Acceleration of the kernel herding algorithm by improved gradient approximation

Kazuma Tsuji
The University of Tokyo
kazuma_tsuji@mist.i.u-tokyo.ac.jp

Ken’ichiro Tanaka
The University of Tokyo
PRESTO, Japan Science and Technological Agency (JST), Japan
kenichiro@mist.i.u-tokyo.ac.jp

Abstract

Kernel herding is a method used to construct quadrature formulas in a reproducing kernel Hilbert space. Although there are some advantages of kernel herding, such as numerical stability of quadrature and effective outputs of nodes and weights, the convergence speed of worst-case integration error is slow in comparison to other quadrature methods. To address this problem, we propose two improved versions of the kernel herding algorithm. The fundamental concept of both algorithms involves approximating negative gradients with a positive linear combination of vertex directions. We analyzed the convergence and validity of both algorithms theoretically; in particular, we showed that the approximation of negative gradients directly influences the convergence speed. In addition, we confirmed the accelerated convergence of the worst-case integration error with respect to the number of nodes and computational time through numerical experiments.

1 Introduction

The numerical integration of multivariate functions is indispensable in various fields, such as statistics, economics, and physics. In statistical machine learning, the numerical integration of multivariate functions is a commonly used tool. Specifically, in Bayesian inference, numerical integration is required in several situations, such as the marginalization of distribution and computation of expectations.

Kernel quadrature is a type of numerical integration method. It is the quadrature formula for functions in a reproducing kernel Hilbert space (RKHS). One of the advantages of this method is the flexibility of choice of RKHS. By fixing an appropriate RKHS for functions we want to integrate, we can construct an effective integration formula for them.

Various methods are used to construct kernel quadrature rules, such as sequential Bayesian quadrature [12] and orthogonal matching pursuit [17]. In addition, we can employ kernel interpolation methods, such as P-greedy algorithm [8], because kernel quadrature rules can be derived by integrating the kernel interpolation function with respect to a measure. Several methods, including the aforementioned algorithms, compute the optimized weight for a fixed set of nodes in each iteration. Although fast convergence can be expected for the optimized weights, the computation of weights is a computationally exhausting process because the inverse matrix of kernel matrix \((K(x_i, x_j))\) with \(1 \leq i, j \leq m\) must be computed in each iteration.

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We evaluate the numerical integration formula. In addition, kernel quadrature is closely related to Bayesian quadrature. Bayesian quadrature lies in the context of probabilistic numerics and it is closely related to uncertainty quantification. In the context of Bayesian quadrature, convergence analysis has been studied.

In this study, we focused on the kernel herding method that can be considered as an infinite-dimensional Frank Wolfe method, which is a continuous optimization method. This method constructs a stable numerical integration formula that is computationally tractable because inverse matrix computation is not required. However, the convergence speed of the worst-case integration error is slow. The exponential convergence is confirmed in a finite dimensional RKHS when the step size \( \alpha_t \) is determined by line search; however, only \( O(\frac{1}{\sqrt{t}}) \) convergence can be determined in an infinite-dimensional RKHS, where \( t \) is the number of nodes of the quadrature formula.

We approach this problem with the perspective of continuous optimization. We note that there are few studies that attempted to improve the kernel herding algorithm considering continuous optimization. Accordingly, we propose two improved versions of the kernel herding algorithm. The fundamental concept common in both methods involves approximating the negative gradient of the objective function, \( F(\nu) = \frac{1}{2} \| \mu_K - \nu \|_K^2 \), by several vertex directions. This concept is derived from the study that proposed an improved Frank Wolfe method in Euclidean space. We theoretically demonstrate that the convergence speed of the worst integration error is directly influenced by \( \cos \theta_i \), where \( \theta_i \) is the angle between the negative gradient of \( F(\nu) \) and \( i \)-th approximate descent direction. This indicates that approximation is significant for constructing a good numerical integration formula. The difference between the two proposed algorithms lies in their approximation method. The first algorithm approximates negative gradients by positive matching pursuit, a procedure similar to [7]. We guarantee the convergence of positive matching pursuit and consider the behavior of \( \cos \theta_i \) when \( i \) increases. The second algorithm is an improved version of the first algorithm that directly maximizes \( \cos \theta_i \). This is a more straightforward approach than the first method. We ensure the validity of the maximization method theoretically. In addition, we confirmed through numerical experiments that the proposed algorithms improve the convergence speed of kernel herding considering the number of nodes and computational time.

The contributions of this work can be summarized as follows:

- We demonstrated that the convergence speed of the worst integration error is directly influenced by \( \cos \theta_i \).
- We proposed two improved kernel herding algorithms. The first algorithm used positive matching pursuit for the approximation of negative gradients. We determined the convergence speed of the approximation and considered the behavior of \( \cos \theta_i \) when \( i \) increased. The second algorithm directly maximizes \( \cos \theta_i \). We verified this algorithm for the maximization of \( \cos \theta_i \).
- Through numerical experiments, we confirmed that the convergence speed of the proposed algorithms is faster than that of ordinary kernel herding methods with respect to the number of nodes and computational time.

2 Mathematical preparations

2.1 Kernel Quadrature

In this section, we introduce the problem setting of this study. Let \( \Omega \) be a compact subset in \( \mathbb{R}^d \) and \( K : \Omega \times \Omega \rightarrow \mathbb{R} \) be a positive definite kernel. In this paper, we assume that \( K \) is a continuous function on \( \Omega \times \Omega \). The function space \( H_K(\Omega) \) is the RKHS induced by \( K \). For \( f_1, f_2 \in H_K \), we denote the inner product of \( f_1 \) and \( f_2 \) by \( \langle f_1, f_2 \rangle_K \) and the norm of \( f_1 \) by \( \| f_1 \|_K \). For a Borel probability measure \( \mu \) defined on \( \Omega \) and \( f \in H_K(\Omega) \), we aim to approximate \( \int_{\Omega} f(x) \mu(dx) \) by the numerical integration formula \( Q_n(f) := \sum_{i=1}^{n} \omega_i f(x_i) \), where \( \{ x_i \}_{i=1}^{n} \subset \Omega \) is a set of nodes and \( \{ \omega_i \}_{i=1}^{n} \subset \mathbb{R} \) is a set of weights. We denote the embeddings of probability measures \( \mu \) and discrete measure \( \sum_{i=1}^{n} \omega_i \delta_{x_i} \) to \( H_K \) by \( \mu_K := \int_{\Omega} K(., ) \mu(dx) \) and \( \nu_K := \sum_{i=1}^{n} \omega_i K(., x_i) \), respectively. We evaluate the numerical integration formula, \( Q_n \), using the following worst-case error:

\[
\text{(the worst case error)} := \sup_{\| f \|_K \leq 1} \left| \int_{\Omega} f(x) \mu(dx) - \sum_{i=1}^{n} \omega_i f(x_i) \right| = \| \mu_K - \nu_K \|_K.
\]
The algorithm is given in Algorithm 1. In each iteration, a point, output determined by \( \alpha \) the inner product (2.2); it moves from \( \nu \) in some manner. Kernel herding \([1, 6, 21]\) is a typical method based on this principle. In the kernel problem of \( F \) \( \mu \) can be considered: \( \nu \). Let \( V := \{K(x, \cdot) \mid x \in \Omega \} \) and \( M := \text{conv}(V) \), where the closure is taken with respect to \( \| \cdot \|_K \).

In this study, we assume that \( \mu_K \), which is the embedding of a Borel probability measure \( \mu \), belongs to \( M \). This assumption is very weak. In subsection A.3, we show \( \mu_K \in M \) in a mild assumption.

Let \( F(\nu) := \frac{1}{2} \| \mu_K - \nu \|_K^2 \). The problem setting of kernel quadrature is rewritten as the minimization problem of \( F \) for the embeddings of discrete measures to \( H_K \). By simple calculation, we can derive the Fréchet derivative \( \nabla_\nu F(\nu) = \nu - \mu_K \). To minimize \( F(\nu) \), the following gradient descent method can be considered: \( \nu_{t+1} := \nu_t - \gamma \nabla_\nu F(\nu_t) = \nu_t + \gamma (\mu_K - \nu_t) \) (\( \gamma > 0 \)). However, because the descent direction \( \mu_K - \nu \) does not necessarily have a form \( \sum_{i=1}^n c_i K(x_i, \cdot) \), gradient descent is not suitable for deriving a numerical integration formula. It is appropriate if we can select a descent direction of the form

\[
K(z_i, \cdot) - \nu_t \quad (z_i \in \Omega)
\]  

(2.1)

in some manner. Kernel herding \([1, 6, 21]\) is a typical method based on this principle. In the kernel herding algorithm, to search a descent direction of the form of (2.1), we consider the maximization of

\[
-\langle (\nu_t - \mu_K), v - \nu_t \rangle_K
\]  

(2.2)

subject to \( v \in V := \{K(z, \cdot) \mid z \in \Omega \} \).

