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Performance analysis of greedy algorithms for minimising a Maximum Mean Discrepancy

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Abstract

We analyse the performance of several iterative algorithms for the quantisation of a probability measure μ , based on the minimisation of a Maximum Mean Discrepancy (MMD). Our analysis includes kernel herding, greedy MMD minimisation and Sequential Bayesian Quadrature (SBQ). We show that the finite-sample-size approximation error, measured by the MMD, decreases as $1/n$ for SBQ and also for kernel herding and greedy MMD minimisation when using a suitable step-size sequence. The upper bound on the approximation error is slightly better for SBQ, but the other methods are significantly faster, with a computational cost that increases only linearly with the number of points selected. This is illustrated by two numerical examples, with the target measure μ being uniform (a space-filling design application) and with μ a Gaussian mixture.

keywords Maximum Mean Discrepancy; quantisation; greedy algorithm; sequential Bayesian quadrature; kernel herding; space-filling design; computer experiments

1 Introduction and motivation

Background. Quantisation of a probability measure μ is a basic task in many fields, such as probabilistic integration (Briol et al., 2019), MCMC computation (Joseph et al., 2015a, 2019) or space-filling design in computer experiments (Joseph et al., 2015b; Mak and Joseph, 2017, 2018; Pronzato and Zhigljavsky, 2020), and minimisation of the Maximum Mean Discrepancy (MMD) defined by a kernel K is a powerful tool for this task¹. In particular, it easily allows iterative constructions that can be stopped when the discrete approximation obtained is deemed sufficient, a situation where the number of support points is not fixed in advance.

Claims and hint of the contents. We derive finite-sample-size errors bounds for iterative methods to quantise a probability measure by minimising the MMD for a given kernel. The

¹We do not consider quantisation methods based on Voronoi partitions, for which one can refer in particular to Graf and Luschgy (2000).

methods considered include gradient-type algorithms (kernel herding), greedy one-step-ahead minimisation, and Sequential Bayesian Quadrature (SBQ) that sets optimal weights on the current support at each iteration. Two variants of SBQ are considered, with and without the constraint that the weights sum to one (the bound for the unconstrained version is markedly pessimistic but our analysis reveals a connection with kernel herding and gives some insight for the reason of this pessimism). We consider the practical situation where the candidate set is finite; it may correspond in particular to points independently sampled with μ , with the possibility to use a different set at every iteration. The context of a finite candidate set is the most widely used in practical situations. It allows us to derive simple proofs that only use (finite-dimensional) linear algebra, but our results can be extended to the infinite-dimensional (Hilbert space) situation, where the new support point selected at each iteration is searched within a continuous set; see, e.g., Chen et al. (2018); Teymur et al. (2020). We show that the error is $\mathcal{O}(n^{-1})$ for SBQ and for algorithms that use a suitable step-size sequence and construct nonuniform discrete measures (with a slightly better constant for SBQ). We show that it is also $\mathcal{O}(n^{-1})$ for the construction of uniform (empirical) measures provided that the measure with total mass one minimising the MMD over the candidate set is a probability measure. We show that the complexity of gradient and greedy one-step-ahead methods grows linearly with n . Two variants of kernel herding are considered, with performance similar to SBQ but less costly in terms of calculation.

Paper organisation. Section 2 recalls the background on MMD and Bayesian quadrature. It defines the notation and introduces the methods that are considered in the rest of the paper. The performance of kernel herding is analysed in Section 3. The results presented in Sections 3.1 and 3.2 are not new, but the analysis of this basic gradient-type algorithm is central to the investigation of the convergence rate for the other methods, more sophisticated, that we consider in Sections 3.3 (variants of kernel herding), 4 (greedy MMD minimisation) and 5 (SBQ). Section 6 extends the results of previous sections to the case where the candidate set corresponds to points independently sampled with μ . Two illustrative examples are presented in Section 7, one with μ uniform (space-filling design), the other with μ a Gaussian mixture. Section 8 concludes briefly.

2 Maximum Mean Discrepancy and Bayesian quadrature

2.1 Maximum Mean Discrepancy (MMD)

Let \mathcal{X} be a measurable set, equipped with a probability measure μ . For instance, for application to space-filling design for computer experiments \mathcal{X} is typically a compact subset of \mathbb{R}^d and μ is proportional to the Lebesgue measure on \mathcal{X} . Let K be a symmetric strictly positive definite (s.p.d.) kernel defined on $\mathcal{X} \times \mathcal{X}$, uniformly bounded on \mathcal{X} ; that is,

$$K(\mathbf{x}, \mathbf{x}) \leq \bar{K} < +\infty, \quad \text{for all } \mathbf{x} \in \mathcal{X}, \quad (1)$$

and for any $n \in \mathbb{N}$ and any $\mathbf{x}_1, \dots, \mathbf{x}_n$ in \mathcal{X} , the $n \times n$ matrix \mathbf{K}_n with element i, j equal to $K(\mathbf{x}_i, \mathbf{x}_j)$ is p.d. and s.p.d. when the \mathbf{x}_i are all pairwise different. Note that K being s.p.d. implies that $K^2(\mathbf{x}, \mathbf{x}') \leq K(\mathbf{x}, \mathbf{x})K(\mathbf{x}', \mathbf{x}')$ for all \mathbf{x} and \mathbf{x}' in \mathcal{X} with the inequality being strict when $\mathbf{x} \neq \mathbf{x}'$. Moreover, (1) implies

$$\tau_\gamma(\mu) = \int_{\mathcal{X}} K^\gamma(\mathbf{x}, \mathbf{x}) \, d\mu(\mathbf{x}) \leq \bar{K}^\gamma < +\infty \quad \text{for any } \gamma \geq 0.$$

K defines a Reproducing Kernel Hilbert Space (RKHS) \mathcal{H}_K , and we respectively denote by $\langle \cdot, \cdot \rangle_K$ and $\|\cdot\|_{\mathcal{H}_K}$ the scalar product and norm in \mathcal{H}_K . We do not assume that \mathcal{H}_K is finite-dimensional. We say that K is positive ($K \geq 0$) when $K(\mathbf{x}, \mathbf{x}') \geq 0$ for all \mathbf{x} and \mathbf{x}' in \mathcal{X} .

We denote by $\mathcal{M}(\mathcal{X})$ the set of finite signed measures on \mathcal{X} , by $\mathcal{M}_{[q]}(\mathcal{X})$ the set of signed measures with total mass q , by $\mathcal{M}^+(\mathcal{X})$ the set of positive measures and by $\mathcal{M}_{[1]}^+(\mathcal{X})$ the set of probability measures on \mathcal{X} (with thus $\mu \in \mathcal{M}_{[1]}^+(\mathcal{X})$). The reproducing property implies that, for any $\nu \in \mathcal{M}(\mathcal{X})$, the *energy* of ν , defined by $\mathcal{E}_K(\nu) = \int_{\mathcal{X}^2} K(\mathbf{x}, \mathbf{x}') d\nu(\mathbf{x}) d\nu(\mathbf{x}')$, satisfies

$$\begin{aligned} \mathcal{E}_K(\nu) &= \int_{\mathcal{X}^2} \langle K(\mathbf{x}, \cdot), K(\mathbf{x}', \cdot) \rangle_K d\nu(\mathbf{x}) d\nu(\mathbf{x}') \leq \int_{\mathcal{X}^2} \|K(\mathbf{x}, \cdot)\|_{\mathcal{H}_K} \|K(\mathbf{x}', \cdot)\|_{\mathcal{H}_K} d\nu(\mathbf{x}) d\nu(\mathbf{x}') \\ &= \left[\int_{\mathcal{X}} K^{1/2}(\mathbf{x}, \mathbf{x}) d\nu(\mathbf{x}) \right]^2 = \tau_{1/2}^2(\nu) < +\infty. \end{aligned}$$

For any $\nu \in \mathcal{M}(\mathcal{X})$ and any $\mathbf{x} \in \mathcal{X}$, we denote by

$$P_{K,\nu}(\mathbf{x}) = \int_{\mathcal{X}} K(\mathbf{x}, \mathbf{x}') d\nu(\mathbf{x}')$$

the *potential* of ν at \mathbf{x} ; $P_{K,\nu}(\cdot)$ is also called the *kernel imbedding* of ν into \mathcal{H}_K .

For μ and ν in $\mathcal{M}_{[1]}^+(\mathcal{X})$, any $f \in \mathcal{H}_K$ satisfies the following (Koksma-Hlawka type) inequality: $|\int_{\mathcal{X}} f(\mathbf{x}) d\nu(\mathbf{x}) - \int_{\mathcal{X}} f(\mathbf{x}) d\mu(\mathbf{x})| = |\langle f, P_{K,\nu} - P_{K,\mu} \rangle_K| \leq \|f\|_{\mathcal{H}_K} \text{MMD}_K(\mu, \nu)$, where

$$\begin{aligned} \text{MMD}_K(\mu, \nu) &= \sup_{\|f\|_{\mathcal{H}_K}=1} \left| \int_{\mathcal{X}} f(\mathbf{x}) d\nu(\mathbf{x}) - \int_{\mathcal{X}} f(\mathbf{x}) d\mu(\mathbf{x}) \right| = \|P_{K,\nu} - P_{K,\mu}\|_{\mathcal{H}_K} \\ &= \mathcal{E}_K^{1/2}(\nu - \mu) = \left[\int_{\mathcal{X}^2} K(\mathbf{x}, \mathbf{x}') d(\nu - \mu)(\mathbf{x}) d(\nu - \mu)(\mathbf{x}') \right]^{1/2} \\ &= \left[\mathcal{E}_K(\mu) + \mathcal{E}_K(\nu) - 2 \int_{\mathcal{X}} P_{K,\mu}(\mathbf{x}) d\nu(\mathbf{x}) \right]^{1/2} \end{aligned} \quad (2)$$

is called the *Maximum-Mean-Discrepancy* (MMD) between ν and μ ; see Sejdinovic et al. (2013, Def. 10). $\text{MMD}_K(\mu, \nu)$ defines an integral pseudometric between probability distributions and a pseudometric between kernel imbeddings. It defines a metric on $\mathcal{M}_{[1]}^+(\mathcal{X})$, when K is characteristic².

Analytic expressions of $\mathcal{E}_K(\mu)$ and $P_{K,\mu}(\cdot)$ are available for particular measures and particular kernels, see Table 1 of Briol et al. (2019). This includes the case when μ is uniform on $\mathcal{X} = [0, 1]^d$ and K is separable, see for example Table 3.1 of (Pronzato and Zhigljavsky, 2020), and separable kernels K based on variants of Brownian motion covariance yield L_2 discrepancies (symmetric, centred, wrap-around and so on); see Hickernell (1998), Fang et al. (2006, Chap. 3). $\mathcal{E}_K(\mu)$ and $P_{K,\mu}(\cdot)$ are not available when μ is a posterior distribution with unknown normalising constant; in that case, Joseph et al. (2015a, 2019) suggest to construct minimum-energy designs that minimise $\mathcal{E}_K(\xi_{n,e})$ for a particular kernel K . Another way is to minimise a kernel Stein discrepancy, that is, to minimise MMD for the image K' of a kernel K under a Stein operator,

²Since K is uniformly bounded, this is equivalent to the condition that K be Conditionally Integrally Strictly Positive Definite (CISPD), that is, $\mathcal{E}_K(\nu) > 0$ for all nonzero signed measure $\nu \in \mathcal{M}_{[0]}(\mathcal{X})$; see Sriperumbudur et al. (2010, Def. 6 and Lemma 8); see also Pronzato and Zhigljavsky (2020) for a comprehensive survey including the case of singular kernels.

so that $\mathcal{E}_{K'}(\mu) = 0$ and $P_{K',\mu}(\mathbf{x}) = 0$ for any \mathbf{x} ; see Chen et al. (2018); Detommaso et al. (2018); Gorham and MacKey (2017); Liu and Wang (2016); Oates et al. (2017). In the rest of the paper we consider the general framework where \mathcal{H}_K is an infinite-dimensional RKHS and assume that $\mathcal{E}_K(\mu)$ and $P_{K,\mu}(\mathbf{x})$ can be easily computed for any $\mathbf{x} \in \mathcal{X}$ (Monte-Carlo methods can always be used as a last resort).

2.2 MMD for discrete measures

For a collection $\mathbf{X}_n = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ of n points in \mathcal{X} , called n -point design, we denote by $\xi_{n,e} = (1/n) \sum_{i=1}^n \delta_{\mathbf{x}_i}$ the associated empirical measure, with $\delta_{\mathbf{x}}$ the Dirac delta measure at \mathbf{x} . For $\mathbf{w}_n = (\{\mathbf{w}_n\}_1, \dots, \{\mathbf{w}_n\}_n)^\top \in \mathbb{R}^n$ a vector of n weights, we denote by $\xi_n = \xi(\mathbf{w}_n)$ the signed measure

$$\xi(\mathbf{w}_n) = \sum_{i=1}^n \{\mathbf{w}_n\}_i \delta_{\mathbf{x}_i} \quad (3)$$

(so that $\xi_{n,e} = \xi(\mathbf{1}_n/n)$, with $\mathbf{1}_n$ the n -dimensional vector with all components equal to 1). An important area of application for MMD minimisation is space-filling design, where the objective is to build evenly distributed designs on a compact \mathcal{X} ; see, for example, Pronzato and Müller (2012); Pronzato (2017). Minimising $\text{MMD}_K(\mu, \xi_{n,e})$ with μ uniform over \mathcal{X} is then an effective approach to achieve this goal. One may also minimise $\text{MMD}_K(\mu, \xi(\mathbf{w}_n))$ with respect to \mathbf{X}_n and \mathbf{w}_n , and the designs obtained differ depending on the chosen kernel K , the constraints set on \mathbf{w}_n and on the optimisation method that is used.

In this paper, we focuss our attention on the construction of extensive point sequences $\mathbf{X}_n = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n]$, such that $\mathbf{X}_{k+1} = [\mathbf{X}_k, \mathbf{x}_{k+1}]$ for all k , with the property that \mathbf{X}_n is the support of a measure ξ_n which approximates μ well in the sense of the MMD criterion for a given K . For a given design \mathbf{X}_n , the optimal weights \mathbf{w}_n minimising $\text{MMD}_K(\mu, \xi_n)$ are easily obtained. Indeed, (2) gives

$$\begin{aligned} \text{MMD}_K^2(\mu, \xi_n) = \mathcal{E}_K(\xi_n - \mu) &= \sum_{i,j=1}^n \{\mathbf{w}_n\}_i \{\mathbf{w}_n\}_j K(\mathbf{x}_i, \mathbf{x}_j) - 2 \sum_{i=1}^n \{\mathbf{w}_n\}_i P_{K,\mu}(\mathbf{x}_i) + \mathcal{E}_K(\mu), \\ &= \mathbf{w}_n^\top \mathbf{K}_n \mathbf{w}_n - 2 \mathbf{w}_n^\top \mathbf{p}_n(\mu) + \mathcal{E}_K(\mu), \end{aligned} \quad (4)$$

where $\mathbf{p}_n(\mu) = [P_{K,\mu}(\mathbf{x}_1), \dots, P_{K,\mu}(\mathbf{x}_n)]^\top$, and \mathbf{w}_n^* that minimises $\text{MMD}_K^2(\mu, \xi_n)$ under the constraints $\{\mathbf{w}_n\}_i \geq 0$ and $\mathbf{1}_n^\top \mathbf{w}_n = 1$ is solution of a Quadratic Programming (QP) problem. Releasing the positivity constraints, $\widehat{\mathbf{w}}_n$ that minimises $\text{MMD}_K^2(\mu, \xi_n)$ with $\mathbf{1}_n^\top \mathbf{w}_n = 1$ is obtained explicitly as

$$\widehat{\mathbf{w}}_n = \left(\mathbf{K}_n^{-1} - \frac{\mathbf{K}_n^{-1} \mathbf{1}_n \mathbf{1}_n^\top \mathbf{K}_n^{-1}}{\mathbf{1}_n^\top \mathbf{K}_n^{-1} \mathbf{1}_n} \right) \mathbf{p}_n(\mu) + \frac{\mathbf{K}_n^{-1} \mathbf{1}_n}{\mathbf{1}_n^\top \mathbf{K}_n^{-1} \mathbf{1}_n} \quad (5)$$

(and $\mathbf{w}_n^* = \widehat{\mathbf{w}}_n$ when all components of $\widehat{\mathbf{w}}_n$ are nonnegative). The unconstrained weights that minimise $\text{MMD}_K^2(\mu, \xi_n)$ are given by

$$\widetilde{\mathbf{w}}_n = \mathbf{K}_n^{-1} \mathbf{p}_n(\mu). \quad (6)$$

Throughout the paper, for any measure ξ_n supported on \mathbf{X}_n , we shall denote by ξ_n^* , $\widehat{\xi}_n$ and $\widetilde{\xi}_n$ the measures with the same support and respective weights \mathbf{w}_n^* , $\widehat{\mathbf{w}}_n$ and $\widetilde{\mathbf{w}}_n$. The measures ξ_n

and $\tilde{\xi}_n$ satisfy

$$\begin{aligned}\text{MMD}_K^2(\mu, \hat{\xi}_n) &= \mathcal{E}_K(\mu) - \mathbf{p}_n^\top(\mu) \mathbf{K}_n^{-1} \mathbf{p}_n(\mu) + \frac{(1 - \mathbf{p}_n^\top(\mu) \mathbf{K}_n^{-1} \mathbf{1}_n)^2}{\mathbf{1}_n^\top \mathbf{K}_n^{-1} \mathbf{1}_n}, \\ \text{MMD}_K^2(\mu, \tilde{\xi}_n) &= \mathcal{E}_K(\mu) - \mathbf{p}_n^\top(\mu) \mathbf{K}_n^{-1} \mathbf{p}_n(\mu),\end{aligned}\quad (7)$$

and we also have

$$\text{MMD}_K^2(\mu, \xi_n) = (\mathbf{w}_n - \tilde{\mathbf{w}}_n)^\top \mathbf{K}_n (\mathbf{w}_n - \tilde{\mathbf{w}}_n) + \text{MMD}_K^2(\mu, \tilde{\xi}_n) \text{ for any } \xi_n \in \mathcal{M}(\mathbf{X}_n), \quad (8)$$

$$\text{MMD}_K^2(\mu, \xi_n) = (\mathbf{w}_n - \hat{\mathbf{w}}_n)^\top \mathbf{K}_n (\mathbf{w}_n - \hat{\mathbf{w}}_n) + \text{MMD}_K^2(\mu, \hat{\xi}_n) \text{ for any } \xi_n \in \mathcal{M}_{[1]}(\mathbf{X}_n), \quad (9)$$

see Pronzato and Zhigljavsky (2020, Th. 4.3). Moreover, $\text{MMD}_K^2(\mu, \xi_n) = \mathbf{w}_n^\top \mathbf{K}_{\mu_n} \mathbf{w}_n$ for any $\xi_n \in \mathcal{M}_{[1]}(\mathbf{X}_n)$ and

$$\text{MMD}_K^2(\mu, \hat{\xi}_n) = (\mathbf{1}_n^\top \mathbf{K}_{\mu_n}^{-1} \mathbf{1}_n)^{-1}, \quad (10)$$

where $\{\mathbf{K}_{\mu_n}\}_{i,j} = K_\mu(\mathbf{x}_i, \mathbf{x}_j)$, $i, j = 1, \dots, n$, and K_μ is the reduced kernel defined by

$$K_\mu(\mathbf{x}, \mathbf{x}') = K(\mathbf{x}, \mathbf{x}') - P_{K,\mu}(\mathbf{x}) - P_{K,\mu}(\mathbf{x}') + \mathcal{E}_K(\mu), \quad \mathbf{x}, \mathbf{x}' \in \mathcal{X}, \quad (11)$$

see Pronzato and Zhigljavsky (2020, Th. 4.4), with the property that \mathbf{K}_{μ_n} is s.p.d. when μ is not fully supported on \mathbf{X}_n and all \mathbf{x}_i are pairwise different.

We consider three families of incremental constructions.

2.3 Incremental MMD minimisation

2.3.1 Sequential Bayesian Quadrature (SBQ)

The construction of a design \mathbf{X}_n that minimises $\text{MMD}_K^2(\mu, \tilde{\xi}_n)$ or $\text{MMD}_K^2(\mu, \hat{\xi}_n)$ is called Bayesian quadrature (BQ); it can be Sequential (SBQ), see Briol et al. (2015), and we shall consider two versions of SBQ. Bounds on their finite-sample-size error are given in Section 5.

