
Bounce: Reliable High-Dimensional Bayesian Optimization for Combinatorial and Mixed Spaces

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Abstract

Impactful applications such as materials discovery, hardware design, neural architecture search, or portfolio optimization require optimizing high-dimensional black-box functions with mixed and combinatorial input spaces. While Bayesian optimization has recently made significant progress in solving such problems, an in-depth analysis reveals that the current state-of-the-art methods are not reliable. Their performances degrade substantially when the unknown optima of the function do not have a certain structure. To fill the need for a reliable algorithm for combinatorial and mixed spaces, this paper proposes Bounce that relies on a novel map of various variable types into nested embeddings of increasing dimensionality. Comprehensive experiments show that Bounce reliably achieves and often even improves upon state-of-the-art performance on a variety of high-dimensional problems.

1 Introduction

Bayesian optimization (BO) has become a ‘go-to’ method for optimizing expensive-to-evaluate black-box functions [27, 83] that have numerous important applications, including hyperparameter optimization for machine learning models [9, 27], portfolio optimization in finance [7], chemical engineering and materials discovery [13, 15, 26, 33, 37, 38, 40, 57, 68, 71, 81], hardware design [22, 36, 51], or scheduling problems [42]. These problems are challenging for a variety of reasons. Most importantly, they may expose hundreds of tunable parameters that allow for granular optimization of the underlying design but also lead to high-dimensional optimization tasks and the ‘curses of dimensionality’ [10, 63]. Typical examples are drug design [53, 76] and combinatorial testing [55]. Moreover, real-world applications often have categorical or ordinal tunable parameters, in addition to the real-valued parameters that BO has traditionally focused on [10, 27, 70]. Recent efforts have thus extended BO to combinatorial and mixed spaces. `Casmpolitan` of Wan et al. [79] uses trust regions (TRs) to accommodate high dimensionality, building upon prior work of Eriksson et al. [25] for continuous spaces. `COMBO` of Oh et al. [56] constructs a surrogate model based on a combinatorial graph representation of the function. Recently, Deshwal et al. [21] presented `BODi` that employs a novel type of dictionary-based embedding and showed that it outperforms the prior work. However, the causes for `BODi`’s excellent performance are not yet well-understood and require a closer examination. Moreover, the ability of methods for mixed spaces to scale to higher dimensionalities trails behind BO for continuous domains. In particular, Papenmeier et al. [60] showed that nested embeddings allow BO to handle a thousand input dimensions, thus outperforming vanilla TR-based approaches and raising the question of whether similar performance gains are feasible for combinatorial domains.

In this work, we assess and improve upon the state-of-the-art in combinatorial BO. In particular, we make the following contributions:

1. We conduct an in-depth analysis of two state-of-the-art algorithms for combinatorial BO, COMBO [56] and BODi [21]. The analysis reveals that their performances often degrade considerably when the optimum of the optimization problem does not exhibit a particular structure common for synthetic test problems.
2. We propose Bounce (**B**ayesian **o**ptimization using **i**ncreasingly high-dimensional combinatorial and continuous **e**MBEDDINGS), a novel high-dimensional Bayesian optimization (HDBO) method that effectively optimizes over combinatorial, continuous, and mixed spaces. Bounce leverages parallel function evaluations efficiently and uses nested random embeddings to scale to high-dimensional problems.
3. We provide a comprehensive evaluation on a representative collection of combinatorial, continuous, and mixed-space benchmarks, demonstrating that Bounce is on par with or outperforms state-of-the-art methods.

2 Background and related work

Bayesian optimization. Bayesian optimization aims to find the global optimum $\mathbf{x}^* \in \mathcal{X}$ of a black-box function $f : \mathcal{X} \rightarrow \mathbb{R}$, where \mathcal{X} is the D -dimensional search space or *input space*. Throughout this paper, we consider minimization problems, i.e., we aim to find $\mathbf{x}^* \in \mathcal{X}$ such that $f(\mathbf{x}^*) \leq f(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}$. The search space \mathcal{X} may contain variables of different types: continuous, categorical, and ordinal. We denote the number of continuous variables in \mathcal{X} by n_{cont} and the number of combinatorial variables by $n_{\text{comb}} = n_{\text{cat}} + n_{\text{ord}} = D - n_{\text{cont}}$, where we denote the number of categorical variables by n_{cat} and the number of ordinal variables by n_{ord} .

Combinatorial domains. Extending BO to combinatorial spaces is challenging, for example, because the acquisition function is only defined at discrete locations or the dimensionality of the space grows drastically when using one-hot encoding for categorical variables. Due to its numerous applications, combinatorial BO has received increased attention in recent years. BOCS [6] handles the exponential explosion of combinations by only modeling lower-order interactions of combinatorial variables and imposing a sparse prior on the interaction terms. COMBO [56] models each variable as a graph and uses the graph-Cartesian product to represent the search space. We revisit COMBO’s performance on categorical problems in Appendix D.1. CoCaBo [67] combines multi-armed bandits and BO to allow for optimization in mixed spaces. It uses two separate kernels for continuous and combinatorial variables and proposes a weighted average of a product and a sum kernel to model mixed spaces. Liu and Wang [47] show that certain, possibly combinatorial functions can be modeled by parametric function approximators such as neural networks or random forests. As a general method to optimize the acquisition function with gradient-based methods, Daulton et al. [19] propose probabilistic reparametrization.