The algorithm is given in Algorithm 1. In each iteration, a point, \( \nu_{t+1} \in V \), is selected to maximize the inner product (2.2); it moves from \( \nu_t \) to \( \nu_{t+1} \) with a step size of \( \alpha_t \). The step size \( \alpha_t \) is usually determined by \( \alpha_t = \frac{1}{t+1} \) or line search: \( \alpha_t = \arg \min_{0 \leq \alpha \leq 1} \| (1 - \alpha) \nu_t + \alpha \nu_{t+1} \|_K \). Eventually, the output \( \nu_t \) has the form \( \sum_{i=1}^n \omega_i K(x, \cdot) \), which corresponds to the numerical integration formula \( \sum_{i=1}^n \omega_i f(x_i) \).

**Algorithm 1** kernel herding

1: select initial point \( \nu_1 \in V \)
2: for \( t = 1 \) to \( n - 1 \) do
3: \( \nu_{t+1} = \arg \max_{v \in V} \langle \mu_K - \nu_t, v - \nu_t \rangle_K \)
4: determine the step size \( 0 < \alpha_t \leq 1 \)
5: \( \nu_{t+1} = (1 - \alpha_t) \nu_t + \alpha_t \nu_{t+1} \)
6: end for
7: return \( \nu_n \)

**Algorithm 2** Frank Wolfe

1: select initial point \( \xi_1 \in C \)
2: for \( t = 1 \) to \( n - 1 \) do
3: \( \nu_{t+1} = \arg \max_{v \in V} \langle -\nabla f(\xi_t), v - \xi_t \rangle \)
4: determine the step size \( 0 < \alpha_t \leq 1 \)
5: \( \xi_{t+1} = (1 - \alpha_t) \xi_t + \alpha_t \nu_{t+1} \)
6: end for
7: return \( \xi_n \)

**Remark 2.1.** When \( \nu_t(x) = \sum_{j=1}^n \omega_i K(x, x_j) \) and \( v(x) = K(x, z_i) \), the inner product in (2.2) is written in the following form:

\[
-\langle (\nu_t - \mu_K), v - \nu_t \rangle_K = \int_{\Omega} K(z_i, y) \mu(dy) - \sum_{j=1}^n \omega_j K(z_i, x_j)
\]
\[-\sum_{j=1}^{n} \omega_j \int_{\Omega} K(x_j, y) \mu(dy) + \sum_{i=1}^{n} \sum_{j=1}^{n} \omega_i \omega_j K(x_i, x_j).\]

Therefore, this value must be maximized with respect to \( z_t \in \Omega \). Because this maximization problem is not convex, we prepare several candidate points and select the maximum point from them.

Kernel herding outputs a stable quadrature rule with \( \sum_{i=1}^{n} \omega_i = 1 \) and \( \omega_i \geq 0 \) \( (i = 1, \ldots, n) \). This is an advantage because it is known that some construction methods of kernel quadrature result in an unstable quadrature formula [12]; moreover, there are not many methods of kernel quadrature whose numerical stability is guaranteed theoretically. In addition, we need not compute the inverse matrix of kernel matrix \( (K(x_i, x_j))_{1 \leq i,j \leq t} \) in each iteration.

Although kernel herding is numerically stable and computationally tractable, its convergence speed to true integral values is slower in comparison to that of other effective methods. This has been confirmed experimentally, for example, in [1][12]. In this study, we attempted to improve the kernel herding algorithm to improve the convergence speed by preserving the aforementioned benefits of kernel herding. To realize this, we employed an improvement concept derived from the Frank-Wolfe method [11]. Kernel herding can be considered to be an infinite-dimensional Frank-Wolfe method. There are several approaches to improve the Frank-Wolfe method, and they can be applied to construct a good numerical integration formula.

### 2.3 Frank-Wolfe method and its improvement

The Frank-Wolfe method [11] is a convex optimization method with a convex constraint. We denote a convex objective function by \( f \) and convex constraint by \( C \). For simplicity, we assume that \( C \) is a polytope and \( V_C \) is a set of vertices of \( C \). Kernel herding is a special case of the Frank-Wolfe method, with convex function \( \frac{1}{2} \| \mu_K - \nu \|_F^2 \) and convex constraint \( M \), which has infinite dimension.

It is well known that the Frank-Wolfe method has slow convergence speed owing to its zig-zagging trajectory (Figure 1). This zig-zagging trajectory arises in the Frank-Wolfe method when a point \( \xi_t \) moves toward the vertex in each iteration and the direction does not approximate the negative gradient \( -\nabla f(\xi_t) \), efficiently in some case. To overcome this, several methods have been examined, such as the away step method [14][22]. This method introduces the “away step,” i.e., \( \xi_t - s_t \) \( (s_t \in \arg \max \langle \nabla f(\xi_t), s_t \rangle, \) where \( S^{(t)} \) is the set of vertices selected in previous steps. We select the direction \( s_t - \xi_t \) or \( \xi_t - v_t \), and move the point to this direction.

We consider that the same zig-zagging trajectory problem exists in kernel herding. This is because it becomes difficult to approximate the negative gradient \( \mu_K - \nu_t \), using only one direction \( v_{t+1} - \nu_t \), as \( t \) increases. Figure 3 shows the decrease in \( \cos \theta_t \) as \( t \) increases, where \( \theta_t \) is the angle between \( \mu_K - \nu_t \) and \( v_{t+1} - \nu_t \). It can be observed in Figure 3 that the approximation of the negative gradient, \( \mu_K - \nu_t \) by \( v_{t+1} - \nu_t \), is not enough. Therefore, in this study, we focused on [7]. The main idea of [7] is approximating the negative gradient \( -\nabla f(\xi_t) \), by the linear combination of vertex directions with positive coefficients, that is, solving \( \min_{d \in \text{cone}(V - \xi_t)} \| -\nabla f(\xi_t) - d \|^2 \) in each iteration. Figure 2 is an example; \( -\nabla f(\xi_t) \) is approximated by \( d_2 \), which is the linear combination of two vertex directions. This helps in avoiding zig-zagging trajectories. For the constrained convex optimization problem in Euclidean space, the proposed algorithms improved the convergence speed with respect to the number of iterations and computational time.
3 New algorithms of kernel herding

In this section, we present the improved version of the kernel herding algorithm, given in Algorithm 3. The algorithm approximates the negative gradient $-\nabla_{\nu} F(\nu_t) = \mu_K - \nu_t$ by $g_t$, which is a component of $\text{cone}(V - \nu_t)$, and updates $\nu_t$ with $\nu_{t+1} = \nu_t + \gamma_t g_t$. This concept has already been used to improve the Frank-Wolfe method in [7]. The negative gradient is approximated by either Algorithm 4 or Algorithm 5.

