Bayesian Optimization over Sets

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Abstract

We propose a Bayesian optimization method over sets, to minimize a black-box function that can take a set as single input. Because set inputs are permutation-invariant and variable-length, traditional Gaussian process-based Bayesian optimization strategies which assume vector inputs can fall short. To address this, we develop a Bayesian optimization method with set kernel that is used to build surrogate functions. This kernel accumulates similarity over set elements to enforce permutation-invariance and permit sets of variable size, but this comes at a greater computational cost. To reduce this burden, we propose a more efficient probabilistic approximation which we prove is still positive definite and is an unbiased estimator of the true set kernel. Finally, we present several numerical experiments which demonstrate that our method outperforms other methods in various applications.

1 Introduction

Bayesian optimization (BO) is an effective method to optimize a black-box function which is expensive to evaluate. It has proven useful in several applications, including hyperparameter optimization [27,17], neural architecture search [29,18], material design [8], and synthetic gene design [13]. Classic BO assumes that a search region \( X \subset \mathbb{R}^d \) is defined and that the black-box function \( f \) can only produce scalar output in the presence of additive noise \( \epsilon \), i.e., \( y = f(x) + \epsilon \) for \( x \in X \).

Unlike this standard BO formulation, in this article we assume that our search region is \( X_{\text{set}} = \{\{x_1, \ldots, x_m\} \mid x_i \in \mathbb{R}^d\} \) for a fixed positive integer \( m \). Thus, for \( X \in X_{\text{set}} \), \( f \) would take in a set containing \( m \) elements, all of length \( d \), and return a noisy function value \( y \):

\[
y = f(X) + \epsilon. \tag{1}
\]

Our motivating example comes from the soft \( k \)-means clustering algorithm over a dataset \( \mathcal{P} = \{p_1, \ldots, p_N\} \); in particular, we want to find the optimal initialization of such an algorithm. The objective function for this problem is a squared loss function which takes in the cluster initialization points \( \{x_1, \ldots, x_k\} \) and returns the weighted distance between the points in \( \mathcal{P} \) and the converged cluster centers \( \{c_1, \ldots, c_k\} \). See [19] for more details.

Some previous research has tried to build Gaussian process (GP) models on set data. [10] proposes a method over discrete sets using stationary kernels over the first Wasserstein distance between two sets, though the power set of fixed discrete sets as domain space is not our interest. However, this method needs the complexity \( \mathcal{O}(n^2m^3d) \), to compute a covariance matrix with respect to \( n \) sets.

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Moreover, because it only considers stationary kernels, GP regression is restricted to the form that cannot express non-stationary models [22]. More detailed explanations can be found in Section 2.3. Therefore, we instead adapt and augment a strategy proposed by [11] involving the creation of a specific \textit{set kernel}. This set kernel uses a kernel defined on the elements $x \in \mathbb{R}^d$ of the sets to build up its own sense of covariance between sets. In turn, then, it can be directly used to build surrogate functions through GP regression, which then can power BO, by Lemma 1.

A key contribution of this article is the development of a computationally efficient approximation to this set kernel. Given $n$ total observed function values, the cost of constructing the matrix required for fitting the GP is $O(n^2m^2d)$ where $m \geq n$ approximately (see the complexity analysis in Section 3.3). We propose the use of random subsampling to reduce the computational cost to $O(n^2L^2d)$ for $L < m$ while still producing an unbiased estimate of the expected value of the true kernel.

We summarize our contributions as follows.

- We propose Bayesian optimization over sets, using a set kernel to define covariance for our Gaussian process-based surrogate function.
- We produce a novel estimator of the set kernel, prove key properties about the bias and variance of this estimator, and analyze its superior computational efficiency relative to the true set kernel.
- We empirically show our estimator retains the necessary theoretical properties enjoyed by the original kernel to effectively perform in our application.

2 Background

In this section, we introduce ideas and notations necessary to understand BO, as well as the notations and previous research on kernels for sets.

2.1 Bayesian Optimization

BO seeks to minimize an unknown function $f$ which is expensive to evaluate:

$$x^* = \arg \min_{x \in \mathcal{X}} f(x) \tag{2}$$

where $\mathcal{X} \subset \mathbb{R}^d$ is a compact space. It is a sequential optimization strategy which, at each iteration, performs the following three computations:

1. Using the $n$ pieces of data presently available, $\{(x_i, y_i)\}$ for $1 \leq i \leq n$, build a probabilistic surrogate model $s_n$, meant to approximate $f$.
2. Using the surrogate model, compute an acquisition function $a_n$, which represents the utility of next acquiring data at some new point $x$.
3. Observe $y_{n+1}$ from a true function $f$ at the location $x_{n+1} = \arg \max_{x \in \mathcal{X}} a_n(x)$.

After exhausting a predefined observation budget $T$, BO returns the best point $x^*$ that has the minimum observation. The benefit of this process is that the optimization of the expensive function $f$ has been replaced by the optimization of much cheaper and more well-understood acquisition functions $a_n$.

In this paper, we use GP regression [24] to produce the surrogate function $s_n$; from $s_n$, we use the standard acquisition function expected improvement [20]:

$$a_n(x) = \mathbb{E}[(y_n^\dagger - s_n(x))]_+,$$

where $y_n^\dagger = \min_{1 \leq i \leq n} y_i$. See [2, 26, 7] for further details on BO.

2.2 Set Kernel

We start by introducing notation which is required for performing kernel approximation of functions on set data. A set of $m$ vectors is denoted $\mathbf{X} = \{x_1, \ldots, x_m\}$. In a collection of $n$ such sets (as will
occur in the BO setting), the $k$th set would be denoted $\mathbf{X}^{(k)} = \{x^{(k)}_1, \ldots, x^{(k)}_m\}$. Note that we are restricting all sets to be of the same size $|\mathbf{X}^{(k)}| = m$ here.