High-dimensional continuous spaces. Subspace-based methods are primarily used for continuous spaces. Wang et al. [84] propose REMBO for HDBO in continuous spaces using Gaussian random projection matrices. REMBO suffers from distortions and projections outside the search domains that the corrections of Binois et al. [11, 12] address. The HeSB0 algorithm of Nayebi et al. [52] avoids the need for corrections by using the CountSketch embedding [87]. Alebo of Letham et al. [46] builds upon REMBO, learning suitable corrections of distortions. TuRB0 [25] is a method that operates in the full-dimensional input space \mathcal{X} , relying on trust region (TR) to focus the search on promising regions of the search space. BAXUS of Papenmeier et al. [60] combines the trust region approach of TuRB0 with the random subspace idea of HeSB0. BAXUS uses a novel family of *nested* random subspaces that exhibit better theoretical guarantees than the CountSketch embedding. While BAXUS handled a $1000D$ problem, it only considers continuous problems and cannot leverage parallel function evaluations. GTB0 [35] assumes the existence of an axis-aligned active subspace. The algorithm first identifies “active” variables and optimizes in the full-dimensional space by placing separate strong length scale priors onto active and inactive variables. Another line of recent approaches employs Monte-Carlo tree search (MCTS) to reduce the complexity of the problem. Wang et al. [82] use MCTS to learn a partitioning of the continuous search space to focus the search on promising regions in the search space. Song et al. [74] use a similar approach, but instead of learning promising regions in the search space, they assume an axis-aligned active subspace and use MCTS to select important variables. Linear embeddings and random linear embeddings [14, 46, 52, 60, 84] require little or no training data to construct the embedding but assume a linear subspace.

Algorithm 1 The Bounce algorithm

Input: initial target dimensionality d_{init} , evaluation budget m , batch size B , evaluation budget to input dimensionality m_D , # new bins added per dimension b , number design of experiment (DOE) points n_{init}

Output: optimizer $\mathbf{x}^* \in \arg \min_{\mathbf{x} \in \mathcal{D}} f(\mathbf{x})$.

- 1: $i \leftarrow 0, d \leftarrow d_{\text{init}}$
- 2: $b \leftarrow \text{ADJUSTBINS}(b, d_{\text{init}}, m_D)$ ▷ Section 3
- 3: $m_i \leftarrow \left\lfloor \frac{b \cdot m_D \cdot d_{\text{init}}}{d_{\text{init}} \cdot (1 - (b+1)^{k+1})} \right\rfloor$
- 4: $S \leftarrow \text{INITIALEMMBEDDING}(d_0, n_{\text{cont}}, n_{\text{cat}}, n_{\text{comb}}, n_{\text{bin}})$ ▷ Section 3.1
- 5: $\mathcal{D} \leftarrow \{(z_k, f(S^{-1}(z_k)))\}_{k \in n_{\text{init}}}$ ▷ Sample and evaluate initial points.
- 6: **for** $j = 1, \dots, m$ **do**
- 7: $L_{\text{cont}} \leftarrow 0.8, L_{\text{comb}} \leftarrow \min(40, n_{\text{comb}})$
- 8: **while** $L_{\text{cont}} > L_{\text{min}}^{\text{cont}} \wedge L_{\text{comb}} > L_{\text{min}}^{\text{comb}}$ **do**
- 9: Find B candidates according to Sec. 3.2
- 10: Evaluate f at B and update \mathcal{D} : $\mathcal{D} \leftarrow \mathcal{D} \cup \{(z_k, f(S^{-1}(z_k)))\}_{k \in B}$
- 11: Update L_{cont} and L_{comb} ▷ Section 3
- 12: **if** $d < D$ **then**
- 13: $i \leftarrow i + 1$ ▷ Increase index for target dimensionality.
- 14: $S \leftarrow \text{INCREASEEMBEDDING}(S, b)$ ▷ Section 3.1
- 15: $d \leftarrow \#$ target variables in S
- 16: $m_i \leftarrow \left\lfloor \frac{b \cdot m_D \cdot d}{d_{\text{init}} \cdot (1 - (b+1)^{k+1})} \right\rfloor$
- 17: **else**
- 18: Reset \mathcal{D} by resampling and evaluating new initial points
- 19: Resample S , reset L_{cont} and L_{comb} , $j \leftarrow j + n_{\text{init}}$

Combinatorial high-dimensional domains. These works optimize black-box functions defined over a combinatorial or mixed space with dozens of input variables. Thebelt et al. [77] use a tree-ensemble kernel to model the Gaussian process (GP) prior and derive a formulation of the upper-confidence bound (UCB) that allows it to be optimized globally and to incorporate constraints. RDUCB [88] relies on random additive decompositions of the GP kernel to model the correlation between variables. Casmpolitan [79] follows TuRBO in using TRs to focus the search on promising regions of the search space and uses the Hamming distance to model TRs for combinatorial variables. For mixed spaces, Casmpolitan uses interleaved search and models continuous and categorical variables with two separate TRs. Kim et al. [44] use a random projection matrix to approach combinatorial problems in a continuous embedded subspace. When evaluating a point, their approach projects the continuous candidate point to the high-dimensional search space and then rounds to the next feasible combinatorial solution. Deshwal et al. [20] propose two algorithms for *permutation spaces*, which occur in problems such as compiler optimization [36] and pose special challenges due to the superexponential explosion of solutions. BODi [21] proposes an embedding type based on a dictionary of anchor points in the search space. The pairwise Hamming distances between the point and each anchor point \mathbf{a}_i in the dictionary represent a point in the search space. The anchor points in the dictionary change at each iteration of the algorithm. They are sampled from the search space to cover a wide range of ‘sequencies’, i.e., the number of changes from 0 to 1 (and vice versa) in the binary vector. The authors hypothesize that the diverse sampling procedure leads to BODi’s remarkable performance in combinatorial spaces with up to 60 dimensions. To our knowledge, BODi is the only other method combining embeddings and combinatorial spaces. We show in Section 4.6 that BODi’s reported good performance relies on an artificial structure of the optimizer \mathbf{x}^* and that its performance degrades considerably when this structure is violated.