(i) Direct calculation using (7) and block matrix inversion gives

$$\text{MMD}_K^2(\mu, \tilde{\xi}_{k+1}) = \text{MMD}_K^2(\mu, \tilde{\xi}_k) - \frac{[\mathbf{p}_k^\top(\mu) \mathbf{K}_k^{-1} \mathbf{k}_k(\mathbf{x}_{k+1}) - P_{K,\mu}(\mathbf{x}_{k+1})]^2}{K(\mathbf{x}_{k+1}, \mathbf{x}_{k+1}) - \mathbf{k}_k^\top(\mathbf{x}_{k+1}) \mathbf{K}_k^{-1} \mathbf{k}_k(\mathbf{x}_{k+1})}.$$

Since $\tilde{\mathbf{w}}_k$ satisfies (6), we get

$$\text{MMD}_K^2(\mu, \tilde{\xi}_{k+1}) = \text{MMD}_K^2(\mu, \tilde{\xi}_k) - \frac{[P_{K,\tilde{\xi}_k}(\mathbf{x}_{k+1}) - P_{K,\mu}(\mathbf{x}_{k+1})]^2}{\min_{\mathbf{w} \in \mathbb{R}^k} \|K(\mathbf{x}_{k+1}, \cdot) - \mathbf{w}^\top \mathbf{k}_k(\cdot)\|_{\mathcal{H}_K}^2}. \quad (12)$$

This corresponds to the ‘‘standard’’ version of SBQ, which uses general signed measures $\tilde{\xi}_k$ in $\mathcal{M}(\mathcal{X})$: it selects $\mathbf{x}_1 \in \text{Arg max}_{\mathbf{x} \in \mathcal{X}} P_{K,\mu}^2(\mathbf{x})/K(\mathbf{x}, \mathbf{x})$ and then

$$\mathbf{x}_{k+1} \in \text{Arg max}_{\mathbf{x} \in \mathcal{X}} \frac{[P_{K,\tilde{\xi}_k}(\mathbf{x}_{k+1}) - P_{K,\mu}(\mathbf{x}_{k+1})]^2}{K(\mathbf{x}, \mathbf{x}) - \mathbf{k}_k^\top(\mathbf{x}) \mathbf{K}_k^{-1} \mathbf{k}_k(\mathbf{x})}, \quad k \geq 1. \quad (13)$$

(ii) We shall also consider a second version that uses measures $\widehat{\xi}_k$ in $\mathcal{M}_{[1]}(\mathcal{X})$. Equation (10) gives

$$\text{MMD}_K^2(\mu, \widehat{\xi}_{k+1}) = \left\{ \mathbf{1}_k^\top \mathbf{K}_{\mu_k}^{-1} \mathbf{1}_k + \frac{[\mathbf{1}_k^\top \mathbf{K}_{\mu_k}^{-1} \mathbf{k}_{\mu_k}(\mathbf{x}_{k+1}) - 1]^2}{K_\mu(\mathbf{x}_{k+1}, \mathbf{x}_{k+1}) - \mathbf{k}_{\mu_k}^\top(\mathbf{x}_{k+1}) \mathbf{K}_{\mu_k}^{-1} \mathbf{k}_{\mu_k}(\mathbf{x}_{k+1})} \right\}^{-1},$$

where $\mathbf{k}_{\mu_k}(\mathbf{x}) = [K_\mu(\mathbf{x}_1, \mathbf{x}), \dots, K_\mu(\mathbf{x}_k, \mathbf{x})]^\top$, $\mathbf{x} \in \mathcal{X}$, and where K_μ is defined by (11). Direct calculation using (5) gives

$$\text{MMD}_K^2(\mu, \widehat{\xi}_{k+1}) = \text{MMD}_K^2(\mu, \widehat{\xi}_k) - \frac{[P_{K, \widehat{\xi}_k}(\mathbf{x}_{k+1}) - P_{K, \mu}(\mathbf{x}_{k+1}) + \widehat{\mathbf{w}}_k^\top \mathbf{p}_k(\mu) - \mathcal{E}_K(\widehat{\xi}_k)]^2}{\min_{\substack{\mathbf{w} \in \mathbb{R}^k \\ \mathbf{1}_k^\top \mathbf{w} = 1}} \|K(\mathbf{x}_{k+1}, \cdot) - \mathbf{w}^\top \mathbf{k}_k(\cdot)\|_{\mathcal{H}_K}^2}. \quad (14)$$

This version of SBQ selects $\mathbf{x}_1 \in \text{Arg min}_{\mathbf{x} \in \mathcal{X}} K_\mu(\mathbf{x}, \mathbf{x})$ and then

$$\mathbf{x}_{k+1} \in \text{Arg max}_{\mathbf{x} \in \mathcal{X}} \frac{[P_{K, \widehat{\xi}_k}(\mathbf{x}_{k+1}) - P_{K, \mu}(\mathbf{x}_{k+1}) + \widehat{\mathbf{w}}_k^\top \mathbf{p}_k(\mu) - \widehat{\mathbf{w}}_k^\top \mathbf{K}_k \widehat{\mathbf{w}}_k]^2}{K(\mathbf{x}, \mathbf{x}) - \mathbf{k}_k^\top(\mathbf{x}) \mathbf{K}_k^{-1} \mathbf{k}_k(\mathbf{x}) + \frac{[1 - \mathbf{1}_k^\top \mathbf{K}_k^{-1} \mathbf{k}_k(\mathbf{x})]^2}{\mathbf{1}_k^\top \mathbf{K}_k^{-1} \mathbf{1}_k}}, \quad k \geq 1. \quad (15)$$

Remark 1. When using unconstrained weights $\widetilde{\mathbf{w}}_k$, we can also consider a sequential construction where all previous weights $\{\widetilde{\mathbf{w}}_i\}_i$ are kept fixed, $i = 1, \dots, k$, and only the next one is optimised (without constraint) when choosing \mathbf{x}_{k+1} . Since $\text{MMD}_K^2(\mu, \xi_k + w \delta_{\mathbf{x}}) = \text{MMD}_K^2(\mu, \xi_k) + w^2 K(\mathbf{x}, \mathbf{x}) + 2w [P_{K, \xi_k}(\mathbf{x}) - P_{K, \mu}(\mathbf{x})]$, the optimal w is $w^* = [P_{K, \mu}(\mathbf{x}) - P_{K, \xi_k}(\mathbf{x})]/K(\mathbf{x}, \mathbf{x})$; the algorithm selects $\mathbf{x}_1 \in \text{Arg max}_{\mathbf{x} \in \mathcal{X}} P_{K, \mu}^2(\mathbf{x})/K(\mathbf{x}, \mathbf{x})$ and then

$$\mathbf{x}_{k+1} \in \text{Arg max}_{\mathbf{x} \in \mathcal{X}} \frac{[P_{K, \widetilde{\xi}_k}(\mathbf{x}) - P_{K, \mu}(\mathbf{x})]^2}{K(\mathbf{x}, \mathbf{x})}, \quad k \geq 1. \quad (16)$$

(Note the coincidence with the choice made by kernel herding when $K(\mathbf{x}, \mathbf{x})$ is a constant, see (18).) When a finite set \mathcal{X}_C is substituted for \mathcal{X} , (16) corresponds to a coordinate-descent algorithm (see, e.g., Wright (2015)) operating on the weights $\omega = (\omega_1, \dots, \omega_C) \in \mathbb{R}^C$; see Section 2.4.

2.3.2 Greedy MMD Minimisation (GM)

To lighten the computations required by SBQ, we can consider the optimal choice of successive \mathbf{x}_k for a predefined sequence of weights \mathbf{w}_k . The standard version of Greedy MMD Minimisation (GM) uses $\mathbf{w}_k = \mathbf{1}_k/k$ for all k . It selects $\mathbf{x}_1 \in \text{Arg min}_{\mathbf{x} \in \mathcal{X}} K(\mathbf{x}, \mathbf{x}) - 2P_{K, \mu}(\mathbf{x}) = \text{Arg min}_{\mathbf{x} \in \mathcal{X}} K_\mu(\mathbf{x}, \mathbf{x})$ and then minimises $\text{MMD}_K(\mu, \xi_{k+1, e})$ incrementally, which gives

$$\mathbf{x}_{k+1} \in \text{Arg min}_{\mathbf{x} \in \mathcal{X}} \sum_{i=1}^k K(\mathbf{x}_i, \mathbf{x}) + \frac{1}{2} K(\mathbf{x}, \mathbf{x}) - (k+1) P_{K, \mu}(\mathbf{x}), \quad k \geq 1. \quad (17)$$

GM will be considered in Section 4. In Section 4.2 we also consider versions with nonuniform weights: one must then define the weight w_{k+1} to be allocated to the next point \mathbf{x}_{k+1} , not selected yet. A convenient way to proceed, usual in the area of optimal design of experiments, is to take $\xi_{k+1} = (1 - \alpha_{k+1}) \xi_k + \alpha_{k+1} \delta_{\mathbf{x}_{k+1}}$, for some $\alpha_{k+1} \in [0, 1]$. This construction guarantees that $\xi_{k+1} \in \mathcal{M}_{[1]}^+(\mathcal{X})$ when $\xi_k \in \mathcal{M}_{[1]}^+(\mathcal{X})$, the choice of α_{k+1} defines the sequence of weights \mathbf{w}_k and the point \mathbf{x}_{k+1} is chosen to minimise $\text{MMD}_K(\mu, \xi_{k+1})$.

2.3.3 The Frank-Wolfe algorithm and Kernel Herding (KH)

A further simplification is obtained by considering a steepest-descent type approach. For any $\xi, \nu \in \mathcal{M}(\mathcal{X})$, the directional derivative of the functional $\xi \rightarrow \mathcal{E}_K(\xi - \mu)$ at ξ in the direction ν equals

$$F_{\text{MMD}_K^2}(\xi, \nu) = 2 \left[\int_{\mathcal{X}^2} K_\mu(\mathbf{x}, \mathbf{x}') d\nu(\mathbf{x}) d\xi(\mathbf{x}') - \mathcal{E}_{K_\mu}(\xi) + \int_{\mathcal{X}} P_{K,\mu}(\mathbf{x}) d(\xi - \nu)(\mathbf{x}) \right],$$

so that $F_{\text{MMD}_K^2}(\xi, \delta_{\mathbf{x}}) = 2 [P_{K,\xi}(\mathbf{x}) - P_{K,\mu}(\mathbf{x}) + \int_{\mathcal{X}} P_{K,\mu}(\mathbf{x}') d\xi(\mathbf{x}') - \mathcal{E}_K(\xi)]$. Iterations of the Frank-Wolfe algorithm (Frank and Wolfe, 1956) correspond to $\xi_{k+1} = (1 - \alpha_{k+1}) \xi_k + \alpha_{k+1} \nu_{k+1}$, where $\nu_{k+1} \in \text{Arg min}_{\nu \in \mathcal{M}_{[1]}^+(\mathcal{X})} F_{\text{MMD}_K^2}(\xi_k, \nu)$, for some $\alpha_{k+1} \in [0, 1]$. This gives $\nu_{k+1} = \delta_{\mathbf{x}_{k+1}}$, with

$$\mathbf{x}_{k+1} \in \text{Arg min}_{\mathbf{x} \in \mathcal{X}} F_{\text{MMD}_K^2}(\xi_k, \delta_{\mathbf{x}}) = \text{Arg min}_{\mathbf{x} \in \mathcal{X}} [P_{K,\xi_k}(\mathbf{x}) - P_{K,\mu}(\mathbf{x})]. \quad (18)$$

When $\alpha_k = 1/k$ for all k , ξ_k remains uniform on its support (unless the same \mathbf{x} is chosen several times); see Wynn (1970) for an early contribution in optimal design of experiments. The method is also called conditional-gradient and corresponds to kernel herding (KH) used in machine learning (Bach et al., 2012). The algorithm selects $\mathbf{x}_1 \in \text{Arg max}_{\mathbf{x} \in \mathcal{X}} P_{K,\mu}(\mathbf{x})$ and then

$$\mathbf{x}_{k+1} \in \text{Arg min}_{\mathbf{x} \in \mathcal{X}} \sum_{i=1}^k K(\mathbf{x}_i, \mathbf{x}) - k P_{K,\mu}(\mathbf{x}), \quad k \geq 1, \quad (19)$$

notice the similarity (but not full agreement) with (17). In particular, (19) can be used with singular kernels, which have an intrinsic repelling property (Pronzato and Zhigljavsky, 2021) but for which $K(\mathbf{x}, \mathbf{x})$ is not defined, whereas (17) cannot. In Section 3.2 we shall also consider nonuniform weights, including the case where α_{k+1} is chosen optimally in $\xi_{k+1} = (1 - \alpha_{k+1}) \xi_k + \alpha_{k+1} \delta_{\mathbf{x}_{k+1}}$. In the area of optimal design of experiments, this corresponds to Fedorov's algorithm (1972).

We shall also consider two variants of KH (Section 3.3). First, in a Bayesian integration application, at iteration k of the algorithm we can exploit the support of ξ_k only, and use one of the optimal measures ξ_k^* , $\widehat{\xi}_k$, or $\widetilde{\xi}_k$, with respective weights \mathbf{w}_k^* , $\widehat{\mathbf{w}}_k$ and $\widetilde{\mathbf{w}}_k$, for integration; we shall call this variant *Off-Line Weight Optimisation* (OLWO)³. Second, we can replace ξ_k by ξ_k^* , $\widehat{\xi}_k$, or $\widetilde{\xi}_k$, *in the algorithm itself* before next iteration; we shall call this variant, closely related to SBQ, *Integrated Weight Optimisation* (IWO)⁴.

In the rest of the paper we derive finite-sample-size error bounds for each of the constructions above and give a numerical illustration in Section 7. We start with the simplest method, the Frank-Wolfe algorithm, which has already been much studied in the literature (Section 3). The derivation of the upper bound closely follows Clarkson (2010), and those arguments will be central for the derivation of the bounds for GM and SBQ presented in Sections 4 and 5.

³It is called Frank-Wolfe Bayesian quadrature in (Briol et al., 2015).

⁴Depending how the 'optimal' measure is constructed, this includes the minimum-norm point (Bach et al., 2012) and fully-corrective Frank-Wolfe (Lacoste-Julien and Jaggi, 2015) algorithms; see Remark 3.

2.4 Notation

At each iteration, instead of searching \mathbf{x} in the whole set \mathcal{X} , we shall use a finite subset $\mathcal{X}_C = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(C)}\}$ of candidate points in \mathcal{X} (typically, C points independently sampled from μ ; see Section 6). We assume that μ is not fully supported on \mathcal{X}_C . We denote $\mathbb{I}_C = \{1, \dots, C\}$,

$$\begin{aligned}\bar{K}_C &= \max_{\mathbf{x} \in \mathcal{X}_C} K(\mathbf{x}, \mathbf{x}) \leq \bar{K}, \\ \bar{K}_{\mu, C} &= \max_{\mathbf{x} \in \mathcal{X}_C} K_\mu(\mathbf{x}, \mathbf{x}) = \max_{\mathbf{x} \in \mathcal{X}_C} K(\mathbf{x}, \mathbf{x}) - 2P_{K, \mu}(\mathbf{x}) + \mathcal{E}_K(\mu) \\ &\leq \bar{K}_C + 2\bar{K}_C^{1/2} \tau_{1/2}(\mu) + \tau_{1/2}^2(\mu) = \left[\bar{K}_C^{1/2} + \tau_{1/2}(\mu) \right]^2\end{aligned}\quad (20)$$

(and $\bar{K}_{\mu, C} \leq \bar{K}_C + \tau_{1/2}^2(\mu)$ when $K \geq 0$). We also denote by \mathbf{K}_C and $\mathbf{K}_{\mu C}$ the $C \times C$ matrices with i, j elements respectively equal to $K(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$ and $K_\mu(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$, for $\mathbf{x}^{(i)}, \mathbf{x}^{(j)}$ in \mathcal{X}_C , with K_μ given by (11); \mathbf{e}_j is the j -th canonical basis vector of \mathbb{R}^C .

Any probability measure ξ in $\mathcal{M}_{[1]}^+(\mathcal{X}_C)$, i.e., supported on \mathcal{X}_C , can be represented as a vector of weights ω in the probability simplex

$$\mathcal{P}_C = \left\{ \omega \in \mathbb{R}^C : \sum_{j=1}^C \omega_j = 1, \omega_j \geq 0 \text{ for all } j \right\}.$$

In particular, any empirical probability measure $\xi_{n,e}$ is such that all components of the associated vector $\omega_n \in \mathcal{P}_C$ have the form j_n/n , for $j = 1, \dots, C$, with $j_n \in \{0, 1, \dots, n\}$ and $\sum_{j=1}^C j_n = n$.

For any $\xi \in \mathcal{M}(\mathcal{X})$, any $\mathbf{x} \in \mathcal{X}$ and any $\alpha \in [0, 1]$, we define

$$\xi^+(\mathbf{x}, \alpha) = (1 - \alpha)\xi + \alpha\delta_{\mathbf{x}}, \quad (21)$$

so that $\xi^+(\mathbf{x}, \alpha) \in \mathcal{M}_{[1]}^+(\mathcal{X}_C)$ (respectively, $\mathcal{M}_{[1]}(\mathcal{X}_C)$) when $\mathbf{x} \in \mathcal{X}_C$ and $\xi \in \mathcal{M}_{[1]}^+(\mathcal{X}_C)$ (respectively, $\mathcal{M}_{[1]}(\mathcal{X}_C)$). For any $\mathbf{x}^{(j)} \in \mathcal{X}_C$ and any $\xi \in \mathcal{M}(\mathcal{X}_C)$ with weights ω , the vector of weights associated with $\xi^+(\mathbf{x}^{(j)}, \alpha)$ equals $\omega^+(\mathbf{x}^{(j)}, \alpha) = (1 - \alpha)\omega + \alpha\mathbf{e}_j$. Any measure ξ_n with n support points in \mathcal{X}_C can thus be represented as in (3), with \mathbf{w}_n a n -dimensional vector of weights attached to its support ($\mathbf{w}_n \in \mathcal{P}_n$ when $\xi_n \in \mathcal{M}_{[1]}^+(\mathcal{X}_C)$), and as a vector $\omega_n \in \mathbb{R}^C$ ($\omega_n \in \mathcal{P}_C$ when $\xi_n \in \mathcal{M}_{[1]}^+(\mathcal{X}_C)$). We shall denote

- ξ_*^C the minimum-MMD measure in $\mathcal{M}_{[1]}^+(\mathcal{X}_C)$, with weights $\omega_*^C = \arg \min_{\omega \in \mathcal{P}_C} \omega^\top \mathbf{K}_{\mu C} \omega$;
- $\hat{\xi}^C$ the minimum-MMD measure in $\mathcal{M}_{[1]}(\mathcal{X}_C)$, its weights $\hat{\omega}^C$ are optimal under the total mass constraint $\mathbf{1}_C^\top \hat{\omega}^C$ only: $\hat{\omega}^C$ is given by (5) where $\mathbf{1}_n$, \mathbf{K}_n and $\mathbf{p}_n(\mu)$ are respectively replaced by $\mathbf{1}_C$, \mathbf{K}_C and $\mathbf{p}_C(\mu) = [P_{K, \mu}(\mathbf{x}^{(1)}), \dots, P_{K, \mu}(\mathbf{x}^{(C)})]^\top$;
- $\tilde{\xi}^C$ the minimum-MMD unconstrained measure in $\mathcal{M}(\mathcal{X}_C)$ with weights $\tilde{\omega}^C = \mathbf{K}_C^{-1} \mathbf{p}_C(\mu)$, see (6).

According to (8), any measure ξ in $\mathcal{M}(\mathcal{X}_C)$ with associated weights ω satisfies

$$\text{MMD}_K^2(\mu, \xi) = \tilde{g}_C(\omega) + \text{MMD}_K^2(\mu, \tilde{\xi}^C), \quad (22)$$

where, for any $\omega \in \mathbb{R}^C$, we denote

$$\tilde{g}_C(\omega) = \|\omega - \tilde{\omega}^C\|_{\mathbf{K}_C}^2 = (\omega - \tilde{\omega}^C)^\top \mathbf{K}_C (\omega - \tilde{\omega}^C) \quad (= \text{MMD}_K^2(\xi, \tilde{\xi}^C)). \quad (23)$$

Similarly, from (9), any measure ξ in $\mathcal{M}_{[1]}(\mathcal{X}_C)$ with associated weights ω satisfies

$$\text{MMD}_K^2(\mu, \xi) = \hat{g}_C(\omega) + \text{MMD}_K^2(\mu, \hat{\xi}^C), \quad (24)$$

where

$$\hat{g}_C(\omega) = \|\omega - \hat{\omega}^C\|_{\mathbf{K}_C}^2 = (\omega - \hat{\omega}^C)^\top \mathbf{K}_C (\omega - \hat{\omega}^C) \quad (= \text{MMD}_K^2(\xi, \hat{\xi}^C)). \quad (25)$$

Denoting

$$M_C^2 = \text{MMD}_K^2(\mu, \xi_*^C) = \omega_*^{C\top} \mathbf{K}_{\mu_C} \omega_*^C, \quad (26)$$

for any measure $\xi \in \mathcal{M}(\mathcal{X}_C)$ with associated weights $\omega \in \mathcal{P}_C$, we define

$$\Delta_C(\xi) = \text{MMD}_K^2(\mu, \xi) - M_C^2; \quad (27)$$

the equation (22) implies $\Delta_C(\xi) = \tilde{g}_C(\omega) - \tilde{g}_C(\omega_*^C)$, and when $\xi \in \mathcal{M}_{[1]}(\mathcal{X}_C)$ the equation (24) gives $\Delta_C(\xi) = \hat{g}_C(\omega) - \hat{g}_C(\omega_*^C)$.

