex-concave procedures for constructing MMD coresets but do not establish their optimality and do not analyze their quality.

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3. To bound MMD\(_k\) using Chen et al. (2019, Thm. 1), choose \(k_0(x, y) = k(x, y) - \mathbb{P}k(x) - \mathbb{P}k(y) + \mathbb{P}\mathbb{P}k\).
4. The statement of Karnin and Liberty (2019, Thm. 24) bounds \(||||_{\infty}\), but the proof bounds MMD\(_k\).
1.2 Related work on weighted MMD coresets

While coresets satisfy a number of valuable constraints that are critical for some downstream applications—exact approximation of constants, automatic preservation of convex integrand constraints, compatibility with unweighted downstream tasks, easy visualization, straightforward sampling, and increased numerical stability against errors in integral evaluations (Karvonen et al., 2019)—some applications also support weighted coreset approximations of $P$ of the form $\sum_{i=1}^{\sqrt{n}} w_i \delta_{x_i}$ for weights $w_i \in \mathbb{R}$ that need not be equal, need not be nonnegative, or need not sum to 1. Notably, weighted coresets that depend on $P$ only through an i.i.d. sample of size $n$ are subject to the same $\Omega(n^{-\frac{1}{2}})$ MMD lower bounds of Tolstikhin et al. (2017) described in Sec. 1.1. Any constructions that violate these bounds do so only by exploiting additional information about $P$ (for example, exact knowledge of $P_k$) that is not generally available and not required for our kernel thinning guarantees. Moreover, while weighted coresets need not provide satisfactory solutions to the unweighted coreset problem studied in this work, kernel thinning coreset points can be converted into an optimally weighted coreset of no worse quality by explicitly minimizing $\text{MMD}_k(P, \sum_{i=1}^{\sqrt{n}} w_i \delta_{x_i})$ or, if computable, $\text{MMD}_k(P, \sum_{i=1}^{\sqrt{n}} w_i \delta_{x_i})$ over the weights $w_i$ in $O(n^{3/2})$ time.

With this context, we now review known weighted MMD coreset guarantees. We highlight that only one of the weighted $(n^{\frac{1}{2}}, o(n^{-\frac{1}{4}}))$-MMD guarantees covers the unbounded distributions addressed in this work and that the single unbounded guarantee relies on a restrictive uniformly bounded eigenfunction assumption that is typically not satisfied. In other words, our analysis establishes MMD improvements for practical $(k, P)$ pairings not covered by prior weighted analyses.

**$P$ with bounded support** If $P$ has bounded density and bounded, regular support and $k$ is a Gaussian or Matérn kernel, then Bayesian quadrature (O’Hagan, 1991) and Bayes-Sard cubature (Karvonen et al., 2018) with quasi-uniform unisolvent point sets yield weighted $(n^{\frac{1}{2}}, o(n^{-\frac{1}{4}}))$-MMD coresets by Wendland (2004, Thm. 11.22 and Cor. 11.33). If $P$ has bounded support, and $k$ has more than $d$ continuous derivatives, then the $P$-greedy algorithm (De Marchi et al., 2005) also yields weighted $(n^{\frac{1}{2}}, o(n^{-\frac{1}{4}}))$-MMD coresets by Santin and Haasdonk (2017, Thm. 4.1). For $(k, P)$ pairs with compact support and sufficiently rapid eigenvalue decay, approximate continuous volume sampling kernel quadrature (Belhadji et al., 2020) using the Gibbs sampler of Rezaei and Gharan (2019) yields weighted coresets with $o(n^{-\frac{1}{4}})$ root mean squared MMD.

**Finite-dimensional kernels with compactly supported $P$** For compactly supported $P$, Briol et al. (2015, Thm. 1) and Bach et al. (2012, Prop. 1) showed that Frank-Wolfe Bayesian quadrature and weighted variants of kernel herding respectively yield weighted $(n^{\frac{1}{2}}, o(n^{-\frac{1}{4}}))$-MMD coresets for continuous finite-dimensional kernels, but, by Bach et al. (2012, Prop. 2), these analyses do not extend to infinite-dimensional kernels, like the Gaussian, Matérn, and B-spline kernels studied in this work.

**Eigenfunction restrictions** For $(k, P)$ pairs with known Mercer eigenfunctions, Belhadji et al. (2019) bound the expected squared MMD of determinantal point process (DPP) kernel quadrature in terms of kernel eigenvalue decay and provide explicit rates for univariate Gaussian $P$ and uniform $P$ on $[0,1]$. Their construction makes explicit use of the
kernel eigenfunctions which are not available for most \((k, P)\) pairings. For \((k, P)\) pairs with \(P k = 0\), uniformly bounded eigenfunctions, and rapidly decaying eigenvalues, Liu and Lee (2017) prove that black-box importance sampling generates an \(\left(n^{\frac{1}{2}}, o(n^{-\frac{1}{4}})\right)\)-MMD probability-weighted coreset but do not provide any examples verifying their assumptions. The uniformly bounded eigenfunction condition is considered particularly difficult to check (Steinwart and Scovel, 2012), does not hold for Gaussian kernels with Gaussian \(P\) (Minh, 2010, Thm. 1), and need not hold even for infinitely univariate smooth kernels on \([0, 1]\) (Zhou, 2002, Ex. 1).

**Unknown coreset quality** Khabara and Mahoney (2019, Thm. 2) prove that weighted kernel herding yields a weighted \(\left(n^{\frac{1}{2}}, \exp\left(-n^{\frac{1}{4}}/\kappa_n\right)\right)\)-MMD coreset. However, the \(\kappa_n\) term in Khabara and Mahoney (2019, Thm. 3, Assum. 2) is at least as large as the condition number of an \(\sqrt{n} \times \sqrt{n}\) kernel matrix, which for typical kernels (including the Gaussian and Matérn kernels) is \(\Omega(\sqrt{n})\) (Koltchinskii and Giné, 2000; El Karoui, 2010); the resulting MMD error bound therefore does not decay with \(n\). The ProtoGreedy and ProtoDash algorithms of Gurumoorthy et al. (2019, Thm. IV.3, IV.5) yield nonnegative weighted coresets \(\hat{S}\) of size \(n^{\frac{1}{2}}\) satisfying \(\text{MMD}_k^n(\mathbb{P}_n, \hat{S}) \leq \text{MMD}_k^n + (\mathbb{P}_n, \mathbb{P}_n) k - \text{MMD}_k^n e^{-\lambda \sqrt{n}}\) where \(\text{MMD}_*\) is the optimal MMD error to \(\mathbb{P}_n\) for a nonnegatively weighted coreset of size \(n^{\frac{1}{2}}\). However, careful inspection reveals that \(\lambda \sqrt{n} \leq 1\) for any kernel and any \(n\). Hence, in the usual case in which \(\mathbb{P}_n, \mathbb{P}_n k = \Omega(1)\), this error bound does not decay to 0 with \(n\). Campbell and Broderick (2019, Thm. 4.4) prove that Hilbert coresets via Frank-Wolfe with \(n\) input points yield weighted order \(\left(n^{\frac{1}{2}}, \nu_n^{\sqrt{n}}\right)\)-MMD coresets for some \(\nu_n < 1\) but do not analyze the dependence of \(\nu_n\) on \(n\).

**Non-MMD guarantees** For \(P\) with continuously differentiable Lebesgue density and \(k\) a bounded Langevin Stein kernel with \(P k = 0\), Thm. 2 of Oates et al. (2017) does not bound MMD but does prove that a randomized control functionals weighted coreset satisfies

\[
\sqrt{\mathbb{E}[\left|\mathbb{P} f - \sum_{i=1}^{\sqrt{n}} w_i f(x_i)\right|^2]} \leq C_{P,k,d,f}/n^{\frac{1}{3}}
\]

for each \(f\) in the RKHS of \(k\) and an unspecified \(C_{P,k,d,f}\). This bound is asymptotically better than the \(\Theta(n^{-\frac{1}{2}})\) guarantee for unweighted i.i.d. coresets but worse than the unweighted kernel thinning guarantees of Thm. 1. On compact domains, Thm. 1 of Oates et al. (2019) establishes improved rates for the same weighted coreset when both \(P\) and \(k\) are sufficiently smooth. Bardenet and Hardy (2020) establish an \(n^{-\frac{1}{2}} - \frac{1}{4}\) asymptotic decay of \(\mathbb{P} f - \sum_{i=1}^{\sqrt{n}} w_i f(x_i)\) for DPP kernel quadrature with \(P\) on \([-1, 1]^d\) and each \(f\) in the RKHS of a particular kernel.

2. Problem Setup

Given a target distribution \(P\) on \(\mathbb{R}^d\), a reproducing kernel \(k: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}\), and a sequence of \(\mathbb{R}^d\)-valued input points \(S_{in} = (x_i)_{i=1}^n\), our goal is to identify a thinned MMD coreset, a subsequence \(S_{out}\) of size \(n^{\frac{1}{2}}\) satisfying \(\text{MMD}_k^n(\mathbb{P}, S_{out}) = o(n^{-\frac{1}{4}})\).

2.1 Input sequence requirements

To achieve our goal, we will require the input sequence to have quality \(\text{MMD}_k^n(\mathbb{P}, S_{in}) = \mathcal{O}(n^{-\frac{1}{2}})\) and to be oblivious, that is, generated independently of any randomness in the
Proposition 1 (MMD guarantee for MCMC). By Meyn and Tweedie (2012, Thm. 15.0.1), if \((x_i)_{i=1}^n\) are the iterates of a homogeneous geometrically ergodic Markov chain with stationary distribution \(\mathbb{P}\), then, for some constant \(\rho \in (0,1)\) and function \(V \geq 1\),

\[
\sup_{h: \mathbb{R}^d \to [-1,1]} |\mathbb{E}[h(x_{i+1}) \mid x_1] - \mathbb{P}h| \leq V(x_1)\rho^i \quad \text{for all} \quad x_1 \in \mathbb{R}^d. \tag{2}
\]

If \(\mathbb{P}V < \infty\), then, with probability at least \(1 - \delta\), \(\text{MMD}_k(\mathbb{P}, S_n) \leq c \sqrt{n} \frac{\|k\|_{\infty} \log(1/\delta)}{\sqrt{2}}\), for \(c > 0\) depending only on the Markov transition probabilities.

2.2 Kernel requirements

We will use the terms reproducing kernel and kernel interchangeably to indicate that \(k\) is symmetric and positive definite, i.e., that the kernel matrix \((k(z_i,z_j))_{i,j=1}^l\) is symmetric and positive semidefinite for any evaluation points \((z_i)_{i=1}^l\) (Berlinet and Thomas-Agnan, 2011).

In addition to \(k\), our algorithm will take as input a square-root kernel for \(k\):

Definition 1 (Square-root kernel). We say a reproducing kernel \(k_{rt}: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}\) is a square-root kernel for \(k: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}\) if

\[
k(x,y) = \int_{\mathbb{R}^d} k_{rt}(x,z)k_{rt}(y,z)dz.
\tag{3}
\]

We highlight that a square-root kernel need not be unique and that its existence is an indication of a certain degree of smoothness in the target kernel \(k\). For example, the following result (proved in App. B) derives square-root kernels for sufficiently-smooth shift-invariant \(k\).

Proposition 2 (Shift-invariant square-root kernels). If \(k(x,y) = \kappa(x-y)\) is continuous and \(\kappa\) has generalized Fourier transform (Wendland, 2004, Def. 8.9) \(\hat{\kappa}\) with \(\int \sqrt{\hat{\kappa}(\omega)}d\omega < \infty\), then \(k_{rt}(x,y) = \frac{1}{(2\pi)^d/2} \kappa_{rt}(x-y)\) is a square-root kernel of \(k\) for \(\kappa_{rt}\) the Fourier transform of \(\sqrt{\kappa}\).

Tab. 1 gives several examples of common kernels satisfying the conditions of Prop. 2 along with their associated square-root kernels. For example, if \(k\) is Gaussian with bandwidth \(\sigma\), then a rescaled Gaussian kernel with bandwidth \(\sigma / \sqrt{2}\) is a valid choice for \(k_{rt}\).

Most of our results will assume that \(k_{rt}\) is bounded with finite Lipschitz constant

\[
L_{k_{rt}} \triangleq \sup_{x,y,z} \frac{|k_{rt}(x,y) - k_{rt}(x,z)|}{\|y-z\|_2},
\tag{4}
\]

although both assumptions can be relaxed at the expense of a more complex presentation. We will also make use of the kernel and distribution tail decay parameters

\[
\tau_{k_{rt}}(R) \triangleq (\sup_x \int_{\|y\|_2 \geq R} k_{rt}^2(x,x-y)dy)^{1/2} \quad \text{and} \quad \tau_{\mathbb{P}}(R) \triangleq \mathbb{P}(B^c(0,R)) \quad \text{for all} \quad R \geq 0. \tag{5}
\]
matrix (of kernel thinning is dominated by coresets, each of size \(n\)). This impact on Alg. 1, so the kernels need only be specified up to arbitrary rescalings. Notably, each halving decision is based on the square-root kernel \(k\). Our solution to the thinned coreset problem is 3. Kernel Thinning inverse multiquadric, sech, and Wendland’s compactly supported kernels \(k\). In Tab. 6 of App. L, we also derive convenient tailored square-root dominating kernels for any sufficiently-smooth shift-invariant and absolutely integrable kernel \(k\). For simplicity, our results will assume the use of an exact square-root kernel \(k\). In the positive-definite order (see Def. 2). For example, \(k\) in terms of inverse multiquadric, sech, and Wendland’s compactly supported kernels \(k\). In Tab. 6 of App. L, we also derive convenient tailored square-root dominating kernels for inverse multiquadric, sech, and Wendland’s compactly supported kernels \(k\).

### 3. Kernel Thinning

Our solution to the thinned coreset problem is kernel thinning, described in Alg. 1. Given a thinning parameter \(m \in \mathbb{N}\), kernel thinning proceeds in two steps: KT-SPLIT and KT-SWAP. In the KT-SPLIT step, the input sequence \(S_{in} = (x_i)_{i=1}^n\) is divided into \(2^m\) candidate coresets, each of size \(n/2^m\). This partitioning is carried out recursively, first dividing the input sequence in half, then halving those halves into quarters, and so on until coresets of size \(n/2^m\) are produced as in Fig. 1. The iterative halving is also conducted in an online fashion using non-uniform randomness to encourage balance across the halved coresets. Notably, each halving decision is based on the square-root kernel \(k_{rt}\) rather than the target kernel \(k\). We will explore and interpret the KT-SPLIT step in more detail in Sec. 4. The KT-SWAP step adds a baseline coreset to the candidate list (for example, one produced by standard thinning or uniform subsampling), selects the candidate closest to \(S_{in}\) in terms of MMD\(_k\), and refines the selected coreset by swapping each input point into the coreset if it offers an improvement in MMD\(_k\). When computable, the exact target MMD\(_k(P, S)\) can be substituted for the surrogate MMD\(_k(S_{in}, S)\) in this step. For any \(m\), the time complexity of kernel thinning is dominated by \(O(n^2)\) kernel evaluations, while the space complexity is \(O(n \min(d, n))\), achieved by storing the smaller of the input sequence \((x_i)_{i=1}^n\) and the kernel matrix \((k_{rt}(x_i, x_j))_{i,j=1}^n\). In addition, scaling either \(k\) or \(k_{rt}\) by a positive multiplier has no impact on Alg. 1, so the kernels need only be specified up to arbitrary rescalings.
Figure 1: Overview of kt-split. (Left) KT-SPLIT recursively partitions its input $S_{in}$ into $2^m$ balanced coresets $S^{(m,ℓ)}$ of size $\frac{n}{2^m}$. (Right) In Sec. 5, we interpret each coreset $S^{(m,ℓ)}$ as the output of repeated kernel halving: on each halving round, remaining points are paired, and one point from each pair is selected using non-uniform randomness.

Algorithm 1: Kernel Thinning – Return coreset of size $\lfloor n/2^m \rfloor$ with small MMD$_k$

Input: kernels $(k, k_{rt})$, point sequence $S_{in} = (x_i)_{i=1}^n$, thinning parameter $m \in \mathbb{N}$, probabilities $(\delta_i)_{i=1}^2$

$(S^{(m,ℓ)})_{ℓ=1}^{2^n} \leftarrow$ KT-SPLIT $(k_{rt}, S_{in}, m, (\delta_i)_{i=1}^2)$ // Split $S_{in}$ into $2^m$ candidate coresets of size $\lfloor \frac{n}{2^m} \rfloor$

$S_{KT} \leftarrow$ KT-SWAP $(k, S_{in}, (S^{(m,ℓ)})_{ℓ=1}^{2^n})$ // Select best coreset and iteratively refine

return coreset $S_{KT}$ of size $\lfloor n/2^m \rfloor$

3.1 MMD guarantee for kernel thinning

Our first main result, proved in App. C, bounds the MMD of the returned kernel thinning coreset in terms of $k_{rt}$ tail decay (5), the $k_{rt}$ and $S_{in}$ radii

$$\mathcal{M}_{k_{rt}}(n, m, d, δ', R) \triangleq 37 \sqrt{\log(\frac{6m}{2^m})} \left[ \sqrt{\log\left(\frac{d}{\sqrt{m}}\right)} + 5 \sqrt{d \log\left(2 + 2 \frac{L_{k_{rt}}}{\|k_{rt}\|_\infty} (\mathcal{R}_{k_{rt}, n} + R)\right)} \right].$$

Theorem 1 (MMD guarantee for kernel thinning). Consider kernel thinning (Alg. 1) with $k_{rt}$ a square-root kernel of $k$, oblivious input sequences $S_{in}$ and probabilities $(\delta_i)_{i=1}^{[n/2]}$ with $δ^* \triangleq \min_i δ_i$. If $\frac{n}{2^m} \in \mathbb{N}$, then for any fixed $δ' \in (0, 1)$, Alg. 1 returns a coreset $S_{KT}$ of size $\lfloor n/2^m \rfloor$ satisfying

$$\text{MMD}_k(S_{in}, S_{KT}) \leq \frac{2^m}{m} \|k_{rt}\|_\infty \left[ 2 + \sqrt{\frac{(4\pi)^{d/2}}{Γ(\frac{d+1}{2})}} \cdot \mathcal{R}_{\max}^d \cdot \mathcal{M}_{k_{rt}}(n, m, d, δ^*, δ', R_{S_{in}, k_{rt}, n}) \right],$$

with probability at least $1 - δ' - \sum_{j=1}^m \frac{2^{j-1}}{m} \sum_{i=1}^{n/2j} δ_i$, where $\mathcal{R}_{\max} \triangleq \max(\mathcal{R}_{S_{in}, k_{rt}, n/2^m})$. 

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Algorithm 1a: KT-SPLIT – Divide points into candidate coresets of size \([n/2^m]\]

**Input:** kernel \(k_\text{rt}\), point sequence \(S_m = (x_i)_{i=1}^n\), thinning parameter \(m \in \mathbb{N}\), probabilities \((\delta_i)_{i=1}^{[n/2]}\)

\(S^{(j,\ell)} = \{\}\) for \(0 < j \leq m\) and \(1 \leq \ell < 2^j\) // Empty coresets: \(S^{(j,\ell)}\) has size \([\frac{n}{2^j-1}]\) after \(i\) rounds

\(\sigma_j, \ell \leftarrow 0\) for \(0 < j \leq m\) and \(1 \leq \ell \leq 2^j\) // Swapping parameters

for \(i = 1, \ldots, [n/2]\) do

\(S^{(0,1)}\).append\((x_{2i-1})\); \(S^{(0,1)}\).append\((x_{2i})\)

// Every \(2^{j-1}\) rounds add point from parent coreset \(S^{(j-1,\ell)}\) to each child \(S^{(j,2\ell-1)}, S^{(j,2\ell)}\)

for \((j = 1; j \leq m \text{ and } i/2^j - 1 \in \mathbb{N}; j = j + 1)\) do

for \(\ell = 1, \ldots, 2^{j-1}\) do

\((S, S') \leftarrow (S^{(j-1,\ell)}, S^{(j,2\ell-1)}); \ (x, x') \leftarrow \text{get_last_two_points}(S)\)

// Compute swapping threshold \(a\)

\(a, \sigma_j, \ell \leftarrow \text{get_swap_params}(\sigma_j, \ell, b, \delta_{[S/2 \cdot 2^{\ell-1}]})\) for \(b^2 = k_\text{rt}(x, x) + k_\text{rt}(x', x') - 2k_\text{rt}(x, x')\)

// Assign one point to each child after probabilistic swapping

\(\alpha \leftarrow k_\text{rt}(x', x') - k_\text{rt}(x, x) + \sum_{y \in S}(k_\text{rt}(y, y') - k_\text{rt}(y, y')) - 2\sum_{z \in S'}(k_\text{rt}(z, z') - k_\text{rt}(z, x'))\)

\((x, x') \leftarrow (x', x)\) with probability \(\min(1, \frac{1}{2}(1 - \frac{\alpha}{a}))\)

\(S^{(j,2\ell-1)}\).append\((x)\); \(S^{(j,2\ell)}\).append\((x')\)

end

end

return \((S^{(m,1)}{^2}_m)_{i=1}^m\), candidate coresets of size \([n/2^m]\)

---

**Remark 1** (Guarantee for any \(\mathbb{P}\)). A guarantee for any target distribution \(\mathbb{P}\) follows directly from the triangle inequality, \(\text{MMD}_k(\mathbb{P}, S_{\text{KT}}) \leq \text{MMD}_k(\mathbb{P}, S_m) + \text{MMD}_k(S_m, S_{\text{KT}})\).

**Remark 2** (Comparison with baseline thinning). The \(\text{KT-swap}\) step ensures that, deterministically, \(\text{MMD}_k(S_m, S_{\text{KT}}) \leq \text{MMD}_k(S_m, S_{\text{base}})\) for \(S_{\text{base}}\) a baseline thinned coreset of size \(\frac{n}{2^m}\). Therefore, we additionally have \(\text{MMD}_k(\mathbb{P}, S_{\text{KT}}) \leq 2\text{MMD}_k(\mathbb{P}, S_m) + \text{MMD}_k(S_m, S_{\text{base}})\).

**Remark 3** (Finite-time and anytime guarantees). To obtain a success probability of at least \(1 - \delta\) with \(\delta' = \frac{\delta}{2}\), it suffices to choose \(\delta_i = \frac{\delta}{n}\) when the stopping time \(n\) is known in advance, and \(\delta_i = \frac{m \log^2(\delta(1+\frac{1}{d}))}{m + 2n(d+1) \log^2(\delta(1+1))}\) when terminating the algorithm at an arbitrary oblivious stopping time \(n\). See App. D for the proof.

The implications of Thm. 1 depend on the radii \((R_S, R_{K_m}, R_{K_m}^{1/2}/K_m,n/2^m)\) which in turn depend on the tail decay of \(\mathbb{P}\) and \(k_\text{rt}\). Consider running Alg. 1 with thinning parameter \(m = \frac{1}{2} \log_2(n)\), probabilities \((\delta', \delta) = (\frac{\delta}{2}, \frac{\delta}{2})\), and an order \((n, n^{-\frac{1}{2}})-\text{MMD}\) input sequence \(S_m\). If \(\mathbb{P}\) and \(k_\text{rt}\) are compactly supported, then the radii are \(O_d(1)\) and kernel thinning returns a \((n^{\frac{1}{2}}, O_d(n^{-\frac{1}{2}} \sqrt{\log n}))-\text{MMD}\) coreset with probability at least \(1 - \delta\). For fixed \(d\), this guarantee significantly improves upon the baseline \(\Theta(n^{-\frac{1}{2}})\) rates of i.i.d. sampling and
standard MCMC thinning and matches the lower bounds of Sec. 1.1 up to a $\sqrt{\log n}$ term and constants depending on $d$. Hence, in this setting, kernel thinning provides a nearly minimax optimal coreset of size $n^{\frac{d}{2}}$ (Phillips and Tai, 2020, Thm. 3.1). Moreover, when $S_{in}$ is drawn i.i.d. from $\mathbb{P}$, kernel thinning is nearly minimax optimal amongst all distributional approximations (even weighted coresets) that depend on $\mathbb{P}$ only through $n$ i.i.d. input points (Tolstikhin et al., 2017, Thms. 1 and 6).

More generally, when $\mathbb{P}$ and $k_{rt}^2$ have sub-Gaussian tails, sub-exponential tails, or simply $\rho > 2d$ moments, we expect the radii to exhibit $O_d(\sqrt{\log n})$, $O_d(\log n)$, and $O_d(n^{\frac{d}{2}})$ growth rates respectively. Under these respective settings, Thm. 1 provides a guarantee of $O_d(n^{-\frac{1}{2}}\sqrt{(\log n)^{d/2+1}\log\log n})$, $O_d(n^{-\frac{1}{2}}\sqrt{(\log n)^{d+1}\log\log n})$, and $O_d(n^{-\frac{1}{2}}n^{\frac{d}{2}}\log n)$ MMD with high probability for kernel thinning coresets of size $\sqrt{n}$ (see Tab. 2). In each case, we find that kernel thinning significantly improves upon an $\Omega(n^{-\frac{d}{2}})$ baseline when $n$ is sufficiently large relative to $d$ and, by Rem. 2, is never significantly worse than the baseline when $n$ is small. Thm. 1 also allows us to derive more precise, explicit error bounds for specific kernels. For example, for the popular Gaussian, Matérn, and B-spline kernels, Tab. 3 provides explicit bounds on each kernel-dependent quantity in Thm. 1: $\|k_{rt}\|_{\infty}$, the kernel radii $(\rho_{k_{rt},n},\rho_{k_{rt},\sqrt{n}})$, and the inflation factor $M_{k_{rt}}$.

### 3.2 MMD coresets from $L^\infty$ coresets

Our proof of Thm. 1 relies on the following key result, proved in App. E, demonstrating that any $L^\infty$ coreset for the square-root kernel $k_{rt}$ is also an MMD coreset for the target $k$ with quality that depends on the tail decay of $k_{rt}$ and $\mathbb{P}$.

**Theorem 2** ($L^\infty$ coresets for $(k_{rt},\mathbb{P})$ are MMD coresets for $(k,\mathbb{P})$). If $k_{rt}$ is a square-root kernel for $k$, then for any distributions $\mathbb{P}$ and $\mathbb{Q}$ and scalars $R, a, b \geq 0$ with $a + b = 1$,

$$\text{MMD}_k(\mathbb{P}, \mathbb{Q}) \leq v_d R^d \cdot \|P k_{rt} - Q k_{rt}\|_{\infty} + 2\tau_{k_{rt}}(aR) + 2\|k\|_{\infty} \cdot \max\{\tau_{\mathbb{P}}(bR), \tau_{\mathbb{Q}}(bR)\}, \quad (10)$$

where $v_d \triangleq (\pi^{d/2}/\Gamma(d/2 + 1))^{\frac{1}{2}}$ decreases super-exponentially in $d$.

In Secs. 4 and 5, we show that, with high probability, KT-SPLIT provides a high-quality $L^\infty$ coreset for $k_{rt}$ and hence, by Thm. 2, also provides a high-quality MMD coreset for $k$.