3 The Bounce algorithm

To overcome the aforementioned challenges in HDBo for real-world applications, we propose Bounce, a new algorithm for continuous, combinatorial, and mixed spaces. Bounce uses a GP [85] surrogate in a lower-dimensional subspace, the *target space*, that is realized by partitioning input variables into ‘bins’, the so-called *target dimensions*. Bounce only bins variables of the same type (categorical, binary, ordinal, and continuous). When selecting new points to evaluate, Bounce sets

all input variables within the same bin to a single value. It thus operates in a subspace of lower dimensionality than the input space and, in particular, maximizes the acquisition function in a subspace of lower dimensionality. Bounce iteratively refines its subspace embedding by splitting bins into smaller bins, allowing for a more granular optimization at the expense of higher dimensionality. Note that by splitting up bins, Bounce asserts that observations taken in earlier subspaces are contained in the current subspace; see Papenmeier et al. [60] for details. Thus, Bounce operates in a series of nested subspaces. It uses a novel TR management to leverage batch parallelism efficiently, improving over the single point acquisition of BAXUS [60].

The nested subspaces. To model the GP in low-dimensional subspaces, Bounce leverages BAXUS’ family of nested random embeddings [60]. In particular, Bounce employs the sparse count-sketch embedding [87] in which each input dimension is assigned to exactly one target dimension. When increasing the target dimensionality, Bounce creates b new bins for every existing bin and re-distributes the input dimensions that had previously been assigned to that bin across the now $b + 1$ bins. Bounce allocates an individual evaluation budget m_i to the current target space \mathcal{X}_i that is proportional to the dimensionality of \mathcal{X}_i . When the budget for the current target space is depleted, and Bounce has not found a better solution, Bounce will increase the dimension of the target space until it reaches the input space of dimensionality D . Let d_{init} denote the dimensionality of the first target space, i.e., the random embedding that Bounce starts with. Then Bounce has to increase the target dimension $\lceil \log_{b+1} D/d_{\text{init}} \rceil =: k$ -times to reach the input dimensionality D . After calculating k , Bounce re-sets the split factor b such that the distance between the predicted final target dimensionality $d_k = d_{\text{init}} \cdot (b + 1)^k$ and the input dimensionality D is minimized: $b = \lfloor \log_k(D/d_{\text{init}}) - 1 \rfloor$, where $\lfloor x \rfloor$ denotes the integer closest to x . This ensures that the predetermined evaluation budget for each subspace will be approximately proportional to its dimensionality. This contrasts to BAXUS [60] that uses a constant split factor b and adjusts the initial target dimensionality d_{init} . The evaluation budget m_i for the i -th subspace \mathcal{X}_i is $m_i := \lfloor \frac{b \cdot m_D \cdot d_i}{d_{\text{init}} \cdot (1 - (b+1)^{k+1})} \rfloor$, where m_D is the budget until D is reached and b is the maximum number of bins added per split.

Trust region management. Bounce follows TuRBO [25] and Casmopolitan [79] in using trust regions (TRs) to efficiently optimize over target spaces of high dimensionality. TRs allow focusing on promising regions of the search space by restricting the next points to evaluate to a region centered at the current best function value [25]. TR-based methods usually expand their TR if they find better points and conversely shrink it if they fail to make progress. If the TR falls below the threshold given by the *base length*, TuRBO and Casmopolitan restart with a fresh TR elsewhere. Casmopolitan [79] uses different base lengths for combinatorial and continuous variables. For combinatorial variables, the distance to the currently best function value is defined in terms of the Hamming distance, and the base length is an integer. For continuous variables, Casmopolitan defines the base length in terms of the Euclidean distance, i.e., a real number. Similarly, Bounce has separate base lengths $L_{\text{min}}^{\text{cont}}$ and $L_{\text{min}}^{\text{comb}}$ for continuous and combinatorial variables but does not fix the factor by which the TR volume is increased or decreased upon successes or failures. Instead, the factor is adjusted dynamically so that the evaluation budget m_i for the current target space \mathcal{X}_i is adhered to. This design is crucial to enable batch parallelism, as we describe next.

Batch parallelism. We allow Bounce to efficiently evaluate batches of points in parallel by using a scalable TR management strategy and q -expected improvement (qEI) [5, 80, 86] as the acquisition function for batches of size $B > 1$. When Bounce starts with a fresh TR, we sample n_{init} initial points to initialize the GP, using a Sobol sequence for continuous variables and uniformly random values for combinatorial variables.