To build a GP surrogate, we require a prior belief of the covariance between elements in $\mathcal{X}_{\text{set}} = \{\{x_1, \ldots, x_m\} | x_i \in \mathbb{R}^d\}$. This belief is imposed in the form of a positive-definite covariance kernel $k_{\text{set}} : \mathcal{X}_{\text{set}} \times \mathcal{X}_{\text{set}} \rightarrow \mathbb{R}$; see [25, 5] for more discussion on approximation with kernels. In addition to the symmetry $k_{\text{set}}(\mathbf{X}^{(i)}, \mathbf{X}^{(j)}) = k_{\text{set}}(\mathbf{X}^{(j)}, \mathbf{X}^{(i)})$ required in standard kernel settings, kernels on sets require an additional property. The ordering of elements in $\mathbf{X}$ should be immaterial (since sets have no inherent ordering).

Given an empirical approximation of the kernel mean $\mu_{\mathbf{X}} \approx |\mathbf{X}|^{-1} \sum_{i=1}^{|\mathbf{X}|} \phi(x_i)$ where $\phi(\cdot)$ is a basis function $\mathbb{R}^d \rightarrow \mathbb{R}$ and $d'$ is a dimension of projected space by $\phi$, a set kernel [11, 21] is defined as

$$k_{\text{set}}(\mathbf{X}^{(1)}, \mathbf{X}^{(2)}) = \langle \mu_{\mathbf{X}^{(1)}}, \mu_{\mathbf{X}^{(2)}} \rangle = \frac{1}{|\mathbf{X}^{(1)}||\mathbf{X}^{(2)}|} \sum_{i=1}^{|\mathbf{X}^{(1)}|} \sum_{j=1}^{|\mathbf{X}^{(2)}|} k(x^{(1)}_i, x^{(2)}_j)$$

(3)

since $k(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle = \phi(x_i)^T \phi(x_j)$. Here, $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is a positive-definite kernel defined to measure the covariance between the $d$-dimensional elements of the sets (e.g., a squared exponential or Matérn kernel).

The kernel [3] arises when comparing a class of functions on different probability measures with the intent of understanding if the measures might be equal [14].

2.3 Related Works

Although it has been raised in different interests, meta-learning approaches dealt with set inputs are promising in machine learning community, because they can generalize distinct tasks with meta-learners [4, 28, 6, 9]. In particular, [4, 28, 9] propose feed-forward neural networks which take permutation-invariant and variable-length inputs: they have the goal of obtaining features derived from the sets with which to input to a standard (meta-)learning routine. Because they consider modeling of set data, they are related to our work, but they are interested in their own specific examples such as point cloud classification, few-shot learning, and image completion.

In BO, [10] suggests a method to find a set that produces a global minimum with respect to discrete sets, each of which is an element of power set of entire set. Because the time complexity of the first Wasserstein distance is $O(n^2 m^3 d)$, they assume a small cardinality of sets and discrete searching space for global optimization method. Furthermore, their method restricts the number of iterations

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1 In principle, sets of varying size can be considered, but we make the restriction to same sized sets to simplify our analysis.
for optimizing an acquisition function, since by the curse of dimensionality the number of iterations should be increased exponentially. However, it implies that the global solution of acquisition function is hard to be found.

Compared to [10], we consider continuous domain space which implies an acquired set can be composed of any instances in a compact space \( \mathcal{X} \). We thus freely use off-the-shelf global optimization method or multi-started local optimization method [26] with relatively large number of instances in sets. In addition, its structure of kernel is \( k_{st}(d(X^{(1)}, X^{(2)})) \) where \( k_{st}(\cdot) \) is a stationary kernel [12] and \( d(\cdot, \cdot) \) is some distance function over two sets (e.g., in [10] the first Wasserstein distance). Using the method proposed in the subsequent section, non-stationary kernels might be considered in modeling a surrogate function.

3 Proposed Method

We first propose and analyze an approximation to the set kernel (3) for GP regression in this section. Then, we present our BO method over sets.

In order for (3) to be a viable covariance kernel of a GP regression, it must be positive-definite. To discuss this topic, we denote a list of \( n \) sets with the notation \( \mathcal{X} = [X^{(1)}, \ldots, X^{(n)}] \in \mathcal{X}^n \); in this notation, the order of the entries matters.

**Lemma 1.** Suppose we have a list \( \mathcal{X} \) which contains distinct sets \( X^{(i)} \) for \( 1 \leq i \leq n \). We define the matrix \( K \in \mathbb{R}^{n \times n} \) as

\[
(K)_{ij} = k_{set}(X^{(i)}, X^{(j)}),
\]

for \( k_{set} \) defined with a chosen inner kernel \( k \) as in (3). Then, \( K \) is a symmetric positive-semidefinite matrix if \( k \) is a symmetric positive-definite kernel.

This proof appears in [16] Lemma 1], and is also discussed in [11].

3.1 Approximation of the Set Kernel

Computing (4) requires pairwise comparisons between all sets present in \( \mathcal{X} \), which has computational complexity \( \mathcal{O}(n^2 m^2 d) \). To alleviate this cost, we propose to approximate (3) with

\[
\tilde{k}_{set}(X^{(1)}, X^{(2)}; \pi, w, L) = k_{set}(\tilde{X}^{(1)}, \tilde{X}^{(2)})
\]

(5)

where \( \pi : [1, \ldots, m] \to [1, \ldots, m] \), \( w \in \mathbb{R}^d \) and \( L \in \mathbb{Z}_+ \) and \( \tilde{X}^{(i)} \) is a subset of \( X^{(i)} \) which is defined by those three quantities (we omit explicitly listing them in \( \tilde{X}^{(i)} \) to ease the notation).