Algorithm 3 accelerated kernel herding algorithm

Input: Input point $\nu_t \in V$
Output: $\nu_T \in M$
1: for $t = 1$ to $T - 1$ do
2: derive the approximate gradient $g_t \in \text{cone}(V - \nu_t)$ using Algorithm 4 or Algorithm 5
3: determine the step size $\gamma_t \in (0, 1)$ by line search
4: $\nu_{t+1} \leftarrow \nu_t + \gamma_t g_t$
5: end for
6: return $\nu_T$

Algorithm 4 positive matching pursuit

Input: Input $\nu_t \in C$, $d_0 = 0$, maximum number of rounds $K_{\text{max}} \in \mathbb{N}$, truncation parameter $\delta < 1$, and $\Lambda_t = 0$.
Output: approximate direction $g_t$
1: for $k = 0$ to $K_{\text{max}} - 1$ do
2: $r_k \leftarrow -(\nu_t - \mu_K) - d_k$
3: $v_k \leftarrow \arg\max_{v \in \mathcal{V}} \langle r_k, v \rangle$
4: $u_k \leftarrow \arg\max_{u \in \mathcal{V}} \langle r_k, u \rangle$ (if $k = 0$, $(r_k, -d_k) / \|d_k\|_K : = -\infty$)
5: $d'_k = d_k + \frac{(r_k, u_k)}{\|u_k\|_K} \mu_k$ ($\mu_k := \frac{(r_k, u_k)}{\|u_k\|_K}$)
6: if align($-(\nu_t - \mu_K), d'_k$) - align($-(\nu_t - \mu_K), d_k$) $> \delta$ then
7: $d_{k+1} \leftarrow d'_k$
8: $\Lambda_t \leftarrow \begin{cases} \Lambda_t + \mu_k & \text{(if } u_k = v_k - \nu_t) \\ \Lambda_t (1 - \mu_k /\|d_k\|) & \text{(if } u_k = -d_k /\|d_k\|) \end{cases}$
9: else
10: break
11: end if
12: end for
13: $K_t \leftarrow k$
14: return $g_t := d_k /\Lambda_t$

Algorithm 5 greedy maximization of $\cos \theta_t$

Input: Input $\nu_t \in C$, maximum number of rounds $K_{\text{max}} \in \mathbb{N}$, and truncation parameter $\delta \geq 0$.
Output: approximate direction $g_t$
1: $d_1 \leftarrow \arg\max_{v \in \mathcal{V} - \nu_t} \frac{\langle v - \mu_K, v \rangle}{\|v - \mu_K\| \|v\|}$
2: $\Lambda_t \leftarrow 1$
3: for $k = 1$ to $K_{\text{max}} - 1$ do
4: $c_k, v_k \leftarrow \arg\max_{c \geq 0, v \in \mathcal{V} - \nu_t} \frac{\langle (v - \mu_K), d_k + cv \rangle}{\|d_k + cv\|}$
5: $d'_k = d_k + c_k v_k$
6: if align($-(\nu_t - \mu_K), d'_k$) - align($-(\nu_t - \mu_K), d_k$) $> \delta$ then
7: $d_{k+1} \leftarrow d'_k$
8: $\Lambda_t \leftarrow \Lambda_t + c_k$
9: else
10: break
11: end if
12: end for
13: $K_t \leftarrow k$
14: return $g_t := d_k /\Lambda_t$

In subsection 3.1, we discuss Algorithm 3 that uses Algorithm 4. The algorithm is a natural extension of the improved Frank-Wolfe method proposed in [7]. In subsection 3.2, we improve the algorithm of subsection 3.1. This algorithm mainly involves the maximization of $\cos \theta_t$, where $\theta_t$ is the angle between the negative gradient $-\nabla_{\nu} F(\nu_t)$ and approximated gradient.

3.1 Positive matching pursuit

We define $\text{align}(f_1, f_2)$ for $f_1, f_2 \in \mathcal{H}_K(\Omega)$ as follows: for $f_1, f_2 \neq 0$, $\text{align}(f_1, f_2) := \frac{\langle f_1, f_2 \rangle_K}{\|f_1\|_K \|f_2\|_K}$ and otherwise, $\text{align}(f_1, f_2) = -1$. 


In the following, we discuss **Algorithm 3** that uses positive matching pursuit (**Algorithm 4**). Positive matching pursuit was introduced in [16]. This is a greedy approximation algorithm for a function in an inner product space. The function is approximated by a positive linear combination of elements in a cone. In line 4 the backward direction \(-d_k/\|d_k\|_K\) may be sometimes selected as a modifier of the approximate direction. In addition, in line 6 we check whether the updated direction increases \(\cos \theta_t\), where \(\theta_t\) is the angle between the approximate direction and \(-\nabla \nu F(\nu_t)\). If the increase is smaller than \(\delta\), the iteration is stopped. In general, \(\cos \theta_t\) does not increase monotonically. Therefore, \(\delta\) is admitted to take a negative value.

In [7], \(K_{\text{max}}\) was taken as a significantly large number, and only the convergence speed with respect to \(T\) was considered. However, in this study, the total number of iterations must be managed, including \(\sum_{t=1}^T K_t\), which is an upper bound of the total number of nodes generated by kernel herding. This is the main difference between this work and [7]. If \(K_{\text{max}}\) is too large, the negative gradient \(-\nabla \nu F(\nu_t)\) is approximated well, but the convergence speed for the number of nodes may be slow. Conversely, if \(K_{\text{max}}\) is too small, \(g_t\) cannot approximate \(-\nabla \nu F(\nu_t)\) sufficiently; thus, the convergence speed may not differ from ordinary kernel herding. Therefore, \(K_{\text{max}}\) should be selected carefully.

In this subsection, we analyze **Algorithm 3** that implements **Algorithm 4** theoretically. Some results from [7] can be referred; however, [7] only treats the Frank-Wolfe method in Euclidean space.

Let us introduce some notations. For \(a, b \in \mathbb{Z}\), we denote \(\{i \in \mathbb{Z} \mid a \leq i \leq b\}\) by \([a, b]\). In addition, we define \(\epsilon_t := \frac{1}{2}\|\mu_K - \nu_t\|_{K}^2\). This is the square of the worst-case error at the \(t\)-th iteration.

First, we confirm that the algorithm works as required using a similar method as Proposition 3.1 in [7].

**Proposition 3.1.** Let \(t \in [1, T - 1]\), and \(\nu_t \in M\). Then,

(i) \(d_1\) is well defined and \(K_t \geq 1\),

(ii) \(\lambda_0, \ldots, \lambda_{K_t-1} \geq 0\),

(iii) For \(k \in [0, K_t]\), \(d_k \in \text{cone}(M - \nu_t)\),

(iv) \(\nu_t + g_t \in M\) and \(\nu_{t+1} \in M\),

(v) \(\text{align}(-\nu_t - \mu_K, g_t) \geq \text{align}(-\nu_t - \mu_K, \nu_0 - \nu_t) + (K_t - 1)\delta\), where \(\nu_0 \in \arg \max_{v \in M} \langle -(\nu_t - \mu_K), v \rangle\).

In addition, \(\text{align}(-\nu_t - \mu_K, \nu_0 - \nu_t) \geq 0\)

We define \(\cos \theta_t := \langle -(\nu_t - \mu_K), g_t \rangle_K / \|\mu_K - \nu_t\|_K \|g_t\|_K\). The following proposition shows that the convergence speed of the worst-case error is influenced by \(\cos \theta_t\).

**Proposition 3.2.** Let \(A_t := \{i \in [1, t - 1] \mid \gamma_{i} \neq 1\}\). Then, it becomes valid for all \(t \in [1, T]\),

\[
\epsilon_t \leq \epsilon_1 \prod_{i \in A_t} (1 - \cos^2 \theta_i).
\]

In particular, if \(\gamma_{i} < 1\) in each iteration, \(\epsilon_t = \epsilon_1 \prod_{1 \leq i \leq t-1} (1 - \cos^2 \theta_i)\). In numerical experiments, \(\gamma_{i} < 1\) most of the time; thus, the convergence speed of the worst-case error is directly determined by \(\cos \theta_i\).

To consider the convergence of the worst-case error for the number of nodes, we use Proposition 3.2. It is evident that the convergence speed is directly influenced by \(\cos \theta_t\). Therefore, we analyze the behavior of \(\cos \theta_t\). First, we state the convergence speed of positive matching pursuit.

We prove the following proposition that states the convergence speed of positive matching pursuit. To discuss the approximation of **Algorithm 4**, we treat the case \(\delta = -\infty\), i.e., we do not consider the truncation in line 6 in **Algorithm 4**. Proposition 3.3 below states the convergence speed of the positive matching pursuit algorithm at \(t\)-th iteration. The procedure of the proof is similar to that in [16].

**Proposition 3.3.** Let \(\delta = -\infty\). If we solve \(\min_{d_k \in M - \nu_t} \|-(\nu_t - \mu_K) - d_k\|_K^2\) by positive matching pursuit,

\[
\|-(\nu_t - \mu_K) - d_k\|_K^2 \leq \frac{\|\nu_t - \mu_K\|_K^2}{1 + Ck\|\nu_t - \mu_K\|_K^2},
\]

holds true.