---

5. $\mathcal{R}_{S_{in}}$ exhibits these growth rates in expectation and with high probability if $S_{in}$ is drawn i.i.d. from $\mathbb{P}$ (see App. I).
kernel thinning in Sec. 5. We dedicate this section to constructing high-quality thinned coresets. For example, when \(\mathbb{P}, \mathbb{Q}\), and \(k_{rt}\) have light tails. For example, when \(\mathbb{P}, \mathbb{Q}\), and \(k_{rt}\) are compactly supported so that the tail integrals \(\tau_\mathbb{P}(R), \tau_{\mathbb{Q}}(R)\), and \(\tau_{k_{rt}}(R)\) vanish for \(R\) sufficiently large, Thm. 2 yields the strong guarantee

\[
\text{MMD}_k(\mathbb{P}, \mathbb{Q}) = O_\mathcal{d}(\|\mathbb{P}k_{rt} - \mathbb{Q}k_{rt}\|_\infty).
\]

4. Self-balancing Hilbert Walk

To exploit the \(L^\infty\)-MMD connection revealed in Thm. 2, we now turn our attention to constructing high-quality thinned \(L^\infty\) coresets. Our strategy relies on a new Hilbert space generalization of the self-balancing walk of Alweiss et al. (2021). We dedicate this section to defining and analyzing this self-balancing Hilbert walk, and we detail its connection to kernel thinning in Sec. 5.

| \(\mathbb{R}_{\text{S}_{\text{in}}} \sim_d \) | \(\mathbb{R}_{\text{k}_{rt}} \sim_d 1\) | \(\text{Compact } \mathbb{P}\) | \(\text{SubGauss } \mathbb{P}\) | \(\text{SubExp } \mathbb{P}\) | \(\text{HeavyTail } \mathbb{P}\) |
|---|---|---|---|---|---|
| \(\sqrt{\log n}\) | \(\log n\) | \(\log n\) | \(\log n\) | \(\log n\) | \(\log n\) |

Table 2: Kernel thinning MMD guarantee under \(\mathbb{P}\) and \(k_{rt}\) tail decay. For \(n\) input points and \(\sqrt{n}\) thinned points, we report the MMD\(_k(\mathbb{S}_{\text{in}}, S_{\text{KT}})\) bound of Thm. 1 up to constants depending on \(d, \delta, \delta', \|k_{rt}\|_\infty\), and \(L_{k_{rt}}/\|k_{rt}\|_\infty\). Here, \(\mathbb{R}_{k_{rt}} \triangleq \max(\mathbb{R}_{k_{rt}, n}, \mathbb{R}_{k_{rt}, v/R})\) and the radii \(\mathbb{R}_{\text{S}_{\text{in}}}, \mathbb{R}_{k_{rt}, n}, \mathbb{R}_{k_{rt}, v/R}\) are defined in (6) and (7). See App. I for our derivation.

| Square-root kernel \(k_{rt}\) | \(\|k_{rt}\|_\infty\) | \(\mathbb{R}_{k_{rt}, n}, \mathbb{R}_{k_{rt}, v/R}\) bound of Thm. 1 up to constants | \(\mathbb{R}_{k_{rt}} (n, \frac{1}{2} \log_2 n, d, \frac{\delta}{\delta'}, R)\) |
|---|---|---|---|
| \(\left(\frac{2}{\pi^2}\right)^\frac{1}{2}\text{Gaussian} \left(\frac{2}{\pi^2}\right)\) | \(\left(\sigma \sqrt{\log n}, \sigma \sqrt{d + \log n}\right)\) | \(\sqrt{\log \left(\frac{n}{d}\right) + d \log \left(\sqrt{\log n} + \frac{d}{2}\right)}\) | \(\mathbb{R}_{k_{rt}} (n, \frac{1}{2} \log_2 n, d, \frac{\delta}{\delta'}, R)\) |
| \(A_{\nu, \gamma,d}\text{Matérn} \left(\frac{\gamma^2}{\pi(a-1)}\right)\) | \(\left(\gamma^{-1}(\log n + a \log(1 + a)), \gamma^{-1}(a + \log n + E)\right)\) | \(\sqrt{\log \left(\frac{n}{d}\right) + d \log \left(\log n + B + \gamma R\right)}\) | \(\mathbb{R}_{k_{rt}} (n, \frac{1}{2} \log_2 n, d, \frac{\delta}{\delta'}, R)\) |
| \(\tilde{S}_{\beta,d}\text{B-spline} \left(\beta\right)\) | \(c_\beta\) | \(\sqrt{\log \left(\frac{n}{d}\right) + d \log \left(\beta + \sqrt{d R}\right)}\) | \(\mathbb{R}_{k_{rt}} (n, \frac{1}{2} \log_2 n, d, \frac{\delta}{\delta'}, R)\) |

Table 3: Explicit bounds on Thm. 1 quantities for common kernels. Here, \(A_{\nu, \gamma,d}\), and \(\tilde{S}_{\beta,d}\) are as in Tab. 1. \(a = 1 - \frac{\nu - d}{2}(\nu - d) > 1)\), \(B = a \log(1 + a)\), \(E = d \log \left(\frac{\nu \pi}{\gamma}\right) + \log \left(\frac{(\nu - 2)^{\frac{\nu - 2}{2}}}{(2(\nu - 1))^\frac{\nu - 1}{2} - 1}\right)\), \(c_1 = \frac{\beta}{\sqrt{3}}\), and \(c_\beta < 1\) for \(\beta > 1\) (see (106)). See App. J for our derivation.

As indicated in Thm. 2, the coreset quality is especially well preserved when \(\mathbb{P}, \mathbb{Q}\), and \(k_{rt}\) have light tails. For example, when \(\mathbb{P}, \mathbb{Q}\), and \(k_{rt}\) are compactly supported so that the tail integrals \(\tau_{\mathbb{P}}(R), \tau_{\mathbb{Q}}(R)\), and \(\tau_{k_{rt}}(R)\) vanish for \(R\) sufficiently large, Thm. 2 yields the strong guarantee

\[
\text{MMD}_k(\mathbb{P}, \mathbb{Q}) = O_\mathcal{d}(\|\mathbb{P}k_{rt} - \mathbb{Q}k_{rt}\|_\infty).
\]
Alweiss et al. (2021, Thm. 1.2) introduced a randomized algorithm called the self-balancing walk that takes as input a streaming sequence of oblivious Euclidean vectors $x_i \in \mathbb{R}^d$ with $\|x_i\|_2 \leq 1$ and outputs a online sequence of random assignments $\eta_i \in \{-1, 1\}$ satisfying

$$\|\sum_{i=1}^n \eta_i x_i\|_\infty \lesssim \sqrt{\log(d/\delta) \log(n/\delta)}$$

with probability at least $1 - \delta$. (11)

Since our ultimate aim is to combine kernel functions, we define a suitable Hilbert space generalization in Alg. 2.

### Algorithm 2: Self-balancing Hilbert Walk

**Input:** sequence of functions $(f_i)_{i=1}^n$ in Hilbert space $\mathcal{H}$, threshold sequence $(a_i)_{i=1}^n$

$$\psi_0 \leftarrow 0 \in \mathcal{H}$$

for $i = 1, 2, \ldots, n$ do

- $\alpha_i \leftarrow \langle \psi_{i-1}, f_i \rangle_{\mathcal{H}}$ \ // Compute Hilbert space inner product
  - if $|\alpha_i| > a_i$:
    - $\psi_i \leftarrow \psi_{i-1} - f_i \cdot \alpha_i / a_i$
  - else:
    - $\eta_i \leftarrow 1$ with probability $\frac{1}{2}(1 - \alpha_i / a_i)$ and $\eta_i \leftarrow -1$ otherwise
    - $\psi_i \leftarrow \psi_{i-1} + \eta_i f_i$

end

**return** $\psi_n$, combination of signed input functions

Given a streaming sequence of functions $f_i$ in an arbitrary Hilbert space $\mathcal{H}$ with a norm $\|\cdot\|_{\mathcal{H}}$, this self-balancing Hilbert walk outputs a streaming sequence of signed function combinations $\psi_i$ satisfying the following desirable properties established in App. F.

### Theorem 3 (Self-balancing Hilbert walk properties).

Consider the self-balancing Hilbert walk (Alg. 2) with $\mathcal{F}_i \triangleq (f_1, a_1, f_2, a_2, \ldots, f_i, a_i)$ and sub-Gaussian constants

$$\sigma_0^2 \triangleq 0 \quad \text{and} \quad \sigma_i^2 \triangleq \sigma_{i-1}^2 + \|f_i\|_{\mathcal{H}}^2 \left(1 + \frac{\sigma_{i-1}^2}{\sigma_i^2}(\|f_i\|_{\mathcal{H}}^2 - 2a_i)\right) + \forall i \geq 1. \quad (12)$$

If $\mathcal{F}_n$ is oblivious, then the following properties hold:

(i) **Functional sub-Gaussianity:** For each $i \in [n]$, $\psi_i$ is $\sigma_i$ sub-Gaussian conditional on $\mathcal{F}_i$:

$$\mathbb{E}[\exp(\langle \psi_i, u \rangle_{\mathcal{H}}) \mid \mathcal{F}_i] \leq \exp\left(\frac{\sigma_i^2\|u\|_{\mathcal{H}}^2}{2}\right) \quad \text{for all} \quad u \in \mathcal{H}. \quad (13)$$

(ii) **Signed sum representation:** If $a_i \geq \sigma_{i-1}\|f_i\|_{\mathcal{H}}^2 \sqrt{2\log(2/\delta_i)}$ for $\delta_i \in (0, 1]$, then, with probability at least $1 - \sum_{i=1}^n \delta_i$ given $\mathcal{F}_n$,

$$|\alpha_i| \leq a_i, \forall i \in [n], \quad \text{and} \quad \psi_n = \sum_{i=1}^n \eta_i f_i. \quad (14)$$

(iii) **Exact two-thinning via symmetrization:** If $a_i \geq \sigma_{i-1}\|f_i\|_{\mathcal{H}}^2 \sqrt{2\log(2/\delta_i)}$ for $\delta_i \in (0, 1]$ and each $f_i = g_{2i-1} - g_{2i}$ for $g_1, \ldots, g_{2n} \in \mathcal{H}$, then, with prob. at least $1 - \sum_{i=1}^n \delta_i$ given $\mathcal{F}_n$,

$$|\alpha_i| \leq a_i, \forall i \in [n], \quad \text{and} \quad \frac{1}{2n}\psi_n = \frac{1}{2n}\sum_{i=1}^{2n} g_i - \frac{1}{n}\sum_{i \in I} g_i \quad \text{for} \quad I = \{2i - \frac{n-1}{2} : i \in [n]\}.
(iv) **Pointwise sub-Gaussianity in RKHS:** If \( \mathcal{H} \) is the RKHS of a kernel \( k : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \), then, for each \( i \in [n] \) and \( x \in \mathcal{X} \), \( \psi_i(x) \) is \( \sigma_i \sqrt{k(x,x)} \) sub-Gaussian conditional on \( \mathcal{F}_i \):

\[
\mathbb{E}[\exp(\psi_i(x)) \mid \mathcal{F}_i] \leq \exp\left(\frac{\sigma_i^2 k(x,x)}{2}\right).
\]

(v) **Sub-Gaussian constant bound:** Fix any \( q \in [0,1) \), and suppose \( \frac{1}{2} \| f_i \|_{\mathcal{H}}^2 \leq a_i \) for all \( i \in [n] \). If \( \frac{\| f_i \|_{\mathcal{H}}^2}{1+q} \leq a_i \leq \frac{\| f_i \|_{\mathcal{H}}^2}{1-q} \) whenever both \( \sigma_{i-1}^2 < \frac{\sigma_i^2}{2a_i-\| f_i \|_{\mathcal{H}}} \) and \( \| f_i \|_{\mathcal{H}} > 0 \), then

\[
\sigma_i^2 \leq \frac{\max_{i \in [n]} \| f_i \|_{\mathcal{H}}^2}{1-q^2} \quad \text{for all} \quad i \in [n].
\]

(vi) **Adaptive thresholding:** If \( a_i = \max(c_i \sigma_{i-1} \| f_i \|_{\mathcal{H}}, \| f_i \|_{\mathcal{H}}^2) \) for \( c_i \geq 0 \), then

\[
\sigma_n^2 \leq \frac{\max_{i \in [n]} \| f_i \|_{\mathcal{H}}^2}{4} (c^* + 1/c^*)^2 \quad \text{for} \quad c^* \triangleq \max_{i \in [n]} c_i.
\]

**Remark 4.** The kernel \( k \) in Property (iv) can be arbitrary and need not be bounded.

Property (i), ensures that the functions \( \psi_i \) produced by Alg. 2 are mean zero and unlikely to be large in any particular direction \( u \). Property (ii), builds on this functional sub-Gaussianity to ensure that \( \psi_i \) is precisely a sum of the signed input functions \( \pm f_i \) with high probability. The two properties together imply that, with high probability and an appropriate setting of \( a_i \), Alg. 2 partitions the input functions \( f_i \) into two groups such that the function sums are nearly balanced across the two groups. Property (iii), uses the signed sum representation to construct a two-thinned coreset for any input function sequence \((g_i)_{i=1}^{2n}\). This is achieved by offering the consecutive function differences \( g_{2i-1} - g_{2i} \) as the inputs \( f_i \) to Alg. 2. Property (iv) highlights that functional sub-Gaussianity also implies sub-Gaussianity of the function values \( \psi_i(x) \) whenever the Hilbert space \( \mathcal{H} \) is an RKHS. Finally, Properties (v) and (vi) provide explicit bounds on the sub-Gaussian constants \( \sigma_i \) when adaptive settings of the thresholds \( a_i \) are employed. In Sec. 5, we will use Properties (iii), (iv), and (vi) together to provably construct thinned coresets with small \( L^\infty \) kernel error.

**Comparison with the self-balancing walk of Alweiss et al. (2021)** In the Euclidean setting with \( \mathcal{H} = \mathbb{R}^d \), constant thresholds \( a_i = 30 \log(n/\delta) \), and \( \langle \psi_i-1, f_i \rangle_{\mathcal{H}} \) the usual Euclidean dot product, Alg. 2 recovers a slight variant of the Euclidean self-balancing walk of Alweiss et al. (2021, Proof of Thm. 1.2). The original algorithm differs only superficially by terminating with failure whenever \( |\alpha_i| > a_i \). We allow the walk to continue with the update \( \psi_i \leftarrow \psi_{i-1} - f_i \cdot \alpha_i/a_i \), as it streamlines our sub-Gaussianity analysis and avoids the reliance on distributional symmetry present in Sec. 2.1 of Alweiss et al. (2021). We show in App. M that Thm. 3 recovers the guarantee (11) of Alweiss et al. (2021, Thm. 1.2) with improved constants and a less conservative setting of \( a_i \).

5. From Kernel Halving to Kernel Thinning

To provide a stepping stone between the self-balancing Hilbert walk of Alg. 2 and kernel thinning in Alg. 1, we next introduce kernel halving (Alg. 3).
5.1 Kernel halving

Kernel halving (Alg. 3) is an instance of the self-balancing Hilbert walk in which each input function \( f_i \) is a difference of kernel functions, \( k(x_{2i-1}, \cdot) - k(x_{2i}, \cdot) \), evaluated at a pair of candidate points \((x_{2i-1}, x_{2i})\). Like KT-SPLIT with \( m = 1 \), Alg. 3 partitions the input points into two equal-sized coresets \( S^{(1)} \) and \( S^{(2)} \). (Note that the subroutine `get_swap_params` was defined in KT-SPLIT Alg. 1a.) To highlight the correspondence with Alg. 2, our presentation of Alg. 3 also redundantly maintains the signed function combinations \( \psi_i \). At each iteration, kernel halving either triggers a failure condition (when \( |\alpha_i| \) exceeds the threshold \( a \)) or adds one of two candidate points to each coreset in a probabilistic manner. Notably, if the failure condition is not triggered, the inner product \( \langle \psi_i, f_i \rangle \) has a simple explicit form in terms of kernel evaluations due to our choice of \( f_i \). Our next result shows that with high probability the failure condition is never triggered, and kernel halving returns valid coresets of size \( \lfloor n/2 \rfloor \) with high probability. The proof (in App. G) builds on the sub-Gaussianity of self-balancing Hilbert walk iterates.

**Algorithm 3: Kernel Halving**

**Input:** kernel \( k \), point sequence \( S_m = (x_i)_{i=1}^n \), probability sequence \( (\delta_i)_{i=1}^{\lfloor n/2 \rfloor} \)

\( S^{(1)}, S^{(2)} \leftarrow \{\}; \quad \psi_0 \leftarrow \emptyset \in H \quad \text{// Initialize empty coresets: } S^{(1)}, S^{(2)} \text{ have size } i \text{ after round } i \)

\( \sigma \leftarrow 0 \quad \text{// Swapping parameter} \)

**for** \( i = 1, 2, \ldots, \lfloor n/2 \rfloor \) **do**

\( (x, x') \leftarrow (x_{2i-1}, x_{2i}); \quad f_i \leftarrow k(x_{2i-1}, \cdot) - k(x_{2i}, \cdot); \quad \eta_i \leftarrow -1 \quad \text{// Construct kernel difference function using next two points} \)

\( a, \sigma \leftarrow \text{get_swap_params}(\sigma, b, 2\delta_i) \text{ with } b^2 = ||f_i||_k^2 = k(x, x) + k(x', x') - 2k(x, x') \quad \text{// Compute swapping threshold } a \)

**if** \( S^{(1)}.\text{contains}(\text{Failure}) \):

\( \alpha_i = \langle \psi_{i-1}, f_i \rangle_k \quad \text{// Inner product } \langle \psi_{i-1}, f_i \rangle_k \text{ has a simple form} \)

\( \alpha_i \leftarrow \sum_{j=1}^{2^{i-1}} (k(x_j, x) - k(x_j, x')) - 2 \sum_{z \in S^{(2)}} (k(z, x) - k(z, x')) \quad \text{// Compute RKHS inner product} \)

**if** \( |\alpha_i| > a \):

**Threshold exceeded: will ultimately return failure**

\( S^{(1)}.\text{append}(\text{Failure}); \quad S^{(2)}.\text{append}(\text{Failure}); \quad \psi_i \leftarrow \psi_{i-1} - f_i \cdot \alpha_i/a \quad \text{// Assign one point to each child after probabilistic swapping} \)

**else:**

\( (x, x') \leftarrow (x', x) \text{ and } \eta_i \leftarrow 1 \quad \text{with probability } \frac{1}{2}(1 - \alpha_i/a_i) \quad \text{// Threshold exceeded: will ultimately return failure} \)

\( S^{(1)}.\text{append}(x); \quad S^{(2)}.\text{append}(x'); \quad \psi_i \leftarrow \psi_{i-1} + \eta_i f_i \quad \text{// Assign one point to each child after probabilistic swapping} \)

**end**

**if** \( S^{(1)}.\text{contains}(\text{Failure}) \):

**return** Failure

**else:**

**return** \( S^{(1)}, \text{coreset of size } \lfloor n/2 \rfloor \)

---

**Theorem 4** (\( L^\infty \) guarantees for kernel halving). Let \( S_{KH}(k, S, \Delta) \) denote the output returned by kernel halving (Alg. 3) with kernel \( k \), input point sequence \( S \), and probability sequence \( \Delta \). For oblivious \( S_m = (x_i)_{i=1}^n \) and \( (\delta_i)_{i=1}^{\lfloor n/2 \rfloor} \) with \( \delta^* \triangleq \min_i \delta_i \) and any \( \delta' \in (0, 1) \),
let $\mathbb{P}_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i}$, and recall the definitions (7) and (8) of $\mathcal{M}_k$ and $\mathcal{R}_{\text{in},k,n}$ (obtained by replacing $k_{rt}$ with $k$).

(a) **Kernel halving yields a 2-thinned $L^\infty$ coreset:** If $\frac{n}{2} \in \mathbb{N}$, then $S^{(1)} = S_{KH}(k, S_{\text{in}}, (\delta_i)_{i=1}^{n/2})$ is a valid coreset of size $\frac{n}{2}$ with $Q^{(1)}_{KH} = \frac{1}{n/2} \sum_{x \in S^{(1)}} \delta_x$ satisfying

$$\|P_1 k - Q^{(1)}_{KH} k\|_\infty \leq \|k\|_\infty \cdot \frac{2}{n} \mathcal{M}_k(n, 1, d, \delta^*, \delta', \mathcal{R}_{\text{in},k,n})$$

with probability at least $1 - \delta' - \sum_{i=1}^{n/2} \delta_i$.

(b) **Repeated kernel halving yields a $2^m$-thinned $L^\infty$ coreset:** For each $j > 1$, let $S^{(j)} = S_{KH}(k, S^{(j-1)}, (\frac{2^{j-1} \delta_i}{m})_{i=1}^{n/2m})$ be the output of kernel halving recursively applied for $m$ rounds. If $\frac{n}{2^m} \in \mathbb{N}$, then $S^{(m)}$ is valid coreset of size $\frac{n}{2^m}$ with $Q^{(m)}_{KH} = \frac{1}{2^m} \sum_{x \in S^{(m)}} \delta_x$ satisfying

$$\|P_1 k - Q^{(m)}_{KH} k\|_\infty \leq \|k\|_\infty \cdot \frac{2^m}{n} \mathcal{M}_k(n, m, \delta^*, \delta', \mathcal{R}_{\text{in},k,n})$$

with probability at least $1 - \delta' - \sum_{j=1}^{m} \frac{2^{j-1}}{m} \sum_{i=1}^{n/2^j} \delta_i$.

**Remark 5** (Near-optimal $L^\infty$ coresets). Suppose $L_k/\|k\|_\infty = O(1)$. By part (b) of Thm. 4 and the definition (8) of $\mathcal{M}_k$, with high probability repeated kernel halving delivers order $(n^{1/2}, \sqrt{\log n})$-$L^\infty$ coresets for compactly supported $\mathbb{P}_n$ and $k$ with $\log(\mathcal{R}_{\text{in},k,n}) = O(1)$ and order $(n^{1/2}, \sqrt{\log n})$-$L^\infty$ coresets for any $\mathbb{P}_n$ and any subpolynomial decay kernel $k$ (i.e., $\log(\mathcal{R}_{\text{in},k,n}) = O(1)$). For any bounded, radial $k$ satisfying mild decay and smoothness conditions, Phillips and Tai (2020, Thm. 3.1) proved that any procedure outputting a coreset of size $n^{1/2}$ must suffer $\Omega(\min(\sqrt{dn^{-1/2}}, n^{-1}))$ $L^\infty$ error for some $\mathbb{P}_n$. Hence, the kernel halving quality guarantees are within a $\log n$ factor of optimal for this kernel family which includes Gaussian and Matérn kernels.

**Remark 6** (Online vector balancing in an RKHS). In the online vector balancing problem of Spencer (1977) one must assign signs $\eta_i$ to Euclidean vectors $f_i$ in an online fashion while keeping the norm of the signed sum $\|\sum_{i=1}^{n} \eta_i f_i\|_\infty$ as small as possible. By part (a) of Thm. 4, kernel halving solves an RKHS generalization of the online vector balancing problem by guaranteeing $\|\sum_{i=1}^{n} \eta_i f_i\|_\infty = O(\sqrt{d} \log n)$ with high probability for all subpolynomial decay kernels with $L_k/\|k\|_\infty = O(1)$. Notably, these conditions are satisfied by common kernels like Gaussian, Matérn and B-spline.

### 5.2 KT-SPLIT is repeated kernel halving

We now connect kernel halving and kernel thinning by observing that, with high probability, the KT-SPLIT step of kernel thinning is identical to repeated kernel halving with the square-root kernel $k_{rt}$. Consider running Alg. 3 and KT-SPLIT with the kernel $k_{rt}$. When the thinning parameter $m = 1$, a careful comparison reveals that the two algorithms are identical whenever $|\alpha_i| \leq a_i$ for all iterations $i$, that is, whenever kernel halving returns a valid coreset instead of returning Failure. Hence, part (a) of Thm. 4 applies equally to the coreset $S^{(1,1)}$ returned by KT-SPLIT with $m = 1$. Similarly, when $m > 1$, the coreset $S^{(m,1)}$ produced
by KT-SPLIT is identical to the output of repeated kernel halving whenever each of the $m$ halving rounds returns a valid coreset instead of Failure. Hence, part (b) of Thm. 4 applies equally to the coreset $S^{(m,1)}$ returned by KT-SPLIT, establishing the following corollary.

**Corollary 1 (KT-SPLIT yields a $2^m$-thinned $L^\infty$ coreset).** Consider KT-SPLIT with oblivious input sequences $S_{in}$ and $(\delta_i)^{[n/2]}$, $\delta^* \triangleq \min_i \delta_i$, and $P_n = \frac{1}{n} \sum_{i=1}^n \delta_i$. If $\frac{n}{2^m} \in \mathbb{N}$, then for any fixed $\delta' \in (0,1)$, KT-SPLIT returns a coreset $S^{(m,1)}$ with $Q^{(m,1)}_K \triangleq \frac{1}{\lfloor n/2^m \rfloor} \sum_{x \in S^{(m,1)}} \delta_x$ satisfying

$$
\|P_n k_{rt} - Q^{(m,1)}_K k_{rt}\|_{\infty} \leq \|k_{rt}\|_{\infty} \cdot \frac{2^m}{n} \mathfrak{M}(n, m, d, \delta^*, \delta', \mathfrak{M}_{S_{in}, k_{rt}, n}),
$$

with probability at least $1 - \delta' - \sum_{j=1}^m \frac{2^{j-1}}{m} \sum_{i=1}^{n/2^j} \delta_i$.

Cor. 1 and Thm. 2 together ensure that, with high probability, KT-SPLIT produces at least one thinned coreset that approximates $P_n$ well in MMD$_K$. The subsequent KT-SWAP step of kernel thinning serves to refine that coreset and can only improve the MMD quality by directly minimizing the MMD$_K$ to $P_n$.

### 5.3 Prior constructive $L^\infty$ coresets

A number of alternative strategies are available for constructing coresets with $L^\infty$ guarantees. For example, for any bounded $k_{rt}$, Cauchy-Schwarz and the reproducing property imply that

$$
\|(P - P_n)k_{rt}\|_{\infty} = \sup_{z \in \mathbb{R}^d} \|\langle k_{rt}(z, \cdot) \rangle P_k_{rt} - P_n k_{rt} \|_K \leq \text{MMD}_k(P, P_n) \cdot \|k_{rt}\|_{\infty},
$$

so that all of the order $(n^{1/2}, n^{-1/2})$-MMD coreset constructions discussed in Sec. 1.1 also yield order $(n^{1/2}, n^{-1/4})$-$L^\infty$ coresets. However, none of those constructions is known to provide a $(n^{1/4}, o(n^{-1/4}))$-$L^\infty$ coreset.

A series of breakthroughs due to Joshi et al. (2011); Phillips (2013); Phillips and Tai (2018, 2020); Tai (2020) has led to a sequence of increasingly compressed $(n^{1/4}, o(n^{-1/4}))$-$L^\infty$ coreset constructions, with the best known guarantees currently due to Phillips and Tai (2020) and Tai (2020). Given $n$ input points, Phillips and Tai (2020) developed an offline, polynomial-time construction to find an $(n^{1/4}, \sqrt{dn}^{-1/4} \sqrt{\log n})$-$L^\infty$ coreset with high probability for Lipschitz kernels exhibiting suitable decay, while Tai (2020) developed an offline construction for Gaussian kernels that runs in $\Omega(d^d)$ time and yields an order $(n^{1/4}, 2^d n^{-1/4} \sqrt{\log(d \log n)})$-$L^\infty$ coreset with high probability. More details on these constructions based on the Gram-Schmidt walk of Bansal et al. (2018) can be found in App. N. Notably, the Phillips and Tai (hereafter, PT) guarantee is tighter than that of Thm. 4 by a factor of $\sqrt{\log n}$ for sub-Gaussian kernels and input points, and $\sqrt{\log n}$ for heavy-tailed kernels and input points. Similarly, the Tai guarantee provides an improvement when $n$ is doubly-exponential in the dimension, that is, when $\sqrt{d \log n} = \Omega(2^d)$.