In the next sections we derive bounds on $\Delta_C(\xi_k)$ for the different constructions of ξ_k considered. Note that we are interested in situations where $k \ll C$. Those derivations will rely on the convexity of $\hat{g}_C(\cdot)$ and $\tilde{g}_C(\cdot)$ and on the following lemma. The proof is given in the Appendix.

Lemma 1. *Let $(t_k)_k$ and $(\alpha_k)_k$ be two real positive sequences and A be a strictly positive real.*
(i) If t_k satisfies

$$t_1 \leq A \quad \text{and} \quad t_{k+1} \leq (1 - \alpha_{k+1}) t_k + A \alpha_{k+1}^2, \quad k \geq 1, \quad (28)$$

with $\alpha_k = 1/k$ for all k , then $t_k \leq A(2 + \log k)/(k + 1)$ for all $k \geq 1$.

(ii) If t_k satisfies (28) with $\alpha_k = 2/(k + 1)$ for all k , then $t_k \leq 4A/(k + 3)$ for all $k \geq 1$.

(iii) If t_k satisfies

$$t_1 \leq A \quad \text{and} \quad t_{k+1} \leq (1 - 2\alpha_{k+1}) t_k + A \alpha_{k+1}^2, \quad k \geq 1, \quad (29)$$

with $\alpha_k = 1/k$ for all k , then $t_k \leq A/k$ for all $k \geq 1$.

(iv) If t_k satisfies

$$t_1 \leq A \quad \text{and} \quad t_{k+1} \leq t_k - \frac{t_k^2}{A}, \quad k \geq 1, \quad (30)$$

then, $t_k \leq A/(k + p_2)$ for all $k \geq 2$, with $p_2 = A/t_2 - 2 \geq 2$; moreover, when $t_1 \leq A/2$, $t_k \leq A/(k + p_1)$ for all $k \geq 1$, with $p_1 = A/t_1 - 1 \geq 1$.

Algorithm 1 Kernel herding, predefined step sizes α_k : $\xi_{k+1} = \text{KH}(\xi_k, \alpha_{k+1})$

Require: $\mu \in \mathcal{M}_{[1]}^+(\mathcal{X}) \cap \mathcal{M}_K^{1/2}(\mathcal{X})$, $\mathcal{X}_C \subset \mathcal{X}$, $n \in \mathbb{N}$;

1: set $S_0(\cdot) \equiv 0$ and $\xi_0 = 0$; compute $P_{K,\mu}(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}_C$;

2: a sequence $(\alpha_k)_k$ in $[0, 1]$ with $\alpha_1 = 1$;

3: $k \leftarrow 1$

4: **while** $k \leq n$ **do**

5: find $\mathbf{x}_k \in \text{Arg min}_{\mathbf{x} \in \mathcal{X}_C} S_{k-1}(\mathbf{x}) - P_{K,\mu}(\mathbf{x})$;

6: $S_k(\mathbf{x}) \leftarrow (1 - \alpha_k) S_{k-1}(\mathbf{x}) + \alpha_k K(\mathbf{x}_k, \mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}_C$;

7: $\xi_k \leftarrow (1 - \alpha_k) \xi_{k-1} + \alpha_k \delta_{\mathbf{x}_k}$;

8: $k \leftarrow k + 1$

9: **end while**

10: **return** $\mathbf{X}_n = [\mathbf{x}_1, \dots, \mathbf{x}_n]$, ξ_n .

3 Performance analysis of Kernel Herding (KH) and its variants

3.1 Empirical measures

Consider first the case of standard KH, corresponding to Algorithm 1 with $\alpha_k = 1/k$. It selects $\xi_1 = \delta_{\mathbf{x}_1}$, $\mathbf{x}_1 \in \text{Arg max}_{\mathbf{x} \in \mathcal{X}_C} P_{K,\mu}(\mathbf{x})$, and then $\xi_{k+1} = \xi_k^+[\mathbf{x}_{k+1}, 1/(k+1)]$ with \mathbf{x}_{k+1} given by (19) where \mathcal{X}_C is substituted for \mathcal{X} . This choice of α_k implies that $\mathbf{w}_k = \mathbf{1}_k/k$ for all k ; that is, $\xi_k = \xi_{k,e}$, the empirical measure on \mathbf{X}_k . The complexity only grows linearly and is $\mathcal{O}(nC)$ for n iterations (the $P_{K,\mu}(\mathbf{x}^{(i)})$ are only computed once for all at the beginning, with complexity $\mathcal{O}(C)$; $S_k(\mathbf{x}^{(i)}) = P_{K,\xi_k}(\mathbf{x}^{(i)})$ is updated at each iteration for each $\mathbf{x}^{(i)}$ in \mathcal{X}_C , again with complexity $\mathcal{O}(C)$). The finite-sample-size error can be bounded as indicated in Theorem 1. The proof is given in the Appendix.

Theorem 1. *The empirical measure ξ_n generated by Algorithm 1 with $\alpha_k = 1/k$ for all k satisfies*

$$\text{MMD}_K^2(\mu, \xi_n) \leq M_C^2 + B_C \frac{2 + \log n}{n + 1}, \quad n \geq 1, \quad (31)$$

where $B_C = 4\bar{K}_C$ ($B_C = 2\bar{K}_C$ when K is positive) and M_C^2 is given by (26). When $\hat{\xi}^C = \xi_*^C$, ξ_n satisfies

$$\text{MMD}_K^2(\mu, \xi_n) \leq M_C^2 + \frac{B_C}{n}, \quad n \geq 1. \quad (32)$$

It may happen that the same $\mathbf{x}^{(j)}$ is selected several (possibly consecutive) times at line 5 of Algorithm 1. One may refer to Chen et al. (2018) for the extension to the case where \mathbf{x}_{k+1} is searched within the whole set \mathcal{X} and the selection is suboptimal with some bounded error. Chen et al. (2010) show that the error can decrease as $\mathcal{O}(n^{-2})$ when \mathcal{H}_K is finite-dimensional, but Bach et al. (2012) indicate that one can only expect the rate $\mathcal{O}(n^{-1})$ in the infinite-dimensional situation; see also Pronzato and Zhigljavsky (2020, Appendix A). In the next section, we show that a better convergence rate than (31), without the log term, can be obtained in general (without the assumption that $\hat{\xi}^C = \xi_*^C$) when we allow ξ_k to be nonuniform on \mathbf{X}_k .

Algorithm 2 Kernel herding, optimal step sizes: $\xi_{k+1} = \text{KH}(\xi_k, \alpha_{k+1}^*)$

Require: $\mu \in \mathcal{M}_{[1]}^+(\mathcal{X}) \cap \mathcal{M}_K^{1/2}(\mathcal{X})$, $\mathcal{X}_C \subset \mathcal{X}$, $n \in \mathbb{N}$;

- 1: set $S_0(\cdot) \equiv 0$ and $\xi_0 = 0$; compute $P_{K,\mu}(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}_C$;
- 2: $k \leftarrow 1$
- 3: **while** $k \leq n$ **do**
- 4: find $\mathbf{x}_k \in \text{Arg min}_{\mathbf{x} \in \mathcal{X}_C} S_{k-1}(\mathbf{x}) - P_{K,\mu}(\mathbf{x})$;
- 5: **if** $k = 1$ **then** set $\alpha_k^* = 1$, $Q_1 = K(\mathbf{x}_1, \mathbf{x}_1)$, $R_1 = P_{K,\mu}(\mathbf{x}_1)$;
- 6: **else** compute $A_k = Q_{k-1} - R_{k-1} + P_{K,\mu}(\mathbf{x}_k) - S_{k-1}(\mathbf{x}_k)$,
- 7: $B_k = Q_{k-1} - 2S_{k-1}(\mathbf{x}_k) + K(\mathbf{x}_k, \mathbf{x}_k)$,
- 8: and $\alpha_k^* = \min\{A_k/B_k, 1\}$
- 9: **end if**
- 10: **if** $\alpha_k^* = 0$ **then return** $\mathbf{X}_{k-1} = [\mathbf{x}_1, \dots, \mathbf{x}_{k-1}]$, ξ_{k-1} and stop;
- 11: **end if**
- 12: $R_k \leftarrow (1 - \alpha_k^*)R_{k-1} + \alpha_k^*P_{K,\mu}(\mathbf{x}_k)$;
- 13: $Q_k \leftarrow (1 - \alpha_k^*)^2 Q_{k-1} + 2\alpha_k^*(1 - \alpha_k^*)S_{k-1}(\mathbf{x}_k) + (\alpha_k^*)^2 K(\mathbf{x}_k, \mathbf{x}_k)$;
- 14: $S_k(\mathbf{x}) \leftarrow (1 - \alpha_k^*)S_{k-1}(\mathbf{x}) + \alpha_k^*K(\mathbf{x}_k, \mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}_C$;
- 15: $\xi_k \leftarrow (1 - \alpha_k^*)\xi_{k-1} + \alpha_k^*\delta_{\mathbf{x}_k}$;
- 16: $k \leftarrow k + 1$
- 17: **end while**
- 18: **return** $\mathbf{X}_n = [\mathbf{x}_1, \dots, \mathbf{x}_n]$, ξ_n .

3.2 Nonuniform weights

Next theorem shows that for a suitable predefined step-size sequence $(\alpha_k)_k$ in Algorithm 1, the squared MMD decreases as $\mathcal{O}(n^{-1})$. The proof is in the Appendix.

Theorem 2. *The measure ξ_n generated with Algorithm 1 with $\alpha_k = 2/(k+1)$ for all k satisfies*

$$\text{MMD}_K^2(\mu, \xi_n) \leq M_C^2 + \frac{4B_C}{n+3}, \quad n \geq 1. \quad (33)$$

Again, it may happen that the same $\mathbf{x}^{(j)}$ is selected several times at line 5 of Algorithm 1; that is, there may exist repetitions in \mathbf{X}_k . The weights $\{\mathbf{w}_n\}_i$ that ξ_n allocates to the \mathbf{x}_i , $i = 1, \dots, n$, can be computed explicitly. When $\alpha_k = 2/(k+1)$ for all k , we have $\xi_n = \sum_{i=1}^n 2i/[n(n+1)] \delta_{\mathbf{x}_i}$. The distribution is thus far from being uniform, as it is the case with $\alpha_k = 1/k$; see the right panel of Figure 1. When the condition $\widehat{\xi}^C = \xi_*^C$ is satisfied in Theorem 1, the bound (32) is better than (33) and there is no point in using $\alpha_k = 2/(k+1)$ rather than $\alpha_k = 1/k$. Example 1 will illustrate that the decrease of $\text{MMD}_K(\mu, \xi_k)$ may be worse for nonuniform weights; see Figure 1-left.

As a further attempt to improve performance, we can select $\mathbf{x}_{k+1} \in \text{Arg min}_{\mathbf{x} \in \mathcal{X}_C} [P_{K,\xi_k}(\mathbf{x}) - P_{K,\mu}(\mathbf{x})]$ as previously, and then optimise $\text{MMD}_K[\mu, \xi_k^+(\mathbf{x}_{k+1}, \alpha)]$ with respect to α in $[0, 1]$. Due to the quadratic form of $\widehat{g}(\cdot)$, the optimal value $\alpha_{k+1}^* = \alpha_{k+1}^*(\mathbf{x}_{k+1})$ is obtained explicitly. The construction is summarised in Algorithm 2 (see the proof of Theorem 3 in the Appendix for details). Again, the complexity grows linearly with n . The use of the optimal α implies that the same $\mathbf{x}^{(j)}$ cannot be selected two consecutive times at line 4 of Algorithm 2.

Theorem 3. *The measure ξ_n generated with Algorithm 2 satisfies (33); when $\widehat{\xi}^C = \xi_*^C$ it satisfies (32). The optimal α at iteration k is $\alpha_{k+1}^* = \min\{\widehat{\alpha}_{k+1}, 1\}$ with*

$$\widehat{\alpha}_{k+1} = \widehat{\alpha}_{k+1}(\mathbf{x}_{k+1}) = \frac{\sum_{i=1}^k \{\mathbf{w}_k\}_i [P_{K,\xi_k}(\mathbf{x}_i) - P_{K,\mu}(\mathbf{x}_i)] + P_{K,\mu}(\mathbf{x}_{k+1}) - P_{K,\xi_k}(\mathbf{x}_{k+1})}{\sum_{i=1}^k \{\mathbf{w}_k\}_i P_{K,\xi_k}(\mathbf{x}_i) - 2P_{K,\xi_k}(\mathbf{x}_{k+1}) + K(\mathbf{x}_{k+1}, \mathbf{x}_{k+1})} \quad (34)$$

where $\mathbf{x}_{k+1} \in \text{Arg min}_{\mathbf{x} \in \mathcal{X}_C} [P_{K,\xi_n}(\mathbf{x}) - P_{K,\mu}(\mathbf{x})]$. If the algorithm stops at iteration k with $\widehat{\alpha}_{k+1} = 0$, then $\text{MMD}_K(\mu, \xi_k) = \text{MMD}_K(\mu, \xi_*^C)$.

It may seem surprising that the bound obtained with optimal step sizes is not better than when $\alpha_k = 2/(k+1)$ for all k in Algorithm 1, since at any given iteration the decrease of MMD is larger in the former case. However, the global decrease over many iterations with the optimal α is not necessarily better than with a predefined step-size sequence; one can refer to Dunn (1980) for a discussion. A numerical comparison is provided in Section 7, showing that Algorithm 2 may perform worse than Algorithm 1; see the left panel of Figure 1.

Remark 2. *Dunn and Harshbarger (1978) and Dunn (1980) propose other choices of step-size sequences which we do not consider here. We also do not consider Frank-Wolfe algorithm with away steps (Wolfe, 1970; Atwood, 1973)⁵, for which $\xi_{k+1} = \xi_k + \alpha_{k+1}(\xi_k - \delta_{\mathbf{x}_{j_k}})$ moves away from one of its support points \mathbf{x}_{j_k} . Here \mathbf{x}_{j_k} is taken in $\text{Arg max}_{\mathbf{x} \in \text{supp}(\xi_k)} F_{\text{MMD}_K^2}(\xi_k, \delta_{\mathbf{x}}) = \text{Arg max}_{\mathbf{x} \in \mathcal{X}} [P_{K,\xi_k}(\mathbf{x}) - P_{K,\mu}(\mathbf{x})]$ and $\alpha_{k+1} \in [0, \xi_k(\mathbf{x}_{j_k})/[1 - \xi_k(\mathbf{x}_{j_k})]]$ to ensure that $\xi_{k+1}(\mathbf{x}_{j_k}) \geq 0$; the decision to use an away step instead of $\xi_{k+1} = \xi_k^+(\mathbf{x}_{k+1}, \alpha)$ with \mathbf{x}_{k+1} given by (18) can rely on the comparison between the criterion values obtained, or on the comparison between the absolute values of the directional derivatives $|F_{\text{MMD}_K^2}(\xi_k, \delta_{\mathbf{x}_{j_k}})|$ and $|F_{\text{MMD}_K^2}(\xi_k, \delta_{\mathbf{x}_{k+1}})|$. Neither do we consider vertex-exchange methods, for which $\xi_{k+1} = \xi_k + \alpha_{k+1}(\delta_{\mathbf{x}_{k+1}} - \delta_{\mathbf{x}_{j_k}})$ for $\alpha_{k+1} \in [0, \xi_k(\mathbf{x}_{j_k})]$; see for instance Pronzato and Zhigljavsky (2020, Appendix A.3), Pronzato and Pázmán (2013, Chap. 9) and the references therein. These methods prove especially efficient for design problems for which the optimal solution is attained on the boundary of \mathcal{P}_C , with many components equal to zero, in particular due to their ability to reduce the support of the current measure (when $\alpha_{k+1} = 1$). The situation is different for the type of problems we have in mind here, and we can only expect a rate of decrease of the finite-sample-size error similar to Algorithm 2. Lacoste-Julien and Jaggi (2015) give a precise analysis of the convergence of these variants of Frank-Wolfe algorithm and prove that they have a global linear convergence rate (contrary to the original Frank-Wolfe algorithm⁶). However, the pyramidal width defined in the same paper (eq. (9)) decreases as $C^{-1/2}$ and the constant ρ in the linear convergence factor $\exp(-\rho k)$ decreases as $1/C$.*

3.3 KH with off-line and integrated weight optimisation

3.3.1 Off-Line Weight Optimisation (OLWO)

The first KH variant mentioned in Section 2.3.2 (Frank-Wolfe Bayesian quadrature, Briol et al. (2015)) uses the support $\mathbf{X}_k = [\mathbf{x}_1, \dots, \mathbf{x}_k]$ obtained at iteration k with Algorithm 1 or 2 and

⁵See also Todd and Yildirim (2007); Ahipasaoglu et al. (2008) for a recent use in the minimum-volume ellipsoid problem.

⁶Linear convergence is obtained for the Frank-Wolfe algorithm under the condition that $\widehat{\omega}^C$ is in the interior of \mathcal{P}_C ; but even in this favourable case the result has no practical interest for large C ; see Pronzato and Zhigljavsky (2020, Lemma A4).

Algorithm 3 Kernel herding + IWO (i), (ii) and (iii)

Require: $\mu \in \mathcal{M}_{[1]}^+(\mathcal{X}) \cap \mathcal{M}_K^{1/2}(\mathcal{X})$, $\mathcal{X}_C \subset \mathcal{X}$, $n \in \mathbb{N}$;

- 1: set $S_0(\cdot) \equiv 0$ and $\xi_0 = 0$; compute $P_{K,\mu}(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}_C$;
 - 2: $k \leftarrow 1$
 - 3: **while** $k \leq n$ **do**
 - 4: find $\mathbf{x}_k \in \text{Arg min}_{\mathbf{x} \in \mathcal{X}_C} S_{k-1}(\mathbf{x}) - P_{K,\mu}(\mathbf{x})$;
 - 5: compute (i) $\mathbf{w}_k = \mathbf{w}_k^*$ (a QP problem), or (ii) $\mathbf{w}_k = \widehat{\mathbf{w}}_k$ (5), or (iii) $\mathbf{w}_k = \widetilde{\mathbf{w}}_k$ (6),
 - 6: compute $S_k(\mathbf{x}) = \sum_{i=1}^k \{\mathbf{w}_k\}_i K(\mathbf{x}, \mathbf{x}_i)$ for all $\mathbf{x} \in \mathcal{X}_C$;
 - 7: $\xi_k = \sum_{i=1}^k \{\mathbf{w}_k\}_i \delta_{\mathbf{x}_i}$;
 - 8: $k \leftarrow k + 1$
 - 9: **end while**
 - 10: **return** $\mathbf{X}_n = [\mathbf{x}_1, \dots, \mathbf{x}_n]$, ξ_n .
-

constructs an optimal measure ξ_k^* , $\widehat{\xi}_k$, or $\widetilde{\xi}_k$, respectively in $\mathcal{M}_{[1]}^+(\mathbf{X}_k)$, $\mathcal{M}_{[1]}(\mathbf{X}_k)$ or $\mathcal{M}(\mathbf{X}_k)$, with respective weights \mathbf{w}_k^* , obtained as solution of a QP problem, $\widehat{\mathbf{w}}_k$ given by (5) and $\widetilde{\mathbf{w}}_k$ given by (6). By construction, $\text{MMD}_K^2(\mu, \xi_k^*) \leq \text{MMD}_K^2(\mu, \xi_k)$, $\text{MMD}_K^2(\mu, \widehat{\xi}_k) \leq \text{MMD}_K^2(\mu, \xi_k)$ and $\text{MMD}_K^2(\mu, \widetilde{\xi}_k) \leq \text{MMD}_K^2(\mu, \xi_k)$ for all k , so that the bounds of Theorems 1-3 remain valid.

3.3.2 Integrated Weight Optimisation (IWO)

The situation is more complicated for the second variant of Section 2.3.2, where we substitute $\nu_k \in \{\xi_k^*, \widehat{\xi}_k, \widetilde{\xi}_k\}$ for ξ_k at every iteration (the case $\nu_k = \xi_k^*$ corresponds to the fully-corrective Frank-Wolfe algorithm, we do not detail the minimum-norm point algorithm, see Remark 3 below). We only consider the situation where the same choice is applied for all iterations and denote respectively by (i), (ii) and (iii) the three cases $\nu_k = \xi_k^*$, $\nu_k = \widehat{\xi}_k$ and $\nu_k = \widetilde{\xi}_k$ for all k . The choice of \mathbf{x}_{k+1} is the same as for KH, but now there is no α_{k+1} to choose. The construction is summarised in Algorithm 3.