The goal of the approximation strategy is to convert from \( X^{(i)} \) (of size \( m \)) to \( \tilde{X}^{(i)} \) (of size \( L \)) in a consistent fashion during all the \( k_{set} \) computations comprising \( K \). We accomplish this in two steps:

1. Use a randomly generated vector \( w \) to impose an (arbitrary) ordering of the elements of all sets \( X^{(i)} \), and
2. Randomly permute the indices \( [1, \ldots, m] \) via a function \( \pi \).

These random strategies are defined once before computing the \( K \) matrix, and then used consistently throughout the entire computation.

To impose an ordering of the elements, we use a random scalar projection \( w \in \mathbb{R}^d \) such that the elements of \( w \) are drawn from the standard normal distribution. If the scalar projections of each \( x_i \) are computed, this produces the set of scalar values \( \{ w^\top x_1, \ldots, w^\top x_m \} \), which can be sorted to generate an ordered list of

\[
[\ell_1, \ldots, \ell_m], \quad w^\top x_{\ell_1} \leq \ldots \leq w^\top x_{\ell_m},
\]

(6)

for an ordering of distinct indices \( \ell_1, \ldots, \ell_m \in [1, \ldots, m] \). Ties between \( w^\top x_i \) values can be dealt with arbitrarily.

The function \( \pi \) then is simply a random bijection of the integers \( [1, \ldots, m] \) onto themselves. Using this, we can sample \( L \) vectors from \( X^{(i)} \):

\[
\tilde{X}^{(i)} = \{ x_{\ell_j} \mid \ell_j = \pi(j) \text{ for } 1 \leq j \leq L \}.
\]

(7)

This process, given \( w \), \( \pi \) and \( L \) is sufficient for computing \( k_{set} \).
Algorithm 1 Forforming the K approximation to K

Input: A list of sets \( X = [X^{(1)}, \ldots, X^{(n)}], L \in \mathbb{Z}_+ \).

Output: A matrix \( \tilde{K} \).

1: Draw a random vector \( w \) from \( \mathcal{N}(0, I_d) \).
2: Create a random permutation of the integers \([1, \ldots, m]\) with which to define \( \pi \).
3: Using \( w \), assign the ordering of elements in \( X^{(i)} \) according to (6).
4: Using \( \pi \), determine the subsets \( X^{(i)} \) as selected according to (7).
5: Using these subsets and (5), populate the matrix with values \((\tilde{K})_{ij} = \tilde{k}_{set}(X^{(i)}, X^{(j)}; w, \pi, L)\).

3.2 Properties of the Approximation

The covariance matrix for this approximation of the set kernel, which we denote by \((\tilde{K})_{ij} = \tilde{k}_{set}(X^{(i)}, X^{(j)}; w, \pi, L)\), should approximate the full version of covariance matrix, \( K \) from (4).

Because of the random structure introduced in Section 3.1, the matrix \( \tilde{K} \) will be random. This will be addressed in Theorem 1 but for now, \( \tilde{K} \) represents a single realization of that random variable, not the random variable itself. To be viable, this approximation must satisfy the following requirements:

Property 1. The approximation satisfies pairwise symmetry:

\[
\tilde{k}_{set}(X^{(i)}, X^{(j)}; w, \pi, L) = \tilde{k}_{set}(X^{(j)}, X^{(i)}; w, \pi, L). \tag{8}
\]

Because \( \tilde{X}^{(i)} \) is uniquely defined given \( w, \pi, L \), this simplifies to \( \tilde{k}_{set}(\tilde{X}^{(i)}, \tilde{X}^{(j)}) = \tilde{k}_{set}(\tilde{X}^{(j)}, \tilde{X}^{(i)}) \), which is true because \( \tilde{k}_{set} \) is symmetric.

Property 2. The “ordering” of the elements in the sets \( X^{(i)}, X^{(j)} \) should not matter when computing \( \tilde{k}_{set} \). Indeed, because (6) enforces ordering based on \( w \) and not whatever arbitrary indexing is imposed in defining the elements of the set, the kernel will be permutation invariant.

Property 3. The kernel approximation (5) reduces to computing \( k_{set} \) on a lower cardinality version of the data (with \( L \) elements selected from \( m \)). Because \( k_{set} \) is positive-definite on these \( L \)-element sets, we know that \( \tilde{k}_{set} \) is also positive-definite.

Property 4. Since the approximation method aims to choose subsets of input sets, the computational cost becomes lower than the original formulation.

Missing from these four properties is a statement regarding the quality of the approximation. We address this in Theorem 1, though we first start by stating Lemma 1. Moreover, using Theorem 1, we can also obtain the variance of our estimate, as shown in Theorem 2.

Lemma 2. Suppose there are two sets \( X, Y \in \mathcal{X}_{set} \). Without loss of generality, let \( X^{(i)} \) and \( Y^{(j)} \) denote the \( i \)th and \( j \)th of \( \binom{m}{L} \) possible subsets containing \( L \) elements of \( X \) and \( Y \), respectively, in an arbitrary ordering. For \( 1 \leq L \leq m \),

\[
\sum_{i=1}^{\binom{m}{L}} \sum_{j=1}^{\binom{m}{L}} \sum_{a=1}^{L} \sum_{b=1}^{L} k(x^{(i)}_a, y^{(j)}_b) = \frac{L^2 \binom{m}{L}^2}{m^2} \sum_{c=1}^{m} \sum_{d=1}^{m} k(x_c, y_d), \tag{9}
\]

where \( x^{(i)}_a \) and \( y^{(j)}_b \) are the \( a \)th and \( b \)th elements of \( X^{(i)} \) and \( Y^{(j)} \), respectively, in an arbitrary ordering.