We define \(\cos \theta_{t,k} := \langle -(\nu_t - \mu_K), d_k \rangle_K / \|\mu_K - \nu_t\|_K \|d_k\|_K\). Using Proposition 3.3, we can derive the lower bound of \(\cos \theta_{t,k}\).
Corollary 3.1. For the same condition as Proposition 3.3

\[ \cos \theta_{t,k} \geq 1 - \frac{1}{2} \frac{\| \mu_k - \nu_t \|_K}{\| \Delta_k \|_K} \]

holds true.

By applying a triangle inequality, we have \( \| \mu_k - \nu_t \|_K \leq \frac{\sqrt{1 + C \epsilon t K}}{\sqrt{1 + C \epsilon t K - 1}} \). Using this inequality, we have \( \cos \theta_{t,k} \geq 1 - \frac{1}{2} \frac{\| \mu_k - \nu_t \|_K}{\| \Delta_k \|_K} \). From this inequality, it can be observed that as \( \epsilon_t \) decreases, the growth of the lower bound of \( k \) becomes slower because \( k \) is multiplied by \( \epsilon_t \). Because Corollary 3.1 only yields the lower bound, we cannot conclude that it is difficult to increase \( \cos \theta_t \) as \( \| \mu_k - \nu_t \|_K \) decreases; however, this gives some insight into the convergence speed. As the worst-case error decreases, more points are required to approximate the direction of \( - (\nu_t - \mu_k) \). In the experiment, it become difficult to increase \( \cos \theta_t \) as \( \| \mu_k - \nu_t \|_K \) decreases. Considering this property, we propose a method that directly maximizes \( \cos \theta_t \).

3.2 Greedy maximization of \( \cos \theta_t \) method

Proposition 3.2 suggests that \( \cos \theta_t \) is directly related to the convergence speed of the worst-case error \( \| \mu_k - \nu_t \|_K \). Then, if we can maximize \( \cos \theta_t \) effectively, we can expect faster convergence speed. We propose an improved kernel herding algorithm that uses the greedy maximizing method of \( \cos \theta_t \) instead of positive matching pursuit. The algorithm is Algorithm 5. In Algorithm 5, we greedily add \( c(K(\cdot, y) - \nu_t) \) to the present descent direction \( d_k \) to maximize \( \cos \theta_{t,k+1} \). We note that Proposition 3.1 and Proposition 3.2 also hold true if we use Algorithm 5 instead of Algorithm 4 for the approximation of \( \mu_k - \nu_t \). For Proposition 3.1, because \( c_k \geq 0 \), it can be ensured that the coefficients of \( \nu_k \) are non-negative. Thus, we can confirm the properties in Proposition 3.1 by following the same argument. In addition, for the proof of Proposition 3.2, we only use the properties of Algorithm 3 and the truncation by \( \delta \). Therefore, they are also applicable to Algorithm 5. We state this in the form of a theorem:

Theorem 3.1. Proposition 3.1 and Proposition 3.2 hold true if we apply Algorithm 5 instead of Algorithm 4 to Algorithm 3.

However, it is not evident that the optimization in line 4 has a solution with \( c > 0 \). In addition, the optimization procedure in line 4 is unclear. In the following argument, we discuss these problems.

Note that we assume \( \cos \theta_{t,k} = \frac{1}{\| \mu_k - \nu_t \|_K} \) never takes its maximum at \( \nu_t \neq \mu_k \) for simplicity.

We consider an optimization problem

\[ \arg \max_{c \geq 0, \nu \in V - \nu_t} \frac{\langle - (\nu_t - \mu_k), d_k + cv \rangle_K}{\| \mu_k - \nu_t \|_K \| d_k + cv \|_K} \]

in Algorithm 5. For \( y \in \Omega \), we denote \( \frac{\langle - (\nu_t - \mu_K), d_k + c (K(\cdot, y) - \nu_t) \rangle_K}{\| d_k + c (K(\cdot, y) - \nu_t) \|_K} \) by \( g(c, y) \). The function \( g(c, y) \) can be written as

\[ g(c, y) = \frac{c \langle - (\nu_t - \mu_K), K(\cdot, y) - \nu_t \rangle_K + \langle - (\nu_t - \mu_K), d_k \rangle_K}{\sqrt{c^2 \| K(\cdot, y) - \nu_t \|_K^2 + 2c (K(\cdot, y) - \nu_t, d_k)_K + \| d_k \|_K^2}} = \frac{cp + q}{\sqrt{\alpha c^2 + 2 \beta c + \gamma}}, \]

where \( p := \langle - (\nu_t - \mu_K), K(\cdot, y) - \nu_t \rangle_K, q := \langle - (\nu_t - \mu_K), d_k \rangle_K, \alpha := \| K(\cdot, y) - \nu_t \|_K^2, \beta := (K(\cdot, y) - \nu_t, d_k)_K, \) and \( \gamma := \| d_k \|_K^2 \). We remark that \( p, \alpha, \beta \) are functions of \( y \).

Because \( \frac{\partial g}{\partial c} = \frac{(p^2 - qa)(q^2 - p^2)}{(\alpha c^2 + 2 \beta c + \gamma)^{3/2}} \), for a fixed \( y \), \( g(c, y) \) takes the extreme value at \( c = \frac{q^2 - p^2}{p^2 - qa} \) if \( p^2 - qa \neq 0 \).

We fix \( y \in \Omega \) and discuss the maximum point of \( g(c, y) \) in \( c \geq 0 \). Proposition 3.4 describes the possibility of the maximum point of \( g(c, y) \) for each \( y \in \Omega \) and \( g(c, y) \) never takes its maximum at \( c = \infty \).

Proposition 3.4. For each \( y \in \Omega \), \( g(c, y) \) takes its maximum value in \( c \geq 0 \) at \( c = 0 \) or \( c = \frac{q^2 - p^2}{p^2 - qa} \).

Now, we consider if there exists \( y \) such that the function \( g(c, y) \) takes its maximum at \( c = \frac{q^2 - p^2}{p^2 - qa} > 0 \). The following Theorem 3.2 suggests a positive result.
We also performed an experiment for integration on a sphere in \( \mathbb{R}^3 \).

We performed numerical experiments to evaluate the performance of the proposed methods. The concrete optimization procedure of Algorithm 4, if we set \( \delta > 0 \), is as follows:

1. Prepare the candidate set of sample points.
2. Select a point \( y_k \in \Omega \) that maximizes \( g(\frac{q^2 - p^2}{p^2 - q^2}, y) \) from the restricted candidate set and let \( v_k = K(\cdot, y_k) - \nu_t \) and \( c = g(\frac{q^2 - p^2}{p^2 - q^2}, y_k) \), where \( \alpha, \beta, \gamma, p, q \) are computed for \( y_k \).

Remark 3.1. We note that the aforementioned algorithm is not computationally exhausting. Proposition 3.4 requires the computation of \( p, q, \alpha, \beta, \gamma \) at each iteration along with the inner products and norms. By memorizing the previous values of \( p, q, \alpha, \beta, \gamma \), we can reduce the cost of such computation; moreover, the computational complexity of Algorithm 5 is not significantly different from that of the ordinary kernel herding. Concretely, the computational cost at each iteration is \( O(m + t + k) \), where \( m \) is the number of candidate points.