Note that $S_k(\cdot) = P_{K,\nu_k}(\cdot)$ can no longer be computed recursively, so that the complexity grows faster than $\mathcal{O}(nC)$. The complexity of iteration k equals $\mathcal{O}(m(k)C)$, with $m(k)$ the complexity of the determination of \mathbf{w}_k^* , $\widehat{\mathbf{w}}_k$ or $\widetilde{\mathbf{w}}_k$ – in the last two cases, $m(k) = k^3$ in general, and $m(k) = k^2$ if rank-one updating is used to compute \mathbf{K}_k^{-1} in (5) and (6); see Remark 4. Kernel herding with IWO satisfies the following error bounds (the bounds for cases (ii) and (iii) are obviously pessimistic since we can have $\text{MMD}_K^2(\mu, \xi_k) < M_C^2$). The proof is in the Appendix.

Theorem 4. *The measure ξ_n generated by Algorithm 3-(i) satisfies (33); when $\widehat{\xi}^C = \xi_*^C$, it satisfies (32). When using Algorithm 3-(ii), ξ_n satisfies (33); when $\widehat{\xi}^C = \xi_*^C$, it satisfies*

$$\text{MMD}_K^2(\mu, \xi_n) \leq M_C^2 + \frac{B_C}{n+2}, \quad n \geq 2, \quad (35)$$

where $B_C = 4\overline{K}_C$ ($B_C = 2\overline{K}_C$ when K is positive) and M_C^2 is given by (26). When using Algorithm 3-(iii), ξ_n satisfies

$$\text{MMD}_K^2(\mu, \xi_n) \leq M_C^2 + \min \left\{ \frac{4\overline{K}}{n + \frac{4\overline{K}}{\text{MMD}_K^2(\mu, \xi_1)} - 1}, \frac{4\overline{K}}{n + 13/3} \right\}, \quad n \geq 1. \quad (36)$$

Stopping conditions. The measures used in Algorithms 3-(ii) and (iii) are not constrained to belong to $\mathcal{M}_{[1]}^+(\mathcal{X}_C)$, so that the algorithm can still progress when $\text{MMD}_K^2(\mu, \xi_k) \leq \text{MMD}_K^2(\mu, \xi_*^C)$.

Let $\widehat{\mathbf{g}}_k = 2 \mathbf{K}_C(\widehat{\omega}_k - \widehat{\omega}^C)$ denote the gradient of $\widehat{g}(\cdot)$ at $\widehat{\omega}_k$. By construction, $(\mathbf{e}_j - \widehat{\omega}_k)^\top \widehat{\mathbf{g}}_k = 0$ for all j such that $\mathbf{x}^{(j)} \in \text{supp}(\widehat{\xi}^k)$, with

$$(\mathbf{e}_j - \widehat{\omega}_k)^\top \widehat{\mathbf{g}}_k = 2 \left\{ P_{K, \widehat{\xi}^k}(\mathbf{x}^{(j)}) - P_{K, \mu}(\mathbf{x}^{(j)}) + \sum_{i=1}^k \{\widehat{\mathbf{w}}_k\}_i \left[P_{K, \mu}(\mathbf{x}_i) - P_{K, \widehat{\xi}^k}(\mathbf{x}_i) \right] \right\}.$$

Therefore, $P_{K, \widehat{\xi}^k}(\mathbf{x}^{(j)}) - P_{K, \mu}(\mathbf{x}^{(j)})$ equals a constant c_k for all $\mathbf{x}^{(j)} \in \text{supp}(\widehat{\xi}^k)$, and the existence of an $\mathbf{x} \in \mathcal{X}_C$ such that $P_{K, \widehat{\xi}^k}(\mathbf{x}) - P_{K, \mu}(\mathbf{x}) < c_k$ implies that Algorithm 3-(ii) can still progress. Conversely, if $P_{K, \widehat{\xi}^k}(\mathbf{x}) - P_{K, \mu}(\mathbf{x}) \geq c_k$ for all $\mathbf{x} \in \mathcal{X}_C$, the algorithm can be stopped. We can thus add the following line to Algorithm 3-(ii):

4³-(ii): if $S_{k-1}(\mathbf{x}_k) - P_{K, \mu}(\mathbf{x}_k) \geq S_{k-1}(\mathbf{x}_{k-1}) - P_{K, \mu}(\mathbf{x}_{k-1})$ then return $\mathbf{X}_{k-1}, \xi_{k-1}$ and stop;

Similarly, let $\widetilde{\mathbf{g}}_k = 2 \mathbf{K}_C(\widetilde{\omega}_k - \widetilde{\omega}^C)$ denote the gradient of $\widetilde{g}(\cdot)$ at $\widetilde{\omega}_k$. By construction, $\mathbf{e}_j^\top \widetilde{\mathbf{g}}_k = 0$ for all j with $\mathbf{x}^{(j)} \in \text{supp}(\widetilde{\xi}^k)$, with $\mathbf{e}_j^\top \widetilde{\mathbf{g}}_k = 2 \left[P_{K, \widetilde{\xi}^k}(\mathbf{x}^{(j)}) - P_{K, \mu}(\mathbf{x}^{(j)}) \right]$. We thus have $P_{K, \widetilde{\xi}^k}(\mathbf{x}^{(j)}) = P_{K, \mu}(\mathbf{x}^{(j)})$ for all $\mathbf{x}^{(j)} \in \text{supp}(\widetilde{\xi}^k)$; Algorithm 3-(iii) can be stopped when $P_{K, \widetilde{\xi}^k}(\mathbf{x}) \geq P_{K, \mu}(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}_C$ and we can add the following line:

4³-(iii): if $S_{k-1}(\mathbf{x}_k) - P_{K, \mu}(\mathbf{x}_k) \geq 0$ then return $\mathbf{X}_{k-1}, \xi_{k-1}$ and stop;

Remark 3. Algorithm 3-(i) corresponds to the fully-corrective Frank-Wolfe algorithm analysed in (Lacoste-Julien and Jaggi, 2015). The Minimum-norm point variant, based on (Wolfe, 1976), uses a sequence of affine projections based on the calculation of a sequence $\widehat{\omega}_{k_i}$ restricted to give nonzero weights to subsets \mathcal{S}_{k_i} of $\mathcal{S}_{k_0} = \text{supp}(\xi_k)$ (at most k weights $\widehat{\omega}_{k_i}$ need to be calculated); see Algorithm 5 in (Lacoste-Julien and Jaggi, 2015). Since the $\widehat{\omega}_{k_i}$ can be obtained explicitly through (5), this construction is simpler than the fully-corrective Frank-Wolfe algorithm. The bounds in Theorem 4 indicated for Algorithm 3-(i) continue to apply, since we still have $\Delta_C(\xi_{k+1}) \leq (1 - \alpha_{k+1}) \Delta_C(\xi_k) + B_C \alpha_{k+1}^2$, $k \geq 1$, for $\alpha_{k+1} = 2/(k+2)$, and $\Delta_C(\xi_{k+1}) \leq (1 - 2\alpha_{k+1}) \Delta_C(\xi_k) + B_C \alpha_{k+1}^2$, $k \geq 1$, for $\alpha_{k+1} = 1/(k+1)$ when $\widehat{\xi}^C = \xi_*^C$; see the proofs of Theorems 1 and 4.

Remark 4. OLWO and IWO requires the repeated computation of optimal weights $\widehat{\mathbf{w}}_n$ or $\widetilde{\mathbf{w}}_n$, respectively given by (5) and (6). To lighten the calculation, it is advantageous to directly update the inverse matrix \mathbf{K}_n^{-1} as

$$\mathbf{K}_{n+1}^{-1} = \begin{pmatrix} \mathbf{K}_n^{-1} + \beta_{n+1} \mathbf{u}_{n+1} \mathbf{u}_{n+1}^\top & -\beta_{n+1} \mathbf{u}_{n+1} \\ -\beta_{n+1} \mathbf{u}_{n+1}^\top & \beta_{n+1} \end{pmatrix},$$

where $\mathbf{u}_{n+1} = \mathbf{K}_n^{-1} \mathbf{k}_n(\mathbf{x}_{n+1})$ and $\beta_{n+1} = [K(\mathbf{x}_{n+1}, \mathbf{x}_{n+1}) - \mathbf{k}_n^\top(\mathbf{x}_{n+1}) \mathbf{u}_{n+1}]^{-1}$. Rank-one Cholesky updates can be used too. The details are omitted.

Remark 5. The numerical experiments of Section 7 show that the versions (13) and (15) of SBQ behave respectively like Algorithm 3-(iii) and (ii). They also confirm the well-known fact that the approximation error for SBQ with unconstrained weights (i.e., (13)) decreases noticeably faster than the bound (36) of Theorem 4. A plausible explanation is that (36) ignores the decrease of $K(\mathbf{x}_{k+1}, \mathbf{x}_{k+1}) - \mathbf{k}_k^\top(\mathbf{x}_{k+1}) \mathbf{K}_k^{-1} \mathbf{k}_k(\mathbf{x}_{k+1})$ as k increases in the denominator of (12) (in the proof of Theorem 4 we simply bound the denominator by \overline{K}).

Algorithm 4 Greedy MMD minimisation, predefined step sizes α_k : $\xi_{k+1} = \text{GM}(\xi_k, \alpha_{k+1})$

Require: $\mu \in \mathcal{M}_{[1]}^+(\mathcal{X}) \cap \mathcal{M}_K^{1/2}(\mathcal{X})$, $\mathcal{X}_C \subset \mathcal{X}$, $n \in \mathbb{N}$;

- 1: set $S_0(\cdot) \equiv 0$ and $\xi_0 = 0$; compute $K(\mathbf{x}, \mathbf{x})$ and $P_{K,\mu}(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}_C$;
 - 2: a sequence $(\alpha_k)_k$ in $[0, 1]$ with $\alpha_1 = 1$;
 - 3: $k \leftarrow 1$
 - 4: **while** $k \leq n$ **do**
 - 5: find $\mathbf{x}_k \in \text{Arg min}_{\mathbf{x} \in \mathcal{X}_C} 2(1 - \alpha_k)S_{k-1}(\mathbf{x}) + \alpha_k K(\mathbf{x}, \mathbf{x}) - 2P_{K,\mu}(\mathbf{x})$;
 - 6: $S_k(\mathbf{x}) \leftarrow (1 - \alpha_k)S_{k-1}(\mathbf{x}) + \alpha_k K(\mathbf{x}_k, \mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}_C$;
 - 7: $\xi_k \leftarrow (1 - \alpha_k)\xi_{k-1}(\mathbf{x}) + \alpha_k \delta_{\mathbf{x}_k}$;
 - 8: $k \leftarrow k + 1$
 - 9: **end while**
 - 10: **return** $\mathbf{X}_n = [\mathbf{x}_1, \dots, \mathbf{x}_n]$, ξ_n .
-

4 Performance analysis of Greedy MMD Minimisation (GM)

4.1 Empirical measures

GM with empirical measures corresponds to Algorithm 4 with $\alpha_k = 1/k$ for all k ; it selects $\mathbf{x}_1 \in \text{Arg min}_{\mathbf{x} \in \mathcal{X}_C} K(\mathbf{x}, \mathbf{x}) - 2P_{K,\mu}(\mathbf{x})$ and then chooses \mathbf{x}_{n+1} according to (17) with \mathcal{X}_C substituted for \mathcal{X} . It corresponds to Algorithm 1 in (Teymur et al., 2020), where the authors derive a finite-sample-size error bound using the RKHS framework. Taking advantage of the finiteness of the candidate set \mathcal{X}_C , we provide a simpler proof using only linear (finite-dimensional) algebra; see the Appendix. Notice that the bound is smaller than for KH in Theorem 1. The complexity of Algorithm 4 only grows linearly and is $\mathcal{O}(nC)$ for n iterations (the $K(\mathbf{x}^{(i)}, \mathbf{x}^{(i)})$ and $P_{K,\mu}(\mathbf{x}^{(i)})$ are only computed once for all at the beginning, with complexity $\mathcal{O}(C)$, the $S_k(\mathbf{x}^{(i)})$ are updated at each iteration for all $\mathbf{x}^{(i)} \in \mathcal{X}_C$, again with complexity $\mathcal{O}(C)$).

Theorem 5. *The measure ξ_n generated by Algorithm 4 with $\alpha_k = 1/k$ for all k satisfies*

$$\text{MMD}_K^2(\mu, \xi_n) \leq M_C^2 + A_C \frac{1 + \log n}{n}, \quad n \geq 1, \quad (37)$$

where M_C^2 is given by (26) and $A_C = [\overline{K}_C^{1/2} + \tau_{1/2}(\mu)]^2$ ($A_C = \overline{K}_C + \tau_{1/2}^2(\mu)$ when K is positive).

4.2 Nonuniform weights

Consider now the case of general discrete measures ξ_n in $\mathcal{M}_{[1]}^+(\mathcal{X}_C)$, see (3). We show that allowing nonuniform weights in GM yields a faster decrease of $\text{MMD}_K(\mu, \xi_n)$. As for KH, we consider iterations of the form $\xi_{k+1} = \xi_k^+(\mathbf{x}_{k+1}, \alpha_{k+1})$, $k \geq 1$, for some $\alpha_{k+1} \in [0, 1]$ and $\mathbf{x}_{k+1} \in \mathcal{X}_C$, where $\xi_k^+(\mathbf{x}, \alpha)$ is defined by (21). We first consider the same choice $\alpha_k = 2/(k+1)$ as in Section 3.2. The proof of Theorem 6 is in the Appendix.

Theorem 6. *The measure ξ_n generated by Algorithm 4 with $\alpha_k = 2/(k+1)$ for all k satisfies (33). When $\widehat{\xi}^C = \xi_*^C$, Algorithm 4 with $\alpha_k = 1/k$ for all k yields (32).*

Remark 6. *As for Algorithm 1, when $\alpha_k = 2/(k+1)$ in Algorithm 4 the measure ξ_n is not uniform on its support \mathbf{X}_n . It is uniform when $\alpha_k = 1/k$ for all k , but the arguments used in the proof of Theorem 6 only give (31), which is worse than (37) obtained by Teymur et al. (2020).*

Consider now GM with optimal step size, which selects α_{k+1} and \mathbf{x}_{k+1} optimally at each iteration: $[\mathbf{x}_{k+1}, \alpha_{k+1}] \in \text{Arg min}_{\mathbf{x} \in \mathcal{X}_C, \alpha \in [0,1]} \text{MMD}_K[\mu, \xi_k^+(\mathbf{x}, \alpha)]$, with $\xi_1 = \delta_{\mathbf{x}_1}$ and $\mathbf{x}_1 \in \text{Arg min}_{\mathbf{x} \in \mathcal{X}_C} K(\mathbf{x}, \mathbf{x}) - 2P_{K,\mu}(\mathbf{x})$. For $\alpha \in [0, 1]$, any $\mathbf{x}^{(j)} \in \mathcal{X}_C$ satisfies

$$\Delta_C[\xi_k^+(\mathbf{x}^{(j)}, \alpha)] = \widehat{g}_C(\omega_k) - \widehat{g}(\omega_*^C) + 2\alpha (\mathbf{e}_j - \omega_k)^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C) + \alpha^2 \|\mathbf{e}_j - \omega_k\|_{\mathbf{K}_C}^2, \quad (38)$$

the right-hand side of which is minimum when

$$\alpha = \widehat{\alpha}_{k+1,j} = \frac{(\mathbf{e}_j - \omega_k)^\top \mathbf{K}_C(\widehat{\omega}^C - \omega_k)}{\|\mathbf{e}_j - \omega_k\|_{\mathbf{K}_C}^2}.$$

By restricting α to $[0, 1]$, we obtain $[\mathbf{x}_{k+1}, \alpha_{k+1}] = [\mathbf{x}^{(j_{k+1}^*)}, \alpha_{k+1,j}^*]$ with

$$\begin{aligned} \alpha_{k+1,j}^* &= \max\{0, \min\{\widehat{\alpha}_{k+1,j}, 1\}\} \\ j_{k+1}^* &= \arg \min_{j \in \mathbb{I}_C} 2\alpha_{k+1,j}^* (\mathbf{e}_j - \omega_k)^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C) + (\alpha_{k+1,j}^*)^2 \|\mathbf{e}_j - \omega_k\|_{\mathbf{K}_C}^2. \end{aligned}$$

Using (46) and (47), we obtain that $\widehat{\alpha}_{k+1,j}$ is given by (34) with $\mathbf{x}^{(j)}$ substituted for \mathbf{x}_{k+1} . The recursive updating of $Q_k = \sum_{i,\ell=1}^k \{\mathbf{w}_k\}_i \{\mathbf{w}_k\}_\ell K(\mathbf{x}_i, \mathbf{x}_\ell)$, $R_k = \sum_{i=1}^k \{\mathbf{w}_k\}_i P_{K,\mu}(\mathbf{x}_i)$ and $S_k(\mathbf{x}) = P_{K,\xi_k}(\mathbf{x})$ gives Algorithm 5. As in the proof of Theorem 3, $\text{MMD}_K(\mu, \xi_k) > \text{MMD}_K(\mu, \xi_*^C)$ implies that there exists $j \in \mathbb{I}_C$ such that $(\mathbf{e}_j - \omega_k)^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C) < 0$, and therefore $\widehat{\alpha}_{k+1,j} = \alpha(\mathbf{x}^{(j)}) > 0$. Conversely, $\alpha(\mathbf{x}) = 0$ for all $\mathbf{x} \in \mathcal{X}_C$ implies that $\text{MMD}_K(\mu, \xi_k) = \text{MMD}_K(\mu, \xi_*^C)$ and Algorithm 5 can be stopped. As for Algorithm 4, the complexity is $\mathcal{O}(nC)$ for n iterations (it is larger than for Algorithm 2 as $\alpha(\mathbf{x})$ must be calculated for all $\mathbf{x} \in \mathcal{X}_C$). The proof of Theorem 7 is in the Appendix.

Theorem 7. *The measure ξ_n generated with Algorithm 5 satisfies (33). When $\widehat{\xi}^C = \xi_*^C$, it satisfies (32).*

Remark 7. *As for KH, one may also consider OLWO and IWO variants of GM; see Section 3.3. The OLWO variant does not raise any particular difficulty as it runs in parallel and does not affect the algorithm: like in Section 3.3.1 for KH, OLWO can only improve performance. The situation is different for IWO: the fact that the next point \mathbf{x}_{k+1} and the step size α_{k+1} must be selected simultaneously render its use less adapted than with KH. Indeed, the presence of gradient terms in the updating equations (12) and (14), see Section 3.3.2, establishes a direct connection between KH and SBQ.*

5 Performance analysis of SBQ

We suppose again that the successive support points are searched within a finite candidate set \mathcal{X}_C and consider the two versions of SBQ presented in Section 2.3.1, with \mathcal{X}_C substituted for \mathcal{X} . We do not detail the algorithm which simply implements (13) or (15) – with \mathbf{K}_k^{-1} calculated recursively as indicated in Remark 4. For any ξ_k , the value of $\Delta_C(\xi_{k+1})$ obtained by SBQ cannot exceed that obtained by IWO applied to KH, and we get the following bounds on the finite-sample-size error.