Theorem 1. Suppose that we are given two sets \( X, Y \in \mathcal{X}_{set} \) and \( L \in \mathbb{Z}_+ \). Suppose, furthermore, that \( w \) and \( \pi \) can be generated randomly as defined in Section 3.1 to form subsets \( \tilde{X} \) and \( \tilde{Y} \). The value of \( \tilde{k}_{set}(X, Y; w, \pi, L) \) is an unbiased estimator of the value of \( k_{set}(X, Y) \).

Theorem 2. Suppose the same conditions as in Theorem 1. Suppose, furthermore, that \( k(x, x') \geq 0 \) for all \( x, x' \in \mathcal{X} \). The variance of \( \tilde{k}_{set}(X, Y; w, \pi, L) \) is bounded by a function of \( m, L \) and \( k_{set}(X, Y) \):

\[
\text{Var} \left[ \tilde{k}_{set}(X, Y; w, \pi, L) \right] \leq \left( \frac{m^4}{L^4} - 1 \right) k_{set}(X, Y)^2. \tag{10}
\]

Proof. To accommodate the page limit, the proofs of Lemma 2, Theorem 1 and Theorem 2 are provided in the supplementary material. \( \square \)
Algorithm 2 Bayesian Optimization over Sets

**Input:** A domain \( \mathcal{X}_{\text{set}} \), a function \( f : \mathcal{X}_{\text{set}} \rightarrow \mathbb{R} \), a budget \( T \in \mathbb{Z}_+ \).

**Output:** Best acquired set \( X^\dagger \)

1: Choose an initial point \( X^{(1)} \) randomly from \( \mathcal{X}_{\text{set}} \) and evaluate \( y_1 = f(X^{(1)}) + \epsilon_1 \).
2: for \( k \) from 1 to \( T - 1 \) do
3: Fit the surrogate model \( s_k \) to all available data \( \{(X^{(i)}, y_i)\}_{i=1}^k \).
4: Compute the acquisition function \( a_k \) from \( s_k \).
5: Identify \( X^{(k+1)} = \arg \max_{X \in \mathcal{X}_{\text{set}}} a_k(X) \).
6: Evaluate \( y_{k+1} = f(X^{(k+1)}) + \epsilon_k \).
7: end for
8: return \( X^\dagger = X^{(i)} \) if \( y_i = \max_{1 \leq j \leq T} y_j \).

By Theorem \([2]\) we can naturally infer the fact that the upper bound of the variance is small, if \( L \) is close to \( m \). This result is confirmed in Section \([4.1]\).

### 3.3 Bayesian Optimization over Sets

For BO over \( \mathcal{X}_{\text{set}} \), the goal is to identify the set \( X \in \mathcal{X}_{\text{set}} \) such that a given function \( f : \mathcal{X}_{\text{set}} \rightarrow \mathbb{R} \) is minimized. As shown in Algorithm \([2]\), BO over sets follows similar steps as laid out in Section \([2.1]\) except that it involves the space of set inputs and requires a surrogate function on \( \mathcal{X}_{\text{set}} \). As we have already indicated, we plan to use a GP surrogate function, with prior covariance defined either with \([5]\) or \([5]\) and a Matérn 5/2 inner kernel \( k \).

Using a GP model requires computation on the order of \( \mathcal{O}(n^3) \) at the \( n \)th step of the BO because the \( K \) matrix must be inverted. Compared to the complexity for computing a full version of the set kernel \( \mathcal{O}(n^2m^2d) \), the complexity of computing the inverse is smaller if roughly \( m \geq n \) (that is, computing the matrix can be as costly or more costly than inverting it). Because BO is efficient sampling-based global optimization, \( n \) is small and the situation \( m \geq n \) is reasonable. Therefore, the reduction proposed by the approximation in Section \([5.1]\) can be effective in reducing complexity of all steps for BO over sets.

In addition, since the Cholesky decomposition, instead of matrix inverse is widely used to compute posterior mean and variance functions \([24]\), the time complexity for inverting a covariance matrix can be reduced. But still, if \( m \) is relatively large, our approximation is effective. In this paper, we compute GP surrogate using the Cholesky decomposition. See the effects of \( L \) in Section \([4]\).

### 4 Experiments

In this section, we present various experiments to show our method can be employed in the applications. Before showing those examples, we describe the baseline methods:

**Vector** A standard BO is performed over a \( md \)-dimensional space where, at the \( n \)th step, the available data \( X_n \in \mathcal{X}_{\text{set}}^n \) is vectorized to \([x_1, \ldots, x_n]\) for \( x_i \in \mathbb{R}^{md} \) with associated function values. At each step, the vectorized next location \( x_{n+1} \) is converted into a set \( X_{n+1} \).

**Split** Individual BO strategies are executed on the \( m \) components comprising \( X \). At the \( n \)th step, the available data \( X_n \in \mathcal{X}_{\text{set}}^n \) is decomposed into \( m \) sets of data, the \( i \)th of which consists of \([x_1^{(i)}, \ldots, x_n^{(i)}]\) with associated data. The \( m \) vectors produced during each step of the optimization are then collected to form \( X_{n+1} \) at which to evaluate \( f \).

All codes and scripts used to implement our methods will be released as open source software. The full implementation details are provided in the supplementary material.
While not our concern here, it is possible that some amount of distance between points in the set $X$ would be desired. If that were the case, such a desire could be enforced in the function $f$.  

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Figure 3: Results on two synthetic functions. First three columns depict one of the best acquisition examples (i.e., purple stars indicate instances in the acquired set) via three methods: (i) Vector, (ii) Split, and (iii) Ours (w/o approximation). The last column plots minimum function value over iterations. For Synthetic 1 (first row) and Synthetic 2 (second row), $m = 20$. All experiments are repeated 10 times. Because the experiments with approximation show similar results with the one without approximation, we omit those acquisition examples.