The TR management strategy of Bounce differs from previous strategies [25, 60, 65, 79] in that it uses a dynamic factor to determine the TR base length. Recall that Bounce shrinks the TR if it fails to make progress and starts a fresh TR if the TR falls below the threshold given by the base length. Bounce’s rule is based on the idea that the minimum admissible TR base length should be reached when the current evaluation budget is exhausted. If one employed the strategies of TuRBO [25], Casmopolitan [79], or BAXUS [60] for larger batch sizes B and Bounce’s nested subspaces, then one would spend a large part of the evaluation budget in early target spaces. For example, suppose a continuous problem, the common values for the initial, minimum, and maximum TR base length, and the constant shrinkage factor of [65]. Then, such a method has to shrink the TR base length at least seven times (i.e., evaluate f $7B$ -times) before it would increase the dimensionality of the target space. Thus, the method would risk depleting its budget before reaching a target space suitable

for the problem. On the other hand, we will see that Bounce chooses an evaluation budget that is smaller in low-dimensional target spaces and higher for later target spaces of higher dimensionality. Considering a 1000-dimensional problem with an evaluation budget of 1000, it uses only 3, 12, and 47 samples for the first three target spaces of dimensionalities 2, 8, and 32.

Bounce’s strategy permits flexible TR shrinkage factors and base lengths, i.e., TR base lengths to vary within the range $[L_{\min}, L_{\max}]$. This allows Bounce to comply with the evaluation budget m_i for the current target space \mathcal{X}_i . Suppose that Bounce has evaluated j batches of B points each since it last increased the dimensionality of the target space, and let L_j denote the current TR base length. Observe that hence $m_i - jB$ evaluations remain for \mathcal{X}_i . Then Bounce sets the TR base length to $L_{j+1} := \lambda_j^{-B} L_j$ with $\lambda_j < 1$, if it found a new best point whose objective value improves upon the incumbent by at least ε . We call this a ‘success’. Otherwise, Bounce observes a ‘failure’ and sets $L_{j+1} := \lambda_j^{+B} L_j$. The rationale of this rule is that if the algorithm is in iteration j and only observes failures subsequently, then we apply this factor $(m_i - jB)$ -times, which is the remaining number of function evaluations in the current subspace \mathcal{X}_i . Hence, the last batch of the i -th target space \mathcal{X}_i will have the minimum TR base length, and Bounce will increase the target dimensionality afterward. If the TR is expanded upon a ‘success’, we need to adjust λ_j not to use more than the allocated number of function evaluations in a target space. At each iteration, we therefore set adjustment factor $\lambda_j = (L_{\min}/L_j)^{1/(m_i-jB)}$. Note that λ_j remains unchanged under this rule unless the TR expanded in the previous iteration.

The kernel choice. To harvest the sample efficiency of a low-dimensional target space, we would like to combine categorical variables into a single bin, even if they vary in the number of categories. This is not straightforward. For example, note that the popular one-hot encoding of categorical variables would give rise to multiple binary input dimensions, which would not be compatible with the above strategy of binning variables to form nested subspaces. Bounce overcomes these obstacles and allows variables of the same type to share a representation in the target space. We provide the details in Sect. 3.1.

For the GP model, we use the CoCaBo kernel [67]. In particular, we model the continuous and combinatorial variables with two separate $5/2$ -Matérn kernels where we use automatic relevance determination (ARD) for the continuous variables and share one length scale for all combinatorial variables. Following Ru et al. [67], we use a mixture of the sum and the product kernel:

$$k(\mathbf{x}, \mathbf{x}') = \sigma_f^2 (\rho k_{\text{cmb}}(\mathbf{x}_{\text{cmb}}, \mathbf{x}'_{\text{cmb}}) k_{\text{cnt}}(\mathbf{x}_{\text{cnt}}, \mathbf{x}'_{\text{cnt}}) + (1 - \rho)(k_{\text{cmb}}(\mathbf{x}_{\text{cmb}}, \mathbf{x}'_{\text{cmb}}) + k_{\text{cnt}}(\mathbf{x}_{\text{cnt}}, \mathbf{x}'_{\text{cnt}}))),$$

where \mathbf{x}_{cnt} and \mathbf{x}_{cmb} are the continuous and combinatorial variables in \mathbf{x} , respectively, and σ_f^2 is the signal variance. The trade-off parameter $\rho \in [0, 1]$ is learned jointly with the other hyperparameters *via* likelihood maximization. See Appendix C.2 for additional details.

Algorithm 1 gives a high-level overview of Bounce. In Appendix A, we prove that Bounce converges to the global optimum under mild assumptions. We now explain the different components of Bounce in detail.

3.1 The subspace embedding of mixed spaces

Bounce supports mixed spaces of four types of input variables: categorical, ordinal, binary, and continuous variables. We discuss binary and categorical variables separately because we model them differently. The proposed embedding maps only variables of a single type to each ‘bin’, i.e., no target dimension of the embedding has variables of different types. Thus, target dimensions are homogeneous in this regard. Note that the number of target dimensions of each type is implied by the current bin size of the embedding that may grow during the execution. The proposed embedding can handle categorical or ordinal input variables that differ in the number of discrete values they can take.

Continuous variables. As common in BO, we suppose that each continuous variable takes values in a bounded interval. Thus, we may normalize each interval to $[-1, 1]$. The embedding of continuous variables, i.e., input dimensions, follows BAXUS [60]: each input dimension D_i is associated with a random sign $s_i \in \{-1, +1\}$ and one or multiple input dimensions can be mapped to the same target dimension of the low-dimensional embedded subspace. Recall that Bounce works on the low-dimensional subspace and thus decides an assignment v_j for every target dimension d_j of the embedding. Then, all input variables mapped to this particular target dimension are set to this value v_j .