Theorem 8. *When ξ_n is generated with (13) (respectively, (15)) where \mathcal{X}_C is substituted for \mathcal{X} , $\text{MMD}_K^2(\mu, \xi_n)$ satisfies the same bounds as those indicated in Theorem 4 for Algorithm 3-(iii) (respectively, Algorithm 3-(ii)).*

Algorithm 5 Greedy MMD minimisation, optimal step sizes: $\xi_{k+1} \mathbf{GM}(\xi_k, \alpha_{k+1}^*)$

Require: $\mu \in \mathcal{M}_{[1]}^+(\mathcal{X}) \cap \mathcal{M}_K^{1/2}(\mathcal{X})$, $\mathcal{X}_C \subset \mathcal{X}$, $n \in \mathbb{N}$;

- 1: compute $K(\mathbf{x}, \mathbf{x})$ and $P_{K,\mu}(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}_C$;
 - 2: set $S_0(\cdot) \equiv 0$, $Q_0 = R_0 = 0$, $\alpha_1(\cdot) \equiv 1$ and $\xi_0 = 0$;
 - 3: set $A_0(\mathbf{x}) = P_{K,\mu}(\mathbf{x})$, $B_0(\mathbf{x}) = K(\mathbf{x}, \mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}_C$;
 - 4: $k \leftarrow 1$
 - 5: **while** $k \leq n$ **do**
 - 6: find $\mathbf{x}_k \in \text{Arg min}_{\mathbf{x} \in \mathcal{X}_C} \alpha^2(\mathbf{x})B_{k-1}(\mathbf{x}) - 2\alpha(\mathbf{x})A_{k-1}(\mathbf{x})$;
 - 7: $\alpha_k \leftarrow \alpha(\mathbf{x}_k)$
 - 8: $R_k \leftarrow (1 - \alpha_k)R_{k-1} + \alpha_k P_{K,\mu}(\mathbf{x}_k)$;
 - 9: $Q_k \leftarrow (1 - \alpha_k)^2 Q_{k-1} + 2\alpha_k(1 - \alpha_k)S_{k-1}(\mathbf{x}_k) + \alpha_k^2 K(\mathbf{x}_k, \mathbf{x}_k)$;
 - 10: $S_k(\mathbf{x}) \leftarrow (1 - \alpha_k)S_{k-1}(\mathbf{x}) + \alpha_k K(\mathbf{x}_k, \mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}_C$;
 - 11: $\xi_k \leftarrow (1 - \alpha_k)\xi_k + \alpha_k \delta_{\mathbf{x}_k}$;
 - 12: compute $A_k(\mathbf{x}) = Q_k - R_k + P_{K,\mu}(\mathbf{x}) - S_k(\mathbf{x})$, $B_k(\mathbf{x}) = Q_k - 2S_k(\mathbf{x}) + K(\mathbf{x}, \mathbf{x})$
 - 13: and $\alpha(\mathbf{x}) = \max\{0, \min\{A(\mathbf{x})/B(\mathbf{x}), 1\}\}$ for all $\mathbf{x} \in \mathcal{X}_C$;
 - 14: **if** all $\alpha(\mathbf{x})$ equal = 0 **then return** $\mathbf{X}_k = [\mathbf{x}_1, \dots, \mathbf{x}_k]$, ξ_k and stop;
 - 15: **end if**
 - 16: $k \leftarrow k + 1$
 - 17: **end while**
 - 18: **return** $\mathbf{X}_n = [\mathbf{x}_1, \dots, \mathbf{x}_n]$, ξ_n .
-

Consider now the version of SBQ presented in Remark 1. For any measure $\xi \in \mathcal{M}(\mathcal{X}_C)$, any $\mathbf{x} \in \mathcal{X}_C$ and any $\alpha \in \mathbb{R}$, denote $\xi^{++}(\mathbf{x}, \alpha) = \xi + \alpha\delta_{\mathbf{x}}$. Then, the construction (16) corresponds to $\xi_{k+1} = \xi_k^{++}(\mathbf{x}_{k+1}, \alpha_{k+1})$, where $[\mathbf{x}_{k+1}, \alpha_{k+1}] \in \text{Arg min}_{\mathbf{x} \in \mathcal{X}_C, \alpha} \text{MMD}_K^2[\xi_k^{++}(\mathbf{x}, \alpha)]$. We can show that $\text{MMD}_K^2(\mu, \xi_n) \leq M_C^2 + A_C \exp(-n/C)$, $n \geq 1$, with A_C and M_C as in Theorem 5. Indeed, for any signed measure ξ with weights ω and any $\mathbf{x}^{(j)} \in \mathcal{X}_C$, we have

$$\begin{aligned} \Delta_C[\xi^{++}(\mathbf{x}^{(j)}, \alpha)] &= \Delta_C(\xi) + 2\alpha \mathbf{e}_j^\top \mathbf{K}_C(\omega - \tilde{\omega}^C) + \alpha^2 K(\mathbf{x}^{(j)}, \mathbf{x}^{(j)}) \\ &\leq \Delta_C(\xi) + 2\alpha \mathbf{e}_j^\top \mathbf{K}_C(\omega - \tilde{\omega}^C) + \alpha^2 \bar{K}_C, \end{aligned}$$

where $\Delta_C(\xi)$ is defined in (27). Therefore, $\min_{\alpha} \Delta_C[\xi_k^{++}(\mathbf{x}^{(j)}, \alpha)] \leq \Delta_C(\xi_k) - [\mathbf{e}_j^\top \mathbf{K}_C(\omega_k - \tilde{\omega}^C)]^2 / \bar{K}_C$ and

$$\begin{aligned} \Delta_C(\xi_{k+1}) &\leq \Delta_C(\xi_k) - \max_{j \in \mathbb{I}_C} [\mathbf{e}_j^\top \mathbf{K}_C(\omega_k - \tilde{\omega}^C)]^2 / \bar{K}_C \\ &\leq \Delta_C(\xi_k) - \max_{\mathbf{u} \in \mathcal{B}(\mathbf{0}_C, r_C)} [\mathbf{u}^\top \mathbf{K}_C(\omega_k - \tilde{\omega}^C)]^2 / \bar{K}_C, \end{aligned}$$

with $\mathcal{B}(\mathbf{0}, r_C)$ the ball centered at the origin $\mathbf{0}_C$ with radius $r_C = C^{-1/2}$. From the definition (23) of $\tilde{g}(\cdot)$, we obtain $\tilde{g}(\omega_{k+1}) \leq \tilde{g}(\omega_k) - [\lambda_{\max}(\mathbf{K}_C)/(C\bar{K}_C)] \tilde{g}(\omega_k) \leq (1 - 1/C) \tilde{g}(\omega_k)$, and thus, for all $n \geq 1$, $\tilde{g}(\omega_n) \leq \tilde{g}(\omega_1) (1 - 1/C)^n \leq A_C (1 - 1/C)^n$, since $\tilde{g}(\omega_1) \leq \text{MMD}_K^2(\mu, \xi_1) \leq A_C$, see (20); (22) and $\text{MMD}_K^2(\mu, \xi^C) \leq M_C^2$ give $\text{MMD}_K^2(\mu, \xi_n) \leq M_C^2 + A_C \exp(-n/C)$. Although the decrease is exponential, for $n < C$ this bound is much worse than those obtained for the other constructions considered in the paper.

6 Random candidate sets

The extension of the results in previous sections to the case where \mathcal{X}_C corresponds to C points independently sampled from μ is fairly simple; see Teymur et al. (2020). For instance, (33) becomes

$$\mathbb{E}_\mu\{\text{MMD}_K^2(\mu, \xi_n)\} \leq \mathbb{E}_\mu\{M_C^2\} + \frac{4\mathbb{E}_\mu\{B_C\}}{n+3}, \quad n \geq 1.$$

We thus only have to bound the expected values of the constants A_C , B_C and M_C^2 that intervene in the various bounds that have been presented. Their values are given in the following lemma, the proof is in the Appendix.

Lemma 2. *Suppose $\mu \in \mathcal{M}_K^1(\mathcal{X})$ and that the C points in \mathcal{X}_C are independently sampled from μ , then*

$$\begin{aligned} \mathbb{E}_\mu\{A_C\} &\leq A(\mu) = [\bar{K}^{1/2} + \tau_{1/2}(\mu)]^2 \quad (A(\mu) = \bar{K} + \tau_{1/2}^2(\mu) \text{ when } K \text{ is positive}), \\ \mathbb{E}_\mu\{B_C\} &\leq B = 4\bar{K} \quad (B = 2\bar{K} \text{ when } K \text{ is positive}), \\ \mathbb{E}_\mu\{M_C^2\} &\leq M^2(\mu)/C = [\tau_1(\mu) - \mathcal{E}_K(\mu)]/C, \end{aligned}$$

M_C^2 given by (26), $A_C = [\bar{K}_C^{1/2} + \tau_{1/2}(\mu)]^2$ and $B_C = 4\bar{K}_C$ ($A_C = \bar{K}_C + \tau_{1/2}^2(\mu)$ and $B = 2\bar{K}_C$ when K is positive).

Teymur et al. (2020) derive a bound similar to (37) (with A_C and M_C^2 replaced by $\mathbb{E}_\mu\{A_C\}$ and $\mathbb{E}_\mu\{M_C^2\}$) for Algorithm 4 with $\alpha_k = 1/k$ for all k in the situation where a different sample $\mathcal{X}_C[k]$ of C random points is used at each iteration; see also Chen et al. (2019). The extension to this situation of the approach used in previous sections does not seem straightforward as the probability simplex \mathcal{P}_C and matrices \mathbf{K}_C and \mathbf{K}_{μ_C} refer to a fixed set \mathcal{X}_C . In Appendix B we provide arguments explaining how our results extend to the case where $\mathcal{X}_C = \mathcal{X}_C[k]$ depends on k : basically, similar bounds continue to hold provided we consider the expectation of $\text{MMD}_K^2(\mu, \xi_n)$ and bound the expected values of the constants involved as in Lemma 2. Note that changing the candidate set at every iteration implies that we need to calculate $K(\mathbf{x}_i, \mathbf{x})$ for all $\mathbf{x}_i \in \text{supp}(\xi_k)$ and all $\mathbf{x} \in \mathcal{X}_C[k]$, and to recalculate $P_{K,\mu}(\mathbf{x})$ (Algorithms 1 and 2), or $P_{K,\mu}(\mathbf{x})$ and $K(\mathbf{x}, \mathbf{x})$ (Algorithms 4 and 5), for all $\mathbf{x} \in \mathcal{X}_C[k]$ at every iteration, with a computational cost thus growing as $\mathcal{O}(k^2 C)$.

We conclude this section by recalling a result on the MMD of the empirical measure $\xi_{n,e}$ of a random n -point sample from μ ; see Mak and Joseph (2018, Lemma 2). The proof is given in Appendix A.

Theorem 9. *When $\mathbf{x}_1, \dots, \mathbf{x}_n$ are independently sampled from μ , then $n \text{MMD}_K^2(\mu, \xi_{n,e}) \xrightarrow{d} Z = \sum_{i=1}^{\infty} \lambda_i \chi_{1i}^2$, where the λ_i are the eigenvalues of the operator T_{K_μ} on $L_2(\mathcal{X}, \mu)$ defined by $T_{K_\mu} f(\mathbf{x}) = \int_{\mathcal{X}} K_\mu(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') d\mu(\mathbf{x}')$, $f \in L_2(\mathcal{X}, \mu)$, $\mathbf{x} \in \mathcal{X}$, and the χ_{1i}^2 are independent χ_1^2 random variables.*

From Lemma 2 and Theorem 9 we have in particular $\mathbb{E}_\mu\{\text{MMD}_K^2(\mu, \xi_{n,e})\} = M^2(\mu)/n = [\tau_1(\mu) - \mathcal{E}_K(\mu)]/n$ and $n^2 \text{var}_\mu\{\text{MMD}_K^2(\mu, \xi_{n,e})\} \rightarrow 2 \sum_{i=1}^{\infty} \lambda_i^2$ as $n \rightarrow \infty$. Although the bounds obtained in previous sections suggest that the measures obtained with the algorithms that have been considered do not perform necessarily better (asymptotically) than i.i.d. samples from μ , the examples in the next section demonstrate the interest of using KH, GM or SBQ.

7 Numerical study

7.1 Example 1: space-filling design

For illustration purpose we only consider the case $d = 2$ and take μ uniform on $\mathcal{X} = [0, 1]^2$; \mathcal{X}_C corresponds to the first $2^{17} = 131\,072$ points of a scrambled Sobol' sequence in \mathcal{X} . K is a separable kernel given by the product of uni-dimensional Matérn 3/2 covariance functions, that is, $K(\mathbf{x}, \mathbf{x}') = \prod_{i=1}^d K_{3/2,\theta}(x_i, x'_i)$ with

$$K_{3/2,\theta}(x, x') = (1 + \sqrt{3}\theta |x - x'|) \exp(-\sqrt{3}\theta |x - x'|).$$

We have $\mathcal{E}_K(\mu) = \prod_{i=1}^d \mathcal{E}_{K_{3/2,\theta}}(\mu_1)$ and $P_{K,\mu}(\mathbf{x}) = \prod_{i=1}^d P_{K_{3/2,\theta},\mu_1}(x_i)$ with μ_1 the uniform measure on $[0, 1]$, and $\mathcal{E}_{K_{3/2,\theta}}(\mu_1)$ and $P_{K_{3/2,\theta},\mu_1}(x)$ can be computed explicitly; see, e.g., Pronzato and Zhigljavsky (2020, Table 3.1). Examples of space-filling design based on MMD-minimisation with $d = 10$ and recommendations for the choice of θ are given in the same paper. We use $\theta = 10$ throughout the example.

The left panel of Figure 1 shows the evolution of $\text{MMD}_K(\mu, \xi_n)$ as a function of n (log-log plot) when ξ_n is generated with Algorithm 1 with $\alpha_k = 1/k$ and $\alpha_k = 2/(k+1)$, or with Algorithm 2. The bound (33) is also shown (M_C^2 is negligible). Although Algorithm 2 uses optimal step-sizes, its performance is the worst for large n and is never better than that of Algorithm 1 with $\alpha_k = 1/k$ (note that the rate of decrease of $\text{MMD}_K(\mu, \xi_n)$ for Algorithm 2 closely follows $\mathcal{O}(1/n)$ when $n \gtrsim 100$). Although the bound (33) of Theorem 2 is better than (31) of Theorem 1, $\alpha_k = 1/k$ yields better performance than $\alpha_k = 2/(k+1)$ all along the sequence. This suggests that there is little interest in using more sophisticated versions of KH than Algorithm 1 with $\alpha_k = 1/k$. The MMD for the empirical measure of a random n -point design is also presented, showing a decrease that closely follows $\mathcal{O}(1/n)$. The evolution of $\text{MMD}_K(\mu, \xi_n)$ obtained for ξ_n generated with Algorithm 4 with $\alpha_k = 1/k$ and $\alpha_k = 2/(k+1)$ (respectively, with Algorithm 5) is visually hardly distinguishable from that obtained with Algorithm 1 with $\alpha_k = 1/k$ and $\alpha_k = 2/(k+1)$ (respectively, with Algorithm 2) and is not presented.

The right panel of Figure 1 shows the strong non-uniformity of the weights $\{\mathbf{w}_{1000}\}_i$, $i = 1, \dots, 1000$, associated with the measures ξ_{1000} generated by Algorithm 1 with $\alpha_k = 2/(k+1)$ and by Algorithm 2 (note that most recent points are overweighed for the former and downweighed for the latter).

We consider now the variants (ii) and (iii) of IWO in Algorithm 3 (here the weights $\widehat{\mathbf{w}}_k$ are positive for all k , so that variant (ii) coincides with (i), the fully-corrective Frank-Wolfe algorithm, and also with the minimum-norm point algorithm, see Remark 3). Unsurprisingly, $\text{MMD}_K(\mu, \nu_n)$ is smaller for $\nu_n = \widetilde{\xi}_n$ of variant (iii) than for $\nu_n = \widehat{\xi}_n$ of variant (ii) since the weights are unconstrained in the former case, see the left panel of Figure 2. The two variants perform similarly for large n , however. The bound (36) for Algorithm 3-(iii) is accurate for small n but very pessimistic for large n ; see Remark 5. Algorithm 3-(ii) performs as Algorithm 1 with $\alpha_k = 1/k$ for small n ($n \lesssim 30$) but performs significantly better for larger n . The performances are quasi identical when using OLWO of Section 3.3.1 (Frank-Wolfe Bayesian quadrature, not shown). When we stop Algorithm 1 (with $\alpha_k = 1/k$) at $n = 200$, all weights $\{\widehat{\mathbf{w}}_n\}_i$ and $\{\widetilde{\mathbf{w}}_n\}_i$, $i = 1, \dots, n$, are positive. The weights are positive too for Algorithm 3-(ii) and (iii)⁷. The evolution of $\text{MMD}_K(\mu, \xi_n)$ for ξ_n obtained with version (13) of SBQ using unconstrained

⁷Note that the question of positivity of Bayesian quadrature weights $\{\widetilde{\mathbf{w}}_n\}_i$ is far from obvious; see Karvonen et al. (2019).

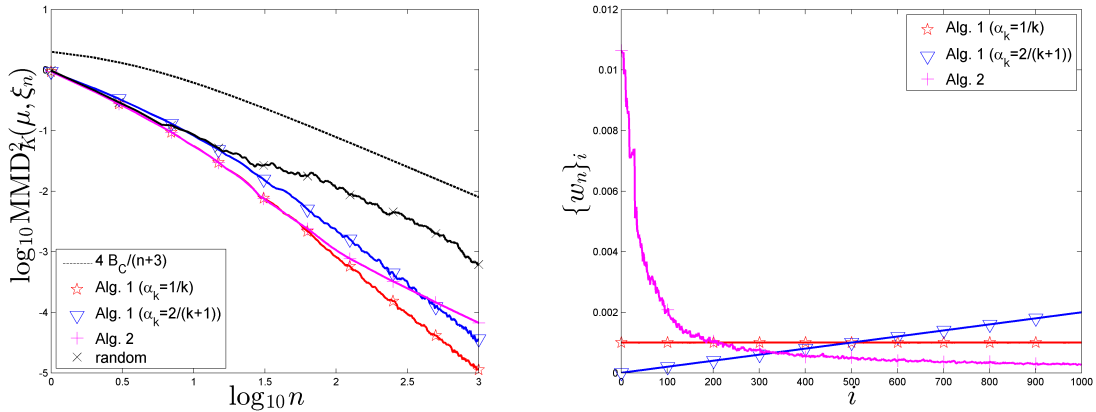


Figure 1: Left: upper bound (33) and $\text{MMD}_K(\mu, \xi_n)$ for ξ_n generated with Algorithm 1 with $\alpha_k = 1/k$ and $\alpha_k = 2/(k+1)$, with Algorithm 2 and for the empirical measure $\xi_n = \xi_{n,e}$ of a random n -point design, $n = 1, \dots, 1000$. Right: weights $\{\mathbf{w}_{1000}\}_i$ of ξ_{1000} .

weights (respectively, with version (15) using weights that sum to one) is indistinguishable from that obtained with Algorithm 3-(iii) (respectively, Algorithm 3-(ii)).

Computational times⁸ are shown on the right panel of Figure 2 for Algorithm 1 with $\alpha_k = 1/k$ and $\alpha_k = 2/(k+1)$, for Algorithm 2 and for Algorithm 3-(ii) and (iii)⁹. The choice of the sequence $(\alpha_k)_k$ has no influence on the computational time of Algorithm 1; Algorithm 2 is slightly more demanding, but its computational time still grows linearly with n ; the higher performance of IWO shown on the left panel comes with a significant increase of computational cost (which is similar for OLWO).

Computational times for Algorithm 4 with $\alpha_k = 1/k$, Algorithm 5 and the two versions (13) and (15) of SBQ are shown on the left panel of Figure 3: Algorithm 4 is as fast as Algorithm 1; Algorithm 5 is slightly slower than Algorithm 3. Note that the two versions of SBQ are much slower than Algorithm 3-(ii) and (iii).

MMD minimisation with μ uniform on \mathcal{X} is an efficient method to construct nested space-filling designs; this is one of the main motivations in (Pronzato and Zhigljavsky, 2020). The right panel of Figure 3 shows the 25-point design corresponding to the support of the measure ξ_n generated with Algorithm 4 with $\alpha_k = 1/k$, with a covering radius $\text{CR}(\mathbf{X}_{25}) \simeq 0.1625$. Algorithm 1 with $\alpha_k = 1/k$ yields a very similar design, but with a different ordering of points and a slightly larger covering radius $\text{CR}(\mathbf{X}_{25}) \simeq 0.1685$. When using Algorithm 3-(ii) (respectively, Algorithm 3-(iii)), the support of ξ_{25} has a covering radius $\text{CR}(\mathbf{X}_{25}) \simeq 0.1677$ (respectively, $\text{CR}(\mathbf{X}_{25}) \simeq 0.2024$). This illustrates the fact that a smaller MMD is not necessarily synonym to better space-filling properties: the optimal weighting of a given design improves its MMD, but space-filling performance, measured for instance by the covering radius, is unweighed. In fact, when allocating uniform weights to the support of ξ_n generated with Algorithm 3-(iii), the MMD obtained is similar to that shown on the left panel of Figure 2 for Algorithm 1 with

⁸All calculations are made with Matlab, on a PC with a clock speed of 1.5 GHz and 16 GB RAM

⁹All computational times start with a positive value at $n = 0$ since we account for the calculation of $P_{K,\mu}(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}_C$.