4.1 Set Kernel Approximation

We study the effect of $L$ for the set kernels introduced in Section 3.1. Using a set generated from standard normal distribution, which has 1,000 50-dimensional instances, we observe the effects of $L$ as shown in Figure 2. $k_{set}$ converges to the value (see the supplementary material for the exact values) as $L$ is increased, and the variance of $k_{set}$ value is large when $L$ is small, as discussed in Section 3.2. Moreover, the consumed time is increased as $L$ is increased. We present the detailed results in the supplementary material.

4.2 Synthetic Functions

We test two synthetic circumstances to show BO over sets is a valid approach to find an optimal set that minimizes an objective function $f : \mathcal{X}_{set} \rightarrow \mathbb{R}$. In each setting, there is an auxiliary function $g : \mathcal{X} \rightarrow \mathbb{R}$, and the function $f$ is defined as

$$f(X) = \frac{1}{m} \sum_{i=1}^{m} g(x_i).$$

(11)

The $g$ functions (see the supplementary material) are designed to be multimodal, giving the opportunity for the set $X$ to contain $x_i$ values from each of the modes in the domain. Additionally, as is expected, $f$ is permutation invariant (any ordering imposed on the elements of $x$ is immaterial).

**Synthetic 1** We consider $d = 1$, $m = 20$ and choose $g$ to be a simple periodic function.

**Synthetic 2** The function $g$ is the summation of probability density functions, where $d = 2$, $m = 20$. As shown in Figure 3, both of these circumstances have a clear multimodal structure, allowing for optimal sets to contain points which are clustered in a single local minima or to be spread out through the domain in several local minima. The first three columns of Figure 3 show that the “Vector” and “Split” strategies have difficulty optimizing functions in both circumstances. On the other hand, our proposed method finds optimal outcomes more effectively.
We study the impact of $L$ when optimizing these two synthetic functions; a smaller $L$ should yield faster computations, but also a worse approximation $K$ to the true $K$ matrix (when $L = m$). Due to the page limit, we present these results in Table 2 located in the supplementary material. The convergence performance does scale as expected, and the computational cost is hurt by the order of the complexities. As we mentioned in Section 3.3, there exists a situation that the complexity for inverting a covariance matrix can be larger than the complexity for computing the covariance matrix.

4.3 Initialization of Clustering Methods

We initialize two clustering methods for dataset $\mathcal{P} = [p_1, \ldots, p_N]$ with BO over sets: (i) $k$-means clustering, and (ii) Gaussian mixture model (GMM). For these experiments, we add four additional baselines for clustering algorithms (see the supplementary material for the additional baselines). To fit a dataset with those four baselines, we use the whole dataset without splitting.

For two clustering algorithms, we generate a dataset where $N = 500$, $d = 5$, and $k = 10$. We split the dataset to training (70%) and test (30%) datasets. In BO settings, after finding the converged cluster centers $\{c_1, \ldots, c_k\}$ with training dataset, the adjusted Rand index (ARI) is computed by test dataset. The algorithms are optimized over $1 - \text{ARI}$. All clustering models are implemented using scikit-learn [23].

The function of interest in the $k$-means clustering setting is the converged clustering residual

$$k\text{-means}\left(\{x_1, \ldots, x_k\}\right) = \sum_{i=1}^{N} \sum_{j=1}^{k} w_{ij} \|p_i - c_j\|^2,$$  \hspace{1cm} (12)

where $\{x_1, \ldots, x_k\}$ is the set of proposed initial cluster centers, $\{c_1, \ldots, c_k\}$ is the set of converged cluster centers [19], and $w_{ij}$ are softmax values from the pairwise distances. Here, the fact that $c_j$ is a function of $X$ and $P$ is omitted for notational simplicity. The set of converged cluster centers is determined through an iterative strategy which is highly dependent on the initial points $X$ to converge to effective centers. As shown in Figure 4(a), our method with $L = 1$ shows the best performance compared to other baselines.

In contrast to $k$-means clustering, the GMM estimates parameters of Gaussian distributions and mixing parameters between the distributions. Because it is difficult to minimize negative log-likelihood of the observed data, we fit the GMM using expectation-maximization (EM) algorithm [3]. Similarly to $k$-means clustering, this requires initial guesses $X$ to converge to cluster centers $\{c_1, \ldots, c_k\}$.

As shown in Figure 4(b) we conduct the experiments to initialize the mixture of Gaussians. Our method shows better performance than other baselines except the “Vector” baseline. Because the “Vector” baseline finds an optimal set under the assumption that we know the structure of sets, it does not directly match to the problem interested in this work, though it can be considered as the baseline.

The computational cost in these experiments is presented as a function of $L$ (see the table in the corresponding section of the supplementary material). Because $d$ in this problem is larger than Section 4.2, the computational cost follows our expectation, which implies that the complexity for computing a covariance matrix over sets is the major computations in the overall procedure.

5 Conclusion

In this paper, we propose the BO method over sets, which takes a set as an input and produces a scalar output. Our method based on GP regression models a surrogate function using set-taking covariance functions, referred to as set kernel. We approximate the set kernel to the efficient positive-definite kernel that is an unbiased estimator of the original set kernel. Our experimental results demonstrate our method can be used in some novel applications for BO.
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Supplementary Material: Bayesian Optimization over Sets

S.A Proof of Lemma

**Proof.** We can rewrite the original summation in a slightly more convoluted form, as

\[
\sum_{i=1}^{m} \sum_{j=1}^{L} \sum_{a=1}^{L} \sum_{b=1}^{L} k(\tilde{x}_a^{(i)}, \tilde{y}_b^{(j)}) = \sum_{i=1}^{m} \sum_{j=1}^{L} \sum_{a=1}^{L} \sum_{b=1}^{L} k(\tilde{x}_a^{(i)}, \tilde{y}_b^{(j)}) \bar{I}_{\tilde{x}_a^{(i)}, \tilde{y}_b^{(j)}}(x_c, y_d),
\]

where \( \bar{I}_{\tilde{x}_a^{(i)}, \tilde{y}_b^{(j)}}(x_c, y_d) = 1 \) if \( \tilde{x}_a^{(i)} = x_c \) and \( \tilde{y}_b^{(j)} = y_d \), and 0 otherwise. As these are finite summations, they can be safely reordered.