4 Numerical experiments

We performed numerical experiments to evaluate the performance of the proposed methods. The first proposed algorithm that uses Algorithm 4 is called “positive matching pursuit” and the second algorithm that uses Algorithm 5 is called “greedy-cos.” We compare the proposed methods with the existing methods, namely, kernel herding with step size determined by line search and \( 1/\|x-y\| \). For simplicity, we refer to the former as “line search” and the latter as “equal weight herding.” First, we compare the convergence speed of the worst-case error with respect to the number of nodes and time. In addition, we compare Algorithm 4 and Algorithm 5 on the growth of \( \cos \theta_{t,k} \) with respect to the total number of iterations \( k + \sum_{i=1}^{t-1} K_i \). The kernel is a Gaussian kernel \( K(x, y) = \exp \left(-\|x-y\|^2\right) \). The domain is \( \Omega = [-1, 1]^d \) and the density function of the distribution on \( \Omega \) is \( \frac{1}{C} \exp \left(-\|x\|^2\right) \), where \( C = \int_{\Omega} \exp \left(-\|x\|^2\right) \) dx. The experiments are performed for \( d = 2, 3 \). Figure 4 shows the results. It can be observed that the proposed algorithms outperformed line search. Thus, we can confirm that the approximation of the negative gradient \( \mu_K - \nu_t \) accelerates convergence. In particular, Algorithm 5 is better than Algorithm 4. This is reasonable because \( \cos \theta_{t,k} \) monotonically increases in Algorithm 5 while it does not in Algorithm 4. It is evident from (b) and (e) that in both methods, \( \cos \theta_{t,k} \) increases in the approximation process. In particular, Algorithm 5 is even better than Algorithm 4. We note that the condition in the numerical experiments for \( d = 2 \) is the same as that in Figure 3. Therefore, (b) and (e) ensure the effectiveness of both methods. The proposed algorithms improved the convergence speed for the computational time in comparison to line search. Moreover, “greedy-cos” outperformed “equal weight herding.”

We also performed an experiment for integration on a sphere in \( \mathbb{R}^3 \). The kernel is \( K(x, y) = \frac{1}{3} - \|x-y\| \). The domain \( \Omega \) is a unit sphere centered at the origin in \( \mathbb{R}^3 \) and the probability distribution is a uniform distribution. It is known that the optimal rate of the worst-case error is \( 1/n^{\frac{2}{3}} \).
Figure 4: Results of numerical experiments for Gaussian kernel \((d = 2, 3)\). (a), (d) represent the convergence speed of the worst-case error with respect to the number of nodes and (c), (f) represent that with respect to the computational time. (b), (e) represent the growth of \(\cos \theta_{t,k}\) in the same condition as (a), (d), respectively. Note that “1/n” and “\((1/n)^{1/2}\)” denote the order for the total number of nodes, \(n\).

as demonstrated by [4]. Figure 5 shows the results. Although the improvements in the proposed methods are smaller than those in the experiments with a Gaussian kernel, the effectiveness of the proposed methods is evident. In this experiment, the two proposed methods exhibit almost the same performance and outperformed line search. Moreover, “equal weight herding” was slightly better than both proposed methods. This can be attributed to the symmetric domain and the uniform distribution.

**Conclusion**

In this study, we improved the kernel herding algorithm to obtain a faster convergence speed while preserving the numerical stability and computational efficiency. The main concept involved approximating the negative gradient \(-\nabla_{\nu} F(\nu_t) = \mu_K - \nu_t\). The first algorithm implemented the algorithm of [7]. We confirmed that the results in [7] are also valid for kernel herding and analyzed the convergence speed of the approximation of \(\mu_K - \nu_t\). The second algorithm involved
the maximization of $\cos \theta_t$, where $\theta_t$ denotes the angle between $\mu_K - \nu_t$ and the approximated direction. We theoretically proved the maximization and proposed the algorithm. Through numerical experiments, we confirmed that the proposed algorithms improve the convergence speed for the number of nodes and computational time; moreover, the improvement in the second proposed algorithm is remarkable.

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We let $k$.

(ii) We let $\nu_t \in N$, $k \geq 0$, and $\lambda_k \geq 0$. Consider $u_k = -\frac{d_k}{\|d_k\|_K}$.

A.1 Proofs of subsection 3.1

Proof of Proposition 3.1

Proof. (i) By definition, $\text{align}(r_0, d_0) = -1$. In addition, because $v_0 \in \arg \max_{v \in M} \langle r_0, v \rangle_K$ and $\nu_t \in M$, the following holds true:

$$\langle r_0, v_0 - \nu_t \rangle_K = \langle r_0, v_0 \rangle_K - \langle r_0, \nu_t \rangle_K \geq 0.$$ 

Therefore, $u_0 = v_0 - \nu_t$ and $\text{align}(r_0, d_0) - \text{align}(r_0, d_0) \geq 1 > \delta$ are valid. Thus, $K_t \geq 1$.

(ii) We let $k \in [0, K_t - 1]$. Because $v_k \in \arg \max_{v \in M} \langle r_k, v \rangle_K$ and $\nu_t \in M$,

$$\langle r_k, v_k - \nu_t \rangle_K = \max_{v \in M} \langle r_k, v \rangle_K - \langle r_k, \nu_t \rangle_K \geq 0.$$ 

In line 4 of Algorithm 4,

$$\langle r_k, u_k \rangle_K \geq \langle r_k, v_k - \nu_t \rangle_K \geq 0.$$ 

Thus, $\lambda_k \geq 0$.

(iii) We prove the following by induction.

(a) $k = 0$

$d_0 = 0 = \nu_t - \nu_t \in \text{cone}(M - x_t)$.

(b) We assume there exist $k \in \mathbb{N}$ and $d_k \in \text{cone}(M - \nu_t)$.

If $u_k = v_k - \nu_t$, because $u_k \in M - \nu_t$ and $\lambda_k \geq 0$,

$$d_{k+1} = d_k + \lambda_k (v_k - \nu_t) \in \text{cone}(M - \nu_t).$$

Consider $u_k = -\frac{d_k}{\|d_k\|_K}$. Because $d_{k+1} = (1 - \frac{\lambda_k}{\|d_k\|_K})d_k$, we must prove that $(1 - \frac{\lambda_k}{\|d_k\|_K}) \geq 0$. It suffices to show that $(1 - \frac{\lambda_k}{\|d_k\|_K}) \geq \frac{1}{2}$. By simple calculation,

$$1 - \frac{\lambda_k}{\|d_k\|_K} \geq \frac{1}{2} \iff \frac{1}{2} \geq \frac{\lambda_k}{\|d_k\|_K} \iff \|d_k\|_K \geq \langle r_k, -d_k \rangle.$$ 

Thus, it suffices to show that $\|d_k\|_K \geq \langle r_k, -d_k \rangle$. This is valid for any $k' \in \mathbb{N}$,

$$\|r_{k'+1}\|_K^2 = \| - (\nu_t - \mu_K) - d_{k'+1} \|_K^2 = \| - (\nu_t - \mu_K) - (d'_k + \lambda_k u_{k'}) \|_K^2 = \|r_{k'} - \lambda_k u_{k'}\|_K^2.$$
\[
\begin{align*}
\|r_k\|^2_K &= 2\lambda_k \langle r_k, u_k \rangle_K + \lambda_k^2 \|u_k\|^2_K \\
&= \|r_k\|^2_K + \frac{\langle r_k, u_k \rangle_K^2}{\|u_k\|^2_K} \\
&\leq \|r_k\|^2_K.
\end{align*}
\]

Note that we used \(\lambda_k = \frac{\langle r_k, u_k \rangle_K}{\|u_k\|^2_K}\). Therefore,

\[
\|r_k\|^2_K \leq \|r_0\|^2_K. \tag{A.1}
\]

Because \(d_0 = 0\), by (A.1), it is evident that

\[
\| - (\nu_t - \mu_K) \|^2_K \geq \| - (\nu_t - \mu_K) - d_k \|^2_K = \| \nu_t - \mu_K \|^2_K + 2 \langle \nu_t - \mu_K, d_k \rangle_K + \| d_k \|^2_K
\]

\[
\Leftrightarrow \langle \nu_t - \mu_K, d_k \rangle_K \leq - \frac{\| d_k \|^2_K}{2}.
\]

Using this,

\[
\langle r_k, -d_k \rangle_K = \langle - (\nu_t - \mu_K) - d_k, -d_k \rangle_K = \langle \nu_t - \mu_K, d_k \rangle_K + \| d_k \|^2_K
\]

\[
\leq \frac{\| d_k \|^2_K}{2}.
\]

Therefore, \(d_{k+1} \in \text{cone}(M - \nu_t)\).

(iv) By (iii), \(d_K, \in \text{cone}(M - \nu_t)\). In addition, from the algorithm and (ii), it is evident that \(g_t \in M - \nu_t\). Therefore, \(\nu_t + g_t \in M\) and \(\nu_{t+1} = \nu_t + \gamma_t g_t = (1 - \gamma_t) \nu_t + \gamma_t (\nu_t + g_t) \in M\).