Moreover, by Thm. 2, we may apply the PT and Tai constructions to a square-root kernel $k_{rt}$ to obtain comparable MMD guarantees for the target kernel $k$ with high probability. However, kernel thinning has a number of practical advantages that lead us to recommend it. First with $n$ input points, using standard matrix multiplication, the PT
and Tai constructions have $\Omega(n^4)$ computational complexity and $\Omega(n^2)$ storage costs, a substantial increase over the $O(n^2)$ running time and $O(n \min(d, n))$ storage of kernel thinning. Second, $\text{kt-split}$ is an online algorithm while the PT and Tai constructions require the entire set of input points to be available a priori. Finally, each halving round of $\text{kt-split}$ splits the sample size exactly in half, allowing the user to run all $m$ halving rounds simultaneously; the PT and Tai constructions require a rebalancing step after each round forcing the halving rounds to be conducted sequentially.

6. Vignettes

We complement our primary methodological and theoretical development with two vignettes illustrating the promise of kernel thinning for improving upon (a) i.i.d. sampling in dimensions $d = 2$ through 100 and (b) standard MCMC thinning when targeting challenging differential equation posteriors. See App. K for supplementary details and https://github.com/microsoft/goodpoints for a Python implementation of kernel thinning and code replicating each vignette.

6.1 Common settings

Throughout, we adopt a $\text{Gauss}(\sigma)$ target kernel $k(x, y) = \exp\left(-\frac{1}{2\sigma^2}\|x - y\|^2_2\right)$ and the corresponding square-root kernel $k_{\text{rt}}$ from Tab. 1. To output a coreset of size $n^{1/2}$ with $n$ input points, we (a) take every $n^{1/2}$-th point for standard thinning and (b) run kernel thinning (KT) with $m = \frac{1}{2} \log_2 n$ using a standard thinning coreset as the base coreset in $\text{kt-swap}$. For each input sample size $n \in \{2^4, 2^6, \ldots, 2^{14}, 2^{16}\}$ with $\delta_i = \frac{1}{2n}$, we report the mean coreset error $\text{MMD}_k(\mathcal{P}, \mathcal{S}) \pm 1$ standard error across 10 independent replications of the experiment (the standard errors are too small to be visible in all experiments). We additionally regress the log mean MMD onto the log input size using ordinary least squares and display both the best linear fit and an empirical decay rate based on the slope of that fit, e.g., for a slope of $-0.25$, we report an empirical decay rate of $n^{-0.25}$ for the mean MMD.

Figure 2: Kernel thinning (KT) and i.i.d. coresets for 4- and 8-component mixture of Gaussian targets with equidensity contours of the target underlaid. See Sec. 6.2 for more details.
6.2 Kernel thinning versus i.i.d. sampling

We first illustrate the benefits of kernel thinning over i.i.d. sampling from a target \( \mathbb{P} \). We generate each input sequence \( S \) i.i.d. from \( \mathbb{P} \), use squared kernel bandwidth \( \sigma^2 = 2d \), and consider both Gaussian targets \( \mathbb{P} = \mathcal{N}(0, I_d) \) for \( d \in \{2, 4, 10, 100\} \) and mixture of Gaussians (MoG) targets \( \mathbb{P} = \frac{1}{M} \sum_{j=1}^{M} \mathcal{N}(\mu_j, I_2) \) with \( M \in \{4, 6, 8\} \) component locations \( \mu_j \in \mathbb{R}^2 \) defined in App. K.1.

Fig. 2 highlights the visible differences between the KT and i.i.d. coresets for the MoG targets. Even for small sample sizes, the KT coresets achieves better stratification across components with less clumping and fewer gaps within components, suggestive of a better approximation to \( \mathbb{P} \). Indeed, when we examine MMD error as a function of coreset size in Fig. 3, we observe that kernel thinning provides a significant improvement across all settings. For the Gaussian \( d = 2 \) target and each MoG target, the KT MMD error scales as \( n^{-\frac{1}{2}} \), a quadratic improvement over the \( \Omega(n^{-\frac{1}{4}}) \) MMD error of i.i.d. sampling. Moreover, despite the dimension dependence in our bounds, KT significantly improves upon the MMD of i.i.d. sampling even for high dimensions and small sample sizes. For example, in Fig. 3(b), we observe empirical decay rates of \( n^{-0.49} \) for \( d = 4 \), \( n^{-0.42} \) for \( d = 10 \), and \( n^{-0.33} \) for \( d = 100 \).

![Image](image_url)

(a) Mixture of Gaussians \( \mathbb{P} \)

![Image](image_url)

(b) Gaussian \( \mathbb{P} \)

**Figure 3: Kernel thinning versus i.i.d. sampling.** For (a) mixture of Gaussian targets with \( M \in \{4, 6, 8\} \) components and (b) standard multivariate Gaussian targets in dimension \( d \in \{2, 4, 10, 100\} \), kernel thinning (KT) reduces MMD\(_k(\mathbb{P}, S)\) significantly more quickly than the standard \( n^{-\frac{1}{4}} \) rate for \( n^2 \) i.i.d. points, even in high dimensions.
6.3 Kernel thinning versus standard MCMC thinning

Next, we illustrate the benefits of kernel thinning over standard Markov chain Monte Carlo (MCMC) thinning on twelve posterior inference experiments conducted by Riabiz et al. (2021). We briefly describe each experiment here and refer the reader to Riabiz et al. (2021, Sec. 4) for more details.

**Goodwin and Lotka-Volterra experiments** From Riabiz et al. (2020), we obtain the output of four distinct MCMC procedures targeting each of two $d = 4$-dimensional posterior distributions $\mathbb{P}$: (1) a posterior over the parameters of the *Goodwin model* of oscillatory enzymatic control (Goodwin, 1965) and (2) a posterior over the parameters of the *Lotka-Volterra model* of oscillatory predator-prey evolution (Lotka, 1925; Volterra, 1926). For each target, Riabiz et al. (2020) provide $2 \times 10^6$ sample points from each of four MCMC algorithms: Gaussian random walk (RW), adaptive Gaussian random walk (adaRW, Haario et al., 1999), Metropolis-adjusted Langevin algorithm (MALA, Roberts and Tweedie, 1996), and pre-conditioned MALA (pMALA, Girolami and Calderhead, 2011).

**Hinch experiments** From Riabiz et al. (2020), we also obtain the output of two independent Gaussian random walk MCMC chains for each of two $d = 38$-dimensional posterior distributions $\mathbb{P}$: (1) a posterior over the parameters of the *Hinch model* of calcium signalling in cardiac cells (Hinch et al., 2004) and (2) a tempered version of the same posterior, as defined by Riabiz et al. (2021, App. S5.4). In computational cardiology, the calcium signalling model represents one component of a heart simulator, and one aims to propagate uncertainty in the signalling model through the whole heart simulation, an operation which requires 1000s of CPU hours per sample point (Riabiz et al., 2021). In this setting, the costs of running kernel thinning are dwarfed by the time required to generate the input sample (two weeks) and more than offset by the cost savings in the downstream uncertainty propagation task.

**Pre-processing and kernel settings** We discard the initial points of each chain as burn-in using the maximum burn-in period reported in Riabiz et al. (2021, Tabs. S4 & S6, App. S5.4). and normalize each Hinch chain by subtracting the post-burn-in sample mean and dividing each coordinate by its post-burn-in sample standard deviation. To form an input sequence $\mathcal{S}_{\text{in}}$ of length $n$ for coreset construction, we downsample the remaining points using standard thinning. Since exact computation of $\text{MMD}_k(\mathbb{P}, \mathcal{S})$ is intractable for these posterior targets, we report $\text{MMD}_k(\mathcal{S}_{\text{in}}, \mathcal{S})$—the error that is controlled directly in our theoretical results—for these experiments. We select the kernel bandwidth $\sigma$ using the popular median heuristic (see, e.g., Garreau et al., 2017). Additional details can be found in App. K.2.

**Results** Fig. 4 compares the mean $\text{MMD}_k(\mathcal{S}_{\text{in}}, \mathcal{S})$ error of the generated kernel thinning and standard thinning coresets. In each of the twelve experiments, KT significantly improves both the rate of decay and the order of magnitude of mean MMD, in line with the guarantees of Thm. 1. Notably, in the $d = 38$-dimensional Hinch experiments, standard thinning already improves upon the $n^{-\frac{1}{4}}$ rate of i.i.d. subsampling but is outpaced by KT which consistently provides further improvements.
7. Discussion

We introduced a new, practical solution to the thinned MMD coreset problem that, given $O(n^2)$ time and $O(n \min(d, n))$ storage, improves upon the integration error of i.i.d. sampling and standard MCMC thinning. In recent work, Dwivedi and Mackey (2022) generalize KT to support arbitrary kernels, even those without square-root dominating kernels. Separately, Shetty et al. (2022) have developed a distribution compression meta-algorithm, Compress++, which reduces the runtime of KT to near-linear $O(n \log^3 n)$ time with MMD error that is worse by at most a factor of 4. Hence, KT-Compress++ can be practically deployed even for very large input sizes.

Several other opportunities for future development recommend themselves. First, since our results cover any target $\mathbb{P}$ with at least $2d$ moments—even discrete and other non-smooth targets—a natural question is whether tighter error bounds with better sample complexities are available when $\mathbb{P}$ is also known to have a smooth Lebesgue density. Second, the MMD to $L^\infty$ reduction in Thm. 2 applies also to weighted $L^\infty$ coresets, and, in applications in which weighted point sets are supported, we would expect either quality or compression improvements from employing non-uniform weights (see, e.g. Turner et al., 2021).
Appendix

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A. Proof of Prop. 1: MMD guarantee for MCMC

Fix any \( y_1, \ldots, y_n, z_1, \ldots, z_n \in \mathbb{R}^d \) and any optimal test function \( f^* \in \arg\max \{ f : \|f\|_k \leq 1 \} | \mathbb{P} f - \frac{1}{n} \sum_{i=1}^n f(y_i) | \). The definition of MMD (1), the triangle inequality, and Cauchy-Schwarz together imply the bounded differences property

\[
\begin{align*}
\text{MMD}_k(\mathbb{P}, \frac{1}{n} \sum_{i=1}^n \delta_{y_i}) - \text{MMD}_k(\mathbb{P}, \frac{1}{n} \sum_{i=1}^n \delta_{z_i}) & \leq \frac{1}{n} \sum_{i=1}^n f^*(y_i) - f^*(z_i) \\
& = \frac{1}{n} \sum_{i=1}^n (k(y_i, \cdot) - k(z_i, \cdot), f^*)_k \\
& \leq \frac{1}{n} \sum_{i=1}^n \|k(y_i, \cdot) - k(z_i, \cdot)\|_k \|f^*\|_k \\
& \leq \sum_{i=1}^n \frac{2}{n} \|k\|_k^2 \mathbb{1}[y_i \neq z_i].
\end{align*}
\]

Hence, by McDiarmid’s inequality for geometrically ergodic Markov chains (Dedecker and Gouëzel, 2015, Thm. 0.2),

\[
\text{MMD}_k(\mathbb{P}, \mathbb{P}_n) \leq \mathbb{E}[\text{MMD}_k(\mathbb{P}, \mathbb{P}_n)] + \sqrt{\frac{C_1 \|k\|_\infty \log(1/\delta)}{n}} \text{ with probability at least } 1 - \delta,
\]

where \( C_1 \) is a finite value depending only on the transition probabilities of the homogeneous geometrically ergodic chain.

Now, define the \( \mathbb{P} \) centered kernel \( k_\mathbb{P}(x, y) = k(x, y) - \mathbb{P}k(x) - \mathbb{P}k(y) + \mathbb{P}\mathbb{P}k \). To bound the expectation, we will use a slight modification of Lem. 3 of Riabiz et al. (2021). The
original lemma used the assumption of $V$-uniform ergodicity (Meyn and Tweedie, 2012, Defn. (16.0.1)) and the assumption $V(x) \geq \sqrt{k}\langle x, \hat{x} \rangle$ solely to argue that

$$|E[f(x_{i+1}) | x_1] - Pf| \leq RV(x_1) \rho^i \quad \text{for all} \quad x_1 \in \mathbb{R}^d$$

for some $R > 0$ and all $f$ with $\|f\|_{k_v} = 1$. In our case, since $k_v$ is bounded and any $f$ with $\|f\|_{k_v} = 1$ satisfies

$$|f(x)| = |(k\langle x, \cdot \rangle, f)_{k_v}| \leq \|k\langle x, \cdot \rangle\|_{k_v} \|f\|_{k_v} = \sqrt{k\langle x, x \rangle} \leq \sqrt{\|k\|_{\infty}} \quad \text{for all} \quad x \in \mathbb{R}^d$$

by the reproducing property and Cauchy-Schwarz, our assumed geometric ergodicity condition (2) implies the analogous bound

$$|E[f(x_{i+1}) | x_1] - Pf| \leq \sqrt{\|k\|_{\infty}} V(x_1) \rho^i \quad \text{for all} \quad x_1 \in \mathbb{R}^d.$$ 

Hence, the conclusions of Riabiz et al. (2021, Lem. 3) with $R = \sqrt{\|k\|_{\infty}}$ hold under our assumptions. Jensen’s inequality and the conclusion of Lem. 3 of Riabiz et al. (2021) now yield the bound

$$\mathbb{E}[\text{MMD}_{k}(\mathbb{P}, \mathbb{P}_n)]^2 \leq \mathbb{E}[\text{MMD}_{k}(\mathbb{P}, \mathbb{P}_n)]^2 = \mathbb{E}\left[\frac{1}{\pi} \sum_{i=1}^{n} k\langle x, x_i \rangle + \frac{1}{\pi} \sum_{i=1}^{n} \sum_{j \neq i} k\langle x, x_j \rangle\right] \\
\leq \frac{1}{n} \|k\|_{\infty} (1 + \frac{2\rho}{1-\rho} \sum_{i=1}^{n-1} \mathbb{E}[V(x_i)]) \leq \mathbb{E}[\|k\|_{\infty} (1 + \frac{2\rho}{1-\rho} \sum_{i=1}^{n-1} \mathbb{E}[V(x_i)])].$$

Now, define $C \triangleq \max_{n \in \mathbb{N}} \frac{1}{n} \sum_{i=1}^{n-1} \mathbb{E}[V(x_i)]$. By Meyn and Tweedie (2012, Thm. 17.0.1(i)) $C$ is finite whenever $\mathbb{P}_V < \infty$, and hence our proof is complete.

**B. Proof of Prop. 2: Shift-invariant square-root kernels**

Following the unitary angular frequency convention of Wendland (2004, Def. 5.15), we define the Fourier transform $\mathcal{F}(f)$ of a function $f \in L^1(\mathbb{R}^d)$ via

$$\mathcal{F}(f)(\omega) \triangleq \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} f(x) e^{-i\langle x, \omega \rangle} dx.$$ (16)

Since $k$ is a real continuous shift-invariant kernel, Bochner’s theorem (Bochner, 1933; Wendland, 2004, Thm. 6.6) implies that $k(x, y) = \frac{1}{(2\pi)^{d/2}} \int e^{-i\langle \omega, x-y \rangle} \hat{k}(\omega) d\omega$, that $\hat{k}$ is nonnegative and integrable, and that $k_{\text{rt}}(x, y)$ is a kernel since $\int \sqrt{\hat{k}(\omega)} d\omega < \infty$. Moreover, since $k_{\text{rt}}(x, \cdot) = \frac{1}{(2\pi)^{d/2}} \mathcal{F}(e^{-i\langle \cdot, x \rangle} \sqrt{\hat{k}})$ for $e^{-i\langle \cdot, x \rangle} \sqrt{\hat{k}} \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$, the Plancherel-Parseval identity Wendland (2004, Proof of Thm. 5.23) implies that

$$\int_{\mathbb{R}^d} k_{\text{rt}}(x, z)k_{\text{rt}}(y, z) dz = \int_{\mathbb{R}^d} \frac{1}{(2\pi)^{d/2}} e^{-i\langle \omega, x \rangle} \sqrt{\hat{k}(\omega)} \frac{1}{(2\pi)^{d/2}} e^{i\langle \omega, y \rangle} \sqrt{\hat{k}(\omega)} d\omega \\
= \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{-i\langle \omega, x-y \rangle} \hat{k}(\omega) d\omega = k(x, y)$$

confirming that $k_{\text{rt}}$ is a square-root kernel of $k$. 

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C. Proof of Thm. 1: MMD guarantee for kernel thinning

By design, KT-SWAP ensures
\[ \text{MMD}_k(S_{in}, S_{KT}) \leq \text{MMD}_k(S_{in}, S^{(m,1)}), \]  
(17)
where \( S^{(m,1)} \) denotes the first coreset returned by KT-SPLIT.

Now, applying Thm. 2 with \( P = P_n = \frac{1}{n} \sum_{x \in S_{in}} \delta_x, \) \( Q = Q_{KT}^{(m,1)} = \frac{1}{[n/2^m]} \sum_{x \in S^{(m,1)}} \delta_x, \) \( R = 2 \max(\mathcal{R}_{S_{in}}, \mathcal{R}_{k_{rt,n}^1}), \) and \( a = b = \frac{1}{2}, \) we find that
\[ \text{MMD}_k(S_{in}, S^{(m,1)}) \]
\[ = \text{MMD}_k(P_n, Q_{KT}^{(m,1)}) \]
\[ \leq \left\| P_n k_{rt} - Q_{KT}^{(m,1)} k_{rt} \right\|_{\infty} \]
\[ \leq \left\| P_n k_{rt} - Q_{KT}^{(m,1)} k_{rt} \right\|_{\infty} \]
\[ \leq \frac{1}{\sqrt{n}} \left( \frac{(4\pi)^{d/2}}{\Gamma(\frac{d}{2}+1)} r^2 + \frac{2\|k_{rt}\|_{\infty}}{\sqrt{n}} \right), \]  
(18)
where step (i) uses the following arguments: (a) \( \frac{v_d R^{d/2}}{2} = \frac{(4\pi)^{d/2}}{\Gamma(\frac{d}{2}+1)} r^2; \) (b) \( Q_{KT}^{(m,1)} \) is supported on a subset of points from \( S_{in} \) and hence
\[ \max\{\tau_{P_n}(r), \tau_{Q_{KT}^{(m,1)}}(r)\} = \tau_{P_n}(r) = 0 \]  
for any \( r > \mathcal{R}_{S_{in}}; \)
and (c) \( \tau_{k_{rt}}(r) \leq \frac{\|k_{rt}\|_{\infty}}{\sqrt{n}} \) for any \( r > \mathcal{R}_{k_{rt,n}}^1. \)

Next, invoking Cor. 1 we obtain that
\[ \left\| P_n k_{rt} - Q_{KT}^{(m,1)} k_{rt} \right\|_{\infty} \leq \|k_{rt}\|_{\infty} \cdot \frac{2^m}{n} \cdot \mathcal{M}_{k_{rt}}(n, m, d, \delta^*, \delta', \mathcal{R}_{S_{in}}), \]  
(19)
with probability at least \( 1 - \delta' - \sum_{j=1}^{m} \frac{2^j}{m} \sum_{j=1}^{\delta/2^j} \delta_i. \) Putting the bounds (17) to (19) together yields the result claimed in Thm. 1.

D. Proof of Rem. 3: Finite-time and anytime guarantees

For the case with known \( n, \) the claim follows simply by noting that
\[ \sum_{j=1}^{m} \frac{2^j}{m} \sum_{i=1}^{\delta/2^j} \delta_i = \sum_{j=1}^{m} \frac{2^j}{m} \frac{\delta}{2^j} = \frac{\delta}{2}. \]
For the case of an arbitrary oblivious stopping time \( n, \) first we note that
\[ \sum_{i=1}^{\infty} \frac{1}{(i+1) \log^2(i+1)} \overset{(i)}{\leq} 2, \]  
and \( \sum_{j=1}^{m} 2^j = 2^{m+1} - 2 \leq 2^{m+1}. \)  
(20)
where step (i) can be verified using mathematical programming software. Therefore, for any \( n \in \mathbb{N}, \) with \( \delta_i = \frac{m \delta}{2^m + 2^{i+1} \log^2(i+1)}, \) we have
\[ \sum_{j=1}^{m} \frac{2^j}{m} \sum_{i=1}^{\delta/2^j} \delta_i \leq \sum_{j=1}^{m} \frac{2^j}{m} \sum_{i=1}^{\delta/2^j} \delta_i \]
\[ = \sum_{j=1}^{m} \frac{2^j}{m} \sum_{i=1}^{\delta/2^j} \frac{m \delta}{2^m + 2^{i+1} \log^2(i+1)} \]
\[ \leq \frac{\delta}{2^m + 2^{m+1}} \cdot 2^{m+1} \cdot 2 \leq \frac{\delta}{2}. \]
E. Proof of Thm. 2: $L^\infty$ coresets for $(k_{rt}, \mathbb{P})$ are MMD coresets for $(k, \mathbb{P})$

For a function $g : \mathbb{R}^d \to \mathbb{R}$, let $\|g\|_2 := (\int_{\mathbb{R}^d} g^2(x)dx)^{\frac{1}{2}}$ denote its $L^2$-norm. The proof of Thm. 2 follows from the following two lemmas.

**Lemma 1** (k-MMD in terms of $k_{rt}$). Given a kernel $k$ and its square-root kernel $k_{rt}$ (Def. 1), and any two distributions $\mathbb{P}$ and $\mathbb{Q}$, we have

$$\text{MMD}_k(\mathbb{P}, \mathbb{Q}) = \sup_{g : \|g\|_2 \leq 1} \left| \int_{\mathbb{R}^d} g(y)(\mathbb{P}k_{rt}(y) - \mathbb{Q}k_{rt}(y))dy \right|. \quad (21)$$

See App. E.1 for the proof. Let $\text{Vol}(R) \triangleq \pi^d/\Gamma(d/2 + 1)R^d$ denote the volume of the Euclidean ball $B(0; R)$. Moreover, define the norm

$$\|k\|_2 \triangleq \sup_x \left| \int k^2(x, x - y)dy \right|^{\frac{1}{2}} = \sup_x \|k(x, x - \cdot)\|_2. \quad (22)$$

**Lemma 2** (Relating kernel integral error with $L^\infty$ error). For any kernel $k$, distributions $\mathbb{P}, \mathbb{Q}$, function $g$ with $\|g\|_2 \leq 1$, radius $R \geq 0$ and scalars $a, b \geq 0$ with $a + b = 1$, we have

$$\left| \int_{\mathbb{R}^d} g(y)(\mathbb{P}k(y) - \mathbb{Q}k(y))dy \right| \leq \|\mathbb{P} - \mathbb{Q}\|_\infty \text{Vol}^{\frac{1}{2}}(R) + 2\tau_k(aR) + 2\|k\|_2 \max\{\tau_{\mathbb{P}}(bR), \tau_{\mathbb{Q}}(bR)\}. \quad (23)$$

See App. E.2 for the proof.

Note that Def. 1 and (22) imply that

$$\|k_{rt}(x, \cdot)\|_2 = \sqrt{k(x, x)} \implies \|k_{rt}\|_2 \leq \sqrt{\|k\|_\infty}. \quad (24)$$

Now invoking the bound (23) along with (24) for the kernel $k_{rt}$ and then substituting it back in (21) in Lem. 1 immediately yields the bound (10) of Thm. 2.

**E.1 Proof of Lem. 1: k-MMD in terms of $k_{rt}$**

Applying Saitoh (1999, Thms. 1 and 2), and the definition (3) of $k_{rt}$, we find that for any $f$ in the RKHS of kernel $k$, there exists a function $g \in L^2(\mathbb{R}^d)$ such that

$$f(x) = \int g(y)k_{rt}(x, y)dy \quad \text{and} \quad \|f\|_k = \|g\|_2. \quad (25)$$

Moreover for any $g \in L^2(\mathbb{R}^d)$ there exists an $f \in \mathcal{H}$ (the RKHS of $k$) such that (25) holds. Next, we have

$$\text{MMD}_k(\mathbb{P}, \mathbb{Q}) = \sup_{\|f\|_k \leq 1} |\mathbb{Q}f - \mathbb{P}f| = \sup_{\|g\|_{L^2(\mathbb{R}^d)} \leq 1} \left| \int_x \int_y g(y)k_{rt}(y, x)dyd\mathbb{P}(x) - \int_x \int_y g(y)k_{rt}(x, y)dxd\mathbb{Q}(x) \right|$$

$$\overset{(i)}{=} \sup_{\|g\|_{L^2(\mathbb{R}^d)} \leq 1} \left| \int_y g(y)\mathbb{P}k_{rt}(y)dy - \int_y g(y)\mathbb{Q}k_{rt}(y)dy \right| = \sup_{\|g\|_{L^2(\mathbb{R}^d)} \leq 1} \int_y g(y)\mathbb{P}k_{rt}(y)dy - \int_y g(y)\mathbb{Q}k_{rt}(y)dy$$

where step (i) follows from (25), and we can swap the order of integration to obtain step (ii) using Fubini’s theorem along with the following fact:

$$\int_x \int_y |g(y)k_{rt}(y, x)|dyd\mathbb{P}(x) \leq \|g\|_2 \|k_{rt}\|_2 \int_x d\mathbb{P}(x) < \infty.$$ 

The proof is complete.
E.2 Proof of Lem. 2: Relating kernel integral error with $L^\infty$ error

Throughout the proof we continue to use the shorthand $\mathcal{B}(R) = \mathcal{B}(0; R)$. Given a function $g : \mathbb{R}^d \to \mathbb{R}$, we define restriction $g_R$ as follows:

$$g_R(x) = g(x)1_{\mathcal{B}(R)}(x).$$

Next, we define the bivariate functions $k_R$ and $k_R^{(c)}$:

$$k_R(x, z) \triangleq k(x, z) \cdot 1_{\mathcal{B}(R)}(z) \quad \text{and} \quad k_R^{(c)}(x, z) \triangleq k(x, z) - k_R(x, z) = k(x, z) - (1 - 1_{\mathcal{B}(R)}(z)),$$

so that

$$\mathbb{P} k(z) = \mathbb{P} k_R(z) + \mathbb{P} k_R^{(c)}(z).$$

Now we have

$$\left| \int g(y)(\mathbb{P} k(y) - \mathbb{Q} k(y))dy \right| = \left| \int g(y)(\mathbb{P} k_R(y) - \mathbb{Q} k_R(y))dy + \int g(y)(\mathbb{P} k_R^{(c)}(y) - \mathbb{Q} k_R^{(c)}(y))dy \right|$$

$$= \left| \int g_R(y)(\mathbb{P} k_R(y) - \mathbb{Q} k_R(y))dy \right| + \left| \int_{\|y\| \geq R} g(y)(\mathbb{P} k_R^{(c)}(y) - \mathbb{Q} k_R^{(c)}(y))dy \right|$$

$$\leq \|g_R\|_{L^1} \cdot \|\mathbb{P} k - \mathbb{Q} k\|_{\infty} + \left| \int_{\|y\| \geq R} g(y)(\mathbb{P} k_R^{(c)}(y) - \mathbb{Q} k_R^{(c)}(y))dy \right|,$$  \hspace{1em} (26)

where the last step uses the Hölder’s inequality. For the first term in (26), Cauchy-Schwarz’s inequality implies that

$$\|g_R\|_{L^1} \leq \|g_R\|_{L^2} \cdot \sqrt{\text{Vol}(R)} \leq \|g\|_{L^2} \cdot \sqrt{\text{Vol}(R)}.$$  \hspace{1em} (27)

Next, we bound the second term in (26). Given any $y$ with $\|y\| \geq R$, and any two scalars $a, b \in [0, 1]$ such that $a + b = 1$, one of the following condition holds for an arbitrary $x \in \mathbb{R}^d$:

either $\|x - y\| \geq aR$ or $\|x\| \geq bR$. Consequently, we obtain the following

$$\left| \int_{\|y\| \geq R} g(y)(\mathbb{P} k(y) - \mathbb{Q} k(y))dy \right| = \left| \int_{\|y\| \geq R} g(y) \int_{x \in \mathbb{R}^d} k(x, y)(d\mathbb{P}(x) - d\mathbb{Q}(x))dy \right|$$

$$\leq \left| \int_{\|y\| \geq R} \int_{\|x - y\| \geq aR} g(y)k(x, y)(d\mathbb{P}(x) - d\mathbb{Q}(x))dy \right|$$

$$+ \left| \int_{\|y\| \geq R} \int_{\|x\| \geq bR} g(y)k(x, y)(d\mathbb{P}(x) - d\mathbb{Q}(x))dy \right|$$

$$= T_1 + T_2.$$  \hspace{1em} (28)

We now bound the terms $T_1$ and $T_2$ separately in (29a) and (29b) below. Substituting those bounds in (28), and then putting it together with (26) and (27) yields the bound (23) as claimed in the lemma.