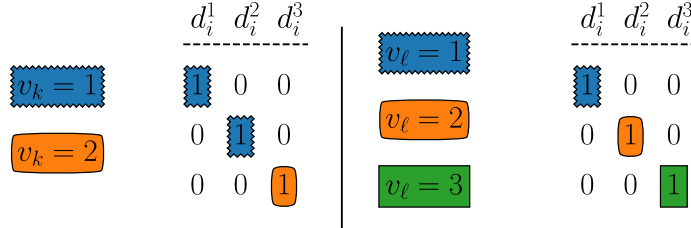


Figure 1: The mapping (or binning) of categorical and ordinal variables. Suppose that variable v_k has two categories and that v_ℓ has three categories. Both are mapped to the target dimension d_i that has cardinality $3 = \max\{2, 3\}$. While the mapping of v_ℓ to d_i is a straightforward bijection, v_k has fewer categories than d_i . Thus, the mapping of v_k to d_i repeats label 1. Ordinal variables are mapped similarly.

Binary variables. Binary dimensions are represented by the values -1 and $+1$. Each input dimension D_i is associated with a random sign $s_i \in \{-1, +1\}$, and the subspace embedding may map one or more binary input dimensions to the same binary target dimension. While the embedding for binary and continuous dimensions is similar, Bounce handles binary dimensions differently when optimizing the acquisition function.

Categorical and ordinal variables. Categorical variables that differ in the number of categories may be mapped to the same target dimension (bin). Suppose that the categorical variables v_1, \dots, v_ℓ with cardinalities c_1, \dots, c_ℓ are mapped to a single bin that is associated with the target dimension d_j of the subspace embedding. Then d_j is of categorical type and has $\max\{c_i \mid 1 \leq i \leq \ell\} =: c_{\max}$ distinct categories, that is, its cardinality is given by the maximum cardinality of any variable mapped to it. Thus, the bin d_j can represent every category of these input variables.

Suppose that Bounce assigns the category $k \in \{1, \dots, c_{\max}\}$ to the categorical bin (target dimension) d_j . We transform this label to a categorical assignment to each input variable v_1, \dots, v_ℓ , setting $v_i = \lceil k \cdot (c_i / c_{\max}) \rceil$. Recall that Bounce may split up bins, i.e., target dimensions, to increase the dimensionality of its subspace embedding. In such an event, every derived bin inherits the cardinality of the parent bin. This allows us to retain any observations the algorithm has taken up to this point. Analogously to the random sign for binary variables, we randomly shuffle the categories before the embedding. This reduces the risk of Bounce being biased towards a specific structure of the optimizer (see Appendix B.4).

We treat ordinal variables as categorical variables whose categories correspond to the discrete values the ordinal variable can take. For the sake of simplicity, we suppose here that an ordinal variable v_i has range $\{1, 2, \dots, c_i\}$ and $c_i \geq 2$ for all $i \in \{1, \dots, \ell\}$. Figure 1 shows examples of the binning of categorical and ordinal variables.

3.2 Maximization of the acquisition function

We use expected improvement (EI) [43] for batches of size $B = 1$ and qEI [5, 80, 86] for larger batches. We optimize the EI using gradient-based methods for continuous problems and local search for combinatorial problems. We interleave gradient-based optimization and local search for functions defined over a mixed space; see Appendix C.1 for details.

4 Experimental evaluation

We evaluate Bounce empirically on various benchmarks whose inputs are combinatorial, continuous, or mixed spaces. The evaluation comprises the state-of-the-art algorithms BODi [21], Casmpolitan [79], COMBO [56], SMAC [41], and RDUCE [88], using code provided by the authors. We also report Random Search [8] as a baseline. For categorical problems, COMBO’s implementation suffers from a bug explained in Appendix D.2. We report the results for COMBO with the correct benchmark implementation as “COMBO (fixed)”.

The experimental setup. We initialize every algorithm with five initial points. The plots show the performances of all algorithms averaged over 50 repetitions except BODi, which has 20 repetitions due to resource constraints caused by its high memory demand. The shaded regions give the standard error of the mean. We use common random seeds for all algorithms and for randomizing the

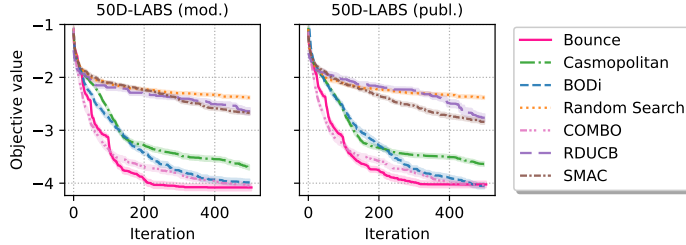


Figure 2: The 50D low-autocorrelation binary sequence problem. Bounce finds the best solutions, followed by COMBO.