(v) By (A.1), align\((- (\nu_t - \mu_K), v_0 - \nu_t) \geq 0\). Because \(g_t = d_K / \lambda_t\) and line 6 of Algorithm 4 the following holds true:

align\((- (\nu_t - \mu), g_t) = align(- (\nu_t - \mu), d_{K_i})
\]

\[
\geq align(- (\nu_t - \mu), d_{K_i-1}) + \delta
\]

\[
\geq align(- (\nu_t - \mu), d_1) + (K_i - 1) \delta
\]

\[
= align(- (\nu_t - \mu), v_0 - \nu_t) + (K_i - 1) \delta.
\]

\[
\square
\]

**Proof of Proposition 3.2**

We remark on the step size, \(\gamma_t\). It can be easily confirmed that \(\arg \min_{\gamma_t \in \mathbb{R}} \| \nu_t + \gamma_t g_t - \mu_K \|^2_K = \gamma_t \in \mathbb{R} \frac{\langle - (\nu_t - \mu_K), g_t \rangle_K}{\| g_t \|^2_K}\). Because \(\| \nu_t + \gamma_t g_t - \mu_K \|^2_K\) is a quadratic function of \(\gamma_t\),

\[
\gamma_t = \arg \min_{0 \leq \gamma_t \leq 1} \| \nu_t + \gamma_t g_t - \mu_K \|^2_K = \min \left\{ \frac{\langle - (\nu_t - \mu_K), g_t \rangle_K}{\| g_t \|^2_K}, 1 \right\}
\]

for each \(t \in [1, T - 1]\).

**Proof.** For each \(i \in [1, t - 1]\), because \(0 \leq \gamma_i \leq 1\), the following is valid:

\[
\frac{1}{2} \| \mu_K - \nu_{i+1} \|^2_K = \frac{1}{2} \| \mu_K - (\nu_i + \gamma_i g_i) \|^2_K \leq \frac{1}{2} \| \mu_K - \nu_i \|^2_K. \tag{A.2}
\]

If \(\gamma_i \neq 1\), \(\gamma_i = \frac{\langle - (\nu_i - \mu_K), g_i \rangle_K}{\| g_i \|^2_K}\). Using this and the definition of \(\cos \theta_i\),

\[
\frac{1}{2} \| \mu_K - \nu_{i+1} \|^2_K = \frac{1}{2} \| \mu_K - (\nu_i + \gamma_i g_i) \|^2_K
\]

\[
= \frac{1}{2} \| \mu_K - \nu_i \|^2_K + \gamma_i \langle \nu_i - \mu_K, g_i \rangle_K + \frac{1}{2} \gamma_i^2 \| g_i \|^2_K
\]

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\[
\frac{1}{2} \|\mu_K - \nu_i\|^2_K - \gamma_i \cos \theta_i \|\nu_i - \mu_K\| K \|\theta_i\|_K + \frac{1}{2} \gamma_i^2 \|\theta_i\|^2_K \\
= \frac{1}{2} \|\mu_K - \nu_i\|^2_K - \cos^2 \theta_i \|\nu_i - \mu_K\|^2_K \\
= (1 - \cos^2 \theta_i) \frac{1}{2} \|\mu_K - \nu_i\|^2_K. \tag{A.3}
\]

Using (A.2) and (A.3), we obtain the desired result. \( \square \)

**Proof of Proposition 3.3**

For preparation, we use the following lemma.

**Lemma A.1** ([2][19]). Let \( \{a_k\}_{k=0}^n \) be a nonnegative sequence of real numbers. If \( \{a_k\}_{k=0}^n \) satisfies \( a_{k+1} \leq a_k - \gamma a_k^2 \) (\( k = 0, \ldots, m-1 \)) for \( \gamma > 0 \),

\[
a_m \leq \frac{a_0}{1 + m \gamma a_0}.
\]

Using the aforementioned lemma, we prove [Proposition 3.3]

**Proof.** We define \( \eta_k = \| - (\nu_t - \mu_K) - d_k \|^2_K \). First, the following equality holds true:

\[
\| - (\nu_t - \mu_K) - d_k \|^2_K = \| - (\nu_t - \mu_K) \|^2_K + 2 \langle d_k + \nu_t - \mu_K, d_k + \nu_t - \mu_K \rangle_K + \| d_k + \nu_t - \mu_K \|^2_K. \tag{A.4}
\]

Here, we divide into cases as for \( u_k \leftarrow \arg \max_{u \in \{v_k - \nu_t - d_k / \|d_k\|_K\}} \langle r_k, u \rangle_K \) in Algorithm 4.

(A) \( u_k = v_k - \nu_t \)

The following is evidently valid: \( \langle \mu_K - \nu_t - d_k, v_k - \nu_t \rangle_K \geq \langle \mu_K - \nu_t - d_k, -d_k / \|d_k\|_K \rangle_K \). In addition,

\[
\langle \mu_K - \nu_t - d_k, v_k - \nu_t \rangle_K = \max_{v \in M} \langle \mu_K - \nu_t - d_k, v - \nu_t \rangle_K \geq \langle \mu_K - \nu_t - d_k, \mu_K - \nu_t \rangle_K.
\]

Therefore,

\[
\langle \mu_K - \nu_t - d_k, \|d_k\|_K + 1 \rangle (v_k - \nu_t) \rangle_K \geq \langle \mu_K - \nu_t - d_k, -d_k \rangle_K + \langle \mu_K - \nu_t - d_k, \mu_K - \nu_t \rangle_K \\
= \|\mu_K - \nu_t - d_k\|^2_K \\
= \eta_k.
\]

Note that this inequality also holds true for \( k = 0 \). By the algorithm, \( d_{k+1} = d_k + \frac{\langle \mu_K - \nu_t - d_k, v_k - \nu_t \rangle_K}{\|v_k - \nu_t\|^2_K} (v_k - \nu_t) \). By substituting this into (A.4), the following holds true:

\[
\eta_{k+1} = \eta_k - \frac{\langle d_k + \nu_t - \mu_K, v_k - \nu_t \rangle^2_K}{\|v_k - \nu_t\|^2_K} \leq \eta_k - \frac{\eta_k^2}{\|v_k - \nu_t\|^2_K (\|d_k\|_K + 1)^2}.
\]

(B) \( u_k = -d_k / \|d_k\|_K \)

By the assumption, it holds that

\[
\langle d_k + \nu_t - \mu_K, -\frac{d_k}{\|d_k\|_K} \rangle_K \leq \langle d_k + \nu_t - \mu_K, v_k - \nu_t \rangle_K \\
= \arg \min_{v \in M} \langle d_k + \nu_t - \mu_K, v - \nu_t \rangle_K \\
\leq \langle d_k + \nu_t - \mu_K, \mu_K - \nu_t \rangle_K.
\]

Therefore,

\[
\langle d_k + \nu_t - \mu_K, -\frac{\|d_k\|_K + 1}{\|d_k\|_K} d_k \rangle_K \leq \langle d_k + \nu_t - \mu_K, \mu_K - \nu_t - d_k \rangle_K = -\eta_k \leq 0 \\
\Rightarrow \langle d_k + \nu_t - \mu_K, -\frac{\|d_k\|_K + 1}{\|d_k\|_K} d_k \rangle^2_K \geq \frac{\eta_k^2}{(\|d_k\|_K + 1)^2} \tag{A.5}
\]

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By substituting $d_{k+1} = d_k + \langle \mu_K - \nu_t - d_k, -\frac{d_k}{\|d_k\|_K} \rangle_K (\frac{d_k}{\|d_k\|_K})$ into (A.4) and using (A.5), we have
\[
\eta_{k+1} \leq \eta_k - \frac{\eta_k^2}{\|d_k\|_K + 1}.
\]
From, (A), (B), the following is valid:
\[
\eta_{k+1} \leq \eta_k - C \eta_k^2,
\]
where $\sup_k\|d_k\|_K + 1)^2 = C_1$, $\max\{1, \sup_{\nu \in M} \|\nu - \nu_t\|_K^2\} = C_2$ and $C_1 C_2 = \frac{1}{\epsilon^2}$. By applying Lemma A.1 to this, we have
\[
\eta_k \leq \frac{\eta_0}{1 + C \eta_k}.
\]
\[\square\]

Remark A.1. Note that the constants $C_1$ and $C_2$ in the proof of Proposition 3.3 are bounded regardless of $k$. We first explain $C_1 = \sup_k\|d_k\|_K + 1)^2$. By the aforementioned proof, $\|d_k - (\mu_K - \nu_t)\|_K$ decreases monotonically. Therefore, the following holds true:
\[
C_1 \leq (1 + \|d_k - (\mu_K - \nu_t)\|_K + \|\mu_K - \nu_t\|_K)^2
\leq (1 + \|d_0 - (\mu_K - \nu_t)\|_K + \|\mu_K - \nu_t\|_K)^2
= (1 + 2\|\mu_K - \nu_t\|_K)^2
\]
\[
\|\mu_K - \nu_t\|_K^2
\]
is bounded because
\[
\|\mu_K - \nu_t\|_K^2 = \int_\Omega \int_\Omega K(\nu, y)(\mu - \nu_t)(d\nu)(\mu - \nu_t)(d\nu)
\leq \int_\Omega \int_\Omega K(\nu, y)(\mu - \nu_t)(d\nu)|\mu - \nu_t|(d\nu)
\leq \int_\Omega \|K\|_\infty |\mu - \nu_t|(d\nu)
\leq 2\|K\|_\infty.
\]

Note that in the above calculation, we consider $\nu_t$ as the discrete measure even though this is abuse of notation. In the same manner, the boundedness of $C_2$ can be proved.