Bounding $T_1$ Substituting $x - y = z$, we have

$$T_1 \leq \int_{\|x - z\| \geq R} \int_{\|z\| \geq aR} |g(x - z)k(x, x - z)||d\mathbb{P}(x) - d\mathbb{Q}(x)|dz$$

$$\leq \int_{x \in \mathbb{R}^d} \int_{\|z\| \geq aR} |g(x - z)k(x, x - z)||dz||d\mathbb{P}(x) - d\mathbb{Q}(x)||$$

$$(i) \leq \int_{x \in \mathbb{R}^d} \|g(x - \cdot)\|_2 \sup_{x'} \left( \int_{\|z\| \geq aR} k^2(x', x' - z)dz \right)^{1/2} |d\mathbb{P}(x) - d\mathbb{Q}(x)|$$

$$(ii) \leq \int_{x \in \mathbb{R}^d} \|g \|_2 \tau_k(aR)||d\mathbb{P}(x) - d\mathbb{Q}(x)|| \leq 2\|g \|_2 \tau_k(aR),$$  \hspace{1em} (29a)

where step (i) follows from Cauchy-Schwarz’s inequality, step (ii) from the definition (5) of $\tau_k$, and step (iii) from the fact $\int |d\mathbb{P}(x) - d\mathbb{Q}(x)| \leq 2$.  \hspace{1em} (29b)
Bounding $T_2$. We have

\[
T_2 \leq \int_{\|x\| \geq bR} \left( \int_{\|y\| \geq R} |g(y)k(x, y)| dy \right) |dP(x) - dQ(x)|
\]

\[
\leq \int_{\|x\| \geq bR} \|g\|_2 \sup_{x'} \|k(x', \cdot)\|_2 |dP(x) - dQ(x)|
\]

\[
\overset{(iv)}{\leq} 2\|g\|_2 \cdot \|k\|_2 \max\{\tau_P(bR), \tau_Q(bR)\}.
\]

(29b)

where step (iv) follows from the definitions (5) and (22) of $\|k\|_2$, $\tau_P$ and $\tau_Q$.

F. Proof of Thm. 3: Self-balancing Hilbert walk properties

We prove each property from Thm. 3 one by one.

F.1 Property (i): Functional sub-Gaussianity

We prove the functional sub-Gaussianity claim (13) by induction on the iteration $i \in \{0, \ldots, n\}$. Our proof uses the obliviousness assumption, which implies that

\[
\psi_{i - 1} \perp (f_i, a_i) | \mathcal{F}_{i - 1} \text{ for all } i,
\]

and the following lemma proved in App. F.7, which supplies a convenient decomposition for the self-balancing Hilbert walk iterates.

Lemma 3 (Alternate representation of $\psi_i$). Each iterate $\psi_i$ of the self-balancing Hilbert walk (Alg. 2) satisfies

\[
\langle \psi_i, u \rangle_{\mathcal{H}} = \left( \langle \psi_{i - 1}, u - f_i \frac{(f_i, u)}{a_i} \rangle_{\mathcal{H}} + \varepsilon_i \langle f_i, u \rangle_{\mathcal{H}} \right) \text{ for all } u \in \mathcal{H}
\]

(31)

for a random variable $\varepsilon_i$ which satisfies

\[
\mathbb{E}[\varepsilon_i | \psi_{i - 1}, \mathcal{F}_i] = 0, \quad \varepsilon_i \in [-2, 2], \quad \text{and } \mathbb{E}[e^{t\varepsilon_i} | \psi_{i - 1}, \mathcal{F}_i] \leq e^{t^2/2} \text{ for all } t \in \mathbb{R}.
\]

(32)

We now proceed with our induction argument.

Base case The base case $i = 0$ is true since $\psi_0 = 0$ and hence is sub-Gaussian with any parameter $\sigma_0 = 0$. 

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Inductive step Fix any $i \in [n]$ and assume that the functional sub-Gaussianity claim (13) holds for $\psi_{i-1}$ with $\sigma_{i-1}$. We have

$$\mathbb{E}[\exp(\langle \psi_i, u \rangle_{\mathcal{H}}) | \mathcal{F}_i] = \mathbb{E}[\mathbb{E}[\exp(\langle \psi_i, u \rangle_{\mathcal{H}}) | \psi_{i-1}, \mathcal{F}_i] | \mathcal{F}_i]$$

(31) $$\leq \mathbb{E} \left[ \exp \left( \left\langle \psi_{i-1}, u - f_i \frac{(f_i, u)_{\mathcal{H}}}{a_i} \right\rangle_{\mathcal{H}} \right) \cdot \mathbb{E}[\exp(\varepsilon_i(\langle f_i, u \rangle_{\mathcal{H}}) | \psi_{i-1}, \mathcal{F}_i) | \mathcal{F}_i] \right]$$

(32) $$= \mathbb{E} \left[ \exp \left( \left\langle \psi_{i-1}, u - f_i \frac{(f_i, u)_{\mathcal{H}}}{a_i} \right\rangle_{\mathcal{H}} \right) \cdot \mathbb{E} \left[ \exp \left( \left\langle \psi_{i-1}, u - f_i \frac{(f_i, u)_{\mathcal{H}}}{a_i} \right\rangle_{\mathcal{H}} \right) | \mathcal{F}_i \right] \right]$$

$$= \mathbb{E} \left[ \exp \left( \frac{1}{2} \langle f_i, u \rangle_{\mathcal{H}}^2 \right) \cdot \mathbb{E} \left[ \exp \left( \left\langle \psi_{i-1}, u - f_i \frac{(f_i, u)_{\mathcal{H}}}{a_i} \right\rangle_{\mathcal{H}} \right) | \mathcal{F}_i \right] \right]$$

$$= \exp \left( \frac{1}{2} \langle f_i, u \rangle_{\mathcal{H}}^2 \right) \cdot \mathbb{E} \left[ \exp \left( \left\langle \psi_{i-1}, u - f_i \frac{(f_i, u)_{\mathcal{H}}}{a_i} \right\rangle_{\mathcal{H}} \right) | \mathcal{F}_i \right]$$

(i) $$\leq \exp \left( \frac{1}{2} \langle f_i, u \rangle_{\mathcal{H}}^2 + \frac{\sigma_{i-1}^2}{2} \left\| u - f_i \frac{(f_i, u)_{\mathcal{H}}}{a_i} \right\|^2_{\mathcal{H}} \right)$$

(33) where step (i) follows from obliviousness (30) and the induction hypothesis. Simplifying the exponent on the right-hand side in the bound (33) using Cauchy-Schwarz and the definition (12) of $\sigma_i$, we have

$$\frac{1}{2} \langle f_i, u \rangle_{\mathcal{H}}^2 + \frac{\sigma_{i-1}^2}{2} \left\| u - f_i \frac{(f_i, u)_{\mathcal{H}}}{a_i} \right\|^2_{\mathcal{H}} = \frac{1}{2} \langle f_i, u \rangle_{\mathcal{H}}^2 + \frac{\sigma_{i-1}^2}{2} \left( \left\| u \right\|_{\mathcal{H}}^2 + \langle f_i, u \rangle_{\mathcal{H}}^2 \left( \frac{\left\| f_i \right\|_{\mathcal{H}}^2}{a_i^2} - \frac{2}{a_i} \right) \right)$$

$$= \frac{\sigma_{i-1}^2}{2} \left\| u \right\|_{\mathcal{H}}^2 + \frac{1}{2} \langle f_i, u \rangle_{\mathcal{H}}^2 \cdot \left( \frac{1}{2} + \frac{\sigma_{i-1}^2}{2a_i^2} - \frac{\sigma_{i-1}^2}{a_i} \right)$$

$$\leq \frac{\sigma_{i-1}^2}{2} \left\| u \right\|_{\mathcal{H}}^2 + \frac{1}{2} \langle f_i, u \rangle_{\mathcal{H}}^2 \cdot \left( \frac{1}{2} + \frac{\sigma_{i-1}^2}{2a_i^2} - \frac{\sigma_{i-1}^2}{a_i} \right)$$

$$= \frac{\sigma_{i-1}^2}{2} \left\| u \right\|_{\mathcal{H}}^2 + \frac{1}{2} \langle f_i, u \rangle_{\mathcal{H}}^2 \left( 1 + \frac{\sigma_{i-1}^2}{a_i^2} \left( \frac{\left\| f_i \right\|_{\mathcal{H}}^2}{a_i} - 2 \right) \right)$$

$$= \frac{\sigma_{i-1}^2}{2} \left\| u \right\|_{\mathcal{H}}^2.$$ 

F.2 Property (ii): Signed sum representation

Since Alg. 2 adds $\pm f_i$ to $\psi$ whenever $|\alpha_i| = |\langle \psi_{i-1}, f_i \rangle_{\mathcal{H}}| \leq a_i$, by the union bound, it suffices to lower bound the probability of this event by $1 - \delta_i$ for each $i$. The following lemma establishes this bound using the functional sub-Gaussianity (13) of each $\psi_i$.

Lemma 4 (Self-balancing Hilbert walk success probability). The self-balancing Hilbert walk (Alg. 2) with oblivious $\mathcal{F}_n \triangleq (f_1, a_1, f_2, a_2, \ldots, f_n, a_n)$ and threshold $a_i \geq \sigma_{i-1} \left\| f_i \right\|_{\mathcal{H}} \sqrt{2 \log(2/\delta_i)}$ for $\delta_i \in (0, 1]$ satisfies

$$\mathbb{P}(E_i | \mathcal{F}_n) \geq 1 - \delta_i \quad \text{for} \quad E_i = \{ |\langle \psi_{i-1}, f_i \rangle_{\mathcal{H}}| \leq a_i \}.$$ 

Proof Instantiate the notation of Thm. 3. Obliviousness implies that $\mathbb{P}(E_i | \mathcal{F}_n) = \mathbb{P}(E_i | \mathcal{F}_i)$. Furthermore, the sub-Gaussian Hoeffding inequality (Wainwright, 2019, Prop. 2.5), the functional sub-Gaussianity of $\psi_i$ (13), and the choice of $a_i$ imply that

$$\mathbb{P}(E_i^c | \mathcal{F}_i) = \mathbb{P}(|\langle \psi_{i-1}, f_i \rangle_{\mathcal{H}}| > a_i | \mathcal{F}_i) \leq 2 \exp(-a_i^2/(2\sigma_{i-1}^2 \left\| f_i \right\|^2_{\mathcal{H}})) \leq 2 \exp(-\log(2/\delta_i)) = \delta_i.$$
F.3 Property (iii): Exact two-thinning via symmetrization
Whenever the signed sum representation (14) holds, we have
\[ \psi_n = \sum_{i=1}^{n} \eta_i f_i = \sum_{i=1}^{n} (\eta_i g_{2i-1} - \eta_i g_{2i}) = \sum_{i=1}^{2n} g_i - 2 \sum_{i \in I} g_i \]
where the last step follows from the definition of \( I \).

F.4 Property (iv): Pointwise sub-Gaussianity in RKHS
The reproducing property of the kernel \( k \) and the established functional sub-Gaussianity (13) yield
\[ \mathbb{E}[\exp(\psi_i(x)) \mid \mathcal{F}_i] = \mathbb{E}[\exp(\langle \psi_i, k(x, \cdot) \rangle_{\mathcal{H}}) \mid \mathcal{F}_i] \leq \exp\left(\frac{\sigma_i^2 \|k(x, \cdot)\|_{\mathcal{H}}^2}{2}\right) = \exp\left(\frac{\sigma_i^2 k(x, x)}{2}\right), \quad \forall x \in \mathcal{X}. \]

F.5 Property (v): Sub-Gaussian constant bound
We will establish the bound (15) for all \( i \in \{0, \ldots, n\} \) by induction on the iteration \( i \).

Base case The claim (15) holds for the base case, \( i = 0 \), since \( \sigma_0 = 0 \).

Inductive step Fix any \( i \in [n] \) and assume that the claim (15) holds for \( \sigma_{i-1} \).
If either \( \|f_i\|_{\mathcal{H}} = 0 \) or \( \sigma_{i-1}^2 \geq \frac{\sigma_i^2}{2a_i \|f_i\|_{\mathcal{H}}} \), then \( \sigma_i^2 = \sigma_{i-1}^2 \) by the definition (12) of \( \sigma_i \) and the assumption that \( \frac{\|f_i\|_{\mathcal{H}}^2}{2a_i} \leq a_i \), completing the inductive step.
If, alternatively, \( \sigma_{i-1}^2 < \frac{\sigma_i^2}{2a_i \|f_i\|_{\mathcal{H}}} \) and \( \|f_i\|_{\mathcal{H}} > 0 \), then our assumptions \( \frac{\|f_i\|_{\mathcal{H}}^2}{1+q} \leq a_i \) imply that \( (\frac{\|f_i\|_{\mathcal{H}}^2}{a_i} - 1)^2 \leq q^2 \). Hence, by the definition (12) of \( \sigma_i \) and the inductive hypothesis,
\[
\sigma_i^2 = \sigma_{i-1}^2 + \|f_i\|_{\mathcal{H}}^2 \left( 1 + \frac{\sigma_{i-1}^2}{\sigma_i^2 - 1} \left(\frac{\|f_i\|_{\mathcal{H}}^2}{2a_i} - 2a_i\right) \right)
= \|f_i\|_{\mathcal{H}}^2 + \sigma_{i-1}^2 \left(\frac{\|f_i\|_{\mathcal{H}}^2}{a_i} - 1\right)^2
\leq (1 - q^2) \frac{\|f_i\|_{\mathcal{H}}^2}{1+q} + q^2 \frac{\max_{j \in [n-1]} \|f_j\|_{\mathcal{H}}^2}{1+q} \leq \frac{\max_{j \in [n]} \|f_j\|_{\mathcal{H}}^2}{1+q},
\]
completing the inductive step.

F.6 Property (vi): Adaptive thresholding
Define \( c_i^* = \max(c^*, 1) \) and let \( q = \frac{(c_i^*)^2 - 1}{(c_i^*)^2 + 1} \in [0, 1] \) so that
\[
\frac{1}{1-q} = 1 + \frac{(c_i^*)^2}{2} \quad \text{and} \quad \frac{1}{1-q^2} = \frac{(c_i^* + 1/c_i^*)^2}{4} \leq \frac{(c^* + 1/c^*)^2}{4},
\]
since \( 1 = \arg\min_{c \geq 0} c + 1/c \). By assumption, \( a_i \geq \|f_i\|_{\mathcal{H}}^2 \geq \frac{\|f_i\|_{\mathcal{H}}^2}{1+q} \) for all \( i \in [n] \).
Now suppose that \( \sigma_{i-1}^2 < \frac{a_i^2}{2a_i - \|f_i\|_q^2} \) and \( \|f_i\|_H > 0 \). If \( a_i \leq \|f_i\|_q^2 \), then \( a_i \leq \frac{\|f_i\|_q^2}{1-q} \). If, alternatively, \( a_i \leq c_i\sigma_{i-1}\|f_i\|_H \), then
\[
a_i < \frac{1}{2}\|f_i\|_H^2(1 + c_i^2) \leq \frac{\|f_i\|_q^2}{1-q}.
\]

The conclusion now follows from the sub-Gaussian constant bound (15).

F.7 Proof of Lem. 3: Alternate representation of \( \psi_i \)
Consider the random variable
\[
\epsilon_i = \begin{cases} 
0 & \text{when } |\alpha_i| > a_i \\
1 + \frac{\alpha_i}{a_i} & \text{when } |\alpha_i| \leq a_i \text{ and } \psi_i = \psi_{i-1} + f_i, \\
-1 + \frac{\alpha_i}{a_i} & \text{when } |\alpha_i| \leq a_i \text{ and } \psi_i = \psi_{i-1} - f_i,
\end{cases}
\]
which satisfies the equalities (31) and the boundedness conditions \( \epsilon_i \in [c_{\min}, c_{\max}] \subseteq [-2, 2] \) for
\[
c_{\min} = \max(-2, \min(0, -1 + \alpha_i/a_i)) \quad \text{and} \quad c_{\max} = \min(2, \max(0, 1 + \alpha_i/a_i))
\]
by construction. Moreover,
\[
\mathbb{E}[\epsilon_i | \psi_{i-1}, \mathcal{F}_i, |\alpha_i| > a_i] = 0
\]
\[
\mathbb{E}[\epsilon_i | \psi_{i-1}, \mathcal{F}_i, |\alpha_i| \leq a_i] = \left(1 + \frac{\alpha_i}{a_i}\right) \cdot \frac{1}{2}\left(1 - \frac{\alpha_i}{a_i}\right) + \left(-1 + \frac{\alpha_i}{a_i}\right) \cdot \frac{1}{2}\left(1 + \frac{\alpha_i}{a_i}\right) = 0,
\]
so that \( \mathbb{E}[\epsilon_i | \psi_{i-1}, \mathcal{F}_i] = 0 \) as claimed. The conditional sub-Gaussianity claim
\[
\mathbb{E}[e^{t\epsilon_i} | \psi_{i-1}, \mathcal{F}_i] \leq e^{t^2/2} \quad \text{for all } t \in \mathbb{R}
\]
now follows from Hoeffding’s lemma (Hoeffding, 1963, (4.16)) since \( \epsilon_i \) is bounded with \( c_{\max} - c_{\min} \leq 2 \) and mean-zero conditional on \( \mathcal{F}_i \).

G. Proof of Thm. 4: \( L^\infty \) guarantees for kernel halving
In App. G.1, we prove the result for the coreset obtained from a single round of kernel halving stated in part (a), and then use it to establish the result for the coreset obtained from recursive kernel halving rounds stated in part (b) in App. G.2.

G.1 Proof of part (a): Kernel halving yields a 2-thinned \( L^\infty \) coreset
Comparison with Alg. 2 reveals that the function \( \psi_{n/2} \) produced by Alg. 3 is the output of the self-balancing Hilbert walk with inputs \( (f_i)_{i=1}^{n/2} \) and \( (a_i)_{i=1}^{n/2} \) with \( a_i = \max(\|f_i\|_H \sigma_{i-1} \sqrt{2 \log(2/\delta_i)}, \|f_i\|_q^2) \) where \( \sigma_i \) was defined in (12). Moreover, when \( |\alpha_i| \leq a_i \) for all \( i \in [n] \), the coreset \( S^{(1)} = (x_i)_{i \in \mathcal{I}} \) for \( \mathcal{I} = \{2i - \eta_{i-1}^{-1} : i \in [n/2]\} \) and \( \eta \) defined in Alg. 2. Next, the property (iii) (exact two-thinning) of Thm. 3 implies that the event
\[
\mathcal{E}_{\text{half}} = \left\{ \frac{1}{n} \psi_{n/2} = \frac{1}{n} \sum_{i=1}^{n} k(x_i, \cdot) - \frac{1}{n^2} \sum_{x \in S^{(1)}} k(x, \cdot) = \mathbb{P}_n k - \mathcal{Q}^{(1)}_{KH} k \right\}
\]
(34)
occurs with probability at least $1 - \sum_{i=1}^{n/2} \delta_i$. Moreover, applying property (vi) of Thm. 3 for $\sigma_{n/2}$ with $c_i = \sqrt{2 \log(2/\delta_i)}$, we obtain that
\[
\sigma_{n/2}^2 \leq \max_{1 \leq i \leq n/2} \|f_i\|_k^2 \cdot 2 \log(\frac{2}{\delta_i})(1 + \frac{1}{2 \log(2/\delta_i)})^2 \leq 4\|k\|_\infty^2 \log(\frac{4}{\delta})
\] (35)
where in step (i), we use the fact that $f_i = k(x_{2i-1}, \cdot) - k(x_{2i}, \cdot)$ satisfies
\[
\|f_i\|_k^2 = k(x_{2i-1}, x_{2i-1}) + k(x_{2i}, x_{2i}) - 2k(x_{2i-1}, x_{2i}) \leq 4\|k\|_\infty.
\]
Recall the definition (7) of $\mathcal{R}_{\text{S},n,k,n}$. Next, we split the proof in two parts: **Case (I)** When $\mathcal{R}_{\text{S},n,k,n} < \mathcal{R}_{\text{S},n}$, and **Case (II)** when $\mathcal{R}_{\text{S},n,k,n} = \mathcal{R}_{\text{S},n}$. We prove the results for these two cases in Apps. G.1.1 and G.1.2 respectively. In the sequel, we make use of the following tail quantity of the kernel:
\[
\overline{\pi}_k(R') \triangleq \sup\{|k(x,y)| : \|x - y\|_2 \geq R'\}.
\] (36)

**G.1.1 Proof for Case (I): When $\mathcal{R}_{\text{S},n,k,n} < \mathcal{R}_{\text{S},n}$**

By definition (7), for this case,
\[
\mathcal{R}_{\text{S},n,k,n} = n^{1 + \frac{1}{d}} \mathcal{R}_{k,n} + n^{\frac{1}{2}} \|k\|_\infty.
\] (37)

On the event $\mathcal{E}_{\text{half}}$, the following lemma provides a high probability bound on $\|\psi_{n/2}\|_\infty$ in terms of the kernel parameters, the sub-Gaussianity parameter $\sigma_{n/2}$ and the size of the cover (Wainwright, 2019, Def. 5.1) of a neighborhood of the input points $(x_i)_{i=1}^n$.

**Lemma 5** (A direct covering bound on $\|\psi_{n/2}\|_\infty$). Fix $R \geq r > 0$ and $\delta' > 0$, and suppose $\mathcal{C}^n(r, R)$ is a set of minimum cardinality satisfying
\[
\bigcup_{i=1}^n B(x_i, R) \subseteq \bigcup_{z \in \mathcal{C}^n(r, R)} B(z, r).
\] (38)

Then, for an $L_k$-Lipschitz kernel $k$, on the event $\mathcal{E}_{\text{half}}$ (34), the event
\[
\mathcal{E}_\infty \triangleq \{ \|\psi_{n/2}\|_\infty \leq \max(n\overline{\pi}_k(R), nL_k r + \sigma_{n/2} \sqrt{2\|k\|_\infty \log(2\|k\|_\infty r)}/\delta') \},
\] (39)
occurs with probability at least $1 - \delta'$, given $\mathcal{F}_n$, where $\overline{\pi}_k$ was defined in (36).

Lem. 5 succeeds in controlling $\psi_{n/2}(x)$ for all $x \in \mathbb{R}^d$ since either $x$ lies far from every input point $x_i$ so that each $k(x_i, x)$ in the expansion (34) is small or $x$ lies near some $x_i$, in which case $\psi_{n/2}(x)$ is well approximated by $\psi_{n/2}(z)$ for $z \in \mathcal{C}^n(r, R)$. The proof inspired by the covering argument of Phillips and Tai (2020, Lem. 2.1) and using the pointwise sub-Gaussianity property of Thm. 3 over the finite cover $\mathcal{C}^n$ can be found in App. G.3.

Now we put together the pieces to prove Thm. 4.

First, (Wainwright, 2019, Lem. 5.7) implies that $|\mathcal{C}^1(r, R)| \leq (1 + 2R/r)^d$ (i.e., any ball of radius $R$ in $\mathbb{R}^d$ can be covered by $(1 + 2R/r)^d$ balls of radius $r$). Thus for an arbitrary $R$, we can conclude that
\[
|\mathcal{C}^n_r| \leq n(1 + 2R/r)^d = (n^{1/d} + 2n^{1/d}R/r)^d.
\] (40)
Second we fix $R$ and $r$ such that $n\tau_k(R) = \|k\|_\infty$ and $nL_k r = \|k\|_\infty$, so that $\frac{R}{r} \leftarrow n\mathcal{R}_{k,n} \frac{L_k}{\|k\|_\infty}$ (c.f. (6) and (36)). Substituting these choices of radii in the bound (39) of Lem. 5, we find that conditional to $\mathcal{E}_{\text{half}} \cap \mathcal{E}_\infty$, we have

$$\|\psi_{n/2}\|_\infty \leq \max(n\tau_k(R), nL_k r + \sigma_{n/2}\sqrt{2\|k\|_\infty \log(2\mathcal{C}(r, R)/\delta')})$$

$$\leq \|k\|_\infty + 2\sqrt{2}\|k\|_\infty \sqrt{\log(\frac{2}{\delta'}) \left[ \log(\frac{2}{\delta'}) + d \log \left( \frac{n}{\delta} + \frac{2L_k}{\|k\|_\infty} \cdot n^{1+\frac{1}{2}} \mathcal{R}_{k,n} \right) \right]}$$

(41)

$$\leq \|k\|_\infty + 2\sqrt{2}\|k\|_\infty \sqrt{\log(\frac{2}{\delta'}) \left[ \log(\frac{2}{\delta'}) + d \log \left( \frac{2L_k}{\|k\|_\infty} (\mathcal{R}_{k,n} + \mathcal{R}_{S_{n,k} n}) \right) \right]}$$

(42)

Putting (34) and (42) together, we conclude

$$\mathbb{P}(\|\mathbb{P}_n k - \mathbb{Q}_{k,H}^{(1)} k\|_\infty > \frac{2}{n} \mathcal{R}_{k,n} (n, 1, d, \delta^*, \delta', \mathcal{R}_{S_{n,k} n})) \leq \mathbb{P}((\mathcal{E}_{\text{half}} \cap \mathcal{E}_\infty))$$

$$\leq \mathbb{P}(\mathcal{E}_{\text{half}}^c) + \mathbb{P}(\mathcal{E}_\infty^c) \leq \delta' + 2\sum_{i=1}^{n/2} \delta_i,$$

as claimed.

G.1.2 PROOF FOR CASE (II): WHEN $\mathcal{R}_{S_{n,k} n} = \mathcal{R}_{S_{n}}$

In this case, we split the proof for bounding $\|\psi_{n/2}\|_\infty$ in two lemmas. First, we relate the $\|\psi_{n/2}\|_\infty$ in terms of the tail behavior of $k$ and the supremum of differences for $\psi_{n/2}$ between any pair points on a Euclidean ball (see App. G.4 for the proof):

**Lemma 6** (A basic bound on $\|\psi_{n/2}\|_\infty$). Conditional on the event $\mathcal{E}_{\text{half}}$ (34), for any fixed $R = R' + \mathcal{R}_{S_{n}}$ with $R' > 0$ and any fixed $\delta' \in (0, 1)$, the event

$$\bar{\mathcal{E}}_\infty = \left\{ \|\psi_{n/2}\|_\infty \leq \max \left( n\tau_k(R'), \sigma_{n/2}\|k\|_\infty \sqrt{2\log(\frac{4}{\delta'}) + \sup_{x,x' \in B(0,R)} \|\psi_{n/2}(x) - \psi_{n/2}(x')\|} \right) \right\},$$

(43)

occurs with probability at least $1 - \delta'/2$, where $\tau_k$ was defined in (36).