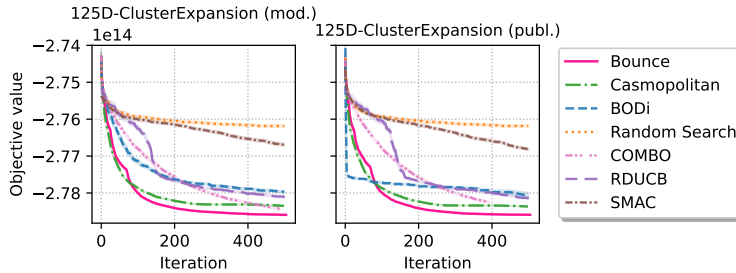


Figure 3: The 125D weighted ClusterExpansion maximum satisfiability problem. We plot the total negative weight of clauses. Bounce produces the best assignments.

benchmark functions. We run all methods for 200 function evaluations unless stated otherwise. The Labs (Section 4.1) and MaxSat125 (Section 4.2) benchmarks are run for 500 evaluations.

The benchmarks. The evaluation uses seven established benchmarks [21]: 53D SVM, 50D LABS, 125D ClusterExpansion [3, 4], 60D MaxSAT60 [21, 56], 25D PestControl, 53D Ackley53, and 25D Contamination [6, 39, 56]. Due to space constraints, we moved the results for the MaxSAT60, Contamination, and Ackley53 benchmarks to Appendix B.1. For each benchmark, we report results for the originally published formulation and for a modification where we move the optimal point to a random location. The randomization procedure is fixed for each benchmark for all algorithms and repetitions. For binary problems, we flip each input variable independently with probability 0.5. For categorical problems, we randomly permute the order of the categories. We motivate this randomization in Section 4.6.

4.1 50D Low-Autocorrelation Binary Sequences (LABS)

LABS has $n = 50$ binary dimensions. It has important applications in communications engineering and mathematics; see [58] for details. LABS is a hard combinatorial problem and currently solved *via* exhaustive search. The goal is to find a sequence $\mathbf{x} \in \{-1, +1\}^n$ with a maximum merit factor $F(\mathbf{x}) = \frac{n^2}{2E(\mathbf{x})}$, where $E(\mathbf{x}) = \sum_{k=1}^{n-1} C_k^2(\mathbf{x})$ and $C_k(\mathbf{x}) = \sum_{i=1}^{n-k} x_i x_{i+k}$ for $k = 0, \dots, n-1$ are the autocorrelations of \mathbf{x} [58]. Figure 2 summarizes the performances. We observe that Bounce outperforms all other algorithms on the benchmark’s original and randomized versions.

4.2 Industrial Maximum Satisfiability: 125D ClusterExpansion benchmark

MaxSat is a notoriously hard problem for which various approximations and exact (exponential time) algorithms have been developed; see [32, 61] for an overview. We evaluate Bounce and the other algorithms on the 125-dimensional ClusterExpansion benchmark, a real-world MaxSAT instance with many applications in materials science [2]. Unlike the MaxSAT60 benchmark (see Appendix B.1.3), ClusterExpansion is not a crafted benchmark, and its optimum has no synthetic structure [1, 3]. We treat the MaxSat problems as black-box problems; hence, algorithms do not have access to the clauses, and we cannot use the usual algorithms.

Figure 3 shows the total negative weight of the satisfied clauses as a function of evaluations. We cannot plot regret curves since the optimum is unknown [4]. We observe that Bounce finds better solutions than all other algorithms. BODi is the only algorithm for which we observe sensitivity to

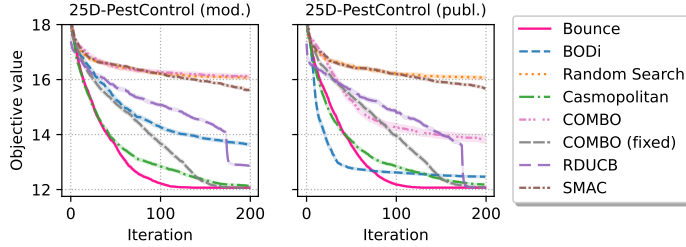


Figure 4: The 25D categorical pest control problem. Bounce obtains the best solutions, followed by Casmpolitan. BODi’s performance degrades significantly when shuffling the order of categories.

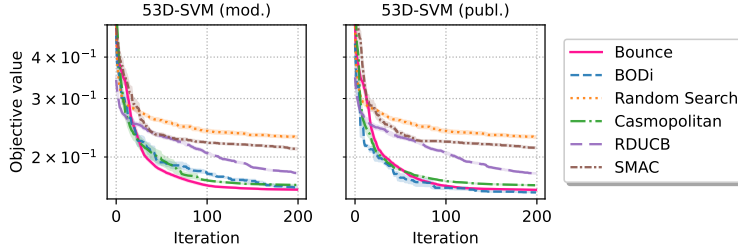


Figure 5: The 53-dimensional SVM benchmark. Bounce, BODi, and Casmpolitan achieve comparable solutions.

the location of the optimal assignment: for the published version of the benchmark, BODi quickly jumps to a moderately good solution but fails to make further progress.

4.3 25D Categorical Pest Control

PestControl is a more complex version of the Contamination benchmark and has 25 categorical variables with five categories each [56]. The task is to select one out of five actions $\{1, 2, \dots, 5\}$ at each of 25 stations to minimize the objective function that combines total cost and a measure of the spread of the pest. We note the setting $\mathbf{x} = (5, 5, \dots, 5)$ achieves a good value of 12.57, while the best value found in our evaluation is 12.07 is $\mathbf{x} = (5, 5, \dots, 5, 1)$ and thus has a Hamming distance of one. The random seed used in our experiments is zero. Figure 4 summarizes the performances of the algorithms. Bounce is robust to the location of the global optimum and consistently obtains the best solutions. In particular, the performances of COMBO and BODi depend on whether the optimum has a certain structure. We discuss this issue in detail in Appendix D.1.