The symmetry in the structure and evaluation of the summation implies that as each \( x_c \) quantity will be paired with each \( y_d \) quantity the same number of times. Therefore, we need only consider the number of times that these quantities appear.

We recognize that this summation follows a pattern related to Pascal’s triangle. Among the \( \binom{m}{L} \) possible subsets \( \tilde{x} \) of \( \mathbf{X} \), only the fraction \( L/m \) of these contain the quantity \( x_c \), for all \( 1 \leq c \leq m \) (irrespective of how that entry may be denoted in \( \tilde{x}_a^{(i)} \) terminology). Because of the symmetry mentioned above, each of those \( x_c \) quantities is paired with each of the \( y_d \) quantities the same \( \frac{L}{m} \binom{m}{L} \) number of times. This result implies that

\[
\sum_{i=1}^{L} \sum_{j=1}^{L} \sum_{a=1}^{L} \sum_{b=1}^{L} k(\tilde{x}_a^{(i)}, \tilde{y}_b^{(j)}) \bar{I}_{\tilde{x}_a^{(i)}, \tilde{y}_b^{(j)}}(x_c, y_d) = \frac{L^2}{m^2} k(x_c, y_d),
\]

where \( \bar{I}_{\tilde{x}_a^{(i)}, \tilde{y}_b^{(j)}}(x_c, y_d) = 1 \) if \( \tilde{x}_a^{(i)} = x_c \) and \( \tilde{y}_b^{(j)} = y_d \), and 0 otherwise. Substituting (s.2) into the bracketed quantity in (s.1) above completes the proof. \( \blacksquare \)

S.B Proofs of Set Kernel Estimator Properties

We start by introducing the notation \( W \) and \( \Pi \) to be random variables such that \( W \sim \mathcal{N}(0, l_x) \) and \( \Pi \) is a uniformly random permutation of the integers between 1 and \( m \). These are the distributions defining the \( w \) and \( \pi \) quantities described above. With this, we note that \( \tilde{k}_{\text{set}}(\mathbf{X}, \mathbf{Y}; W, \Pi, L) \) is a random variable.

We also introduce the notation \( \sigma_L(\mathbf{X}) \) to be the distribution of random subsets of \( \mathbf{X} \) with \( L \) elements selected without replacement, the outcome of the subset selection from Section 3.1. This notation allows us to write the quantities

\[
\mathbb{E}_{W, \Pi}[\tilde{k}_{\text{set}}(\mathbf{X}, \mathbf{Y}; W, \Pi, L)] = \mathbb{E}_{\mathbf{X}, \mathbf{Y}}[k_{\text{set}}(\mathbf{\tilde{X}}, \mathbf{\tilde{Y}})] = \mathbb{E}[k_{\text{set}}(\mathbf{\tilde{X}}, \mathbf{\tilde{Y}})], \quad (s.3)
\]

\[
\text{Var}_{W, \Pi}[\tilde{k}_{\text{set}}(\mathbf{X}, \mathbf{Y}; W, \Pi, L)] = \text{Var}_{\mathbf{X}, \mathbf{Y}}[k_{\text{set}}(\mathbf{\tilde{X}}, \mathbf{\tilde{Y}})] = \text{Var}[k_{\text{set}}(\mathbf{\tilde{X}}, \mathbf{\tilde{Y}})], \quad (s.4)
\]

for \( \mathbf{\tilde{X}} \sim \sigma_L(\mathbf{X}), \mathbf{\tilde{Y}} \sim \sigma_L(\mathbf{Y}) \). We have dropped the random variables from the expectation and variance definitions for ease of notation.

S.B.1 Proof of Theorem

**Proof.** Our goal is to show that \( \mathbb{E}[k_{\text{set}}(\mathbf{\tilde{X}}, \mathbf{\tilde{Y}})] = k_{\text{set}}(\mathbf{X}, \mathbf{Y}) \), where \( \mathbb{E}[k_{\text{set}}(\mathbf{\tilde{X}}, \mathbf{\tilde{Y}})] \) is defined in (s.3).

We first introduce an extreme case: \( L = m \). If \( L = m \), the subsets we are constructing are the full sets, i.e., \( \sigma_m(\mathbf{X}) \) contains only one element, \( \mathbf{X} \). Thus, \( \tilde{k}_{\text{set}}(\mathbf{X}, \mathbf{Y}; W, \Pi, m) = k_{\text{set}}(\mathbf{X}, \mathbf{Y}) \) is not a random variable.
For $1 \leq L < m$, we compute this expected value from the definition (with some abuse of notation):

$$
E[k_{set}(\bar{X}, Y)] = \sum_{X,Y} k_{set}(\bar{X}, Y)p(\bar{X}, Y).
$$

(s.5)

There are $\binom{m}{L}$ subsets, all of which could be indexed (arbitrarily) as $\bar{X}^{(i)}$ for $1 \leq i \leq \binom{m}{L}$. The probability mass function is uniform across all subsets, meaning that $p(\bar{X} = \bar{X}^{(i)}, Y = \bar{Y}^{(j)}) = 1/\binom{m}{L}^2$. Using this, we know

$$
E[k_{set}(\bar{X}, Y)] = \sum_{i=1}^{\binom{m}{L}} \sum_{j=1}^{\binom{m}{L}} k_{set}(\bar{X}^{(i)}, \bar{Y}^{(j)}) \frac{1}{\binom{m}{L}^2}.
$$