Next, to control the supremum term on the RHS of the display (43), we establish a high probability bound in the next lemma. Its proof in App. G.5 proceeds by showing that $\psi_{n/2}$ is an Orlicz process with a suitable metric and then applying standard concentration arguments for such processes.

**Lemma 7** (A high probability bound on supremum of $\psi_{n/2}$ differences). For an $L_k$-Lipschitz kernel $k$, any fixed $R > 0$, $\delta' \in (0, 1)$, given $\mathcal{F}_n$, the event

$$\mathcal{E}_{\sup} \triangleq \left\{ \sup_{x,x' \in B(0,R)} |\psi_{n/2}(x) - \psi_{n/2}(x')| \leq 8D_R \left( \sqrt{\log(\frac{4}{\delta'})} + 6\sqrt{d \log \left( 2 + \frac{L_k R}{\|k\|_\infty} \right)} \right) \right\}$$

(44)

occurs with probability at least $1 - \delta'/2$, where $D_R \triangleq \sqrt{\frac{32}{3}} \sigma_{n/2}\|k\|_\infty \cdot \min(1, \sqrt{\frac{1}{2}L_k R})$. 

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We now turn to the rest of the proof for Thm. 4. We apply both Lem. 6 and 7 with \( R = R_{S_{in}} + R_{k,n} \) (6) and (7). For this \( R \), we have \( R' = R_{k,n} \) in Lem. 6 and hence \( n \tau_k(R') \leq \|k\|_\infty \). Now, condition on the event \( \mathcal{E}_{\text{half}} \cap \mathcal{E}_\infty \cap \mathcal{E}_{\text{sup}} \). Then, we have

\[
\begin{aligned}
n \|p_n k - Q^{(1)}_{KH} k\|_\infty \\
\overset{(34)}{=} & n \|p_n k - Q^{(1)}_{KH} k\|_\infty \\
\overset{(43)}{\leq} & \max(\|k\|_\infty, \sigma_{n/2} \|k\|_\infty \sqrt{2 \log(\frac{4}{\delta'}) + \sup_{x,x' \in B(0,R)} |\psi_{n/2}(x) - \psi_{n/2}(x')|}) \\
\overset{(44)}{\leq} & \max(\|k\|_\infty, \sigma_{n/2} \|k\|_\infty \sqrt{2 \log(\frac{4}{\delta'}) + 
32 \sqrt{\frac{2}{3} \sigma_{n/2} \|k\|_\infty \left( \sqrt{\log(\frac{4}{\delta'})} + 6 \sqrt{d \log(2 + \frac{L_k(R_{S_{in}} + R_{k,n})}{\|k\|_\infty})} \right) \right) \\
\overset{(i)}{\leq} & \max(\|k\|_\infty, 32 \sigma_{n/2} \|k\|_\infty \left( \sqrt{\log(\frac{4}{\delta'})} + 6 \sqrt{d \log(2 + \frac{L_k(R_{S_{in}} + R_{k,n})}{\|k\|_\infty})} \right) \right) \\
\overset{(35)}{\leq} & \|k\|_\infty \cdot 64 \sqrt{\log(\frac{4}{\delta'})} \left( \sqrt{\log(\frac{4}{\delta'})} + 5 \sqrt{d \log(2 + \frac{L_k(R_{S_{in}} + R_{k,n})}{\|k\|_\infty})} \right) \\
\overset{(i)}{\leq} & \|k\|_\infty 2 R_k(n, 1, d, \delta^*, \delta', R_{S_{in}}, k_n),
\end{aligned}
\]

where step (i) follows from the fact that \( D_R \leq \sqrt{\frac{32}{3} \sigma_{n/2} \|k\|_\infty} \), and in step (ii) we have used the working assumption for this case, i.e., \( R_{S_{in}} = R_{S_{in}} \). As a result,

\[
\begin{aligned}
\mathbb{P}(\|p_n k - Q^{(1)}_{KH} k\|_\infty > \frac{2}{n} R_k(n, 1, d, \delta^*, \delta', R_{S_{in}})) \leq & \mathbb{P}(\mathcal{E}_{\text{half}} \cap \mathcal{E}_\infty \cap \mathcal{E}_{\text{sup}}) \\
\leq & \mathbb{P}(\mathcal{E}_\infty^c) + \mathbb{P}(\mathcal{E}_{\text{sup}}^c) + \mathbb{P}(\mathcal{E}_{\text{half}}^c) \leq \delta' + \sum_{i=1}^{n/2} \delta_i,
\end{aligned}
\]

as desired.

**G.2 Proof of part (b): Repeated kernel halving yields a \( 2^m \)-thinned \( L_\infty \) coreset**

The proof follows by applying the arguments from previous section, separately for each round, and then invoking the sub-Gaussianity of a weighted sum of the output functions from each round.

Note that coreset \( S^{(j-1)} \) remains oblivious for the \( j \)-th round of kernel halving. When running kernel halving with the input \( S^{(j-1)} \), let \( f_{i,j}, a_{i,j}, \psi_{i,j}, \alpha_{i,j}, \eta_{i,j} \) denote the analog of the quantities \( f_i, a_i, \psi_i, \alpha_i, \eta_i \) defined in Alg. 3. Thus like in part (a), we can argue that \( \psi_{n/2^j,i} \) is the output of the self-balancing Hilbert walk with oblivious inputs \( (f_{i,j})_{i=1}^{n/2^j} \) and \( (a_{i,j})_{i=1}^{n/2^j} \) with \( a_{i,j} = \max(\|f_{i,j}\|_k \sigma_{i-1,j} \sqrt{2 \log(\frac{4m}{2^{j+1}})}, \|f_{i,j}\|_k^2) \) where we define \( \sigma_{i,j} \) in a recursive manner as in (12) with \( f_{i,j}, a_{i,j}, \sigma_{i,j} \) taking the role of \( f_i, a_i, \sigma_i \) respectively.

With this set-up, first we apply property (i) of Thm. 3 which implies that given \( S^{(j-1)} \), the function \( \psi_{n/2^j,i} \) is \( \sigma_{n/2^j,i} \) sub-Gaussian, where

\[
\sigma_{n/2^j,i}^2 \leq 4 \|k\|_\infty \log(\frac{4m}{2^{j+1}}) \quad \text{with} \quad \delta_j^* = \min(\delta_i)_{i=1}^{n/2^j},
\]

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using an argument similar to (35) with property (vi) of Thm. 3.

Next, we note that for $j$-th round, no Failure occurs when $|a_{i,j}| \leq a_{i,j}$ for all $i \in [n/2^j]$, in which case the coreset $S^{(j)} = (x_i)_{i \in I_j}$ for $I_j = \{2i - \frac{n-j-1}{2} : i \in [n/2^j]\}$, and by property (iii) (exact two-thinning) of Thm. 3 we obtain that the equivalent event

$$E^{(j)}_{\text{half}} = \left\{ \frac{2^j-1}{n} \psi_{n/2^j,j} = \frac{1}{n/2^j} \sum_{x \in S^{(j-1)}} k(x, \cdot) - \frac{1}{n/2^j} \sum_{x \in S^{(j)}} k(x, \cdot) \right\}$$

occurs with probability at least $1 - \sum_{s=1}^{n/2^j} \delta_s \frac{2^j-1}{m}$. Then conditional on the event of no Failure for all $m$ rounds, equivalent to $\cap_{j=1}^m E^{(j)}_{\text{half}}$, we have

$$\Pr_n k - Q^{(m)}_{KH} = \frac{1}{n} \sum_{x \in S_m} k(x, \cdot) - \frac{1}{n/2^m} \sum_{x \in S^{(m)}} k(x, \cdot) = \frac{1}{n} \sum_{j=1}^m \frac{2^j-1}{n} \psi_{n/2^j,j}$$

where we abuse notation $S^{(0)} \equiv S_m$ in step (i) for simplicity of expressions.

Next, we use the following basic fact:

**Lemma 8** (Sub-Gaussian additivity). For a sequence of random variables $(Z_j)_{j=1}^m$ such that $Z_j$ is a $\sigma_j$ sub-Gaussian variable conditional on $(Z_1, \ldots, Z_{j-1})$, the random variable $Z = \sum_{j=1}^m \theta_j Z_j$ is $(\sum_{j=1}^m \theta_j^2 \sigma_j^2)^{1/2}$ sub-Gaussian.

**Proof** We will prove the result for $Z_s = \sum_{j=1}^s \theta_j Z_j$ by induction on $s \leq m$. The result holds for the base case of $s = 0$ as $Z_0 = 0$ is 0 sub-Gaussian. For the inductive case, suppose the result holds for $s$. Then we may apply the tower property, our conditional sub-Gaussianity assumption, and our inductive hypothesis in turn to conclude

$$\mathbb{E}[e^{\sum_{j=1}^{s+1} \theta_j Z_j}] = \mathbb{E}[e^{\sum_{j=1}^{s+1} \theta_j Z_j} | \mathbb{E}[e^{\theta_{s+1} Z_{s+1} | Z_1:s}] \leq \mathbb{E}[e^{\sum_{j=1}^s \theta_j Z_j}] e^{\frac{\sum_{j=1}^{s+1} \theta_j^2 \sigma_j^2}{2}} = e^{\frac{\sum_{j=1}^{s+1} \theta_j^2 \sigma_j^2}{2}}.$$ 

Hence, $Z_{s+1}$ is $(\sum_{j=1}^{s+1} \theta_j^2 \sigma_j^2)^{1/2}$ sub-Gaussian, and the proof is complete. ■

Applying Lem. 8 to the sequence $(\psi_{n/2^j,j})_{j=1}^m$, we conclude that, the random variable

$$W_m \equiv \sum_{j=1}^m \frac{2^j-1}{n} \psi_{n/2^j,j}$$

is sub-Gaussian with parameter

$$\sigma_{W_m} \equiv \frac{2}{\sqrt{3}} \frac{2}{\sqrt{m}} \sqrt{\|k\|_{\infty} \log(\frac{6m^2}{\sigma_{W_m}^2})} \geq \sqrt{\|k\|_{\infty} \sum_{j=1}^m 4^j \log(\frac{4m}{2^{j+1}})} \geq \sqrt{\sum_{j=1}^m (\frac{2^j-1}{n} \sigma_{n/2^j,j}^2)^2},$$

conditional to the input $S_m$, where step (ii) follows since

$$\|k\|_{\infty} \sum_{j=1}^m 4^j \log(\frac{4m}{2^{j+1}}) \geq 4\|k\|_{\infty} \sum_{j=1}^m 4^{j-1} \log(\frac{4m}{2^{j+1}}) \geq \sum_{j=1}^m 4^{j-1} \sigma_{n/2^j,j}^2,$$

and step (iii) follows from the fact that $\delta^* = \min(\delta_j^*)_{j=1}^m$. Now to prove step (i), we note that

$$\mathcal{G}_1 \equiv \sum_{j=1}^m 4^j = \frac{4}{3}(4^m - 1) \leq \frac{4}{3} 4^m, \quad \text{and} \quad \mathcal{G}_2 \equiv \sum_{j=1}^m j 4^j = \frac{4m^2}{3} - \frac{4m}{3},$$
which in turn implies that

\[
\sum_{j=1}^m 4 \psi \log(\frac{4m}{2^j \delta'}) = \mathcal{G}_1 \log(\frac{4m}{\delta^*}) - \log 2 \cdot \mathcal{G}_2 = \mathcal{G}_1 \left( \log(\frac{4m}{\delta^*}) + \frac{\log 2}{3} \right) - \frac{4m \log 2}{3} \cdot 4^m \\
\leq \mathcal{G}_1 \cdot \log(\frac{6m}{\delta^*}) - \frac{4m \log 2}{3} \cdot 4^m \\
\leq \frac{4}{3} 4^m \cdot \log(\frac{6m}{\delta^*}) - \frac{4}{3} 4^m \cdot \log 2 = \frac{4}{3} 4^m \cdot \log(\frac{6m}{2 \delta^*}),
\]

thereby establishing step (i).

Next, analogous to the proof of part (a), we split the proof in two parts: **Case (I)** when \( \mathcal{R}_{S_{m,k,n}} < \mathcal{R}_{S_{m}} \), in which case, we proceed with a direct covering argument to bound \( \|W_m\|_\infty \) using a lemma analogous to Lem. 5; and **Case (II)** when \( \mathcal{R}_{S_{m,k,n}} = \mathcal{R}_{S_{m}} \), in which case, we proceed with a metric-entropy based argument to bound \( \|W_m\|_\infty \) using two lemmas that are analogous Lems. 6 and 7.

**G.2.1 Proof for Case (I): When \( \mathcal{R}_{S_{m,k,n}} < \mathcal{R}_{S_{m}} \)**

Recall that for this case, \( \mathcal{R}_{S_{m,k,n}} \) is given by (37). The next lemma provides a high probability control on \( \|W_m\|_\infty \). Its proof can be derived by replacing \( \psi_n/2 \) with \( nW_n \), and repeating the direct covering argument, and the sub-Gaussian tail bounds from Lem. 5, and is omitted for brevity.

**Lemma 9** (A direct covering bound on \( \|W_m\|_\infty \)). Fix \( R \geq r > 0 \) and \( \delta' > 0 \), and recall the definition (38) of \( C^n(r, R) \). Then, for an \( L_\mathbf{k} \)-Lipschitz kernel \( \mathbf{k} \), on the event \( \bigcap_{j=1}^m \mathcal{E}^{(j)}_{\text{half}} \) (48), the event

\[
\mathcal{E}^{(m)}_\infty \triangleq \left\{ \|W_m\|_\infty \leq \max\left( 2^m \tau_\mathbf{k}(R), 2^m L_\mathbf{k}r + \sigma W_n \sqrt{2\|\mathbf{k}\|_\infty \log(2C^n(r, R)/\delta')} \right) \right\},
\]

occurs with probability at least \( 1 - \delta' \), given \( F_n \), where \( \tau_\mathbf{k} \) was defined in (36).

Next, we repeat arguments similar to those used earlier around the display (41) and (42). Fix \( R \) and \( r \) such that \( \tau_\mathbf{k}(R) = \|\mathbf{k}\|_\infty /n \) and \( L_\mathbf{k}r = \|\mathbf{k}\|_\infty /n \), so that \( R \leftarrow n\mathcal{R}_{k,n} L_\mathbf{k} / \|\mathbf{k}\|_\infty \) (c.f. (6) and (36)). Substituting these choices of radii in the bound (52) of Lem. 9, we find that conditional to \( \bigcap_{j=1}^m \mathcal{E}^{(j)}_{\text{half}} \cap \mathcal{E}^{(m)}_\infty \), we have

\[
\|p_n \mathbf{k} - \mathfrak{Q}_{KH}^{(m)} \mathbf{k}\|_\infty \overset{(49)}{=} \left\| \sum_{j=1}^m \frac{2^{j-1}}{n} \psi_{n/2^j} \right\|_\infty \overset{(50)}{=} \|W_m\|_\infty \overset{(52)}{\leq} \max\left( 2^m \tau_\mathbf{k}(R), 2^m L_\mathbf{k}r + \sigma W_n \sqrt{2\|\mathbf{k}\|_\infty \log(2C^n(r, R)/\delta')} \right) \overset{(i)}{\leq} \frac{2^m}{n} \|\mathbf{k}\|_\infty \left( 1 + 2 \sqrt{\frac{2}{3}} \sqrt{\log\left( \frac{6m}{2 \delta^*} \right) \left[ \log\left( \frac{2}{\delta'} \right) + d \log\left( n^{\frac{1}{2}} + 2L_\mathbf{k} / \|\mathbf{k}\|_\infty \cdot n^{1 + \frac{1}{2}} \mathcal{R}_{k,n} \right) \right]} \right) \overset{(37)}{\leq} \frac{2^m}{n} \|\mathbf{k}\|_\infty \left( 1 + 2 \sqrt{\frac{2}{3}} \sqrt{\log\left( \frac{6m}{2 \delta^*} \right) \left[ \log\left( \frac{2}{\delta'} \right) + d \log\left( \frac{2L_\mathbf{k}}{\|\mathbf{k}\|_\infty} \left( \mathcal{R}_{k,n} + \mathcal{R}_{S_{m,k,n}} \right) \right) \right]} \right) \overset{(8)}{\leq} \|\mathbf{k}\|_\infty \cdot \frac{2^m}{n} \mathcal{M}_\mathbf{k}(n, m, d, \delta^*, \delta', \mathcal{R}_{S_{m,k,n}}),
\]

35
where in step (i), we have used the bounds (40) and (51). Putting the pieces together, we conclude
\[
\mathbb{P}(\|P_n k - Q^{(m)}_{KH} k\|_\infty \leq \|k\|_\infty \cdot \frac{2m}{n} \mathcal{M}_k(n, m, d, \delta^*, \delta', \mathcal{R}_{S_{m,k,n}})) \\
\geq \mathbb{P}(\cap_{j=1}^m \mathcal{E}_{\text{half}}^{(j)} \cap \mathcal{E}_\infty^{(m)}) = 1 - \mathbb{P}(\cap_{j=1}^m \mathcal{E}_{\text{half}}^{(j)} \cap \mathcal{E}_\infty^{(m)})^c \\
\geq 1 - \mathbb{P}((\mathcal{E}_\infty^{(m)})^c) - \sum_{j=1}^m \mathbb{P}((\mathcal{E}_{\text{half}}^{(j)})^c)^{(48)} \leq 1 - \delta' - \sum_{j=1}^m \sum_{i=1}^{n/2^j} \delta_i \cdot \frac{2^{j-1}}{m},
\]
as claimed for this case.

G.2.2 Proof for Case (II): When $\mathcal{R}_{S_{m,k,n}} = \mathcal{R}_{S_{m}}$

In this case, we make use of two lemmas. Their proofs (omitted for brevity) can be derived essentially by replacing $\psi_{n/2}$ and $\sigma_{n/2}$ with $\mathcal{W}_m$ (50) and $\sigma_{\mathcal{W}_m}$ (51) respectively, and repeating the proof arguments from Lems. 6 and 7.

Lemma 10 (A basic bound on $\|\mathcal{W}_m\|_\infty$). Conditional on the event $\cap_{j=1}^m \mathcal{E}_{\text{half}}^{(j)}$ (48), given $\mathcal{F}_n$, for any fixed $R = R' + \mathcal{R}_{S_{m}}$ with $R' > 0$ and any fixed $\delta' \in (0, 1)$, the event
\[
\tilde{\mathcal{E}}_\infty^{(m)} = \left\{ \|\mathcal{W}_m\|_\infty \leq \max \left( 2^m \tau_k(R'), \sigma_{\mathcal{W}_m} \|k\|_k^{1/2} \sqrt{2 \log \left( \frac{4}{\delta} \right)} + \sup_{x,x' \in B(0, R)} |\mathcal{W}_m(x) - \mathcal{W}_m(x')| \right) \right\},
\]
occurs with probability at least $1 - \delta'/2$, where $\tau_k(R') \triangleq \sup \{ |k(x, y)| : \|x - y\|_2 \geq R' \}$.

Lemma 11 (A high probability bound on supremum of $\mathcal{W}_m$ differences). For an $L_k$-Lipschitz kernel $k$, any fixed $R > 0, \delta' \in (0, 1)$, given $\mathcal{S}_{m}$, the event
\[
\mathcal{E}_{\text{sup}}^{(m)} \triangleq \left\{ \sup_{x,x' \in B(0, R)} |\mathcal{W}_m(x) - \mathcal{W}_m(x')| \leq 8D_R \left( \sqrt{\log \left( \frac{4}{\delta'} \right)} + 6 \sqrt{d \log \left( 2 + \frac{L_k R}{\|k\|_\infty} \right)} \right) \right\}
\]
occurs with probability at least $1 - \delta'/2$, where $D_R \triangleq \sqrt{\frac{32}{3} \sigma_{\mathcal{W}_m} \|k\|_k^{1/2} \min \left( 1, \frac{1}{2} \sqrt{L_k R} \right)}$

Mimicking the arguments like those in display (45) and (46), with $R = \mathcal{R}_{S_{m}} + \mathcal{R}_{k,n},$ and $R' = \mathcal{R}_{k,n},$ we find that conditional on the event $\tilde{\mathcal{E}}_\infty^{(m)} \cap \mathcal{E}_{\text{sup}}^{(m)} \cap_{j=1}^m \mathcal{E}_{\text{half}}^{(j)}$, 
\[
\|P_n k - Q^{(m)}_{KH} k\|_\infty \stackrel{(49)}{=} \|\sum_{j=1}^m \frac{2^{j-1}}{n} \psi_{n/2^j} \|_\infty \\
\stackrel{(50)}{=} \|\mathcal{W}_m\|_\infty \\
\leq \max(\frac{2^m}{n} \|k\|_\infty, 32 \sigma_{\mathcal{W}_m} \|k\|_k^{1/2} \left( \sqrt{\log \left( \frac{4}{\delta'} \right)} + 5 \sqrt{d \log \left( 2 + \frac{L_k \mathcal{R}_{S_{m}} + \mathcal{R}_{k,n}}{\|k\|_\infty} \right)} \right)) \\
\stackrel{(51)}{\leq} \|k\|_\infty \cdot \frac{2^m}{n} \cdot 37 \sqrt{\log \left( \frac{6}{\sqrt{2^{m}}} \right)} \left( \sqrt{\log \left( \frac{4}{\delta'} \right)} + 5 \sqrt{d \log \left( 2 + \frac{L_k \mathcal{R}_{S_{m}} + \mathcal{R}_{k,n}}{\|k\|_\infty} \right)} \right) \\
\stackrel{(8)}{=} \|k\|_\infty \cdot \frac{2^m}{n} \mathcal{M}_k(n, m, d, \delta^*, \delta', \mathcal{R}_{S_{m}}),
\]
which happens with probability at least
\[
\mathbb{P}(\tilde{E}^{(m)} \cap E^{(m)} \cap \bigcap_{j=1}^{m} E^{(m)}_{\text{half}}) = 1 - \mathbb{P}(\tilde{E}^{(m)} \cap E^{(m)} \cap \bigcap_{j=1}^{m} E^{(m)}_{\text{half}}^c)
\]
\[
\geq 1 - \mathbb{P}(\tilde{E}^{(m)}_\infty^c) - \mathbb{P}(E^{(m)}_{\text{sup}}^c) - \sum_{j=1}^{m} \mathbb{P}(E^{(m)}_{\text{half}}^c)
\]
\[
\geq 1 - \delta' \frac{n}{2} - \delta' \frac{n}{2} - \sum_{j=1}^{m} \frac{n}{2^j} \delta_i \frac{2^{j-1}}{m},
\]
as claimed. The proof is now complete.

**G.3 Proof of Lem. 5: A direct covering bound on** \( \|\psi_{n/2}\|_\infty \)

We claim that conditional on the event \( \mathcal{E}_{\text{half}} \) (34), we deterministically have

\[
\|\psi_{n/2}\|_\infty \leq \max\{n\tau_k(R), nL_k r + \max_{z \in \mathcal{C}^n(r,R)} |\psi_{n/2}(z)|\}, \tag{53}
\]

and the event

\[
\{\max_{z \in \mathcal{C}^n(r,R)} |\psi_{n/2}(z)| \leq \sigma_{n/2} \sqrt{2\|k\|_\infty \log(2\mathcal{C}(r,R)/\delta')} \}
\]

occurs with probability at least \( 1 - \delta' \), conditional on \( \mathcal{F}_n \). Putting these two claims together yields the lemma. We now prove these two claims separately.

**G.3.1 Proof of (53)**

Note that on the event \( \mathcal{E}_{\text{half}} \) (34) we have

\[
\psi_{n/2} = n(\mathbb{P}_n k - \tilde{Q}_n k) = \sum_{i=1}^{n} \eta_i k(x_i, \cdot) \tag{55}
\]

for some \( \eta_i \in \{-1, 1\} \). Now fix any \( x \in \mathbb{R}^d \), and introduce the shorthand \( \mathcal{C}^n = \mathcal{C}^n(r,R) \). The result follows by considering two cases.

**Case 1** \( x \notin \bigcup_{i=1}^{n} \mathcal{B}(x_i, R) \) In this case, we have \( \|x - x_i\|_2 \geq R \) for all \( i \in [n] \) and therefore, representation (55) yields that

\[
|\psi_{n/2}(x)| = |\sum_{i=1}^{n} \eta_i k(x_i, x)| \leq \sum_{i=1}^{n} |\eta_i| |k(x_i, x)| = \sum_{i=1}^{n} |k(x_i, x)| \leq n\tau_k(R),
\]

by Cauchy-Schwarz’s inequality and the definition (36) of \( \tau_k \).

**Case 2** \( x \in \bigcup_{i=1}^{n} \mathcal{B}(x_i, R) \) By the definition (38) of our cover \( \mathcal{C}^n \), there exists \( z \in \mathcal{C}^n \) such that \( \|x - z\|_2 \leq r \). Therefore, on the event \( \mathcal{E}_{\text{half}} \), using representation (55), we find that

\[
|\psi_{n/2}(x)| \leq |\sum_{i=1}^{n} \eta_i k(x_i, x)| = |\sum_{i=1}^{n} \eta_i (k(x_i, x) - k(x_i, z) + k(x_i, z))|
\]
\[
\leq |\sum_{i=1}^{n} \eta_i (k(x_i, x) - k(x_i, z))| + |\sum_{i=1}^{n} \eta_i k(x_i, z)|
\]
\[
\leq \sum_{i=1}^{n} |k(x_i, x) - k(x_i, z)| + |\psi_{n/2}(z)|
\]
\[
\leq nL_k r + \sup_{z' \in \mathcal{C}^n} |\psi_{n/2}(z')|,
\]

by Cauchy-Schwarz’s inequality.
G.3.2 Proof of (54)

Introduce the shorthand $C^n = C^n(r, R)$. Then applying the union bound, the pointwise sub-Gaussian property (iv) of Thm. 3, and the sub-Gaussian Hoeffding inequality (Wainwright, 2019, Prop. 2.5), we find that

$$
\mathbb{P}(\max_{z \in C^n} |\psi_n/2(z)| > t \mid F_{n/2}) \leq \sum_{z \in C^n} 2\exp(-t^2/(2\sigma_n^2 k(z, z)))
\leq 2|C^n| \exp(-t^2/(2\sigma_n^2 \|k\|_\infty)) = \delta',
$$

for $t = \sigma_n/2\sqrt{2\|k\|_\infty \log(2|C^n|/\delta')}$,

as claimed.

G.4 Proof of Lem. 6: A basic bound on $\|\psi_n/2\|_\infty$

For any $R > 0$, we deterministically have

$$
\|\psi_n/2\|_\infty \leq \max(\sup_{x \in B(0, R)} |\psi_n/2(x)|, \sup_{x \in B^c(0, R)} |\psi_n/2(x)|)
$$

Since $R = R' + 2\delta_n$, for any $x \in B^c(0, R)$, we have $\|x - x_i\|_2 \geq R'$ for all $i \in \{n\}$. Thus conditional on the event $E_{\text{half}}$, applying property (ii) from Thm. 3, we find that

$$
|\psi_n/2(x)| = |\sum_{i=1}^n \eta_i k(x_i, x)| \leq \sum_{i=1}^n |\eta_i| \|k(x_i, x)| = \sum_{i=1}^n |k(x_i, x)| \leq n\pi_k(R'),
$$

by Cauchy-Schwarz's inequality and the definition (36) of $\pi_k$.