4.4 SVM – a 53D AutoML task

In the SVM benchmark, we optimize over a mixed space with 50 binary and 3 continuous parameters to tune an ϵ -support vector regression (SVR) model [72]. The 50 binary parameters determine whether to include or exclude an input feature from the dataset. The 3 continuous parameters correspond to the regularization parameter C , the kernel width γ , and the ϵ parameter of the ϵ -SVR model [72]. Its root mean squared error on a held-out dataset gives the function value. Figure 5 summarizes the performances of the algorithms. We observe that Bounce, BODi, and Casmpolitan achieve comparable solutions. BODi performs slightly worse if the ordering of the categories is shuffled and slightly better if the optimal assignment to all binary variables is one. COMBO does not support continuous variables and thus was omitted.

4.5 Bounce’s efficacy for batch acquisition

We study the sample efficiency of Bounce when it selects a batch of B points in each iteration to evaluate in parallel. Figure 6 shows the results for $B = 1, 3, 5, 10,$ and 20 , where Bounce was run for $\min(2000, 200 \cdot B)$ function evaluations. We configure Bounce to reach the input dimensionality after 100 evaluations for $B = 1, 3, 5$ and after $25B$ for $B = 10, 20$. We observe that Bounce leverages parallel function evaluations effectively: it obtains a comparable function value at a considerably smaller number of iterations, thus saving wall-clock time for applications with time-consuming function evaluations. We also studied batch acquisition for continuous problems

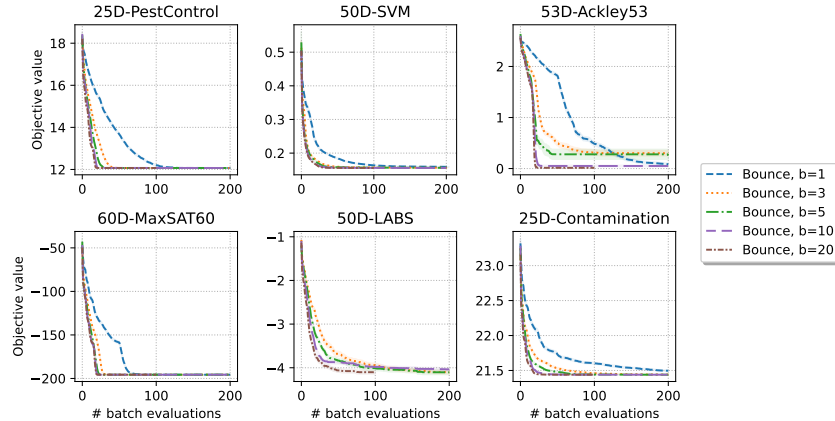


Figure 6: Bounce benefits from the batch acquisition that allows parallelizing function evaluations. We show the best function values obtained after each batch for batch sizes 1, 3, 5, 10, and 20.

and found that Bounce also provides significant speed-up. Due to space constraints, we deferred the discussion to Appendix B.2.

4.6 The sensitivity of BODi and COMBO to the location of the optima

The empirical evaluation reveals that the performances of BODi [21] and COMBO [56] are sensitive to the location of the optima. Both methods degrade on at least one benchmark when the optimum is moved to a randomly chosen point. This is particularly unexpected for categorical variables where moving the optimum to a random location is equivalent to shuffling the labels of the categories of each variable. Such a change of representation should not affect the performance of an algorithm.

BODi is more susceptible to the location of the optimizer than COMBO. The performance of COMBO degrades only on the categorical `PestControl` benchmark, whereas BODi degrades on five out of seven benchmarks. Looking closer, we observe that BODi’s performance degradation is particularly large for synthetic benchmarks like `Ackley53` and `MaxSAT60`, where setting all variables to the same value is optimal. Figure 7 summarizes the effects of moving the optimum on BODi. Due to space constraints, we moved the details and a discussion of categorical variables to the appendix. Similarly, setting all binary variables of the `SVM` benchmark to one produces a good objective value. It is not surprising, given that the all-one assignment corresponds to including all features previously selected for the benchmark because of their high importance.

We prove in Appendix D.1 that BODi adds a point with zero Hamming distance to an all-zero or all-one solution, with a probability that increases with the dictionary size. Deshwal et al. [21, p. 7] reported that BODi’s performance ‘tends to improve’ with the size of the dictionary. Moreover, BODi samples a new dictionary in each iteration, eventually increasing the chance of having such a point in its dictionary. Thus, we hypothesize that BODi benefits from having a near-optimal solution in its dictionary. For COMBO, Figure 4 shows that the performance on `PestControl` degrades substantially if the labels of the categories are shuffled. Then COMBO’s sample-efficiency becomes comparable to Random Search.

5 Discussion

BO in combinatorial spaces has many exciting and impactful applications. Its applicability to real-world problems, such as LABS that defy a closed-form solution, makes it a valuable tool for practitioners. Our empirical evaluation reveals that state-of-the-art methods fail to provide good solutions reliably. In particular, it finds that BODi and COMBO, which performed best in recent publications, are sensitive to the location of the optimizer. We identified design flaws in BODi and an implementation bug in COMBO as the root causes of the performance degradations.