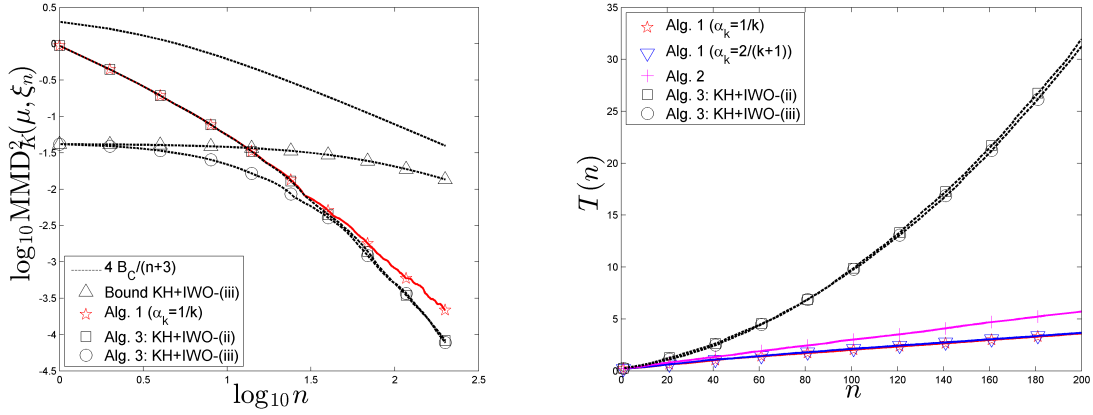


Figure 2: Left: upper bounds (33) and (36), and $\text{MMD}_K(\mu, \xi_n)$ for ξ_n generated with Algorithm 1 with $\alpha_k = 1/k$ and with Algorithm 3-(ii) and (iii), $n = 1, \dots, 200$. Right: computational time $T(n)$ (in s) of ξ_n for Algorithm 1 with $\alpha_k = 1/k$ and $\alpha_k = 2/(k+1)$, for Algorithm 2 and for Algorithm 3-(ii) and (iii), $n = 1, \dots, 200$.

$\alpha_k = 1/k$ (red \star), thus much worse than for the original ξ_n (black \circ).

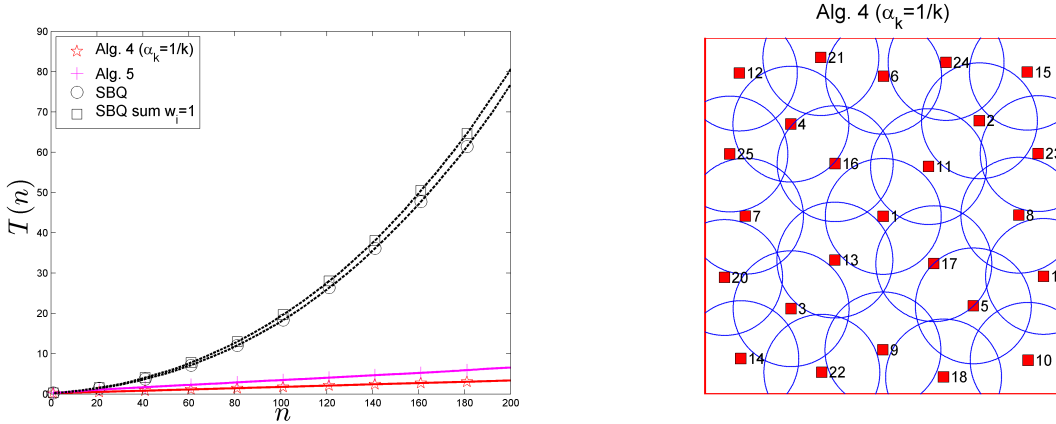


Figure 3: Left: computational time $T(n)$ (in s) of ξ_n for Algorithm 4 with $\alpha_k = 1/k$, Algorithm 5 and for the two versions (13) and (15) of SBQ, $n = 1, \dots, 200$. Right: support \mathbf{X}_n (ordered) of ξ_{25} generated with Algorithm 4 with $\alpha_k = 1/k$; the radius of the circles equals the covering radius of \mathbf{X}_n (the smallest value that permits to cover \mathcal{X}).

7.2 Example 2: Gaussian mixture

Here $\mu = \sum_{j=1}^m \beta_j \mu_{\mathcal{N}}(\mathbf{a}_j, \sigma_j)$ with $\beta_j > 0$, $\sum_{j=1}^m \beta_j = 1$ and $\mu_{\mathcal{N}}(\mathbf{a}_j, \sigma_j)$ corresponding to the normal distribution with mean \mathbf{a}_j and variance $\sigma_j^2 \mathbf{I}_d$, with \mathbf{I}_d the identity matrix. Again, for illustration purpose we take $d = 2$. The difficulty increases with the number m of components,

the problem is also more difficult when the weights and/or variances of the components differ. We take $m = 3$, $\mathbf{a}_1 = (-1, 1)^\top$, $\mathbf{a}_2 = (1, -1)^\top$, $\mathbf{a}_3 = (1, 1)^\top$, $\sigma_j = 1/2$ for all j , and $\beta_1 = \beta_2 = 2/7$, $\beta_3 = 3/7$ (this is a slight variation of the example in Figure 1 of (Teymur et al., 2020) where the three components have equal weights). Figure 4 presents a 3-d plot of the probability density function φ_μ (left) and its contour lines (right) together with the candidate set \mathcal{X}_C formed by $2^{14} = 16\,384$ independent samples, among which we select a subset of n representative points.

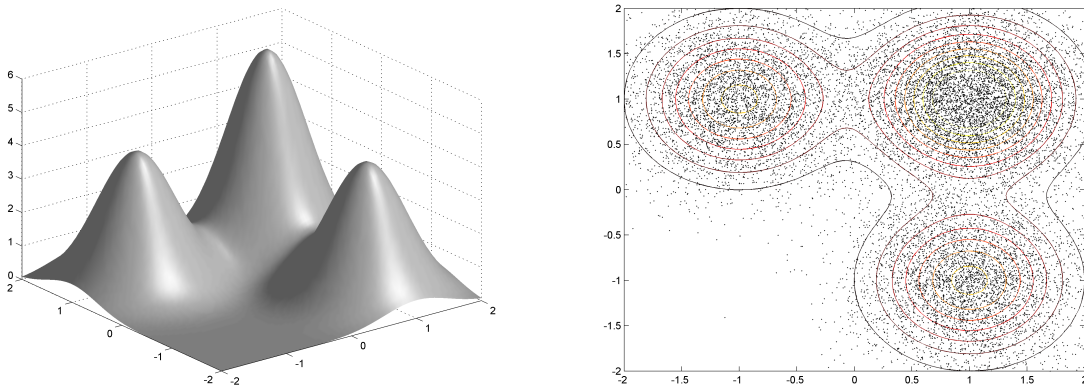


Figure 4: Left: 3d-plot of the p.d.f. φ_μ ; right: contour lines of φ_μ and candidate set \mathcal{X}_C (dots).

We use the Gaussian, or Radial Basis Function, kernel,

$$K_\theta(\mathbf{x}, \mathbf{x}') = \exp(-\theta \|\mathbf{x} - \mathbf{x}'\|^2), \quad (39)$$

for which direct calculation gives¹⁰

$$\begin{aligned} \mathcal{E}_{K_\theta}(\mu) &= \sum_{j,\ell=1}^d \frac{\beta_j \beta_\ell}{(1 + 2\theta\sigma_j^2 + 2\theta\sigma_\ell^2)^{d/2}} \exp\left(-\frac{\theta \|\mathbf{a}_j - \mathbf{a}_\ell\|^2}{1 + 2\theta\sigma_j^2 + 2\theta\sigma_\ell^2}\right) \\ P_{K,\mu}(\mathbf{x}) &= \sum_{j=1}^d \frac{\beta_j}{(1 + 2\theta\sigma_j^2)^{d/2}} \exp\left(-\frac{\theta \|\mathbf{x} - \mathbf{a}_j\|^2}{1 + 2\theta\sigma_j^2}\right), \quad \mathbf{x} \in \mathbb{R}^d. \end{aligned} \quad (40)$$

It is important to choose a suitable order of magnitude for θ , even if a precise tuning is not essential. This issue is frequently mentioned in the literature, see for example Huszár and Duvenaud (2012), but is often overlooked. As for the construction of space-filling designs where the target measure μ is uniform on \mathcal{X} , see Pronzato and Zhigljavsky (2020), we recommend to let θ depend on the number of points to be generated. If the target size is n_{\max} points, each point \mathbf{x}_i will “represent” a fraction $1/n_{\max}$ of the C candidate points, and having a correlation $K_\theta(\mathbf{x}_i, \mathbf{x}_j) > 1/2$ with C/n_{\max} points seems reasonable. We thus choose θ such that $K_\theta(\mathbf{x}_i, \mathbf{x}_j) < 1/2$ for $(100/n_{\max})\%$ of the pairs $(\mathbf{x}^{(j)}, \mathbf{x}^{(k)})$ in a random sample of 1 000 points of \mathcal{X}_C (that is, with obvious notation, $\theta = -\log(0.5)/Q_{1/n_{\max}}(\|\mathbf{x}^{(j)} - \mathbf{x}^{(k)}\|^2)$ for the example considered).

¹⁰The analytic expression of $P_{K,\mu}(\mathbf{x})$ is also available for K the product of uni-dimensional Matérn 3/2 kernels as in Section 7.1, though the expression is more complicated than (40) and involves the error function $\text{erf}(t) = (2/\sqrt{\pi}) \int_0^t \exp(-x^2) dx$; the results obtained are similar to those presented here for the Gaussian kernel.

Figure 5 shows the first n_{\max} points selected by Algorithms 1 and 4, both with $\alpha_k = 1/k$ for all k : $n_{\max} = 25$ ($\theta \simeq 5.7$) on the first row, $n_{\max} = 200$ ($\theta \simeq 46.4$) on the second. The points location looks roughly the same for both algorithms when $n_{\max} = 25$, the ordering being however different starting at $n = 12$; the designs look also similar when $n_{\max} = 200$ and it is difficult to separate them.

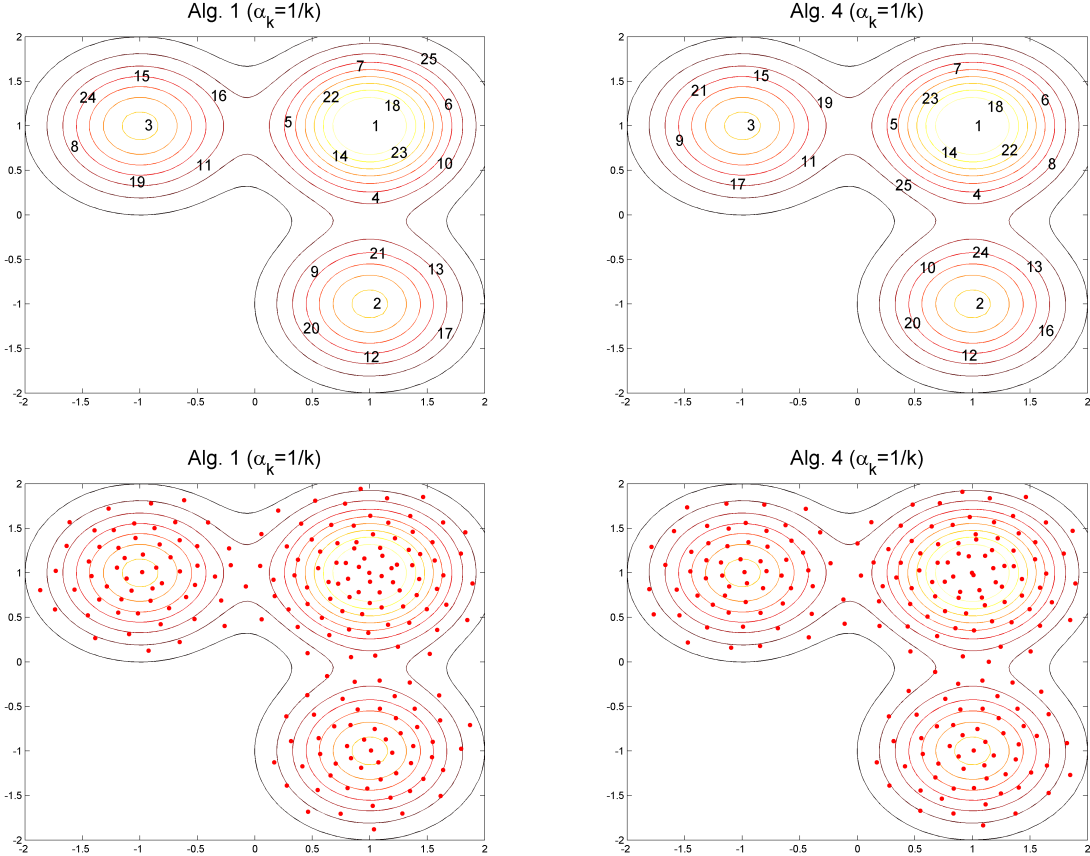


Figure 5: Designs \mathbf{X}_n obtained with Algorithms 1 and 4 (both with $\alpha_k = 1/k$); $n_{\max} = 25$ ($\theta \simeq 5.7$) on the first row, $n_{\max} = 200$ ($\theta \simeq 46.39$) on the second row.

Figure 6 shows the evolution of $\text{MMD}_K(\mu, \xi_n)$ (and its upper bound (33)) for ξ_n generated with Algorithms 1, 2, 3-(ii), 3-(iii), 4 and 5 and for the empirical measure of a random design, when $n_{\max} = 200$ (the designs are not shown, but they all look very similar to those on the second row of Figure 5). Algorithms 1 and 4 (both with $\alpha_k = 1/k$ for all k) and 2 and 5 perform similarly; Algorithm 3-(ii) is only marginally superior; the MMD is significantly smaller for Algorithm 3-(iii) which does not set constraints on ξ_n . The weights that ξ_n allocates to its support points are positive for Algorithm 3-(ii) and (iii), with $\sum_{i=1}^{200} \{\mathbf{w}_{200}\}_i \simeq 0.834$ for Algorithm 3-(iii). The two versions of SBQ perform similarly to Algorithm 3-(ii) and (iii) and their weights $\{\mathbf{w}_{200}\}_i$ are positive too.

Finally, we also evaluate the approximation error by the MMD for the distance kernel $K_D(\mathbf{x}, \mathbf{x}') = -\|\mathbf{x} - \mathbf{x}'\|$ of Székely and Rizzo (2013). Since $P_{K_D, \mu}(\cdot)$ and the energy distance

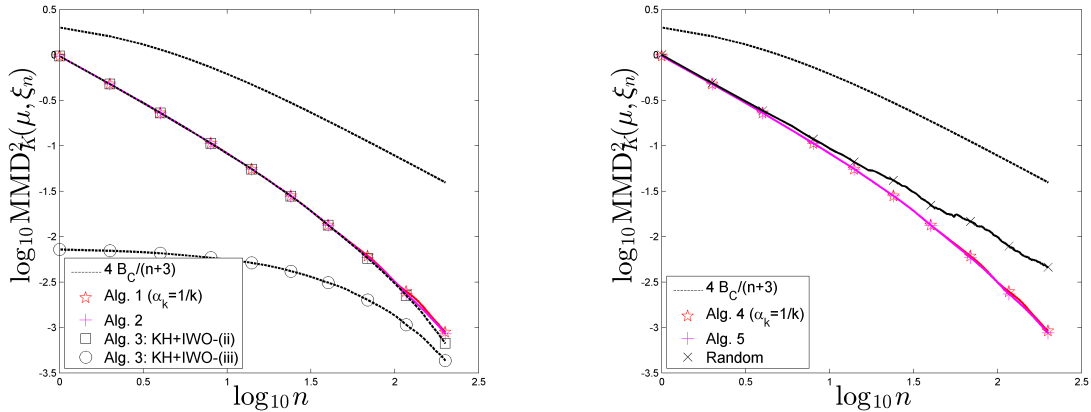


Figure 6: Upper bound (33) and $\text{MMD}_K(\mu, \xi_n)$ for ξ_n generated with Algorithms 1, 2, 3-(ii), 3-(iii) (left), 4 and 5, and for the empirical measure of a random design (right).

$\mathcal{E}_{K_D}(\mu)$ are not known explicitly, we compute $\text{MMD}_{K_D}(\mu_C, \xi_n)$, with μ_C the empirical measure for the candidate set \mathcal{X}_C . Figure 7 shows $\text{MMD}_{K_D}(\mu_C, \xi_n)$ for ξ_n generated with Algorithms 1, 3-(ii) and 4, using the Gaussian kernel (39) – ξ_n generated with Algorithm 3-(iii) cannot be tested since its weights do not sum to one¹¹. The three algorithms appear to perform similarly and provide better approximations of μ than random sampling in terms of $\text{MMD}_{K_D}(\mu_C, \cdot)$. Due to their much smaller computational costs, Algorithms 1 and 4 are preferable to Algorithm 3-(ii) (and version (15) of SBQ) in this example. Algorithm 3-(iii) is preferable to standard SBQ with unconstrained weights (13) due to its smaller computational cost. We also tried to use a Stein kernel, based on the inverse multiquadric kernel $K_{s,\theta}(\mathbf{x}, \mathbf{x}') = 1/(1 + \theta \|\mathbf{x} - \mathbf{x}'\|^2)^s$, $\theta > 0$, $s \in (0, 1)$, instead of (39) to generate ξ_n , but the values obtained for $\text{MMD}_{K_D}(\mu_C, \xi_n)$ were significantly larger than with (39)¹².

8 Conclusions

Bounds on the finite-sample-size approximation error of iterative methods for the minimisation of an MMD discrepancy have been derived and illustrated by numerical experiments. These experiments indicate that the bounds give a fair picture of the decrease of the true MMD for all methods considered, except for SBQ with unconstrained weights (13) for which the bound is markedly pessimistic (the connection with kernel herding used for its derivation gives a plausible explanation for this pessimism; see Remark 5). They also indicate that the performances of kernel herding and greedy MMD minimisation do not improve by considering other step-size sequences than $1/k$ (which generate empirical measures), and that a variant of kernel herding with optimised weights yields performance similar to standard SBQ at a lower computational cost.

We have restricted our attention to finite candidate sets. This situation is at the same time simpler and computationally more efficient in terms of practical implementation, and simpler in

¹¹ K_D is Conditionally Integrally Strictly Positive Definite and defines a metric between measures in $\mathcal{M}_{[1]}(\mathcal{X})$.

¹² We used $s = 1/2$ and θ given by the median heuristic of Garreau et al. (2017); see also Teymur et al. (2020).

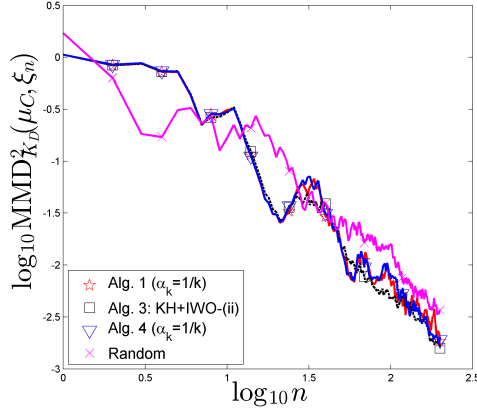


Figure 7: $\text{MMD}_{K_D}(\mu_C, \xi_n)$ for the empirical measure of a random design and for ξ_n generated with Algorithms 1, 3-(ii), and 4, all using the Gaussian kernel (39), with K_D the distance kernel of Székely and Rizzo (2013).

terms of analysis since only finite-dimensional linear algebra is used, but the extension to the Hilbert-space situation remains possible.

Finally, we have only considered the case where one adds one-point-at-a-time to the construction. Less myopic methods that select several (say $m > 1$) points at each iterations could also be considered. The extension of our results to this context, and the development of computationally efficient methods that avoid the combinatorial explosion due to considering all possible $\binom{C}{m}$ subset selections, deserve further studies. One can refer to Teymur et al. (2020) for an exciting contribution in this direction.

Appendix A: proofs

Proof of Lemma 1.

(i) Suppose that t_k satisfies (28) with $\alpha_k = 1/k$ for all k . We show that $t_k \leq A(2 + \log k)/(k + 1)$ by induction on k . The inequality is satisfied for $k = 1$, assume that it is satisfied for $k \geq 1$, we get $A[2 + \log(k + 1)]/(k + 2) - t_{k+1} \geq A a(k)/[(k + 2)(k + 1)^2]$, with $a(k) = (k + 1)^2 \log(1 + 1/k) + \log k - k \geq 0$, implying that the inequality is satisfied for all k .

(ii) Suppose now that t_k satisfies (28) with $\alpha_{k+1} = b/(k + 1 + q)$ for all k , for some $0 < b < q + 2$. We prove that $t_k \leq A a/(k + p)$ for some $a, p > 0$ by induction on k . Not all values of a, b, p, q are legitimate, and a natural objective is to have a and p respectively as small and large as possible. We show that the best choice is that indicated in Lemma 1. For $k = 1$, since $t_1 \leq A$, to ensure that $t_1 \leq A a/(p + 1)$ we need to have $p \leq a - 1$. Assume that $t_k \leq A a/(k + p)$, and denote $\delta_k = A a/(k + 1 + p) - t_{k+1}$. It satisfies

$$\delta_k \geq A \frac{a}{k + 1 + p} - [(1 - \alpha_{k+1}) t_k + B_C \alpha_{k+1}^2] \geq A \frac{a(k)}{(k + p)(k + 1 + p)(k + 1 + q)^2},$$

where $a(k)$ is a second-degree polynomial in k , with leading term $(ab - a - b^2)k^2$. We thus need to choose a pair (a, b) of positive numbers such that $ab - a - b^2 \geq 0$; the pair with the smallest value of a is $(4, 2)$. For this choice of a, b , we get $a(k) = 4[k + 1 + p - (p - q)^2]$, which increases with k . We only need to guarantee that $a(1) \geq 0$, which corresponds to $q + 1/2 - (1/2)\sqrt{4q + 9} \leq p \leq q + 1/2 + (1/2)\sqrt{4q + 9}$.