Proof of Corollary 3.1

Proof. By simple calculation,
\[
\|\mu_K - \nu_t - d_k\|_K^2 = \|\mu_K - \nu_t\|_K^2 + \|d_k\|_K^2 - 2 \langle \mu_K - \nu_t, d_k \rangle_K
\]
\[
\Leftrightarrow \cos \theta_{t, k} = \frac{1}{2} \frac{\|\mu_K - \nu_t\|_K^2 + \frac{1}{2} \|d_k\|_K^2 - \|d_k\|_K - \langle \mu_K - \nu_t, d_k \rangle_K}{\|d_k\|_K}.
\]
Using $\frac{1}{2} \frac{\|\mu_K - \nu_t\|_K^2 + \frac{1}{2} \|d_k\|_K^2}{\|d_k\|_K} \geq 1$,
\[
\cos \theta_{t, k} \geq 1 - \frac{\|d_k\|_K - \langle \mu_K - \nu_t, d_k \rangle_K}{\|d_k\|_K}.
\]
In addition, by applying Proposition 3.3
\[
\frac{\|\mu_K - \nu_t\|_K}{\|d_k\|_K} \geq \frac{\frac{\mu_K - \nu_t}{\|d_k\|_K}}{1 + C \|d_k\|_K - \frac{\mu_K - \|d_k\|_K}{\|d_k\|_K}}.
\]
\[\square\]

A.2 Proofs of subsection 3.2

We remark that $q > 0$. At each iteration, we maximize $\langle (\nu - \mu_K), d_1 + cv \rangle_K$ and thus,
\[
\langle (\nu - \mu_K), d_1 \rangle_K \geq \langle (\nu - \mu_K), u_1 \rangle_K \geq \langle (\nu - \mu_K), \mu_K - \nu_t \rangle_K > 0,
\]
where $u_1 = \arg \max_v (\nu - \mu_K, v)$. Therefore, $q > 0$.  

\[14\]
Proof of Proposition 3.4

Proof. First, we consider the case \( p \beta - q \alpha \neq 0 \). We divide the cases into \( p \geq 0 \) or \( p < 0 \) to clarify the maximum point of \( g(c, y) \).

(i) \( p < 0 \)

Because \( g(0, y) = \frac{q}{\sqrt{\gamma}} > 0 \), \( \lim_{c \to \infty} g(c, y) = -\frac{p}{\sqrt{\alpha}} > 0 \) and \( \lim_{c \to \infty} g(c, y) = \frac{p}{\sqrt{\alpha}} < 0 \),
arg max \( g(c, y) \) is \( c = 0 \) or \( c = \frac{q \beta}{p \beta - q \alpha} \).

(ii) \( p \geq 0 \)

Because \( g(0, y) = \frac{q}{\sqrt{\gamma}} > 0 \), \( \lim_{c \to \infty} g(c, y) = -\frac{p}{\sqrt{\alpha}} \leq 0 \) and \( \lim_{c \to \infty} g(c, y) = \frac{p}{\sqrt{\alpha}} \geq 0 \),
arg max \( g(c, y) \) is \( c = 0 \) or \( c = \infty \) or \( c = \frac{q \beta}{p \beta - q \alpha} \). We show that the following never holds true:
arg max \( g(c, y) = \infty \). If arg max \( g(c, y) = \infty \), \( g(\infty, y) > g(0, y) \), that is,
\[
\begin{align*}
\arg max \frac{-((\nu_t - \mu_K), K(\cdot, y) - \nu_t\nu)}{\|\mu_K - \nu_t\|_K \|K(\cdot, y) - \nu_t\|_K} > \frac{-((\nu_t - \mu_K), d_k)}{\|\mu_K - \nu_t\|_K \|d_k\|_K}.
\end{align*}
\]
In addition, because \( \frac{-((\nu_t - \mu_K), d_k)}{\|\mu_K - \nu_t\|_K \|d_k\|_K} \) monotonically increases,
\[
\frac{-((\nu_t - \mu_K), K(\cdot, y) - \nu_t\nu)}{\|\mu_K - \nu_t\|_K \|K(\cdot, y) - \nu_t\|_K} > \frac{-((\nu_t - \mu_K), d_k)}{\|\mu_K - \nu_t\|_K \|d_k\|_K},
\]
This is the contradiction because \( d_1 = \arg max \frac{-((\nu_t - \mu_K), \nu)}{\|\mu_K - \nu\|_K \|\nu\|_K} \). Thus, arg max \( g(c, y) \) is \( c = 0 \) or 
\[
c = \frac{q \beta}{p \beta - q \alpha}.
\]
If \( p \beta - q \alpha = 0 \), \( g(c, y) \) is monotonically decreasing or increasing. Thus, \( g(c, y) \) takes its maximum at \( c = 0 \) or \( c = \infty \). However, by the argument above, it is evident that \( g(c, y) \) never takes its maximum at \( c = \infty \). Thus, it takes the maximum at \( c = 0 \) \( \square \)

Remark A.2. We mention some remarks on the proof of Proposition 3.4

(i) When \( p < 0 \), \( g(c, y) \) takes the minimum value at \( \frac{q \beta}{p \beta - q \alpha} \), the minimum value is negative. Therefore, if \( \frac{q \beta}{p \beta - q \alpha} > 0 \), we can distinguish if the extreme point is maximum or minimum by the sign.

(ii) When \( p \geq 0 \), if \( \frac{q \beta}{p \beta - q \alpha} > 0 \), this is the maximum point. If \( \frac{q \beta}{p \beta - q \alpha} > 0 \) and this is the minimum value, \( g(c, y) < 0 \) for \( c < 0 \). This is the contradiction because \( g(0, y) > 0 \).

Proof of Theorem 3.2

Proof. From Proposition 3.4 it is sufficient to show that there exists \( y \in \Omega \) such that \( \frac{\partial g(c, y)}{\partial c} |_{c=0} > 0 \); in that case, \( g(c, y) \) does not take its maximum at \( c = 0 \). This can be written as
\[
p \gamma - q \beta = -((\nu_t - \mu_K), K(\cdot, y) - \nu_t\nu) \|d_k\|_K - \langle K(\cdot, y) - \nu_t, d_k \rangle_K < 0.
\]
Therefore, it suffices to show that
\[
\frac{(\mu_K - \nu_t, K(\cdot, y) - \nu_t\nu)}{\|\nu_t - \mu_K\|_K \|K(\cdot, y) - \nu_t\|_K} > \frac{(\nu_t - \mu_K, d_k)}{\|\mu_K - \nu_t\|_K \|d_k\|_K}.
\]
Because \( \frac{(\mu_K - \nu_t, d_k)}{\|\mu_K - \nu_t\|_K \|d_k\|_K} < 1 \), it suffices to show that there exists \( y \in \Omega \) such that
\[
\frac{(\mu_K - \nu_t, K(\cdot, y) - \nu_t\nu)}{\|\nu_t - \mu_K\|_K \|K(\cdot, y) - \nu_t\|_K} > \frac{(K(\cdot, y) - \nu_t, d_k)}{\|\mu_K - \nu_t\|_K \|d_k\|_K}.
\]
To show this, we use the following lemma.