(s.6)

We apply (s.6) to see that

$$
k_{set}(\bar{X}^{(i)}, \bar{Y}^{(j)}) = \frac{1}{L^2} \sum_{a=1}^{L} \sum_{b=1}^{L} k(\bar{x}_a^{(i)}, \bar{y}_b^{(j)}),
$$

(s.7)

following the notational conventions used above. The expectation involves four nested summations,

$$
E[k_{set}(\bar{X}, Y)] = \frac{1}{L^2 \binom{m}{L}^2} \sum_{i=1}^{L} \sum_{j=1}^{\binom{m}{L}} \sum_{a=1}^{L} \sum_{b=1}^{L} k(\bar{x}_a^{(i)}, \bar{y}_b^{(j)}).
$$

(s.8)

We utilize Lemma 2 to rewrite this as

$$
E[k_{set}(\bar{X}, Y)] = \frac{1}{L^2 \binom{m}{L}^2} \sum_{i=1}^{\binom{m}{L}} \sum_{j=1}^{\binom{m}{L}} \sum_{c=1}^{m} \sum_{d=1}^{m} k(x_c, y_d) = \frac{1}{m^2} \sum_{c=1}^{m} \sum_{d=1}^{m} k(x_c, y_d).
$$

(s.9)

S.B.2 Proof of Theorem 2

**Proof.** The variance of $k_{set}(\bar{X}, Y)$, defined in (s.4), is computed as

$$
\text{Var} [k_{set}(\bar{X}, Y)] = E \left[ (k_{set}(\bar{X}, Y) - E [k_{set}(\bar{X}, Y)])^2 \right]
$$

$$
= E \left[ k_{set}(\bar{X}, Y)^2 \right] + k_{set}(\bar{X}, Y)^2 - 2k_{set}(\bar{X}, Y)E [k_{set}(\bar{X}, Y)]
$$

$$
= E \left[ k_{set}(\bar{X}, Y)^2 \right] - k_{set}(\bar{X}, Y)^2,
$$

(s.10)

where Theorem 1 is invoked to produce the final line. Using (s.6) and (s.7), we can express the first term of (s.10) as

$$
E \left[ k_{set}(\bar{X}, Y)^2 \right] = \sum_{i=1}^{\binom{m}{L}} \sum_{j=1}^{\binom{m}{L}} \left( \frac{1}{L^2} \sum_{a=1}^{L} \sum_{b=1}^{L} k(\bar{x}_a^{(i)}, \bar{y}_b^{(j)}) \right)^2 \frac{1}{\binom{m}{L}^2}.
$$

(s.11)

At this point, we invoke the fact that $k(x, x') \geq 0$ to state

$$
0 \leq \sum_{a=1}^{L} \sum_{b=1}^{L} k(\bar{x}_a^{(i)}, \bar{y}_b^{(j)}) \leq \sum_{a=1}^{m} \sum_{b=1}^{m} k(x_a, x_b),
$$

(s.12)

which is true because the summation to $m$ terms contains all of the elements in the summation to $L$ terms, as well as other (nonnegative) elements. Using this, we can bound (s.11) by

$$
E \left[ k_{set}(\bar{X}, Y)^2 \right] \leq \sum_{i=1}^{\binom{m}{L}} \sum_{j=1}^{\binom{m}{L}} \left( \frac{1}{m^2} \sum_{a=1}^{m} \sum_{b=1}^{m} k(x_a, x_b) \right)^2 \frac{1}{\binom{m}{L}^2}
$$

$$
= \frac{m^4 \binom{m}{L}^2 L^4 \sum_{i=1}^{\binom{m}{L}} \sum_{j=1}^{\binom{m}{L}} \left( \frac{1}{m^2} \sum_{a=1}^{m} \sum_{b=1}^{m} k(x_a, x_b) \right)^2}
$$

$$
= \frac{m^4 \binom{m}{L}^2 L^4 \binom{m}{L} \frac{1}{L} k_{set}(\bar{X}, Y)^2}
$$

$$
= \frac{m^4}{L^4} k_{set}(\bar{X}, Y)^2.
$$

(s.13)
We define our synthetic functions as

$$\text{Var} \left[ k_{\text{set}}(\bar{X}, \bar{Y}) \right] \leq \frac{m^4}{L^4} k_{\text{set}}(X, Y)^2 - k_{\text{set}}(X, Y)^2 = \left( \frac{m^4}{L^4} - 1 \right) k_{\text{set}}(X, Y)^2$$

(s.14)

which concludes this proof.

The restriction $k(x, x') \geq 0$ is satisfied by many standard covariance kernels (such as the Gaussian, the Matérn family and the multiquadric) as well as some more interesting choices (such as the Wendland or Wu families of compactly supported kernels). It does, however, exclude some oscillatory kernels such as the Poisson kernel as well as kernels defined implicitly which may have an oscillatory behavior. More discussion on different types of kernels and their properties can be found in the kernel literature [5].

S.C Experiments

In this section, we describe the detailed settings, baselines, and results that are not covered in the main article.

We use Gaussian process regression [24] with a set kernel or Matérn 5/2 kernel as a surrogate function. Because computing the inverse of covariance matrix needs heavy computations, we use the Cholesky decomposition instead [24]. For the experiments with set kernel, Matérn 5/2 kernel is used as a base kernel. All Gaussian process regression models are optimized by marginal likelihood maximization decomposition instead [24]. For the experiments with set kernel, Matérn 5/2 kernel is used as a base kernel. All settings follows the settings in Figure 2. The numerical results are rounded to the three decimals, to show the effects precisely.