Since $a = 4$, the largest p allowed is $p = 3$, which is admissible for $q = 1$. In that case, $a(k) = 4k$ and $\delta_k \geq 0$, showing that $t_k \leq 4A/(k+3)$ for all k when (28) is satisfied with $\alpha_k = 2/(k+1)$ for all k .

(iii) Suppose that t_k satisfies (29) with $\alpha_k = 1/k$ for all k . We have $t_i \leq A$ by hypothesis; the induction hypothesis $t_k \leq A/k$ and (29) give $A/(k+1) - t_{k+1} \geq A/[k(k+1)^2] > 0$, and thus imply that $t_{k+1} \leq A/(k+1)$.

(iv) The function $t \rightarrow f(t) = t - t^2/A$ is increasing on $[0, A/2)$ with a maximum on $[0, A]$ equal to $A/4$ attained for $t = A/2$. We have $t_2 \leq f(A/2) = A/4$, and thus $t_k \leq A/4$ for all $k \geq 2$. Take $p = A/t_2 - 2$, so that $p \geq 2$ and $t_2 = A/(p+2) \leq A/4$. Suppose that $t_k \leq A/(p+k)$; we have $t_{k+1} \leq A[1/(k+p) - 1/(k+p)^2] = A(k+p-1)/(k+p)^2 = A/(k+p+1) - A/[(k+p)^2(k+p+1)] < A/(k+p+1)$, showing that $t_k \leq A/(p+k)$ for all $k \geq 2$.

When $t_1 \leq A/2$, we take $p = A/t_1 - 1$, which gives $p \geq 1$, $t_1 = A/(p+1) \leq A/2$ and $t_k < A/2$ for all $k > 1$. Assuming that $t_k \leq A/(p+k)$, we get $t_{k+1} < A/(k+p+1)$, showing that $t_k \leq A/(p+k)$ for all $k \geq 1$. ■

Proof of Theorem 1. The proof is based on (Clarkson, 2010). The weights ω_k of ξ_k belong to \mathcal{P}_C for all k . For any $\mathbf{x}^{(j)} \in \mathcal{X}_C$, the definition (27) of $\Delta_C(\xi)$ gives

$$\Delta_C[\xi_k^+(\mathbf{x}^{(j)}, \alpha_{k+1})] = \widehat{g}_C(\omega_k) - \widehat{g}_C(\omega_*^C) + 2\alpha_{k+1}(\mathbf{e}_j - \omega_k)^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C) + \alpha_{k+1}^2 \|\mathbf{e}_j - \omega_k\|_{\mathbf{K}_C}^2,$$

where $\alpha_{k+1} = 1/(k+1)$. The definition of $\widehat{\omega}^C$ implies that $\mathbf{u}^\top \mathbf{K}_C \widehat{\omega}^C = \mathbf{u}^\top \mathbf{p}_C(\mu)$ for any $\mathbf{u} \in \mathbb{R}^C$ orthogonal to $\mathbf{1}_C$; therefore $(\mathbf{e}_j - \omega_k)^\top \mathbf{K}_C \widehat{\omega}^C = P_{K,\mu}(\mathbf{x}^{(j)}) - \sum_{i=1}^k \{\mathbf{w}_k\}_i P_{K,\mu}(\mathbf{x}_i)$, and $\mathbf{x}_{k+1} = \mathbf{x}^{(j_{k+1})}$ with

$$j_{k+1} \in \text{Arg min}_{j \in \mathbb{I}_C} P_{K,\xi_k}(\mathbf{x}^{(j)}) - P_{K,\mu}(\mathbf{x}^{(j)}) = \text{Arg min}_{j \in \mathbb{I}_C} (\mathbf{e}_j - \omega_k)^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C),$$

in agreement with (19). The convexity of $\widehat{g}_C(\cdot)$ implies that

$$\begin{aligned} \widehat{g}_C(\omega_*^C) &\geq \widehat{g}_C(\omega_k) + 2(\omega_*^C - \omega_k)^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C) \\ &\geq \widehat{g}_C(\omega_k) + 2 \min_{j \in \mathbb{I}_C} (\mathbf{e}_j - \omega_k)^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C), \end{aligned} \quad (41)$$

where the second inequality follows from $\omega_*^C \in \mathcal{P}_C$, implying that

$$\Delta_C(\xi_{k+1}) = \Delta_C[\xi_{k+1}^+(\mathbf{x}_{k+1}, \alpha_{k+1})] \leq (1 - \alpha_{k+1}) [\widehat{g}_C(\omega_k) - \widehat{g}_C(\omega_*^C)] + \alpha_{k+1}^2 \|\mathbf{e}_{j_{k+1}} - \omega_k\|_{\mathbf{K}_C}^2.$$

The last term can be bounded as follows: for all $j \in \mathbb{I}_C$, we have

$$\begin{aligned} \|\mathbf{e}_j - \omega_k\|_{\mathbf{K}_C}^2 &\leq \max_{\omega, \omega' \in \mathcal{P}_C} (\omega - \omega')^\top \mathbf{K}_C(\omega - \omega') = \max_{i, j \in \mathbb{I}_C} (\mathbf{e}_i - \mathbf{e}_j)^\top \mathbf{K}_C(\mathbf{e}_i - \mathbf{e}_j) \\ &= \max_{i, j \in \mathbb{I}_C} K(\mathbf{x}^{(i)}, \mathbf{x}^{(i)}) + K(\mathbf{x}^{(j)}, \mathbf{x}^{(j)}) - 2K(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) \leq B_C, \end{aligned}$$

with $B_C = 4\overline{K}_C$ ($B_C = 2\overline{K}_C$ when $K \geq 0$). It implies that

$$\Delta_C(\xi_{k+1}) \leq (1 - \alpha_{k+1}) \Delta_C(\xi_k) + B_C \alpha_{k+1}^2. \quad (42)$$

Since $\Delta_C(\xi_1) \leq \text{MMD}_K^2(\mu, \xi_1) = K(\mathbf{x}_1, \mathbf{x}_1) - 2P_{K,\mu}(\mathbf{x}_1) + \mathcal{E}_K(\mu) \leq B_C$, Lemma 1-(i) gives (31) when $\alpha_k = 1/k$ for all k .

When $\widehat{\xi}^C = \xi_*^C$, $\Delta_C(\xi_k) = \widehat{g}_C(\omega_k)$. Therefore,

$$\min_{j \in \mathbb{I}_C} (\mathbf{e}_j - \omega_k)^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C) \leq (\widehat{\omega}^C - \omega_k)^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C) = -\widehat{g}_C(\omega_k), \quad (43)$$

and we get $\Delta_C(\xi_{k+1}) \leq (1 - 2\alpha_{k+1}) \Delta_C(\xi_k) + B_C \alpha_{k+1}^2$ instead of (42). Lemma 1-(iii) gives (32). ■

Proof of Theorem 2. $\Delta_C(\xi_k)$ satisfies (42) with $\alpha_{k+1} = 2/(k+2)$. Lemma 1-(ii) gives (33). ■

Proof of Theorem 3. Consider again the proof of Theorem 1. We have

$$\begin{aligned}\Delta_C(\xi_{k+1}) &= \min_{\alpha \in [0,1]} \Delta_C[\xi_k^+(\mathbf{x}^{(j_{k+1})}), \alpha] \\ &\leq \Delta_C[\xi_k^+(\mathbf{x}^{(j_{k+1})}), \alpha_{k+1}] \leq (1 - \alpha_{k+1}) \Delta_C(\xi_k) + B_C \alpha_{k+1}^2,\end{aligned}\quad (44)$$

for any arbitrary choice of $\alpha_{k+1} \in [0, 1]$, and $\alpha_{k+1} = 2/(k+2)$ for all k has been shown to imply (33) in Theorem 2. When $\widehat{\xi}^C = \xi_*^C$, we get $\Delta_C(\xi_{k+1}) \leq (1 - 2\alpha_{k+1}) \Delta_C(\xi_k) + B_C \alpha_{k+1}^2$, see the proof of Theorem 1. When we use $\alpha_k = 1/k$ for all k , Lemma 1-(iii) implies (32).

The value of α minimising $\Delta_C[\xi_k^+(\mathbf{x}^{(j_{k+1})}), \alpha]$ is

$$\widehat{\alpha}_{k+1} = \frac{(\omega_k - \mathbf{e}_{j_{k+1}})^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C)}{\|\mathbf{e}_{j_{k+1}} - \omega_k\|_{\mathbf{K}_C}^2}, \quad (45)$$

so that (41) implies $\widehat{\alpha}_{k+1} > 0$ when $\text{MMD}_K(\mu, \xi_k) > \text{MMD}_K(\mu, \xi_*^C)$. The algorithm can thus be stopped if $\widehat{\alpha}_{k+1} = 0$. Since $(\omega_k - \mathbf{e}_{j_{k+1}})^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C) = \|\mathbf{e}_{j_{k+1}} - \omega_k\|_{\mathbf{K}_C}^2 + (\mathbf{e}_{j_{k+1}} - \widehat{\omega}^C)^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C) - \|\mathbf{e}_{j_{k+1}} - \widehat{\omega}^C\|_{\mathbf{K}_C}^2$, we have $\widehat{\alpha}_{k+1} \leq 1 + (\mathbf{e}_{j_{k+1}} - \widehat{\omega}^C)^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C) / \|\mathbf{e}_{j_{k+1}} - \omega_k\|_{\mathbf{K}_C}^2$. When $\widehat{\omega}^C \in \mathcal{P}_C$ (that is, when $\widehat{\omega}^C = \omega_*^C$), the definition of j_{k+1} implies that $\widehat{\alpha}_{k+1} \leq 1$ (since $\sum_{j=1}^C \{\widehat{\omega}^C\}_j (\mathbf{e}_j - \widehat{\omega}^C)^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C) = 0$ with all $\{\widehat{\omega}^C\}_j \geq 0$). However, nothing guarantees that $\widehat{\alpha}_{k+1} \leq 1$ in general. Direct calculation gives

$$\begin{aligned}(\omega_k - \mathbf{e}_j)^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C) &= \sum_{i,\ell=1}^k \{\mathbf{w}_k\}_i \{\mathbf{w}_k\}_\ell K(\mathbf{x}_i, \mathbf{x}_\ell) - \sum_{i=1}^k \{\mathbf{w}_k\}_i K(\mathbf{x}_i, \mathbf{x}^{(j)}) \\ &\quad + P_{K,\mu}(\mathbf{x}^{(j)}) - \sum_{i=1}^k \{\mathbf{w}_k\}_i P_{K,\mu}(\mathbf{x}_i),\end{aligned}\quad (46)$$

$$\|\mathbf{e}_j - \omega_k\|_{\mathbf{K}_C}^2 = \sum_{i,\ell=1}^k \{\mathbf{w}_k\}_i \{\mathbf{w}_k\}_\ell K(\mathbf{x}_i, \mathbf{x}_\ell) - 2 \sum_{i=1}^k \{\mathbf{w}_k\}_i K(\mathbf{x}_i, \mathbf{x}^{(j)}) + K(\mathbf{x}^{(j)}, \mathbf{x}^{(j)}), \quad (47)$$

which together with (45) gives (34). The recursive updating of $Q_k = \sum_{i,\ell=1}^k \{\mathbf{w}_k\}_i \{\mathbf{w}_k\}_\ell K(\mathbf{x}_i, \mathbf{x}_\ell)$, $R_k = \sum_{i=1}^k \{\mathbf{w}_k\}_i P_{K,\mu}(\mathbf{x}_i)$ and $S_k(\mathbf{x}) = P_{K,\xi_k}(\mathbf{x})$ gives Algorithm 2. \blacksquare

Proof of Theorem 4.

(i) Consider the proof of Theorem 1. When $\nu_k = \xi_k^*$ is substituted for ξ_k , we have $\mathbf{x}_{k+1} = \mathbf{x}^{(j_{k+1})}$ with $j_{k+1} \in \text{Arg min}_{j \in \mathbb{I}_C} (\mathbf{e}_j - \omega_k^*)^\top \mathbf{K}_C(\omega_k^* - \widehat{\omega}^C)$ and, for any $\alpha \in [0, 1]$,

$$\Delta_C[\nu_k^+(\mathbf{x}^{(j_{k+1})}), \alpha] = \widehat{g}_C(\omega_k^*) - \widehat{g}_C(\omega_*^C) + 2\alpha (\mathbf{e}_{j_{k+1}} - \omega_k^*)^\top \mathbf{K}_C(\omega_k^* - \widehat{\omega}^C) + \alpha^2 \|\mathbf{e}_{j_{k+1}} - \omega_k^*\|_{\mathbf{K}_C}^2,$$

where $\Delta_C(\xi)$ is given by (27) and $\nu_k^+(\mathbf{x}^{(j)}, \alpha) = (1 - \alpha) \xi_k^* + \alpha \delta_{\mathbf{x}^{(j)}}$. Since $\omega_k^* \in \mathcal{P}_C$, $\|\mathbf{e}_j - \omega_k^*\|_{\mathbf{K}_C}^2 \leq B_C$, see the proof of Theorem 1. The convexity of $\widehat{g}_C(\cdot)$ implies

$$\widehat{g}_C(\omega_*^C) \geq \widehat{g}_C(\omega_k^*) + 2(\omega_*^C - \omega_k^*)^\top \mathbf{K}_C(\omega_k^* - \widehat{\omega}^C) \geq \widehat{g}_C(\omega_k^*) + 2(\mathbf{e}_{j_{k+1}} - \omega_k^*)^\top \mathbf{K}_C(\omega_k^* - \widehat{\omega}^C)$$

(since $\omega_*^C \in \mathcal{P}_C$). By construction, $\Delta_C(\xi_{k+1}) \leq \Delta_C[\nu_k^+(\mathbf{x}^{(j_{k+1})}), \alpha]$ for any $\alpha \in [0, 1]$, and therefore

$$\Delta_C(\xi_{k+1}) \leq \Delta_C[\nu_k^+(\mathbf{x}_{k+1}), \alpha_{k+1}] \leq (1 - \alpha_{k+1}) \Delta_C(\nu_k) + B_C \alpha_{k+1}^2, \quad (48)$$

$k \geq 1$, for any predefined α_{k+1} . When $\alpha_{k+1} = 2/(k+2)$, the induction used in the proof of Theorem 2 gives (33). When $\widehat{\xi}^C = \xi_*^C$, the right-hand side of (48) becomes $(1 - 2\alpha_{k+1}) \Delta_C(\nu_k) + B_C \alpha_{k+1}^2$, see the proof of Theorem 1, and if we take $\alpha_k = 1/k$ for all k , Lemma 1-(iii) implies (32).

(ii) Suppose now that $\nu_k = \widehat{\xi}_k$ is substituted for ξ_k at iteration k . Equation (14) gives

$$\Delta_C(\xi_{k+1}) = \Delta_C(\xi_k) - \frac{[(\mathbf{e}_{j_{k+1}} - \widehat{\omega}_k)^\top \mathbf{K}_C(\widehat{\omega}_k - \widehat{\omega}^C)]^2}{\min_{\substack{\mathbf{w} \in \mathbb{R}^k \\ \mathbf{1}_k^\top \mathbf{w} = 1}} \|K(\mathbf{x}_{k+1}, \cdot) - \mathbf{w}^\top \mathbf{k}_k(\cdot)\|_{\mathcal{H}_K}^2}.$$

As long as $\widehat{g}_C(\omega_*^C) \geq \widehat{g}_C(\widehat{\omega}_k)$, we thus have

$$\begin{aligned} \Delta_C(\xi_{k+1}) &\leq \Delta_C(\xi_k) - \frac{[\widehat{g}_C(\widehat{\omega}_k) - \widehat{g}_C(\omega_*^C)]^2}{4 \|K(\mathbf{x}_{k+1}, \cdot) - (\mathbf{1}_k^\top/k)\mathbf{K}_k(\cdot)\|_{\mathcal{H}_K}^2} \\ &= \Delta_C(\xi_k) - \frac{\Delta_C^2(\xi_k)}{4 [K(\mathbf{x}_{k+1}, \mathbf{x}_{k+1}) + \mathbf{1}_k^\top \mathbf{K}_k \mathbf{1}_k/k^2 - 2 \mathbf{1}_k^\top \mathbf{k}_k(\mathbf{x}_{k+1})/k]} \\ &\leq \Delta_C(\xi_k) - \frac{\Delta_C^2(\xi_k)}{4 B_C}, \end{aligned} \quad (49)$$

with $\Delta_C(\xi_1) \leq B_C$. Lemma 1-(iv) with $A = 4 B_C$ and $p_1 = 3$ gives (33). When $\widehat{\xi}^C = \xi_*^C$, (43) gives $\Delta_C(\xi_{k+1}) \leq \Delta_C(\xi_k) - \Delta_C^2(\xi_k)/B_C$, and Lemma 1-(iv) with $A = B_C$ and $p_2 = 2$ gives (35).

(iii) Suppose finally that $\nu_k = \widetilde{\xi}_k$ is substituted for ξ_k at iteration k . Since $\widetilde{\xi}_k$ is not necessarily in $\mathcal{M}_{[1]}(\mathcal{X}_C)$, we need to use (22) instead of (25), which gives

$$\Delta_C[\nu_k^+(\mathbf{x}^{(j)}, \alpha)] = \widetilde{g}_C(\widetilde{\omega}_k) - \widetilde{g}_C(\omega_*^C) + 2\alpha (\mathbf{e}_j - \widetilde{\omega}_k)^\top \mathbf{K}_C(\widetilde{\omega}_k - \widetilde{\omega}^C) + \alpha^2 \|\mathbf{e}_j - \widetilde{\omega}_k\|_{\mathbf{K}_C}^2$$

for all $\mathbf{x}^{(j)}$ in \mathcal{X}_C and any $\alpha \in [0, 1]$. The definition of $\widetilde{\omega}^C$ implies $\mathbf{K}_C \widetilde{\omega}^C = \mathbf{p}_C(\mu)$, and thus $\mathbf{x}_{k+1} = \mathbf{x}^{(j_{k+1})}$ with

$$j_{k+1} \in \text{Arg min}_{j \in \mathcal{I}_C} P_{K, \nu_k}(\mathbf{x}^{(j)}) - P_{K, \mu}(\mathbf{x}^{(j)}) = \text{Arg min}_{j \in \mathcal{I}_C} (\mathbf{e}_j - \widetilde{\omega}_k)^\top \mathbf{K}_C(\widetilde{\omega}_k - \widetilde{\omega}^C).$$

The convexity of $\widetilde{g}(\cdot)$ implies

$$\begin{aligned} \widetilde{g}_C(\omega_*^C) &\geq \widetilde{g}_C(\widetilde{\omega}_k) + 2(\omega_*^C - \widetilde{\omega}_k)^\top \mathbf{K}_C(\widetilde{\omega}_k - \widetilde{\omega}^C) \geq \widetilde{g}_C(\widetilde{\omega}_k) + 2(\mathbf{e}_{j_{k+1}} - \widetilde{\omega}_k)^\top \mathbf{K}_C(\widetilde{\omega}_k - \widetilde{\omega}^C) \\ &\text{(since } \omega_*^C \in \mathcal{P}_C \text{) and } \widetilde{\omega}_k^\top \mathbf{K}_C(\widetilde{\omega}_k - \widetilde{\omega}^C) = 0 \text{ (see Section 3.3.2) gives } \mathbf{e}_{j_{k+1}}^\top \mathbf{K}_C(\widetilde{\omega}_k - \widetilde{\omega}^C) \leq -[\widetilde{g}_C(\widetilde{\omega}_k) - \widetilde{g}_C(\omega_*^C)]/2. \end{aligned}$$

Therefore, as long as $\widetilde{g}_C(\omega_*^C) \geq \widetilde{g}_C(\widetilde{\omega}_k)$, (12) gives

$$\begin{aligned} \Delta_C(\xi_{k+1}) &\leq \Delta_C(\xi_k) - \frac{[\widetilde{g}_C(\widetilde{\omega}_k) - \widetilde{g}_C(\omega_*^C)]^2}{4 [K(\mathbf{x}_{k+1}, \mathbf{x}_{k+1}) - \mathbf{k}_k^\top(\mathbf{x}_{k+1})\mathbf{K}_k^{-1}\mathbf{k}_k(\mathbf{x}_{k+1})]} \\ &= \Delta_C(\xi_k) - \frac{\Delta_C^2(\xi_k)}{4 [K(\mathbf{x}_{k+1}, \mathbf{x}_{k+1}) - \mathbf{k}_k^\top(\mathbf{x}_{k+1})\mathbf{K}_k^{-1}\mathbf{k}_k(\mathbf{x}_{k+1})]} \\ &\leq \Delta_C(\xi_k) - \frac{\Delta_C^2(\xi_k)}{4 \overline{K}_C} \leq \Delta_C(\xi_k) - \frac{\Delta_C^2(\xi_k)}{4 \overline{K}}. \end{aligned} \quad (50)$$