Lemma A.2. Let \( \{f_i\}_{i=1}^{\infty} \subseteq \mathcal{H}_K \). Let \( X := \overline{\text{cone}(\{f_i\}_{i=1}^{\infty})} \), where the closure is taken with respect to \( \|\cdot\|_K \). For any \( z_1, z_2 \in X \) such that \( \|z_1 + z_2\|_K \neq \|z_1\|_K + \|z_2\|_K \), there exists \( i \in \mathbb{N} \) such that
\[
\frac{\langle z_1, f_i \rangle_K}{\|f_i\|_K \|z_1\|_K} > \frac{\langle z_2, f_i \rangle_K}{\|f_i\|_K \|z_2\|_K}.
\]
Since $K$ is continuous and $\Omega \times \Omega$ is compact, $K$ is uniformly continuous on $\Omega \times \Omega$. Therefore, we can prove that there exists $\{x_i\}_{i=1}^\infty \subset \Omega$ such that $d_k, \mu_K - \nu_i \in \text{conv}\{K(x_i, \cdot) - \nu_i\}_{i=1}^\infty$ as shown in subsection A.3. Then, we can apply Lemma A.2 to $z_1 = \mu_K - \nu_i$ and $z_2 = d_k$ and there exists $y \in \Omega$ such that

$$\frac{\langle \mu_K - \nu_i, (K(\cdot, y) - \nu_i) \rangle_K}{\|\nu_i - \mu_K\|_K \|K(\cdot, y) - \nu_i\|_K} > \frac{\langle (K(\cdot, y) - \nu_i, d_k) \rangle_K}{\|d_k\|_K \|K(\cdot, y) - \nu_i\|_K}.$$ 

Thus, we derive the desired result.

Proof of Lemma A.2

Proof. Let $z_1 = \sum_{j=1}^\infty t_j f_j$, $z_2 = \sum_{i=1}^\infty s_i f_i$, where $t_i, s_i \geq 0$ for any $i \in \mathbb{N}$. We prove this lemma by contradiction. We assume that for any $j \in \mathbb{N}$, the following is valid:

$$\frac{\langle z_1, f_j \rangle_K}{\|f_j\|_K \|z_1\|_K} \geq \frac{\langle z_2, f_j \rangle_K}{\|f_j\|_K \|z_2\|_K} \iff \frac{\langle z_1, s_j f_j \rangle_K}{\|z_1\|_K} \geq \frac{\langle z_2, s_j f_j \rangle_K}{\|z_2\|_K}.$$  

(A.6)

By (A.6), for each $j \in \mathbb{N}$, we have

$$\frac{\langle z_1, s_j f_j \rangle_K}{\|z_1\|_K} \geq \frac{\langle z_2, s_j f_j \rangle_K}{\|z_2\|_K}.$$ 

Then, we have

$$\sum_{j=1}^\infty \frac{\langle z_1, s_j f_j \rangle_K}{\|z_1\|_K} \geq \sum_{j=1}^\infty \frac{\langle z_2, s_j f_j \rangle_K}{\|z_2\|_K} \iff \langle z_1, z_2 \rangle_K \geq \|z_1\|_K \|z_2\|_K.$$ 

This contradicts the equality condition of the Cauchy-Schwarz inequality and the assumption of $z_1$ and $z_2$. 

Proof of $\mu_K \in \mathcal{M}$

Lemma A.3. If $K(\cdot, \cdot)$ is uniformly continuous on $\Omega \times \Omega$ and bounded, for any Borel probability measure $\mu$ and $\mu_K$, which is the embedding of $\mu$, there exists $\{x_i\}_{i=1}^\infty \subset \Omega$ such that

$$\mu_K \in \text{conv}\{K(x_i, \cdot)\}_{i=1}^\infty,$$

where closure is considered with respect to $\| \cdot \|_K$.

Proof. Let $\{X_i\}_{i=1}^\infty$ be a sequence of r.v. i.i.d which satisfies $X_i \sim \mu$ (i = 1, 2, ...). By law of large numbers, for any $y \in \Omega$, the following holds true:

$$\lim_{n \to \infty} \sum_{i=1}^n \frac{1}{n} K(X_i, y) \to \int_\Omega K(x, y) \mu(dx)$$  

(A.7)

with a probability of 1. Because $\mathbb{R}^d$ is separable, we can take $\{y_i\}_{i=1}^\infty \subset \Omega$, which is dense in $\Omega$. In addition, because an intersection of the countable sets of measure 1 is measure 1, from (A.7), there exists $\{x_i\}_{i=1}^\infty \subset \Omega$ such that

$$\lim_{n \to \infty} \sum_{i=1}^n \frac{1}{n} K(x_i, y_j) \to \int_\Omega K(x, y_j) \mu(dx)$$  

(A.8)

for any $y_j \in \{y_i\}_{i=1}^\infty$. By the assumption, $K$ is uniformly continuous in $\Omega \times \Omega$. Thus, for any $\epsilon > 0$, there exists $\delta > 0$ such that if $\|x_1, y_1) - (x_2, y_2)\| < \delta$, then $|K(x_1, y_1) - K(x_2, y_2)| < \epsilon$. In addition, for any $y \in \Omega$ and $\delta > 0$, there exists $y_j \in \{y_i\}_{i=1}^\infty$ such that $|y - y_j| < \delta$. Therefore, for any $\epsilon > 0$ and $y \in \Omega$, we take $y_j$ such that $|y - y_j| < \delta$ and the following is valid:

$$\left| \sum_{i=1}^n \frac{1}{n} K(x_i, y_j) - \sum_{i=1}^n \frac{1}{n} K(x_i, y) - \left( \int_\Omega K(x, y_j) \mu(dx) - \int_\Omega K(x, y) \mu(dx) \right) \right| < 2\epsilon.$$
By (A.8), we let \( n \to \infty \) and

\[
\lim_{n \to \infty} \left| \sum_{i=1}^{n} \frac{1}{n} K(x_i, y_j) - \int_{\Omega} K(x, y_j) \mu(dx) \right| < 2\epsilon.
\]

for any \( \epsilon > 0 \). This means that for each \( y \in \Omega \),

\[
\lim_{n \to \infty} \left\langle \sum_{i=1}^{n} \frac{1}{n} K(x_i, \cdot), K(y, \cdot) \right\rangle \to \left\langle K(y, \cdot), \mu_K \right\rangle.
\]

Because the subspace of \( \mathcal{H}_K \) spanned by \( \{K(y, \cdot) : y \in \Omega\} \) is dense in \( \mathcal{H}_K \), \( \mu_K \in \text{conv}(\{K(x_i, \cdot)\}_{i=1}^{\infty}) \).

\[\square\]

### B Supplement of numerical experiments

The conditions for the numerical experiments in Section 4 are as follows:

**Figure 4** The candidate points are in equally spaced grid in \( \Omega \); a total of 6400 \( (d = 2) \) and 8000 \( (d = 3) \) candidate points were used. For (a), (b), (d), and (e), the parameters of Algorithm 4 are \( \delta = 10^{-4}, K_{\text{max}} = 20, T = 35 \ (d = 2), \delta = 10^{-4}, K_{\text{max}} = 20, T = 25 \ (d = 3) \) and those of Algorithm 5 are \( \delta = 0, K_{\text{max}} = 20, T = 15 \ (d = 2), \delta = 0, K_{\text{max}} = 20, T = 16 \ (d = 3) \). For (c), (f), most of the parameters are the same, but there are some differences. We set the parameters in Algorithm 4 as \( T = 28 \ (d = 2), T = 18 \ (d = 3) \) and those in Algorithm 5 as \( T = 12 \ (d = 2), T = 12 \ (d = 3) \). Because the computational time slightly varies in each experiment, we take an average of 10 computations.

**Figure 5** The kernel is \( K(x, y) = \frac{\delta}{3} - \|x - y\| \). \( \Omega \) is a unit sphere centered at the origin in \( \mathbb{R}^3 \) and the probability distribution is a uniform distribution. The parameters of Algorithm 4 are \( \delta = 10^{-4}, K_{\text{max}} = 10, T = 20 \) and those of Algorithm 5 are \( \delta = 0, K_{\text{max}} = 10, T = 20 \).