For the first term on the RHS of (56), we have

$$
\sup_{x \in B(0, R)} |\psi_n/2(x)| \leq |\psi_n/2(0)| + \sup_{x \in B(0, R)} |\psi_n/2(x) - \psi_n/2(0)| \leq |\psi_n/2(0)| + \sup_{x, x' \in B(0, R)} |\psi_n/2(x) - \psi_n/2(x')|.
$$

Now, the sub-Gaussianity of $\psi_n/2$ (property (iv) of Thm. 3) with $x = 0$, and the sub-Gaussian Hoeffding inequality (Wainwright, 2019, Prop. 2.5) imply that

$$
|\psi_n/2(0)| \leq \sigma_n/2\sqrt{2k(0, 0) \log(4/\delta')} \leq \sigma_n/2\sqrt{2\|k\|_\infty \log(4/\delta')},
$$

with probability at least $1 - \delta'/2$, given $F_n$. Putting the pieces together completes the proof.

G.5 Proof of Lem. 7: A high probability bound on supremum of $\psi_n/2$ differences

The proof proceeds by using concentration arguments for Orlicz processes Wainwright (2019, Def. 5.5). Given a set $T \subseteq \mathbb{R}^d$, a random process $\{Z_x, x \in T\}$ is called an Orlicz $\Psi_2$-process with respect to the metric $\rho$ if

$$
\|Z_x - Z_{x'}\|_{\Psi_2} \leq \rho(x, x') \quad \text{for all} \quad x, x' \in T,
$$

where for any random variable $Z$, its Orlicz $\Psi_2$-norm is defined as

$$
\|Z\|_{\Psi_2} = \inf\{\lambda > 0 : \mathbb{E}[\exp(Z^2/\lambda^2)] \leq 2\}.
$$

Our next result (see App. G.6 for the proof) establishes that $\psi_n/2$ is an Orlicz process with respect to a suitable metric. (For clarity, we use $B_2$ to denote the Euclidean ball.)
Lemma 12 (ψ_{n/2} is an Orlicz Ψ_2-process). Given \( \mathcal{F}_n \) and any fixed \( R > 0 \), the random process \( \{ψ_{n/2}(x), x ∈ \mathcal{B}_2(0; R)\} \) is an Orlicz Ψ_2-process with respect to the metric \( ρ \) defined in (58), i.e.,

\[
\|ψ_{n/2}(x) - ψ_{n/2}(x')\|_{\mathcal{F}_n} ≤ ρ(x, x') \text{ for all } x, x' ∈ \mathcal{B}_2(0; R),
\]

where the metric \( ρ \) is defined as

\[
ρ(x, x') = \sqrt{\frac{3}{2}} · σ_{n/2} \cdot \min(√{2L_k \|x - x'\|_2}, 2√{\|k\|_∞}).
\]  

(58)

Given Lem. 12, we can invoke high probability bounds for Orlicz processes. For the Orlicz process \( \{ψ_{n/2}(x), x ∈ \mathcal{T}\} \), given any fixed \( δ' \in (0, 1] \), Wainwright (2019, Thm 5.36) implies that

\[
\sup_{x,x' ∈ \mathcal{T}} |ψ_{n/2}(x) - ψ_{n/2}(x')| ≤ 8\left( J_{T, ρ}(D) + D √{\log(4/δ')} \right),
\]

(59)

with probability at least \( 1 - δ'/2 \) given \( \mathcal{F}_n \), where \( D = \sup_{x,x' ∈ \mathcal{T}} ρ(x, x') \) denotes the \( ρ \)-diameter of \( \mathcal{T} \), and the quantity \( J_{T, ρ}(D) \) is defined as

\[
J_{T, ρ}(D) ≜ \int_0^D √{\log(1 + N_{T, ρ}(u))} du.
\]

(60)

Here \( N_{T, ρ}(u) \) denotes the \( u \)-covering number of \( \mathcal{T} \) with respect to metric \( ρ \), namely the cardinality of the smallest cover \( \mathcal{C}_{T, ρ}(u) ⊆ \mathbb{R}^d \) such that

\[
\mathcal{T} ⊆ \bigcup_{z ∈ \mathcal{C}_{T, ρ}(u)} \mathcal{B}_ρ(z; u) \quad \text{where} \quad \mathcal{B}_ρ(z; u) ≜ \{x ∈ \mathbb{R}^d : ρ(z, x) ≤ u\}.
\]

(61)

To avoid confusion, let \( \mathcal{B}_2 \) denote the Euclidean ball (metric induced by \( \|\cdot\|_2 \)). Then in our setting, we have \( \mathcal{T} = \mathcal{B}_2(0; R) \) and hence

\[
D_R ≜ \sup_{x,x' ∈ \mathcal{B}_2(0; R)} ρ(x, x') = \min\left(√{\frac{3}{2}}, σ_{n/2}√{\frac{32\|k\|_∞}{3}}\right), \text{ with } β_R = \frac{32}{3} σ_{n/2}^2 L_k R.
\]

(62)

Some algebra establishes that this definition of \( D_R \) is identical to that specified in Lem. 7. Next, we derive bounds for \( N_{T, ρ} \) and \( J_{T, ρ} \) (see App. G.7 for the proof).

Lemma 13 (Bounds on \( N_{T, ρ} \) and \( J_{T, ρ} \)). For an \( L_k \)-Lipschitz kernel \( k \), \( \mathcal{T} = \mathcal{B}_2(0; R) \) with \( R > 0 \), and \( ρ \) defined in (58), we have

\[
N_{T, ρ}(u) ≤ (1 + β_R/u^2)^d, \quad \text{and}
\]

\[
J_{T, ρ}(D_R) ≤ \sqrt{d} D_R \left[ 3 + √{2\log(β_R/D_R^2)} \right],
\]

(63)

(64)

where \( D_R \) and \( β_R \) are defined in (62).

Doing some algebra, we find that

\[
β_R = \max\left(2, \frac{L_k R}{\|k\|_∞}\right) ≤ 2 + \frac{L_k R}{\|k\|_∞}.
\]

(65)

Moreover, note that \( 3 + √{2\log(2 + a)} ≤ 6 √{\log(2 + a)} \) for all \( a ≥ 0 \), so that the bound (64) can be simplified to

\[
J_{T, ρ}(D_R) ≤ 6 √{d} D_R √{\log(2 + \frac{L_k R}{\|k\|_∞})}.
\]

(66)

Substituting the bound (66) in (59) yields that the event \( \mathcal{E}_{sup} \) defined in (44) holds with probability at least \( 1 - δ'/2 \) conditional to \( \mathcal{F}_n \), as claimed.
G.6 Proof of Lem. 12: $\psi_{n/2}$ is an Orlicz $\Psi_2$-process

The proof of this lemma follows from the sub-Gaussianity of $\psi_{n/2}$ established in Thm. 3. Introduce the shorthand $Y \triangleq \psi_{n/2}(x) - \psi_{n/2}(x')$. Applying property (i) of Thm. 3 with $u = k(x, \cdot) - k(x', \cdot)$ along with the reproducing property of the kernel $k$, we find that for any $t \in \mathbb{R}$,

$$\mathbb{E}[\exp(tY) \mid \mathcal{F}_n] = \mathbb{E}[\exp(t(\psi_{n/2}(x) - \psi_{n/2}(x'))) \mid \mathcal{F}_n] \leq \exp(\frac{1}{2}t^2\sigma_{n/2}^2\|k(x, \cdot) - k(x', \cdot)\|_k^2).$$

That is, the random variable $Y$ is sub-Gaussian with parameter $\sigma_Y \triangleq \sigma_{n/2}\|k(x, \cdot) - k(x', \cdot)\|_k$, conditional to $\mathcal{F}_n$. Next, (Wainwright, 2019, Thm 2.6 (iv)) yields that $\mathbb{E}[\exp(\frac{3}{8}\sigma_Y^2) \mid \mathcal{F}_n] \leq 2$, which in turn implies that

$$\|Y\|_{\Psi_2} \leq \sqrt{\frac{8}{3}}\sigma_Y.$$

Moreover, we have

$$\|k(x, \cdot) - k(x', \cdot)\|_k^2 = k(x, x) - k(x, x') + k(x', x') - k(x', x) \leq \min(2L_k\|x - x'\|_2, 4\|k\|_\infty),$$

using the Lipschitzness of $k$ and the definition of $\|k\|_\infty$ (4). Putting the pieces together along with the definition (58) of $\rho$, we find that $\|Y\|_{\Psi_2} \leq \rho(x, x')$ thereby yielding the claim (57).

G.7 Proof of Lem. 13: Bounds on $N_{r, \rho}$ and $\mathcal{J}_{r, \rho}$

We use the relation of $\rho$ to the Euclidean norm $\|\cdot\|_2$ to establish the bound (63). The definitions (58) and (61) imply that

$$B_2(z; \frac{u^2}{\alpha}) \subseteq B_\rho(z; u) \quad \text{for} \quad \alpha \triangleq \frac{16}{\pi}\sigma_{n/2}^2L_k,$$

since $\rho(x, x') \leq \sqrt{\alpha\|x - x'\|_2}$. Consequently, any $u^2/\alpha$-cover $C$ of $\mathcal{T}$ in the Euclidean ($\|\cdot\|_2$) metric automatically yields a $u$-cover of $\mathcal{T}$ in $\rho$ metric as we note that

$$B_2(0; R) \subseteq \bigcup_{z \in C}B_2(z; \frac{u^2}{\alpha}) \subseteq \bigcup_{z \in C}B_\rho(z; u).$$

Consequently, the smallest cover $C_{r, \rho}(u)$ would not be larger than than the smallest cover $C_{r, \|\cdot\|_2}(u^2/\alpha)$, or equivalently:

$$N_{r, \rho}(u) \leq N_{r, \|\cdot\|_2}(\frac{u^2}{\alpha}) \leq (1 + 2R\alpha/u^2)^d,$$

where inequality (i) follows from Wainwright (2019, Lem 5.7) using the fact that $\mathcal{T} = B_2(0; R)$. Noting that $\beta_R = 2R\alpha$ yields the bound (63).

We now use the bound (63) on the covering number to establish the bound (64).
Proof of bound on $\mathcal{J}_{\kappa, \rho}$ Applying the definition (60) and the bound (63), we find that

$$\mathcal{J}_{\kappa, \rho}(\kappa) \leq \int_0^{\kappa} \sqrt{\log(1 + (1 + \kappa^2)/u^2)} du$$

where step (i) follows from a change of variable $s \leftarrow \sqrt{s}$. Note that $\log(1 + a) \leq \log a + 1/a$, and $\sqrt{a} + b \leq \sqrt{a} + \sqrt{b}$ for any $a, b \geq 0$. Applying these inequalities, we find that

$$\log(1 + (1 + s)^d) \leq d \log(2 + s) \leq d \log s + \frac{1}{a} + \frac{1}{1+a} \leq d (\log s + \frac{2}{s})$$

for $s \in [\kappa^2 \log^2 \kappa, \infty) \subseteq [2, \infty)$. Consequently,

$$\int_{\kappa^2 \log^2 \kappa}^{\infty} s^{-3/2} \sqrt{\log(1 + (1 + s)^d)} ds \leq \sqrt{d} \int_{\kappa^2 \log^2 \kappa}^{\infty} \left( \frac{\sqrt{\log s}}{\sqrt{2}} + \frac{\sqrt{2}}{s} \right) ds.$$  (68)

Next, we note that

$$\int_{\kappa^2 \log^2 \kappa}^{\infty} \frac{\sqrt{2}}{s^2} ds = \sqrt{2} \sqrt{\log \kappa},$$  (69)

$$\int_{\kappa^2 \log^2 \kappa}^{\infty} \frac{\sqrt{\log s}}{s} ds = -2 \sqrt{\log \kappa} - \frac{1}{\sqrt{2}} \log(\frac{1}{\sqrt{2}} + \frac{1}{\sqrt{2} + \sqrt{\log 2}}),$$  (70)

where step (i) follows from the following bound on the incomplete Gamma function:

$$\Gamma\left(\frac{1}{2}, a\right) = \int_a^{\infty} \frac{1}{\sqrt{t}} e^{-t} dt \leq \frac{1}{\sqrt{a}} \int_a^{\infty} e^{-t} dt = a^{-\frac{1}{2}} e^{-a} \quad \text{for any} \quad a > 0.$$  

Putting the bounds (67) to (70) together, we find that

$$\mathcal{J}_{\kappa, \rho}(\kappa) \leq \sqrt{d} \kappa \left( \frac{\sqrt{\log \kappa}}{\sqrt{2}} + \sqrt{2} \left( \sqrt{\log(\kappa) / \kappa^2} + 1 / \sqrt{\log(\kappa) / \kappa^2} \right) \right).$$

Note that by definition (62) $\frac{\sqrt{\log \kappa}}{\sqrt{2}} \leq \frac{1}{\sqrt{2}}$. Using this observation and the fact that $\frac{1}{\sqrt{2}} + \sqrt{\log 2} \leq 3$ yields the claimed bound (64).

H. Derivation of Tab. 1: Square-root kernels $k_{rt}$ for common kernels $k$

In this appendix, we derive the results stated in Tab. 1.

H.1 General proof strategy

Let $\mathcal{F}$ denote the Fourier operator (16). In Tab. 4, we state the continuous $\kappa$ such that $k(x, y) = \kappa(x - y)$ in the first column, its Fourier transform (16) $\hat{k}$ in the second column, the square-root Fourier transform in the third column, and the square-root kernel in the fourth column, given by $k_{rt}(x, y) = \frac{1}{(2\pi)^{d/2}} \kappa_{rt}(x - y)$ with $\kappa_{rt} = \mathcal{F}(\sqrt{\hat{k}})$. Prop. 2 along with expressions in Tab. 4 directly establishes the validity of the square-root kernels for the Gaussian and (scaled) B-spline kernels. For completeness, we also illustrate the remaining calculus for the B-spline kernels in App. H.3. We do a similar calculation in App. H.2 for the Matérn kernel for better exposition of the involved expressions.


| Expression for \( \kappa(z) \) | Expression for Fourier transform of \( \kappa \cdot \hat{\kappa}(\omega) \) | Square-root Fourier transform: \( \sqrt{\hat{\kappa}(\omega)} \) | Expression for \( \kappa_{rt}(z) \) |
|---------------------------------|-------------------------------------------------|--------------------------|-------------------------------|
| \( \exp\left(-\frac{||z||^2}{2\sigma^2}\right) \) | \( \sigma^d \exp\left(-\frac{\sigma^2||z||^2}{2}\right) \) | \( \sigma^\frac{d}{2} \exp\left(-\frac{\sigma^2||z||^2}{4}\right) \) | \( \left(\frac{2}{\pi\sigma^2}\right)^\frac{d}{2} \exp\left(-\frac{||z||^2}{\sigma^2}\right) \) |
| \( \prod_{j=1}^{d} \otimes^{\beta+d/2} 1_{[-\frac{1}{2}, \frac{1}{2}]}(z_j) \) | \( \left(\frac{4^d+1}{\sqrt{2\pi}}\right) \prod_{j=1}^{d} \sum_{l=1}^{\beta+d/2} \sin^d(l\omega_j/2) \omega_j^{\beta+d/2} \) | \( \left(\frac{4^d+1}{\sqrt{2\pi}}\right) \prod_{j=1}^{d} \sin^d(\omega_j/2) \omega_j^{\beta+d/2} \) | \( \prod_{j=1}^{d} \otimes^{\beta+1} 1_{[-\frac{1}{2}, \frac{1}{2}]}(z_j) \) |

Table 4: Fourier transforms of kernels \( k(x,y) = \kappa(x-y) \) and square-root kernels \( k_{rt}(x,y) = \kappa_{rt}(x-y) \) from Tab. 1. Here \( \mathcal{F} \) denotes the Fourier operator (16), and \( \otimes^d \) denotes the convolution operator applied \( \ell - 1 \) times, with the convention \( \otimes^0 f = f \) and \( \otimes^2 f = f \otimes f \) for \( (f \otimes g)(x) = \int f(y)g(x-y)dy \). Each Fourier transform is derived from (Sriperumbudur et al., 2010, Tab. 2).

### H.2 Deriving \( k_{rt} \) for the Matérn kernel

For \( k = \text{Matérn}(\nu, \gamma) \) from Tab. 1, we have

\[
\kappa(x,y) = \phi_{d,\nu,\gamma} \cdot \Phi_{\nu,\gamma}(x-y) \quad \text{where} \quad \Phi_{\nu,\gamma}(z) = c_{\nu}\left(\frac{\|z\|_2}{\gamma}\right)^{\nu - \frac{d}{2}} K_{\nu - \frac{d}{2}}(\gamma \|z\|_2), \tag{71}
\]

and \( K_a \) denotes the modified Bessel function of third kind of order \( a \) (Wendland, 2004, Def. 5.10). That is, for Matérn kernel with \( k(x,y) = \kappa(x-y) \), the function \( \kappa \) is given by \( \kappa = \phi_{d,\nu,\gamma} \cdot \Phi_{\nu,\gamma} \). Now applying (Wendland, 2004, Thm. 8.15), we find that

\[
\mathcal{F}(\Phi_{\nu,\gamma}) = \frac{1}{(\gamma^2 + \|z\|^2)^\nu} \quad \implies \quad \mathcal{F}(\sqrt{\mathcal{F}(\Phi_{\nu,\gamma})}) = \frac{1}{(2\pi)^{d/2}} \Phi_{\nu/2,\gamma},
\]

where in the last step we also use the facts that \( \Phi_{\nu,\gamma} \) is an even function and \( \sqrt{\mathcal{F}(\Phi_{\nu,\gamma})} \in L^1 \) for all \( \nu > d/2 \). Thus, by Prop. 2, a valid square-root kernel \( k_{rt}(x,y) = \kappa_{rt}(x-y) \) is defined via

\[
\kappa_{rt} = \sqrt{\phi_{d,\nu,\gamma}} \frac{1}{(2\pi)^{d/4}} \Phi_{\nu/2,\gamma}, \quad \implies \quad k_{rt} = A_{\nu,\gamma,d} \cdot \text{Matérn}(\nu/2, \gamma), \tag{72}
\]

where \( A_{\nu,\gamma,d} \triangleq \left(\frac{1}{\pi\gamma^2}\right)^{d/4} \frac{\Gamma(\nu)}{\Gamma(\nu-d/2)} \frac{\Gamma((\nu-d)/2)}{\Gamma(\nu/2)} \). \tag{73}

### H.3 Deriving \( k_{rt} \) for the B-Spline kernel

For positive integers \( \beta, d \), define the constants

\[
\mathfrak{B}_\beta \triangleq \frac{1}{(\beta-1)!} \sum_{j=0}^{\lceil\beta/2\rceil} (-1)^j \binom{\beta}{j} (\beta - j)^{\beta-1}, \quad S_{\beta,d} \triangleq \mathfrak{B}_\beta^{-d}, \quad \text{and} \quad \bar{S}_{\beta,d} \triangleq \frac{\sqrt{S_{2\beta+2,d}}}{S_{\beta+1,d}}. \tag{74}
\]

Define the function \( \chi_\beta : \mathbb{R}^d \to \mathbb{R} \) as follows:

\[
\chi_\beta(z) \triangleq S_{\beta,d} \prod_{i=1}^{d} f_\beta(z_i). \tag{75}
\]
Then for kernel \( k = \text{B-spline}(2\beta + 1) \), we have
\[
k(x, y) = \chi_{2\beta+2}(x - y).
\] (76)

The second row of Tab. 4 implies that
\[
(\frac{d}{2\beta})^{\frac{d}{2}} F(\sqrt{\mathcal{F}(\chi_{2\beta+2})}) = \frac{\sqrt{S_{\beta+2,d}}}{S_{\beta+1,d}} \cdot \chi_{\beta+1} \equiv \overline{S}_{\beta,d} \cdot \chi_{\beta+1},
\] (74)
where we also use the fact that \( \chi_{\beta} \) is an even function. Putting the pieces together with Prop. 2, we conclude that
\[
k_{rt} = \overline{S}_{\beta,d} \cdot \text{B-spline}(\beta),
\] (77)
(with \( \kappa_{rt} = \overline{S}_{\beta,d} \chi_{\beta+1} \)) is a valid square-root kernel for \( k = \text{B-spline}(2\beta + 1) \).

I. Derivation of Tab. 2: Kernel thinning MMD guarantee under \( \mathbb{P} \) and \( k_{rt} \) tail decay

We consider four different growth conditions for the input point radius \( R_{S_{in}} \) arising from four forms of target distribution tail decay: (1) \textbf{Compact} (\( R_{S_{in}} \lesssim \sqrt{\log n} \)), (2) \textbf{SubGauss} (\( R_{S_{in}} \lesssim \log n \)), (3) \textbf{SubExp} (\( R_{S_{in}} \lesssim \log n \)), and (4) \textbf{HeavyTail} (\( R_{S_{in}} \lesssim n^{1/\rho} \)). The first is typical when \( \mathbb{P} \) is supported on a compact set like the unit cube \([0, 1]^d\). The remainder hold in expectation and with high probability when \( \mathbb{P} \) has, respectively, sub-Gaussian tails, sub-exponential tails, or sub-polynomial tails, as the inverse multiquadric kernels of Tab. 6. As we demonstrate in expression (111) of App. H, up to constants depending on \( \delta, \delta', ||k_{rt}||_{\infty}, \) and \( \frac{L_{k_{rt}}}{||k_{rt}||_{\infty}} \), the MMD guarantee of Thm. 1 can be simplified as follows:

\[
\text{MMD}_{k}(S_{in}, S_{KT}) \lesssim ||k_{rt}||_{\infty} \left( C_{\max(\mathcal{R}_{k_{rt,n}}, \mathcal{R}_{S_{in}})}^{d (\frac{||k_{rt}||_{\infty}}{d})^2} d^{\frac{d}{2}} \frac{\log n}{n} \log \left( \frac{L_{k_{rt}}}{||k_{rt}||_{\infty}} \right) \right),
\] (78)

for some universal constant \( C \), where to simplify the expressions, we have used the fact that \( \mathcal{R}_{S_{in}, k_{rt,n}} \leq \mathcal{R}_{S_{in}} \) (7). Tab. 2 now follows from plugging the assumed growth rate bounds into the estimate (78).
J. Derivation of Tab. 3: Explicit bounds on Thm. 1 quantities for common kernels

We start by collecting some common tools in App. J.1 that we later use for our derivations for the Gaussian, Matérn and B-spline kernels in Apps. J.2 to J.4 respectively. Finally, in App. J.5, we put the pieces together to derive explicit MMD rates, as a function of $d$, $n$, $\delta$ and kernel parameters for the three kernels, and summarize the rates in Tab. 5. (This table is complementary to the generic results stated in Tab. 2.)

J.1 Common tools for our derivations

We collect some simplified expressions, and techniques that come handy in our derivations to follow.

Simplified bounds on $\mathcal{M}_{\kappa_{rt}}$ From (8), we have

$$\mathcal{M}_{\kappa_{rt}}(n, \frac{1}{2} \log_2 n, d, \frac{\delta}{n}, \delta', R) \lesssim \sqrt{\log \frac{n}{\delta} \log \left( \frac{L_{\kappa_{rt}}}{\|\kappa_{rt}\|_\infty} \cdot (\mathcal{M}_{\kappa_{rt}}, n + R) \right)}$$

Thus, given (79), to get a bound on $\mathcal{M}_{\kappa_{rt}}$, we need to derive bounds on $(L_{\kappa_{rt}}, \|\kappa_{rt}\|_\infty, \mathcal{M}_{\kappa_{rt}}, n)$ for various kernels to obtain the desired guarantees on MMD and $L^\infty$ coresets.

Bounds on Gamma function Our proofs make use of the bounds from Batir (2017, Thm 2.2) on the Gamma function:

$$\Gamma(b + 1) \geq \frac{b}{e} \sqrt{2\pi b} \text{ for any } b \geq 1, \text{ and } \Gamma(b + 1) \leq \frac{b}{e} \sqrt{2\pi b} \text{ for any } b \geq 1. \quad (80)$$

General tools for bounding Lipschitz constant To bound the Lipschitz constant $L_{\kappa_{rt}}$, the following two observations come in handy. For a radial kernel $\kappa_{rt}(x, y) = \kappa_{rt}(\|x - y\|_2)$ with $\kappa_{rt} : \mathbb{R}_+ \to \mathbb{R}$, we note

$$\sup_{\|y - z\|_2 \leq r} |\kappa_{rt}(x, y) - \kappa_{rt}(x, z)| \leq \sup_{a > 0, b \leq r} |\kappa_{rt}(a) - \kappa_{rt}(a + b)| \leq \|\kappa_{rt}'\|_\infty r$$

$$\implies \quad L_{\kappa_{rt}} \leq \|\kappa_{rt}'\|_\infty. \quad (81)$$

For a translation-invariant kernel $\kappa_{rt}(x, y) = \kappa_{rt}(x - y)$ with $\kappa_{rt} : \mathbb{R}^d \to \mathbb{R}$, we use the bound

$$\sup_{\|y - z\|_2 \leq r} |\kappa_{rt}(x, y) - \kappa_{rt}(x, z)| = \sup_{\|z'\|_2 \leq r} |\kappa_{rt}(z') - \kappa_{rt}(z'')|$$

$$\leq \sup_{z' \in \mathbb{R}^d} \|\nabla \kappa_{rt}(z')\|_2 r,$$

$$\implies \quad L_{\kappa_{rt}} \leq \sup_{z' \in \mathbb{R}^d} \|\nabla \kappa_{rt}(z')\|_2 \leq \sqrt{d} \sup_{z' \in \mathbb{R}^d} \|\nabla \kappa_{rt}(z')\|_\infty, \quad (82)$$

where step (i) follows from Cauchy-Schwarz’s inequality (and is handy when coordinate wise control on $\nabla \kappa_{rt}$ is easier to derive). We later apply the inequality (81) for the Gaussian and Matérn kernels, and (82) for the B-spline kernel.
J.2 Proofs for Gaussian kernel

For the kernel $k = \text{Gauss}(\sigma)$ and its square-root kernel $k_{\text{rt}} = \left(\frac{2}{\pi \sigma^2}\right)^{\frac{d}{2}} \text{Gauss}(\frac{\sigma}{\sqrt{2}})$, we claim the following bounds on various quantities

$$\|k_{\text{rt}}\|_{\infty} = \left(\frac{2}{\pi \sigma^2}\right)^{\frac{d}{2}} \quad \text{and} \quad \|k\|_{\infty} = 1, \quad (83)$$

$$L_{k_{\text{rt}}} \leq \left(\frac{2}{\pi \sigma^2}\right)^{\frac{d}{2}} \frac{\sqrt{2/e}}{\sigma} \implies \frac{L_{k_{\text{rt}}}}{\|k_{\text{rt}}\|_{\infty}} \overset{(83)}{=} \frac{1}{\sigma} \sqrt{2/e} \quad (84)$$

$$R_{k_{\text{rt}},n} = \sigma \sqrt{\log n}, \quad (85)$$

$$R_{k_{\text{rt}},\sqrt{n}}^\dagger = \mathcal{O}(\sigma \sqrt{d + \log n}). \quad (86)$$

Substituting these expressions in (79), we find that

$$\mathfrak{M}_{k_{\text{rt}}} \left(n, \frac{1}{2} \log_2 n, d, \frac{\delta}{2\pi}, \delta', R\right) \lesssim \sqrt{\log(n)} \left[\log \frac{1}{\delta'} + d \log \left(\sqrt{\log n} + \frac{R}{\sigma}\right)\right],$$

as claimed in Tab. 3.