Table 1: The effects of $L$ for set kernels. All settings follows the settings in Figure 2. The numerical results are rounded to the three decimals, to show the effects precisely.

| $L$   | $k_{\text{set}}$          | Time (sec.) |
|-------|---------------------------|-------------|
| 1     | $1.057 \times 10^{-5}$ $\pm$ $1.387 \times 10^{-6}$ | $2.981 \times 10^{-4}$ |
| 2     | $1.045 \times 10^{-5}$ $\pm$ $4.512 \times 10^{-7}$ | $5.440 \times 10^{-4}$ |
| 5     | $1.019 \times 10^{-5}$ $\pm$ $1.68 \times 10^{-7}$ | $7.332 \times 10^{-4}$ |
| 10    | $1.023 \times 10^{-5}$ $\pm$ $9.98 \times 10^{-8}$ | $1.749 \times 10^{-3}$ |
| 20    | $1.025 \times 10^{-5}$ $\pm$ $9.305 \times 10^{-8}$ | $5.204 \times 10^{-3}$ |
| 50    | $1.028 \times 10^{-5}$ $\pm$ $4.955 \times 10^{-8}$ | $3.036 \times 10^{-2}$ |
| 100   | $1.026 \times 10^{-5}$ $\pm$ $3.030 \times 10^{-8}$ | $1.171 \times 10^{-1}$ |
| 200   | $1.027 \times 10^{-5}$ $\pm$ $1.961 \times 10^{-8}$ | $4.798 \times 10^{-1}$ |
| 500   | $1.027 \times 10^{-5}$ $\pm$ $1.372 \times 10^{-8}$ | $3.021 \times 10^{0}$ |
| 1000(= $m$) | $1.027 \times 10^{-5}$ | $1.217 \times 10^{1}$ |

We use Matérn 5/2 kernel as a base kernel. Table 1 shows the effects of $L$ for set kernels. As we mentioned in the main article, as $L$ is increased, $k_{\text{set}}$ value is converged to the true value and execution time is increased.

S.C.2 Synthetic Functions

We define our synthetic functions as
Table 2: Convergence quality and its execution time on the synthetic functions. All settings follow the settings in Figure 4.

| $L$ | Synthetic 1 | Synthetic 2 |
|-----|-------------|-------------|
|     | Min. function value | Time (10^3 sec.) | Min. function value | Time (10^3 sec.) |
| 1   | $-0.466 \pm 0.194$ | $7.17 \pm 0.38$ | $-0.118 \pm 0.018$ | $6.00 \pm 0.82$ |
| 2   | $-0.579 \pm 0.102$ | $6.78 \pm 0.56$ | $-0.118 \pm 0.018$ | $4.18 \pm 1.37$ |
| 5   | $-0.712 \pm 0.117$ | $6.13 \pm 0.91$ | $-0.126 \pm 0.015$ | $4.50 \pm 0.90$ |
| 10  | $-0.658 \pm 0.054$ | $5.02 \pm 1.22$ | $-0.124 \pm 0.019$ | $4.63 \pm 1.08$ |
| 20(= m) | $-0.764 \pm 0.029$ | $7.72 \pm 0.98$ | $-0.133 \pm 0.013$ | $12.28 \pm 0.17$ |

Table 3: Convergence quality and its execution time on $k$-means clustering and GMM. All settings follow the settings in Figure 4.

| $L$ | $k$-means clustering | Gaussian mixture model |
|-----|----------------------|-----------------------|
|     | 1–ARI Time (10^3 sec.) | 1–ARI Time (10^3 sec.) |
| 1   | $0.0681 \pm 0.0391$ | $0.70 \pm 0.22$ | $0.177 \pm 0.058$ | $1.03 \pm 0.34$ |
| 2   | $0.0907 \pm 0.0396$ | $0.94 \pm 0.21$ | $0.204 \pm 0.074$ | $0.94 \pm 0.36$ |
| 5   | $0.0997 \pm 0.0377$ | $2.29 \pm 0.26$ | $0.203 \pm 0.066$ | $2.44 \pm 0.27$ |
| 10(= m) | $0.0921 \pm 0.0405$ | $6.86 \pm 0.70$ | $0.188 \pm 0.062$ | $8.33 \pm 0.73$ |

**Synthetic 1** We consider $d = 1$, $m = 20$ and a $g$ function which is a simple periodic function

$$g(x) = \sin(2\|x\|_2) + |0.05|\|x\|_2|.$$  \hspace{1cm} (s.15)

**Synthetic 2** We consider $d = 2$, $m = 20$ and a $g$ function which is the summation of probability density functions

$$g(x) = -\sum_{i=1}^{8} p(x; \mu_i, \Sigma_i)$$  \hspace{1cm} (s.16)

where $p$ is the normal density function with $\mu_i$ depicted in Figure 5 and $\Sigma_i = I_2$.

Table 2 represents a convergence quality and its execution time for the synthetic functions defined in this work. Because of the order of the complexities induced from various computations, the results on computational cost are saturated from relatively large $L$ (e.g., $L = 10$). See the main article for the detailed explanations.

**S.C.3 Initialization of Clustering Methods**

The four baselines that are additionally used in initializing clustering methods are defined as below:

- **Random** This baseline randomly draws $k$ points from a compact space $\subset \mathbb{R}^d$.
- **Data** This baseline randomly samples $k$ points from a dataset $\mathcal{P}$. It is widely used in initializing a clustering algorithm.

- **(k-means only) k-means++** \hspace{1cm} (11) This is a method for $k$-means clustering with the intuition that spreading out initial cluster centers is better than the “Data” baseline (see [11] for the details).

- **(GMM only) k-means** This baseline sets initial cluster centers as the results of $k$-means clustering.

Table 3 shows convergence qualities and their execution time on $k$-means clustering algorithm and GMM. Similar to Table 1, the computational cost is increased as $L$ is increased. However, the target values do not show the results we expected. We explain these results in the main article.