Since any signed measure supported on \mathcal{X}_C can be used, we may start with $\xi_0 = 0$, with weights $\omega_0 = \mathbf{0}_C$, so that (12) and the inequality above apply from $k = 0$. We have $\Delta_C(\xi_0) \leq \text{MMD}_K^2(\mu, \xi_0) = \mathcal{E}_K(\mu) \leq \overline{K}$; therefore, $\Delta_C(\xi_k) \leq 4 \overline{K}/(k+p)$, $k \geq 1$, for $p = 4 \overline{K}/\text{MMD}_K^2(\mu, \xi_1) - 1 \leq 4 \overline{K}/\Delta_C(\xi_1) - 1$; see the proof of Lemma 1-(iv). Since $\Delta_C(\xi_1) \leq 3 \overline{K}/4$, we can take $p_1 = 13/3$ in Lemma 1-(iv) and we also have $\Delta_C(\xi_k) \leq 4 \overline{K}/(k+13/3)$, $k \geq 1$. This completes the proof of (36). ■

Proof of Theorem 5. We have $\mathcal{E}_K(\nu - \mu) = \mathcal{E}_{K_\mu}(\nu)$ for any $\nu \in \mathcal{M}_{[1]}(\mathcal{X}_C)$ with K_μ the reduced kernel defined by (11); see Damelin et al. (2010), Pronzato and Zhigljavsky (2020, Th. 3.5). Let ω_k be the vector of weights associated with ξ_k at step k . We can write $\text{MMD}_K^2(\mu, \xi_k) = \omega_k^\top \mathbf{K}_{\mu_C} \omega_k$, which gives

$$(k+1)^2 \text{MMD}_K^2(\mu, \xi_{k+1}) = k^2 \text{MMD}_K^2(\mu, \xi_k) + 2k \omega_k^\top \mathbf{K}_{\mu_C} \mathbf{e}_{j_{k+1}} + K_\mu(\mathbf{x}^{(j_{k+1})}, \mathbf{x}^{(j_{k+1})}),$$

where $j_{k+1} \in \text{Arg min}_{j \in \mathcal{I}_C} 2k \omega_k^\top \mathbf{K}_{\mu_C} \mathbf{e}_j + K_\mu(\mathbf{x}^{(j)}, \mathbf{x}^{(j)})$, so that $\mathbf{x}^{(j_{k+1})}$ coincides with (17) when \mathcal{X}_C is substituted for \mathcal{X} . Therefore, for any $\omega \in \mathcal{P}_C$, we have

$$\begin{aligned} (k+1)^2 \text{MMD}_K^2(\mu, \xi_{k+1}) &\leq k^2 \text{MMD}_K^2(\mu, \xi_k) + 2k \omega_k^\top \mathbf{K}_{\mu_C} \omega + \overline{K}_{\mu_C}, \\ &\leq k^2 \text{MMD}_K^2(\mu, \xi_k) + 2k (\omega_k^\top \mathbf{K}_{\mu_C} \omega_k)^{1/2} (\omega^\top \mathbf{K}_{\mu_C} \omega)^{1/2} + \overline{K}_{\mu_C}, \end{aligned} \quad (51)$$

where $\bar{K}_{\mu,C} = \max_{\mathbf{x} \in \mathcal{X}_C} K_\mu(\mathbf{x}, \mathbf{x}) \leq A_C$, see (20). The inequality (51) is satisfied in particular for $\omega_*^C \in \text{Arg min}_{\omega \in \mathcal{P}_C} \omega^\top \mathbf{K}_{\mu_C} \omega$, with $\omega_*^{C\top} \mathbf{K}_{\mu_C} \omega_*^C = M_C^2$, therefore

$$(k+1)^2 \text{MMD}_K^2(\mu, \xi_{k+1}) \leq k^2 \text{MMD}_K^2(\mu, \xi_k) + 2k M_C \text{MMD}_K(\mu, \xi_k) + A_C. \quad (52)$$

We prove (37) by induction on n . For $n = 1$, $\text{MMD}_K^2(\mu, \delta_{\mathbf{x}_1}) = K_\mu(\mathbf{x}_1, \mathbf{x}_1) \leq \bar{K}_{\mu,C} \leq A_C$. Suppose that (37) is true for n . Then, (52) implies

$$\begin{aligned} \text{MMD}_K^2(\mu, \xi_{n+1}) &\leq \frac{1}{(n+1)^2} \left\{ n^2 \left(M_C^2 + A_C \frac{1 + \log n}{n} \right) \right. \\ &\quad \left. + 2n M_C \left(M_C^2 + A_C \frac{1 + \log n}{n} \right)^{1/2} + A_C \right\} \\ &\leq \frac{1}{(n+1)^2} \left\{ n^2 \left(M_C^2 + A_C \frac{1 + \log n}{n} \right) + n \left(2 M_C^2 + A_C \frac{1 + \log n}{n} \right) + A_C \right\} \\ &= M_C^2 + A_C \frac{1 + \log(n+1)}{n+1} - \frac{M_C^2 + A_C [(n+1) \log(1 + 1/n) - 1]}{(n+1)^2} \\ &= M_C^2 + A_C \frac{1 + \log(n+1)}{n+1} - \frac{M_C^2/(n+1) + A_C [-\log(1 - 1/(n+1)) - 1/(n+1)]}{n+1} \\ &\leq M_C^2 + A_C \frac{1 + \log(n+1)}{n+1} \end{aligned}$$

since $\log(1+x) \leq x$ for $x > -1$, which concludes the proof of (37). ■

Proof of Theorem 6. We have, for any $\mathbf{x}^{(j)} \in \mathcal{X}_C$,

$$\Delta_C[\xi_k^+(\mathbf{x}^{(j)}, \alpha_{k+1})] = \widehat{g}_C(\omega_k) - \widehat{g}_C(\omega_*^C) + 2\alpha_{k+1} (\mathbf{e}_j - \omega_k)^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C) + \alpha_{k+1}^2 \|\mathbf{e}_j - \omega_k\|_{\mathbf{K}_C}^2,$$

where $\Delta_C(\xi)$ is given by (27) and $\|\mathbf{e}_j - \omega_k\|_{\mathbf{K}_C}^2 \leq B_C$, see the proof of Theorem 1. Therefore,

$$\min_{\mathbf{x} \in \mathcal{X}_C} \Delta_C[\xi_k^+(\mathbf{x}, \alpha_{k+1})] \leq \widehat{g}_C(\omega_k) - \widehat{g}_C(\omega_*^C) + \min_{j \in \mathbb{I}_C} 2\alpha_{k+1} (\mathbf{e}_j - \omega_k)^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C) + B_C \alpha_{k+1}^2,$$

and, from the same arguments as in the proof of Theorem 1,

$$\Delta_C(\xi_{k+1}) = \min_{\mathbf{x} \in \mathcal{X}_C} \Delta_C[\xi_k^+(\mathbf{x}, \alpha_{k+1})] \leq (1 - \alpha_{k+1}) \Delta_C(\xi_k) + B_C \alpha_{k+1}^2. \quad (53)$$

When $\alpha_k = 2/(k+1)$ for all k , Lemma 1-(ii) gives (33).

Similarly, when $\widehat{\xi}^C = \xi_*^C$, we have

$$\Delta_C(\xi_{k+1}) = \min_{\mathbf{x} \in \mathcal{X}_C} \Delta_C[\xi_k^+(\mathbf{x}, \alpha_{k+1})] \leq (1 - 2\alpha_{k+1}) \Delta_C(\xi_k) + B_C \alpha_{k+1}^2,$$

see the proof of Theorem 1, and Lemma 1-(iii) gives (32). ■

Proof of Theorem 7. $\Delta_C[\xi_k^+(\mathbf{x}^{(j)}, \alpha)]$ satisfies (38) where $\|\mathbf{e}_j - \omega_k\|_{\mathbf{K}_C}^2 \leq B_C$, see the proof of Theorem 1. Therefore,

$$\min_{\mathbf{x} \in \mathcal{X}_C, \alpha \in [0,1]} \Delta_C[\xi_k^+(\mathbf{x}, \alpha)] \leq \widehat{g}_C(\omega_k) - \widehat{g}_C(\omega_*^C) + \min_{j \in \mathbb{I}_C} 2\alpha_{k+1} (\mathbf{e}_j - \omega_k)^\top \mathbf{K}_C(\omega_k - \widehat{\omega}^C) + B_C \alpha_{k+1}^2$$

for any predefined choice of α_{k+1} in $[0, 1]$. The rest of the proof is similar to that of Theorem 3. ■

Proof of Lemma 2. A_C depends on \mathcal{X}_C , but $A_C \leq A(\mu)$; similarly, $B_C \leq B$. Since $M_C^2 \leq \mathbf{1}_C^\top \mathbf{K}_{\mu_C} \mathbf{1}_C / C^2$, we get

$$\begin{aligned}
\mathbb{E}\{M_C^2\} &\leq \frac{1}{C^2} \mathbb{E} \left\{ \sum_{i,j=1}^C K_\mu(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) \right\} \\
&= \frac{1}{C^2} \mathbb{E} \left\{ \sum_{i,j=1}^C K(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) \right\} - \frac{2}{C} \mathbb{E} \left\{ \sum_{i=1}^C P_{K,\mu}(\mathbf{x}^{(i)}) \right\} + \mathcal{E}_K(\mu) \\
&= \frac{1}{C^2} \mathbb{E} \left\{ \sum_{i=1}^C K(\mathbf{x}^{(i)}, \mathbf{x}^{(i)}) \right\} + \frac{1}{C^2} \mathbb{E} \left\{ \sum_{\substack{i,j=1 \\ i \neq j}}^C K(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) \right\} - \mathcal{E}_K(\mu) \\
&= \frac{\tau_1(\mu)}{C} + \frac{C(C-1)}{C^2} \mathcal{E}_K(\mu) - \mathcal{E}_K(\mu) = \frac{\tau_1(\mu) - \mathcal{E}_K(\mu)}{C}. \quad \blacksquare
\end{aligned}$$

Proof of Theorem 9. We have $\text{MMD}_K^2(\mu, \xi_{n,e}) = \mathbf{1}_n^\top \mathbf{K}_{\mu_n} \mathbf{1}_n / n^2$, with $\mathbb{E}_\mu \{K_\mu(\cdot, X)\} \equiv 0$ on \mathcal{X} and $\int_{\mathcal{X}^2} K_\mu(\mathbf{x}, \mathbf{x}') d\mu(\mathbf{x}) d\mu(\mathbf{x}') = \mathcal{E}_{K_\mu}(\mu) = 0$. From Serfling (1980, p. 194), the U-statistic $U_n = 2/[n(n-1)] \sum_{i < j} K_\mu(\mathbf{x}_i, \mathbf{x}_j)$ satisfies $n U_n \xrightarrow{d} Y = \sum_{i=1}^\infty \lambda_i (\chi_{1i}^2 - 1)$. The V-statistic $V_n = (1/n^2) \sum_{i,j} K_\mu(\mathbf{x}_i, \mathbf{x}_j) = \text{MMD}_K^2(\mu, \xi_{n,e})$ satisfies $V_n = (1-1/n) U_n + (1/n^2) \sum_i K_\mu(\mathbf{x}_i, \mathbf{x}_i)$, with $U_n \xrightarrow{\text{a.s.}} 0$ and $(1/n) \sum_i K_\mu(\mathbf{x}_i, \mathbf{x}_i) \xrightarrow{\text{a.s.}} \sum_{i=1}^\infty \lambda_i$. Therefore, $n V_n \xrightarrow{d} Z = \sum_{i=1}^\infty \lambda_i \chi_{1i}^2$. \blacksquare

Appendix B: multiple random candidate sets

Suppose that \mathbf{x}_{k+1} is selected within $\mathcal{X}_C[k+1]$ at iteration k . Denote $\mathcal{X}_{C_{k+1}} = \cup_{i=1}^{k+1} \mathcal{X}_C[i]$ and let $\mathcal{P}_{C_{k+1}}$ be the corresponding probability simplex in $\mathbb{R}^{C_{k+1}}$ (with $C_{k+1} = (k+1)C$ when the $\mathcal{X}_C[i]$ do not intersect). To a measure ξ_k in $\mathcal{M}(\mathcal{X}_{C_k})$ (respectively, in $\mathcal{M}_{[1]}^+(\mathcal{X}_{C_k})$) corresponds a vector of weights ω_k in \mathbb{R}^{C_k} (respectively, in \mathcal{P}_{C_k}), and we denote by ω'_k the same vector plunged into $\mathbb{R}^{C_{k+1}}$ (respectively, into $\mathcal{P}_{C_{k+1}}$); $\xi_*^{C[k+1]}$ is the measure in $\mathcal{M}_{[1]}^+(\mathcal{X}_C[k+1])$ that minimises $\text{MMD}(\mu, \xi)$ and $\omega_*^{C[k+1]}'$ is the vector of associated weights in $\mathcal{P}_{C_{k+1}}$. Similarly, $\hat{\omega}^{C_{k+1}}$ denotes the vector of weights for the optimal measure in $\mathcal{M}_{[1]}^+(\mathcal{X}_{C_{k+1}})$.

Consider one-step-ahead algorithms (Algorithms 1, 2, 4 and 5) and $\xi_k^+[\mathbf{x}_{k+1}, \alpha_{k+1}] = (1 - \alpha_{k+1}) \xi_k + \alpha_{k+1} \delta_{\mathbf{x}_{k+1}}$ constructed at iteration k . We have

$$\begin{aligned}
\text{MMD}_K^2(\mu, \xi_k^+[\mathbf{x}_{k+1}, \alpha_{k+1}]) - \text{MMD}_K^2(\mu, \xi_*^{C[k+1]}) &= \hat{g}_{C_{k+1}}(\omega'_k) - \hat{g}_{C_{k+1}}(\omega_*^{C[k+1]'}) \\
&\quad + 2\alpha_{k+1} (\mathbf{e}_{j_{k+1}} - \omega'_k)^\top \mathbf{K}_{C_{k+1}} (\omega'_k - \hat{\omega}^{C_{k+1}}) + \alpha_{k+1}^2 \|\mathbf{e}_{j_{k+1}} - \omega'_k\|_{\mathbf{K}_{C_{k+1}}}^2,
\end{aligned}$$

with $\mathbf{e}_{j_{k+1}}$ the basis vector in $\mathbb{R}^{C_{k+1}}$ corresponding to $\mathbf{x}_{k+1} \in \mathcal{X}_C[k+1]$, and $\|\mathbf{e}_{j_{k+1}} - \omega'_k\|_{\mathbf{K}_{C_{k+1}}}^2 \leq B$, see the proof of Theorem 1 and Lemma 2. The convexity of $\hat{g}_{C_{k+1}}(\cdot)$ implies

$$\hat{g}_{C_{k+1}}(\omega_*^{C[k+1]'}) \geq \hat{g}_{C_{k+1}}(\omega'_k) + 2(\omega_*^{C[k+1]}' - \omega'_k)^\top \mathbf{K}_{C_{k+1}} (\omega'_k - \hat{\omega}^{C_{k+1}})$$

so that $2(\mathbf{e}_{j_{k+1}} - \omega'_k)^\top \mathbf{K}_{C_{k+1}} (\omega'_k - \hat{\omega}^{C_{k+1}}) \leq \hat{g}_{C_{k+1}}(\omega_*^{C[k+1]'}) - \hat{g}_{C_{k+1}}(\omega'_k)$ when \mathbf{x}_{k+1} is chosen by kernel herding. This gives

$$\begin{aligned}
\text{MMD}_K^2(\mu, \xi_k^+[\mathbf{x}_{k+1}, \alpha_{k+1}]) - \text{MMD}_K^2(\mu, \xi_*^{C[k+1]}) &\leq \\
&\quad (1 - \alpha_{k+1}) \left[\text{MMD}_K^2(\mu, \xi_k) - \text{MMD}_K^2(\mu, \xi_*^{C[k+1]}) \right] + B \alpha_{k+1}^2.
\end{aligned}$$

When each $\mathcal{X}_C[i]$ is made of independent samples from μ , we have $\mathbb{E}_\mu\{\text{MMD}_K^2(\mu, \xi_*^{C[i]})\} = \mathbb{E}_\mu\{M_C^2\}$ for all i , and therefore, when α_{k+1} is predefined (deterministic),

$$\mathbb{E}_\mu\{\Delta(\xi_{k+1})\} \leq (1 - \alpha_{k+1}) \mathbb{E}_\mu\{\Delta(\xi_k)\} + B \alpha_{k+1}^2,$$

where we have denoted $\Delta(\xi) = \Delta_{C[1]}(\xi) = \text{MMD}_K^2(\mu, \xi) - \text{MMD}_K^2(\mu, \xi_*^{C[1]})$. From the same arguments as those used in the proof of Theorem 1, we thus obtain that the measure generated by Algorithm 1 with $\alpha_k = 1/k$ and using a set $\mathcal{X}_C[k]$ composed of C independent samples from μ for all k satisfies $\mathbb{E}_\mu\{\text{MMD}_K^2(\mu, \xi_k)\} \leq \mathbb{E}_\mu\{M_C^2\} + B(2 + \log n)/(n + 1)$, $n \geq 1$, compare with (31). When $\alpha_k = 2/(k + 1)$ in Algorithm 1, then $\mathbb{E}_\mu\{\text{MMD}_K^2(\mu, \xi_k)\} \leq \mathbb{E}_\mu\{M_C^2\} + 4B/(n + 3)$, $n \geq 1$, compare with (33). Following the arguments used in the proof of Theorem 3, see (44), we get the same bound for Algorithm 2. Also, following the arguments in the proofs of Theorems 6 and 7, similar bounds are obtained for Algorithms 4 and 5, which extends the results in those theorems to this situation of multiple random candidate sets. A similar extension applies to Algorithm 3-(i); see the proof of Theorem 4-(i).

Consider now Algorithm 3-(ii) and (iii) and SBQ. For Algorithm 3-(ii), we have

$$\text{MMD}_K^2(\mu, \xi_{k+1}) \leq \text{MMD}_K^2(\mu, \xi_k) - \frac{[(\mathbf{e}_{j_{k+1}} - \omega'_k)^\top \mathbf{K}_{C_{k+1}}(\omega'_k - \widehat{\omega}^{C_{k+1}})]^2}{B}$$

and the convexity of $\widehat{g}_{C_{k+1}}(\cdot)$ gives

$$\text{MMD}_K^2(\mu, \xi_{k+1}) \leq \text{MMD}_K^2(\mu, \xi_k) - \frac{[\widehat{g}_{C_{k+1}}(\omega'_k) - \widehat{g}_{C_{k+1}}(\omega_*^{C[k+1]'})]^2}{4B}.$$

Since $\mathbb{E}_\mu\{\text{MMD}_K^2(\mu, \xi_*^{C[i]})\} = \mathbb{E}_\mu\{M_C^2\}$ for all i , Jensen's inequality gives

$$\begin{aligned} \mathbb{E}_\mu \left\{ \left[\widehat{g}_{C_{k+1}}(\omega'_k) - \widehat{g}_{C_{k+1}}(\omega_*^{C[k+1]'}) \right]^2 \right\} &\geq \left[\mathbb{E}_\mu \left\{ \widehat{g}_{C_{k+1}}(\omega'_k) - \widehat{g}_{C_{k+1}}(\omega_*^{C[k+1]'}) \right\} \right]^2 \\ &= \mathbb{E}_\mu^2\{\text{MMD}_K^2(\mu, \xi_k)\} - \mathbb{E}_\mu\{M_C^2\} = \mathbb{E}_\mu^2\{\Delta(\xi_k)\}. \end{aligned}$$

We thus obtain

$$\mathbb{E}_\mu\{\Delta(\xi_{k+1})\} \leq \mathbb{E}_\mu\{\Delta(\xi_k)\} - \frac{\mathbb{E}_\mu^2\{\Delta(\xi_k)\}}{4B},$$

an inequality similar to (49) in the proof of Theorem 4-(ii), and ξ_n satisfies an inequality of the form (33) where each term is replaced by its expected value.

Similar developments yield an inequality similar to (50), with expected values everywhere, and thus an extension of (36) for Algorithm 3-(iii). Theorem 8, that indicates that the performance of SBQ cannot be worse than that of Algorithm 3, continues to apply; the details are omitted.

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