**Proof of claims (83) to (86)** The claim (83) follows directly from the definition of $k_{\text{rt}}$. The bound (84) on $L_{k_{\text{rt}}}$ follows from the fact $\|d/\sigma^2\|_{\infty} = \sqrt{2/e}$ and invoking the relation (81). Next, recalling the definition (6) and noting that

$$\sup_{x,y: \|x-y\|_2 \geq r} |k_{\text{rt}}(x,y)| \leq \left(\frac{2}{\pi \sigma^2}\right)^{\frac{d}{2}} e^{-r^2/\sigma^2}$$

implies the bound (85) on $R_{k_{\text{rt}},n}$.

Next, we have

$$\tau^2_{k_{\text{rt}}}(R) = \int_{\|z\|_2 \geq R} \left(\frac{2}{\pi \sigma^2}\right)^{\frac{d}{2}} \exp(-2\|z\|_2^2/\sigma^2)dz = \mathbb{P}_{X \sim \mathcal{N}(0, \sigma^2/4, I_d)}(\|X\|_2 \geq R) \overset{(i)}{=} e^{-R^2/\sigma^2}, \quad (87)$$

for $R \geq \sigma \sqrt{2d}$, where step (i) follows from the standard tail bound for a chi-squared random variable $Y$ with $k$ degree of freedom (see (Laurent and Massart, 2000, Lem. 1)): $\mathbb{P}(Y - k > 2\sqrt{kt} + 2t) \leq e^{-t}$, wherein we substitute $k = d$, $Y = \frac{d}{\sigma^2} \|X\|^2$, $t = d\alpha$ with $\alpha \geq 2$, and $R^2 = \sigma^2 t$. Using the tail bound (87), the bound (83) on $\|k_{\text{rt}}\|_{\infty}$ and the definition (6) of $R_{k_{\text{rt}},\sqrt{n}}^\dagger$, we find that

$$R_{k_{\text{rt}},\sqrt{n}}^\dagger = \mathcal{O}(\sigma \max(\sqrt{(\log n - \frac{d}{2} \log(\sigma \sqrt{\frac{\pi}{2}}))_+}, \sqrt{d})) = \mathcal{O}(\sigma \sqrt{d + \log n}).$$

yielding the claim (86).

J.3 Proofs for Matérn kernel

Recall the notations from (71) to (73) for the Matérn kernel related quantities. Let $K_b$ denote the modified Bessel function of the third kind with order $b$ (Wendland, 2004,
Def. 5.10). Let $a \triangleq \frac{\nu - d}{2}$. Then, the kernel $\mathbf{k} = \text{Matérn}(\nu, \gamma)$ and its square-root kernel $\mathbf{k}_{rt} = A_{\nu, \gamma, d} \cdot \text{Matérn}(\nu, \gamma)$ satisfy
\[ \mathbf{k}(x, y) = \tilde{\kappa}_{\nu - d/2}(\gamma \|x - y\|_2), \quad \text{and} \]
\[ \mathbf{k}_{rt}(x, y) = A_{\nu, \gamma, d} \tilde{\kappa}_0(\gamma \|x - y\|_2), \tag{88} \]
where $\tilde{\kappa}_0(r) \triangleq c_b \rho^b K_b(r)$, and $c_b = \frac{2^{1-b}}{\Gamma(b)}$. \[ \tag{89} \]

We claim the following bounds on various quantities assuming $a \geq 2.2$, and $d \geq 2$:
\[ \|\mathbf{k}_{rt}\|_\infty = A_{\nu, \gamma, d} \quad \text{and} \quad \|\mathbf{k}\|_\infty = 1, \tag{91} \]
\[ A_{\nu, \gamma, d} \leq 5\nu \left(\frac{\gamma^2}{2\pi(a-1)}\right)^{\frac{d}{2}}, \tag{92} \]
\[ L_{\mathbf{k}_{rt}} \leq A_{\nu, \gamma, d} \frac{C_1 \gamma}{\sqrt{a} + C_2} \quad \implies \quad \frac{L_{\mathbf{k}_{rt}}}{\|\mathbf{k}_{rt}\|_\infty} \leq \frac{C_1 \gamma}{\sqrt{a} + C_2}, \tag{93} \]
\[ \mathfrak{R}_{\mathbf{k}_{rt}, n} = \frac{1}{\gamma} \mathcal{O}(\max(\log n - a \log(1 + a), C_2 a \log(1 + a))), \tag{94} \]
\[ \mathfrak{R}_{\mathbf{k}_{rt}, \sqrt{n}} = \frac{1}{\gamma} \mathcal{O}(a + \log n + d \log(\frac{\sqrt{2\pi}}{\gamma}) + \log(\frac{(\nu - 2)\nu - 3}{2(a-1)a^2 + 1})) \tag{95} \]

We prove these claims in App. J.3.1 through App. J.3.5. Putting these bounds together with (79) yields that
\[ \mathfrak{m}_{\text{Matérn}}(n, \frac{1}{2} \log_2 n, d, \frac{d}{2\pi}, \delta', R) \preccurlyeq \begin{cases} \sqrt{\log \left(\frac{n}{\delta}\right)} \left[ \log \frac{1}{\delta} + d \log \left(\frac{1}{\sqrt{1 + a}} \cdot (\log n + \gamma R)\right) \right] & \text{if } a = o(\log n) \\ \sqrt{\log \left(\frac{n}{\delta}\right)} \left[ \log \frac{1}{\delta} + d \log(\sqrt{a} \log(1 + a) + \gamma R) \right] & \text{if } a = \Omega(\log n) \end{cases} \]
with $B = a \log(1 + a)$, as claimed in Tab. 3.

J.3.1 SET-UP FOR PROOFS OF MATÉRN KERNEL QUANTITIES

Before proceeding to the proofs of the claims (91) to (95), we collect some handy inequalities. Applying Wendland (2004, Lem. 5.13, 5.14), we have
\[ \tilde{\kappa}_a(\gamma r) \leq \min \left(1, \sqrt{2\pi c_a(\gamma r)^{a-\frac{1}{2}} e^{-\gamma r + \frac{a^2}{2\gamma}}} \right) \quad \text{for} \quad r > 0. \tag{96} \]

For a large enough $r$, we also establish the following bound:
\[ \tilde{\kappa}_a(\gamma r) \leq \min(1, 4c_a(\gamma r)^{a-1} e^{-\gamma r/2}) \quad \text{for} \quad \gamma r \geq 2(a - 1), a \geq 1. \tag{97} \]

6. When $a \in (1, 2.2)$, and $d \in [1, 2)$, analogous bounds with slightly different constants follow from employing the Gamma function upper bound of Batir (2017, Thm 2.3) in place of our upper bound (80). For brevity, we omit these derivations.
Proof of (97) Noting the definition (90) of $\kappa$, it suffices to show the following bound:

$$|K_a(r)| \leq \frac{1}{r}e^{-r/2} \quad \text{for} \quad r/2 \geq a - 1,$$

where $K_a$ is the modified Bessel function of the third kind. Using (Wendland, 2004, Def. 5.10), we have

$$K_a(r) = \frac{1}{2} \int_0^\infty e^{-r \cosh t} \cosh(at) dt \leq \int_0^\infty e^{-\frac{r}{2} e^t} e^{at} dt \equiv \int_{r/2}^\infty e^{-s(\frac{2a}{r})} \cdot \frac{1}{s} ds \leq \frac{1}{r}e^{-r/2}$$

where step (i) uses the following inequalities: $\cosh t \triangleq \frac{1}{2}(e^t + e^{-t}) \geq \frac{1}{2}e^t$ and $\cosh(at) \leq e^{at}$ for $a > 0, t > 0$, step (ii) follows from a change of variable $s \leftarrow \frac{r}{2} e^t$, and finally step (iii) uses the following bound on the incomplete Gamma function obtained by substituting $B = 2$ and $A = a$ in Borwein and Chan (2009, Eq. 1.5):

$$\int_r^\infty t^{a-1}e^{-t} dt \leq 2r^{a-1}e^{-r} \quad \text{for} \quad r \geq a - 1.$$

The proof is now complete.

J.3.2 Proof of the bound (91) on $\|k_r\|_\infty$ and $\|k\|_\infty$

We claim that

$$\|\tilde{k}_b\|_\infty = 1 \quad \text{for all} \quad b > 0.$$  \hspace{1cm} (98)

where was defined in (90). Putting the equality (98) with (88), (89), and (96) immediately implies the bounds (91) on the $\|k_r\|_\infty$ and $\|k\|_\infty$. To prove (98), we follow the steps from the proof of (Wendland, 2004, Lem. 5.14). Using (Wendland, 2004, Def. 5.10), for $b > 0$ we have

$$K_b(r) = \frac{1}{2} \int_{-\infty}^\infty e^{-r \cosh t} e^{bt} dt = \frac{1}{2} \int_{-\infty}^\infty e^{-\frac{r}{2}(e^t + e^{-t})} e^{bt} dt = k^{-b} \frac{1}{2} \int_0^\infty e^{-r/2(u/k+k/u)} u^{b-1} du$$

where the last step follows by substituting $u = ke^t$. Setting $k = r/2$, we find that

$$r^{b} K_b(r) = 2^{b-1} \int_0^\infty e^{-u}e^{r/2(4u)} u^{b-1} du \leq 2^{b-1} \Gamma(b),$$

where we achieve equality in the last step when we take the limit $r \to 0$. Noting that $\tilde{k}_b(r) = \frac{2^{1-b}}{\Gamma(b)} r^{b} K_b(r)$ (90) yields the claim (98).

J.3.3 Proof of the bound (92) on $A_{\nu, \gamma, d}$

Using the definition (73) we have $A_{\nu, \gamma, d} = (\frac{1}{4\pi} \gamma^2)^{\frac{d}{4}} \cdot A'_{\nu, \gamma, d}$, where

$$A'_{\nu, \gamma, d} = \sqrt{\frac{\Gamma(\nu-1/2)}{\Gamma(\nu-d/2)}} \cdot \frac{\Gamma((\nu-d)/2)}{\Gamma(\nu/2)} \leq \sqrt{\frac{e^{\frac{1}{2}(\nu-1)\sqrt{\nu-1}}}{\nu^{\nu/2}} \cdot \sqrt{2\pi}} \cdot \frac{(\nu-d-2)^{\frac{\nu-d-2}{2}}}{(\nu-d)^{\frac{\nu-d-2}{2}}} \cdot \sqrt{\Gamma(\nu-d/2)/(\nu-d-1)}$$

$$\leq \left(\frac{2^3}{(2\pi)^3}\right)^{\frac{3}{4}} \left(\frac{2\sqrt{\nu}}{\nu}\right)^{\nu-2} \cdot \sqrt{\nu-1} \cdot \frac{(\nu-1)^{\frac{1}{4}}}{\nu} \cdot \frac{(\nu-d-2)^{\frac{\nu-d-2}{2}}}{(\nu-d)^{\frac{\nu-d-2}{2}}} \cdot \frac{(\nu-d-2)/(\nu-1)^{\frac{d}{2}}}{\nu-d/2}$$

$$\leq \left(\frac{2^3\sqrt{2\pi}}{(2\pi)^3}\right)^{\frac{3}{4}} \left(\frac{2\sqrt{\nu}}{\nu}\right)^{\nu-2} \cdot \sqrt{\nu} \cdot \sqrt{\nu-2} \cdot (\nu-1)^{\frac{1}{4}} \cdot (\nu-1)^{\frac{d}{2}} + \frac{(\nu-d-2)/(\nu-1)^{\frac{d}{2}}}{\nu-d/2}$$

$$\leq \left(\frac{2^3\sqrt{2\pi}}{(2\pi)^3}\right)^{\frac{3}{4}} \left(\frac{2\sqrt{\nu}}{\nu}\right)^{\nu-2} \cdot (\nu-1)^{\frac{1}{4}} \cdot (\nu-\frac{d}{2} - 1)^{\frac{d}{2}} \cdot (\nu-d/2)^{-\frac{d}{4}}.$$
As a result, we have
\[ A_{\nu,\gamma,d} = \left( \frac{1}{4\pi} \gamma^2 \right)^{d/4}, \quad A'_{\nu,\gamma,d} \leq 5\nu \left( \frac{\gamma^2}{\pi^{(d-2)}} \right)^{\frac{d}{4}} = 5\nu \left( \frac{\gamma^2}{2\pi^{(a-1)}} \right)^{\frac{d}{4}}, \]
as claimed.

**J.3.4 Proof of the bound (93) on \( L_{k_{\alpha}} \)**

To derive a bound on the Lipschitz constant \( L_{k_{\alpha}} \), we bound the derivative of \( \bar{\kappa}_a \). Using \((r^a K_a(r))' = -r^a K_{a-1}(r)\) (Wendland, 2004, Eq. 5.2), we find that
\[ (\bar{\kappa}_a(\gamma r))' = c_a \frac{d}{dr}((\gamma r)^a K_a(\gamma r)) = -\frac{c_a}{c_{a-1}} \gamma^2 r \tilde{\kappa}_{a-1}(\gamma r). \]

Using (96), we have
\[ \frac{c_a}{c_{a-1}} \gamma^2 r \tilde{\kappa}_{a-1}(\gamma r) \leq \frac{c_a}{c_{a-1}} \min \left( r, \sqrt{2\pi c_{a-1}}(\gamma r)^a \frac{1}{2} e^{-r^2/4} \right) \quad \text{for } r > 0. \]

And (97) implies that
\[ \frac{c_a}{c_{a-1}} \gamma^2 r \tilde{\kappa}_{a-1}(\gamma r) \leq \frac{c_a}{c_{a-1}} \min(\gamma r, 4c_{a-1}(\gamma r)^{a-1} e^{-2\gamma r/2}) \quad \text{for } r \geq 2(a-2), a \geq 2. \]

Next, we make use of the following observations: The function \( t^b e^{-t/2} \) achieves its maximum at \( t = 2b \). Then for any function \( f : \mathbb{R}_+ \rightarrow \mathbb{R}_+ \) such that \( f(t) \leq t \) for all \( t \geq 0 \) and \( f(t) \leq \min(t, C t^b e^{-t/2}) \) for \( t > t^\dagger \) with \( t^\dagger < 2b \), we have
\[ \sup_{t \geq 0} f(t) \leq \min(2b, C(2b)^b e^{-b}). \]

As a result, we conclude that
\[ \sup_{t \geq 0} \frac{c_a}{c_{a-1}} \gamma^2 r \tilde{\kappa}_{a-1}(\gamma r) \leq \frac{c_a}{c_{a-1}} \min(2(a-1), 4c_{a-1}(2(a-1))^{a-1} e^{-a+1}). \quad (99) \]

Substituting the value of \( c_{a-1} \) and the bound (80), we can bound the second argument inside the min on the RHS of (99) (for \( a \geq 3 \)) as follows:
\[ 4c_{a-1}(2(a-1))^{a-1} e^{-a+1} \leq 4 \cdot 2^{2-a} \frac{1}{\sqrt{2\pi(a-2)}} \left( \frac{e}{a-2} \right)^{a-2} 2^{a-1} (a-1)^{a-1} e^{1-a} \]
\[ \leq \frac{8}{e^{2\pi}} (1 + (1/a)^{a-2} \left( \sqrt{a-2} + \frac{1}{\sqrt{a-2}} \right)) \leq \frac{8}{\pi^{a-2}} \]
for \( a \geq 3 \). When \( a \in [2,3) \), one can directly show that \( 4c_{a-1}(2(a-1))^{a-1} e^{-a+1} \leq 8/e \). Putting the pieces together, and noting that \( \frac{c_a}{c_{a-1}} = \frac{1}{\max(2(a-1),1)} \), we find that
\[ \sup_{t \geq 0} \frac{c_a}{c_{a-1}} \gamma^2 r \tilde{\kappa}_{a-1}(\gamma r) \leq \frac{c_a}{c_{a-1}} \frac{\gamma}{\max(2(a-1),1)} \min(2(a-1), \frac{8}{e} + \frac{8}{\pi^{a-2}}) \leq \frac{C_1 \gamma}{\sqrt{a+C_2}} \]
for any \( a \geq 2 \). And hence
\[ L_{k_{\alpha}} \leq A_{\nu,\gamma,d} \sup_{t \geq 0} |\kappa'_a(\gamma r)| \leq A_{\nu,\gamma,d} \frac{C_1 \gamma}{\sqrt{a+C_2}} \frac{C_1 \gamma}{\sqrt{a+C_2}} \]
as claimed.
J.3.5 Proof of the bound \((94)\) on \(R_{k_t,n}\)

Using arguments similar to those used to obtain \((100)\), we find that

\[
\max_{\gamma r \geq 2(a-1)} \tilde{\kappa}_a(\gamma r) \leq 4c_a(2(a-1))^{a-1}e^{-(a-1)} \leq \sqrt{\frac{4}{a-1}} = \sqrt{\frac{8}{\nu-d-2}}.
\]

Next, note that

\[
(\gamma r)^{a-\frac{1}{2}}e^{-\gamma r + \frac{a^2}{2\gamma r}} \preceq e^{-\gamma r/2} \quad \text{for} \quad \gamma r \gtrsim a \log(1 + a), \tag{101}
\]

\[
c_a = \frac{2^{1-a}}{\Gamma(a)} \leq \left(\frac{2a}{a-1}\right)^{a-1} \frac{1}{\sqrt{2\pi(a-1)}},
\]

where \((101)\) follows from standard algebra. Thus, we have

\[
\begin{align*}
\max_{\gamma r \geq 2(a-1)} \tilde{\kappa}_a(\gamma r) & \leq c_a \exp(-\gamma r/2) \quad \text{for} \quad \gamma r \gtrsim a \log(1 + a) \\
& \overset{\text{(80)}}{\Rightarrow} R_{k_t,n} \preceq \frac{1}{\gamma} \max(\log n - a \log(1 + a), C_1a \log(1 + a)),
\end{align*}
\]

as claimed.

J.3.6 Proof of the bound \((95)\) on \(R_{k_t,\sqrt{n}}\)

Let \(V_d = \pi^{d/2}/\Gamma(d/2 + 1)\) denote the volume of unit Euclidean ball in \(\mathbb{R}^d\). Using \((89)\), we have

\[
\frac{1}{A_{\nu,\gamma,d}} \tau_{k_t}^2(R) = \int_{\|z\|_2 \geq R} \tilde{\kappa}_a^2(\gamma \|z\|_2)dz = dV_d \int_{r > R} r^{d-1} \tilde{\kappa}_a^2(\gamma r)dr
\]

\[
\overset{\text{(96)}}{\leq} 2\pi c_a^2 dV_d \int_{r > R} r^{d-1}(\gamma r)^2 \exp(-2\gamma r + \frac{a^2}{\gamma r})dr
\]

\[
= 2\pi c_a^2 dV_d \gamma^{1-d} \int_{r > R} (\gamma r)^{\nu-2} \exp(-2\gamma r + \frac{a^2}{\gamma r})dr \tag{102}
\]

where we have also used the fact that \(2a + d = \nu\). Next, we note that

\[
\exp(-2\gamma r + \frac{a^2}{\gamma r}) \leq \exp(-\frac{3}{2}\gamma r) \quad \text{for} \quad \gamma r \geq \sqrt{2a}
\]

For any integer \(b > 1\), noticing that \(f(t) = \frac{1}{\Gamma(b)} t^{b-1}e^{-t}\) is the density function of an Erlang distribution with shape parameter \(b\) and rate parameter 1, and using the expression for its complementary cumulative distribution function, we find that

\[
\int_{t}^{\infty} t^{b-1}e^{-t}dt = \Gamma(b) \sum_{i=0}^{b-1} \frac{r^i}{i!}e^{-r}
\]

\[
\overset{(104)}{\Rightarrow}
\]

Thus, for \(R > \frac{\sqrt{2}}{\gamma} a\), we have

\[
\int_{r > R} (\gamma r)^{\nu-2} \exp(-2\gamma r + \frac{a^2}{\gamma r})dr \overset{(103)}{\leq} \int_{r > R} (\gamma r)^{\nu-2} \exp(-\frac{3}{2}\gamma r)dr
\]

\[
= \frac{1}{\gamma} \left(\frac{3}{2}\right)^{\nu-1} \int_{\gamma R/2}^{\infty} t^{\nu-2}e^{-t}dt
\]

\[
= \frac{1}{\gamma} \left(\frac{3}{2}\right)^{\nu-1} \Gamma(\nu - 1)e^{-\frac{3}{2}\gamma R} \sum_{i=0}^{\nu-1} \left(3\gamma R/2\right)^i
\]

\[
\leq \frac{1}{\gamma} \Gamma(\nu - 1)e^{-\frac{3}{2}\gamma R} c_\gamma R \leq \frac{1}{\gamma} \Gamma(\nu - 1)e^{-\frac{3}{2}\gamma R} \tag{105}
\]

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Putting the bounds (102) and (105) together for \( R \geq \frac{\nu - d}{\sqrt{2\gamma}} \), we find that

\[
\tau_{krt}^2 (R) \leq A_{\nu,\gamma,d}^2 \cdot \gamma^{-d} \cdot 2\pi^{2 - 2a} \cdot \frac{\pi^2}{\Gamma(a)} \cdot \frac{d^2}{\Gamma(\frac{d}{2} + 1)} \cdot \Gamma(\nu - 1) \exp\left(-\frac{1}{2} \gamma R\right).
\]

Using (80), we have

\[
2\pi^{2 - 2a} \cdot \frac{d^2}{\Gamma(\frac{d}{2} + 1)} \cdot \Gamma(\nu - 1) \leq 2\pi \cdot \frac{22 - 2a \cdot e^{2(a - 1)}}{2\pi(a - 1)(a - 1)^{2(a - 1)} \cdot \frac{\pi^2}{\Gamma(a)} \cdot \frac{d^2}{\Gamma(\frac{d}{2} + 1)} \cdot e \sqrt{\nu - 2(\nu - \frac{1}{a})} e^{-2}} \approx \frac{2}{\sqrt{e}} (2a - 2d) + (2\pi \cdot d^2 \cdot (\nu - 2)^{d - 2}) - (2a - 1) \cdot d^2 / (\nu - 2) \cdot \gamma^{-3 / 2}
\]

Putting the bounds (102) and (105) together for \( R \geq \frac{\nu - d}{\sqrt{2\gamma}} \), we find that \( \mathfrak{M}_{\nu,\gamma,d} (6) \) can be bounded as

\[
\mathfrak{M}_{krt,\sqrt{n}}^\dagger \leq \frac{2}{\gamma} \cdot \max\left(\frac{a}{\sqrt{a}}, \log n + \log \left(\frac{2}{\sqrt{e}}\right) + d \log\left(\sqrt{\nu} / \gamma\right) + \log\left(\frac{(\nu - 2)^{\nu - \frac{3}{2}}}{(2(a - 1))^2(a - 1)^2} \right)\right)
\]

\[
\leq \frac{1}{\gamma} \cdot \left(\frac{a}{\log n} + \log \left(\sqrt{\nu} / \gamma\right) + \log\left(\frac{(\nu - 2)^{\nu - \frac{3}{2}}}{(2(a - 1))^2(a - 1)^2} \right)\right),
\]

as claimed.

### J.4 Proofs for B-spline kernel

Recall the notations from (74) to (77). Then, the kernel \( k = \text{B-spline}(2\beta + 1) \) and its square-root kernel \( k_{\text{rt}} = \overline{S}_{\beta,d} \cdot \text{B-spline}(\beta) \) satisfy

\[
\|k\|_{\infty} = \overline{S}_{\beta,d} \Rightarrow c_{\beta} \cdot \text{B-spline}(\beta) \Rightarrow \begin{cases} 
\frac{2}{\sqrt{\beta}} & \text{when } \beta = 1 \\
\leq 1 & \text{when } \beta > 1
\end{cases}
\]

\[
\|k\|_{\infty} = 1,
\]

\[
\mathfrak{M}_{k_{\text{rt}}} \leq \frac{4}{3} \sqrt{\beta},
\]

\[
\mathfrak{M}_{k_{\text{rt}}} \leq \sqrt{d(\beta + 1) / 2}, \quad \text{and} \quad \mathfrak{M}_{k_{\text{rt}}}^\dagger \leq \sqrt{d(\beta + 1) / 2}.
\]

While claims (i) and (ii) follow directly from the definitions in the display (74), claim (iii) can be verified numerically, e.g., using SciPy (Virtanen et al., 2020). From numerical verification, we also find that the constant \( c_{\beta} \) in (106) is decreasing with \( \beta \). See App. J.4.1 for the proofs of the remaining claims. Finally, substituting various quantities from (106), (108), and (109) in (79), we find that

\[
\mathfrak{M}_{k_{\text{rt}}}^{\text{B-spline}} \left(n, \frac{1}{2} \log_2 n, d, \frac{\delta}{2n}, \delta', R\right) \leq \sqrt{\log\left(\frac{n}{\delta}\right) + \log(d \log(d\beta + \sqrt{dR})}. 
\]
J.4.1 Proofs of the bounds on B-spline kernel quantities

We start with some basic set-up. Consider the (unnormalized) univariate B-splines

\[ f_\beta : \mathbb{R} \to [0, 1] \quad \text{with} \quad f_\beta(a) = \oplus_\beta^1 1_{[-\frac{1}{2}, \frac{1}{2}]}(a) = \frac{1}{(\beta-1)!} \sum_{j=0}^{\beta} (-1)^j (\frac{\beta}{2} - j)^{\beta-1} \]

where step (i) follows from Schumaker (2007, Eqn 4.46, 4.47, 4.59, p.135, 138). Noting that \( f_\beta \) is an even function with a unique global maxima at 0 (see Schumaker (2007, Ch 4.) for more details), we find that

\[ \| f_\beta \|_\infty = f_\beta(0) = \frac{1}{(\beta-1)!} \sum_{j=0}^{[\beta/2]} (-1)^j (\frac{\beta}{2} - j)^{\beta-1} \]

(74) \( \mathfrak{B}_\beta \).

Bounds on \( \| k \|_\infty \) and \( \| k_{rt} \|_\infty \) Recalling (75) and (76), we find that

\[ \| k \|_\infty = \| \chi_{2\beta+2} \|_\infty = S_{2\beta+2,d} \| f_{2\beta+2} \|_\infty = S_{2\beta+2,d} \mathfrak{B}_\beta^{d} = 1, \]

thereby establishing (107).

Bounds on \( L_{k_{rt}} \) We have

\[ f'_{\beta+1}(a) = \int f_{\beta}(b) \frac{d}{db} 1_{[-\frac{1}{2}, \frac{1}{2}]}(a - b) dy = f_{\beta}(a - \frac{1}{2}) - f_{\beta}(a + \frac{1}{2}) \]

and hence \( \| f'_{\beta+1} \|_\infty = \sup_a |f_{\beta}(a - \frac{1}{2}) - f_{\beta}(a + \frac{1}{2})| \leq \| f_{\beta} \|_\infty \) since \( f_{\beta} \) is non-negative. Putting the pieces together, we have

\[ \frac{L_{k_{rt}}}{\| k_{rt} \|_\infty} = \frac{1}{S_{\beta,d}} L_{k_{rt}} \leq \sup_z \| \nabla \chi_{\beta+1}(z) \|_2 \leq \sqrt{d} \cdot S_{\beta+1,d} \| f'_{\beta+1} \|_\infty \cdot \| f_{\beta+1} \|_\infty^{d-1} \leq \sqrt{d} \cdot \mathfrak{B}_\beta \cdot \mathfrak{B}_\beta^{d-1} \]

(74,110) \leq \sqrt{d} \cdot \mathfrak{B}_\beta \cdot \mathfrak{B}_\beta \cdot \mathfrak{B}_\beta^{d-1} \]

(74,110)

where step (i) can be verified numerically.

Bounds on \( \mathfrak{R}_{k_{rt},n} \) and \( \mathfrak{R}_{k_{rt},\sqrt{n}}^\dagger \) Using the property of convolution, we find that \( f_{\beta+1}(a) = 0 \) if \( |a| \geq \frac{1}{2}(\beta + 1) \). Hence \( \kappa_{rt}(z) = 0 \) for \( \| z \|_\infty > (\beta + 1)/2 \) and applying the definitions (6), we find that

\[ \mathfrak{R}_{k_{rt},n} \leq \sqrt{d}(\beta + 1)/2 \quad \text{and} \quad \mathfrak{R}_{k_{rt},\sqrt{n}}^\dagger \leq \sqrt{d}(\beta + 1)/2 \]

as claimed in (109).

J.5 Explicit MMD rates for common kernels

Putting the quantities from Tab. 3 together with Thm. 1 (with \( \delta' = \delta \), and \( \delta \) treated as a constant) yields the MMD rates summarized in Tab. 5.

For completeness, we illustrate a key simplification that can readily yield the results stated in Tab. 5. Define \( \zeta_{k_{rt},S_{in}} \) as follows:

\[ \zeta_{k_{rt},S_{in}} \triangleq \frac{1}{d} \max(\mathfrak{R}_{k_{rt},\sqrt{n}}^\dagger, \mathfrak{R}_{S_{in}}), \]

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K. Supplementary Details for Vignettes of Sec. 6

This section provides supplementary details for the vignettes of Sec. 6.

K.1 Mixture of Gaussians target

Our mixture of Gaussians target is given by $\mathbb{P} = \frac{1}{M} \sum_{j=1}^{M} \mathcal{N}(\mu_j, I_d)$ for $M \in \{4, 6, 8\}$ where

$\mu_1 = [-3, 3]^T$, $\mu_2 = [-3, 3]^T$, $\mu_3 = [-3, -3]^T$, $\mu_4 = [3, -3]^T$, $\mu_5 = [0, 6]^T$, $\mu_6 = [-6, 0]^T$, $\mu_7 = [6, 0]^T$, $\mu_8 = [0, -6]^T$.

K.2 MCMC vignette details

For complete details on the targets and sampling algorithms we refer the reader to Riabiz et al. (2021, Sec. 4).

When applying standard thinning to any Markov chain output, we adopt the convention of keeping the final sample point. For all experiments, we used only the odd indices of the post burn-in sample points when thinning to form $S_{in}$.

| Kernel $k$  | $\text{MMD}_k(S_{in}, S_{KRT}) \lesssim$ |
|-------------|---------------------------------|
| Gaussian($\sigma$) | $C_1 \cdot \sqrt{\frac{\log n}{n}} \cdot [(1 + \frac{1}{4}(\log n + (\frac{\|k_{in}\|}{\sigma})^2))] \cdot \log(\sqrt{\log n + \frac{\|k_{in}\|}{\sigma}})$ |
| Matérn($\nu, \gamma$) | $C_2 \cdot \sqrt{\frac{\nu^{\frac{1}{2}} \log n}{n}} \cdot \left[\frac{1}{\Gamma(\alpha-1)}(a + \log^2 n + d^2 \log^2 (\frac{\|k_{in}\|}{\gamma}) + G^2_{\nu,d} + \gamma^2 \|k_{in}\|^2)\right] \cdot \log(\log n + a + \gamma \|k_{in}\|)$ |
| B-spline($2\beta + 1$) | $C_3 \cdot \sqrt{\frac{\log n}{n}} \cdot \left[(\beta^2 + \frac{\|k_{in}\|^2}{\gamma^2})\right] \cdot \log(\beta + \frac{\|k_{in}\|}{\gamma})$ |

Table 5: Explicit kernel thinning MMD guarantees for common kernels. Here, $\alpha \triangleq \frac{1}{2}(\nu - d)$, $G_{\nu,d} \triangleq \log(\frac{\nu - 2 - \frac{3}{2}}{(2\nu - 1)d^2 \pi})$ and each $C_i$ denotes a universal constant. See App. J.5 for more details on deriving these bounds from Thm. 1.

where $\mathcal{R}_{S_{in}}$, and $\mathcal{R}_{k_{in}, \sqrt{n}}$ were defined in (6) and (7) respectively. Then applying Thm. 1, and substituting the simplified bound (79) in (9), we find that

$$\text{MMD}_k(S_{in}, S_{KRT}) \leq 2 \frac{\|k_{in}\|}{\sqrt{n}} + \|k_{in}\|_{\infty} (B \mathcal{C}_{k_{in}, S_{in}})^{\frac{d}{2}} \cdot d^{\frac{1}{2}} \cdot \frac{1}{2} \sqrt{\log \frac{1}{\delta} + \log \left(\frac{L_{k_{in}}(\mathcal{R}_{k_{in}, S_{in}} + R)}{\|k_{in}\|_{\infty}}\right)}$$

(i)

$$\lesssim \delta \frac{2}{\sqrt{n}} \frac{\|k_{in}\|_{\infty}}{\sqrt{n}} + \|k_{in}\|_{\infty} (B \mathcal{C}_{k_{in}, S_{in}})^{\frac{d}{2}} \cdot d^{\frac{1}{2}} \cdot \frac{1}{2} \sqrt{\log \frac{1}{\delta} + \log \left(\frac{L_{k_{in}}(\mathcal{R}_{k_{in}, S_{in}} + \mathcal{R}_{S_{in}})}{\|k_{in}\|_{\infty}}\right)}$$

with probability at least $1 - 2 \delta$, where $B \triangleq 8e\pi$ is a universal constant, and in step (i) we use the following bound: For any $r = \sqrt{\alpha d}$, we have

$$c_d r^2 = \frac{(4\pi)^{\frac{d}{2}}}{(\Gamma(\frac{d}{2}+1))^{\frac{3}{2}}} (\alpha d)^{\frac{d}{2}} \leq \left(\frac{8e\pi}{\pi d}\right)^{\frac{d}{2}} \leq (B \alpha)^{\frac{d}{2}} d^{\frac{1}{2}} \cdot \frac{1}{2}$$

where $B \triangleq 8e\pi$, and step (ii) follows (for $d \geq 2$) from the Gamma function bounds (80). Now the results in Tab. 5 follow by simply substituting the various quantities from Tab. 3 in (111).
The selected burn-in periods for the Goodwin task were 820,000 for RW; 824,000 for adaRW; 1,615,000 for MALA; and 1,475,000 for pMALA. The respective numbers for the Lotka-Volterra task were 1,512,000 for RW; 1,797,000 for adaRW; 1,573,000 for MALA; and 1,251,000 for pMALA. For the Hinch experiments, we discard the first $10^6$ points as burn-in following Riabiz et al. (2021, App. S5.4). For all $n$, the parameter $\sigma$ for the Gaussian kernel is set to the median distance between all pairs of $4^7$ points obtained by standard thinning the post-burn-in odd indices. The resulting values for the Goodwin chains were 0.02 for RW; 0.0201 for adaRW; 0.0171 for MALA; and 0.0205 for pMALA. The respective numbers for Lotka-Volterra task were 0.0274 for RW; 0.0283 for adaRW; 0.023 for MALA; and 0.0288 for pMALA. Finally, the numbers for the Hinch task were 8.0676 for RW; 8.3189 for adaRW; 8.621 for MALA; and 8.6649 for pMALA.

L. Kernel Thinning with Square-root Dominating Kernels

As alluded to in Sec. 2, it is not necessary to identify an exact square-root kernel $k_{rt}$ to run kernel thinning. Rather, it suffices to identify any square-root dominating kernel $\tilde{k}_{rt}$ defined as follows.

**Definition 2** (Square-root dominating kernel). We say a reproducing kernel $\tilde{k}_{rt}: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a square-root dominating kernel for a reproducing kernel $k: \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ if either of the following equivalent conditions hold.

(a) The RKHS of $k$ belongs to the RKHS of $\tilde{k}_{rt}(x,y) \triangleq \int_{\mathbb{R}^d} \tilde{k}_{rt}(x,z)\tilde{k}_{rt}(y,z)dz$.

(b) The function $\tilde{k} - ck$ is positive definite for some $c > 0$.

**Remark 7** (Controlling MMD$_k$). A square-root dominating kernel $\tilde{k}_{rt}$ is a suitable surrogate for $k_{rt}$ as, by Zhang and Zhao (2013, Lem. 2.2, Prop. 2.3), $\text{MMD}_k(P, Q) \leq \sqrt{1/c} \cdot \text{MMD}_{\tilde{k}}(P, Q)$ for $c$ the constant appearing in Def. 2(b) and all distributions $P$ and $Q$.

Def. 2 and Rem. 7 enable us to use convenient dominating surrogates whenever an exact square-root kernel is inconvenient to derive or deploy. For example, our next result, proved in App. L.1, shows that a standard Matérn kernel is a square-root dominating kernel for every sufficiently-smooth shift-invariant and absolutely integrable $k$.

**Proposition 3** (Dominating smooth kernels). If $k(x,y) = \kappa(x - y)$ and $\kappa \in L^1(\mathbb{R}^d) \cap C^{2\nu}(\mathbb{R}^d)$ for $\nu > d$, then, for any $\gamma > 0$, the Matérn($\nu/2, \gamma$) kernel of Tab. 1 is a square-root dominating kernel for $k$.

Checking the square-root dominating condition is also particularly simple for any pair of continuous shift-invariant kernels as the next result, proved in App. L.2, shows.

**Proposition 4** (Dominating shift-invariant kernels). If $k(x,y) = \kappa(x - y)$ and $\tilde{k}_{rt}(x,y) = \tilde{\kappa}_{rt}(x - y)$ are real continuous kernels on $\mathbb{R}^d$ and $\kappa$ and $\tilde{\kappa}_{rt}$ have generalized Fourier transforms (Wendland, 2004, Def. 8.9) $\hat{\kappa}$ and $\hat{\tilde{\kappa}}_{rt}$ respectively with $\hat{\tilde{\kappa}}_{rt} \in L^2(\mathbb{R}^d)$, then $\tilde{k}_{rt}$ is a square-root dominating kernel for $k$ if and only if

$$\text{ess sup}_{\omega \in \mathbb{R}^d: \hat{\kappa}(\omega) > 0} \frac{\hat{\tilde{\kappa}}_{rt}(\omega)}{\hat{\kappa}(\omega)} < \infty.$$  

(112)
In Tab. 6, we use Prop. 4 to derive convenient tailored square-root dominating kernels \( \tilde{k}_{rt} \) for standard inverse multiquadric kernels, hyperbolic secant (sech) kernels, and Wendland’s compactly supported kernels. In each case, we can identify a square-root dominating kernel from the same family.

| Name of kernel \( k(x,y) = \kappa(x-y) \) | Expression for \( \kappa(z) \) | Name of square-root dominating kernel \( \tilde{k}_{rt}(x,y) = \tilde{\kappa}_{rt}(x-y) \) |
|-----------------------------------------|-----------------------------|-----------------------------------------------|
| InverseMultiquadric(\( \nu, \gamma \)) \( \nu > 0, \gamma > 0 \) | \((\gamma^2 + \|z\|^2)^{-\nu}\) | InverseMultiquadric(\( \nu', \gamma' \)) \( (\nu', \gamma') \in \mathcal{C}_{\nu,\gamma,d} \); see (117) |
| Sech(\( a \)) \( a > 0 \) | \( \prod_{j=1}^{d} \text{sech}(\sqrt{\omega}z_j) \) | Sech(\( 2a \)) |
| Wendland(s) \( s \in \mathbb{N}, s \geq \frac{1}{2}(d+1) \) | \( \phi_{d,s}(\|z\|_2) \); see (113) | Wendland(s’) \( s' \in \mathbb{N}_0, s' \leq \frac{1}{2}(2s-1-d) \) |

Table 6: Square-root dominating kernels \( \tilde{k}_{rt} \) for common kernels \( k \) (see Def. 2). Here \( \mathbb{N}_0 \) denotes the non-negative integers. See App. L.3 for our derivation.

**Expressions for Wendland kernels** The Wendland(s) kernel is a compactly-supported radial kernel \( \phi_{d,s}(\|x-y\|_2) \) on \( \mathbb{R}^d \) where \( \phi_{d,s} : \mathbb{R}_+ \to \mathbb{R} \) is a truncated minimal-degree polynomial with 2s continuous derivatives. We collect here the expressions for \( \phi_{d,s} \) for \( s = 0, 1, 2 \) and refer the readers to Wendland (2004, Ch. 9, Thm. 9.13, Tab. 9.1) for more general \( s \). Let \( (r)_+ = \max(0, r) \) and \( \ell \overset{\Delta}{=} \lfloor d/2 \rfloor + 3 \), then we have

\[
\begin{align*}
\phi_{d,0}(r) &= (1-r)^{[d/2]+1}, & \phi_{d,1}(r) &= (1-r)^{[d/2]+2} \lfloor (\lfloor d/2 \rfloor + 2)r + 1 \rfloor \\
\phi_{d,2}(r) &= (1-r)^{[d/2]+3} \lfloor (\ell^2 + 4\ell + 3)r^2 + (3\ell + 6)r + 3 \rfloor .
\end{align*}
\]

(113)

**L.1 Proof of Prop. 3: Dominating smooth kernels**

Since \( \kappa \in L^1(\mathbb{R}^d) \), \( F(\kappa) \) is bounded by the Babenko-Beckner inequality (Beckner, 1975) and nonnegative by Bochner’s theorem (Bochner, 1933; Wendland, 2004, Thm. 6.6). Moreover, since \( \kappa \in C^{2\nu}(\mathbb{R}^d) \), Sun (1993, Thm. 4.1) implies that \( \int \|\omega\|_2^{2\nu} F(\kappa)(\omega) d\omega < \infty \). By Wendland (2004, Theorem 8.15), the Matérn(\( \nu, \gamma \)) kernel \( \tilde{k}(x,y) \propto \Phi_{\nu,\gamma}(x-y) \) for \( \Phi_{\nu,\gamma} \) continuous with \( F(\Phi_{\nu,\gamma})(\omega) = (\gamma^2 + \|\omega\|_2^2)^{-\nu} \). Since we have established that

\[
\int \frac{F(\kappa)(\omega)^2}{F(\Phi_{\nu,\gamma})(\omega)} d\omega = \int (\gamma^2 + \|\omega\|_2^{2\nu}) F(\kappa)(\omega)^2 d\omega \leq \|F(\kappa)\|_\infty \int (\gamma^2 + \|\omega\|_2^{2\nu}) F(\kappa)(\omega) d\omega < \infty ,
\]

Wendland (2004, Thm. 10.12) implies that \( \kappa \) belongs to \( \mathcal{H}_{\kappa} \) and hence that \( \mathcal{H}_k \subseteq \mathcal{H}_{\kappa} \). Finally, by App. H.1, Matérn(\( \frac{1}{2}, \gamma \)) is a valid square-root dominating kernel for \( k \) and therefore for \( \kappa \).
L.2 Proof of Prop. 4: Dominating shift-invariant kernels

Since $k$ and $\tilde{k}_{rt}$ are real continuous translation invariant kernels, applying Bochner’s theorem (Bochner, 1933; Wendland, 2004, Thm. 6.6), we find that

$$k(x, y) = \frac{1}{(2\pi)^{d/2}} \int e^{-i(\omega, x-y)} \check{\kappa}(\omega) d\omega$$ and $$\tilde{k}_{rt}(x, y) = \frac{1}{(2\pi)^{d/2}} \int e^{-i(\omega, x-y)} \check{\kappa}_{rt}(\omega) d\omega,$$

and that $\check{\kappa}$ and $\check{\kappa}_{rt}$ are nonnegative and absolutely integrable. Moreover, since $k_{rt}(x, \cdot) = \mathcal{F}(e^{-i(\cdot, x)} \check{\kappa}_{rt})$ for $e^{-i(\cdot, x)} \check{\kappa}_{rt} \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$, the Plancherel-Parseval identity Wendland (2004, Proof of Thm. 5.23) implies that

$$\int_{\mathbb{R}^d} \kappa_{rt}(x, z) d\omega = \int_{\mathbb{R}^d} \kappa_{rt}(y, z) d\omega = \int_{\mathbb{R}^d} \kappa_{rt}(x-y) d\omega = \int_{\mathbb{R}^d} \kappa_{rt}(x) d\omega.$$

and Bochner’s theorem implies that $\check{\kappa}$ is a kernel. Finally, Prop. 3.1 of Zhang and Zhao (2013) now implies that the RKHS of $k_{rt}$ belongs to the RKHS of $k$ if and only if the ratio condition (112) holds.

L.3 Derivation of Tab. 6: Square-root dominating kernels $\tilde{k}_{rt}$ for common kernels $k$

Thanks to Prop. 4, to establish the validity of the square root dominating kernels stated in Tab. 6, it suffices to verify that

$$\check{\kappa}_{rt} \in L^2(\mathbb{R}^d) \quad \text{and} \quad \check{\kappa}_{rt} \preceq_{d, \nu, \gamma, \nu, \gamma} \check{\kappa}_{rt}^2,$$

where the functions $\kappa$ and $\check{\kappa}_{rt}$ are the generalized Fourier transforms of $\kappa$ and $\check{\kappa}_{rt}$.

**Inverse multiquadric** Consider the positive definite function $\Phi_{\nu, \gamma} (71)$ underlying the Matérn kernel, which is continuous on $\mathbb{R}^d \setminus \{0\}$. When $\kappa(z) = (\gamma^2 + \|z\|_2^2)^{-\nu}$ and $\check{\kappa}_{rt}(z) = (\gamma^2 + \|z\|_2^2)^{-\nu'}$, Wendland (2004, Theorem 8.15) implies that

$$\check{\kappa}(\omega) = \Phi_{\nu, \gamma}(\omega) \quad \text{and} \quad \Phi_{\nu, \gamma}(\omega) = \check{\kappa}_{rt}(\omega)^2.$$

Let $a(\omega) \asymp_{d, \nu, \gamma} b(\omega)$ denote asymptotic equivalence up to a constant depending on $d, \nu, \gamma$. Then, by (DLMF, Eqs. 10.25.3 & 10.30.2), we have

$$\Phi_{\nu, \gamma}(\omega) \asymp_{d, \nu, \gamma} \|\omega\|^{-\frac{d-1}{2}} e^{-\gamma\|\omega\|_2} \quad \text{as} \quad \|\omega\|_2 \to \infty, \quad (115)$$

$$\Phi_{\nu, \gamma}(\omega) \asymp_{d, \nu, \gamma} \|\omega\|^{-\left(d-2\nu+1\right)} \quad \text{as} \quad \|\omega\|_2 \to 0. \quad (116)$$

Hence, $\check{\kappa}_{rt} \in L^2(\mathbb{R}^d)$ whenever $\nu' > \frac{d}{2}$.

Moreover, applying (115), we find that for $\|\omega\|_2 \to \infty$,

$$\frac{\Phi_{\nu, \gamma}(\omega)}{\Phi_{\nu', \gamma'}(\omega)} \asymp_{d, \nu, \gamma, \nu', \gamma'} \|\omega\|^{-\frac{d-1}{2}} e^{-\gamma\|\omega\|_2} \cdot \|\omega\|_2^{-2\nu'+d+1} e^{2\gamma\|\omega\|_2}$$

$$= \|\omega\|^{-\frac{d+1}{2}} e^{(2\gamma'-\gamma)\|\omega\|_2}.$$
If $2\gamma' - \gamma < 0$, this expression is bounded for any value of $\nu'$. If $2\gamma' - \gamma = 0$, this expression is bounded when $\nu' \geq \frac{d}{4} + \frac{d}{2}$. Applying (116), we find that for $\|\omega\|_2 \to 0$, 

$$\Phi_{\nu,\gamma}(\omega) \asymp_{d,\nu,\gamma,\gamma'} \|\omega\|_2^{-(d-2\nu)_+} \cdot \|\omega\|_2^{2(d-2\nu')_+} = \|\omega\|_2^{2(d-2\nu')_+ - (d-2\nu)_+},$$

If $\nu \geq \frac{d}{2}$, this expression is finite for any value of $\nu'$. If $\nu < \frac{d}{2}$, this expression is finite when $\nu' \leq \frac{\nu}{2} + \frac{d}{4}$. Hence, our condition (114) is verified whenever $(\nu', \gamma')$ belongs to the set

$$C_{\nu,\gamma,d} \triangleq \{(\nu', \gamma') : (1) \nu' > \frac{d}{4} \quad \text{and} \quad \gamma' \leq \frac{\gamma}{2}, \quad \text{and} \quad (2) \nu' \leq \frac{d}{4} + \frac{\nu}{2} \quad \text{if} \quad \nu < \frac{d}{2}, \quad \text{and} \quad (3) \nu' \geq \frac{d}{4} + \frac{\nu}{2} + \frac{d}{4} \quad \text{if} \quad \gamma' = \frac{\gamma}{2} \}.$$  

Sech Define $\kappa_a(z) \triangleq \prod_{j=1}^d \sech(\sqrt{\frac{\nu}{a}} z_j)$, and suppose $\kappa = \kappa_a$ and $\tilde{\kappa}_{rt} = \kappa_{2a}$. Huggins and Mackey (2018, Ex. 3.2) yields that 

$$\tilde{\kappa}(\omega) = \mathcal{F}(\kappa_a)(\omega) = \frac{1}{a^d} \prod_{j=1}^d \sech(\sqrt{\frac{\nu}{a}}) = a^{-d} \cdot \kappa_{1/a}(\omega), \quad \text{and} \quad \tilde{\kappa}_{rt}(\omega) = \mathcal{F}(\tilde{\kappa}_{rt})(\omega) = (2a)^{-d} \cdot \kappa_{1/(2a)}(\omega).$$

Since $\sech^2(b/2) = \frac{4}{e^b + e^{-b}} > \frac{4}{e^{b} + e^{-b}} = 2 \sech(b)$, we have

$$\kappa_{1/a}(\omega) \leq 2^{-d} \cdot \kappa_{1/(2a)}(\omega)^2.$$  

Putting the pieces together, we further have

$$\tilde{\kappa}(\omega) \overset{(118)}{=} a^{-d} \cdot \kappa_{1/a}(\omega) \overset{(120)}{=} (2a)^{-d} \cdot \kappa_{1/(2a)}(\omega)^2 \overset{(119)}{=} (2a)^d \cdot \tilde{\kappa}_{rt}(\omega)^2.$$ 

Since $\kappa_{1/(2a)} \in L^2$, we have verified the condition (114).

Wendland When $\kappa(z) = \phi_{d,s,\nu}(\|z\|_2)$ and $\tilde{\kappa}_{rt}(z) = \phi_{d,s,\nu}(\|z\|_2)$, Wendland (2004, Thm. 10.35) implies that

$$\tilde{\kappa}(\omega) \lesssim_{d,s,\nu'} \frac{1}{(1 + \|\omega\|_2^2)^{d+2s+1}} \lesssim_{d,s,\nu'} \tilde{\kappa}_{rt}(\omega) \leq \frac{1}{(1 + \|\omega\|_2^2)^{2d+4s+2}},$$

with $s' \in \mathbb{N}_0$, $s' \leq \frac{(2s + 1 - d)}{4}$, thereby establishing the condition (114).

M. Online Vector Balancing in Euclidean Space

Using Thm. 3, we recover the online vector balancing result of Alweiss et al. (2021, Thm. 1.2) with improved constants and a less conservative setting of the thresholds $a_i$.

**Corollary 2** (Online vector balancing in Euclidean space). If $\mathcal{H} = \mathbb{R}^d$ equipped with the Euclidean dot product, $\mathcal{F}_n$ is oblivious, each $\|f_i\|_2 \leq 1$, and each $a_i = \frac{1}{2} + \log(4n/\delta)$, then, with probability at least $1 - \delta$ given $\mathcal{F}_n$, the self-balancing Hilbert walk (Alg. 2) returns $\psi_n$ satisfying 

$$\|\psi_n\|_\infty = \|\sum_{i=1}^n \eta_i f_i\|_\infty \leq \sqrt{2 \log(4d/\delta)} \log(4n/\delta).$$
Proof Instantiate the notation of Thm. 3. With our choice of \( a_i \), the signed sum representation property (ii) implies that 
\[ \psi_n = \sum_{i=1}^{\eta} f_i \]
with probability at least \( 1 - \delta/2 \) given \( F_n \). Moreover, the union bound, the functional sub-Gaussianity property (i), and the sub-Gaussian Hoeffding inequality (Wainwright, 2019, Prop. 2.5) now imply
\[
P(\|\psi_n\|_\infty > t \mid F_n) \leq \sum_{j=1}^{d} P(|\langle \psi_n, e_j \rangle| > t \mid F_n) \leq 2d \exp(-t^2/(2\sigma_n^2)) = \delta/2
\]
for \( t \triangleq \sigma_n \sqrt{2 \log(4d/\delta)} \).

Since \( a_i \) is non-decreasing in \( i \), and \( \frac{1}{2} + \frac{\log(4/\delta)}{\log(4/\delta)} \) is increasing in \( \delta \in (0, 1] \),
\[
\sigma_n^2 = \max_{j \leq n} \frac{a_j^2}{2a_j - \|J_j\|_1^2} \leq \max_{j \leq n} \frac{a_j^2}{2a_j - 1} = \log(4n/\delta) \left( \frac{1}{2} + \frac{\log(4/\delta)}{2(\log(4/\delta))^2} \right) 
\leq \log(4n/\delta) \left( \frac{1}{2} + \frac{\log(4)}{2(\log(4))^2} \right) \leq \log(4n/\delta).
\]

The advertised result now follows from the union bound.

N. \( L^\infty \) Coresets of Phillips and Tai (2020) and Tai (2020)

Here we provide more details on the \( L^\infty \) coreset construction of Phillips and Tai (2020) and Tai (2020) discussed in Sec. 5.3. Given input points \( (x_i)_{i=1}^{n} \), the Phillips-Tai (PT) construction forms the matrix \( K = (k(x_i, x_j))_{i,j=1}^{n} \) of pairwise kernel evaluations, finds a matrix square-root \( V \in \mathbb{R}^{n \times n} \) satisfying \( K = VV^T \), and augments \( V \) with a row of ones (to encourage near-halving in the next step). Then, the PT construction runs the Gram-Schmidt (GS) walk of Bansal et al. (2018) to identify approximately half of the columns of \( V \) as coreset members and rebalances the coreset until exactly half of the input points belong to the coreset. The GS walk and rebalancing steps are recursively repeated \( \Omega(\log(n)) \) times to obtain a \( (n^{\frac{1}{2}}, \sqrt{dn^{-\frac{1}{2}} \sqrt{\log n}}) \)-\( L^\infty \) coreset with high probability. The low-dimensional Gaussian kernel construction of Tai (2020) first partitions the input points into \( \Omega(\log(n)) \) balls of radius \( 2\sqrt{\log n} \) and then applies the PT construction separately to each ball. The result is a high-probability order \( (n^{\frac{1}{2}}, 2d^{n-\frac{1}{2}} \sqrt{\log(d \log n)}) \)-\( L^\infty \) coreset with an additional superexponential \( \Omega(d^{\Theta(d)}) \) running time dependence.

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