The proposed Bounce algorithm is reliable for high-dimensional black-box optimization in combinatorial, continuous, and mixed spaces. The empirical evaluation demonstrates that Bounce reliably outperforms the state-of-the-art on a diverse set of problems. Using a novel TR management strat-

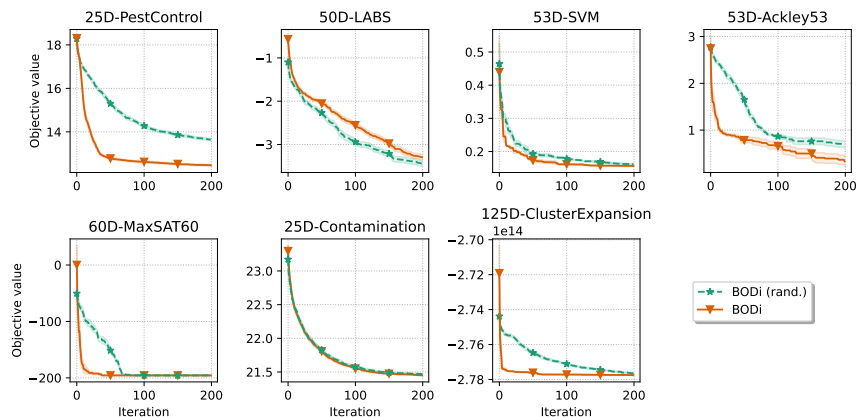


Figure 7: BODi’s performance degrades on five out of seven benchmarks when randomizing the location of the optimal solution: BODi on the default version (orange) of the benchmark and on the modified version (green, dashed) where the optimum was moved.

egy, Bounce leverages parallel evaluations of the objective function to improve its performance. We anticipate headroom by tailoring the modeling of combinatorial objects, e.g., arising in the search for peptides or materials discovery [28, 34, 37, 59, 75, 78]. Here it seems particularly interesting to incorporate prior belief on the importance of decision variables while maintaining the overall scalability. Moreover, extending the present work to black-box constraints [24, 30], multiple objectives, and multiple information sources [18, 31, 62] will considerably expand the applicable use cases.

Limitations. Bounce is not designed to handle noisy evaluations of the objective function. While it seems straightforward to extend Bounce to handle noisy evaluations, e.g., by using a Gaussian process with a noise term and acquisition functions that account for noise [70], we leave this for future work. Moreover, in applications where the categorical or ordinal variables vary substantially in the number of values they can take, there may be better ways to ‘bin’ them.

Societal impact. Bayesian optimization has recently gained wide-spread popularity for tasks in drug discovery [53], chemical engineering [15, 33, 38, 68, 71], materials discovery [28, 34, 37, 59, 75, 78], aerospace engineering [6, 45, 49], robotics [16, 17, 48, 50, 64], and many more. This highlights the Bayesian optimization community’s progress toward providing a reliable ‘off-the-shelf optimizer.’ However, this promise is not yet fulfilled for the newer domain of mixed-variable Bayesian optimization that allows optimization over hundreds of ‘tunable levers’, some of which are discrete, while others are continuous. This domain is of particular relevance for the tasks above. Bounce’s ability to incorporate more such levers in the optimization significantly impacts the above practical applications, allowing for more granular control of a chemical reaction or a processing path, to give some examples. The empirical evaluation shows that the performance of state-of-the-art methods is highly sensitive to the location of the unknown global optima and often degenerates drastically, thus putting practitioners at risk. The proposed algorithm Bounce, however, achieves robust performance over a broad collection of tasks and thus will become a ‘goto’ optimizer for practitioners in other fields. Therefore, we open-source the Bounce code.¹

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¹<https://github.com/LeoIV/bounce>

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A Consistency of Bounce

In this section, we prove the consistency of the Bounce algorithm. The proof is based on Papenmeier et al. [60] and Eriksson and Poloczek [24].

Theorem 1 (Bounce consistency). *With the following definitions*

Def. 1. $(\mathbf{x}_k)_{k=1}^\infty$ is a sequence of points of decreasing function values;

Def. 2. $\mathbf{x}^ \in \arg \min_{\mathbf{x} \in \mathcal{X}}$ is a minimizer of f in \mathcal{X} ;*

and under the following assumptions:

Ass. 1. D is finite;

Ass. 2. f is observed without noise;

Ass. 3. The range of f is bounded in \mathcal{X} , i.e., $\exists C \in \mathbb{R}_{++}$ s.t. $|f(\mathbf{x})| < C \ \forall \mathbf{x} \in \mathcal{X}$;

Ass. 4. For at least one of the minimizers \mathbf{x}_i^ the (partial) assignment corresponding to the continuous variables lies in a (continuous) region with positive measure;*

Ass. 5. One Bounce reached the input dimensionality D , the continuous elements of the initial points $\{\mathbf{x}_{cont_i}\}_{n=1}^{n_{min}}$ after each TR restart are chosen

(a) uniformly at random for continuous variables; and

(b) such that every realization of the combinatorial variables has positive probability;

then the Bounce algorithm finds a global optimum with probability 1, as the number of samples N goes to ∞ .

Proof. The range of f is bounded per Assumption 3, and Bounce only considers a function evaluation a ‘success’ if the improvement over the current best solution exceeds a certain constant threshold. Bounce can only have a finite number of ‘successful’ evaluations because the range of f is bounded per Assumption 3. For the sake of a contradiction, we suppose that Bounce does not obtain an optimal solution as its number of function evaluations $N \rightarrow \infty$. Thus, there must be a sequence of failures, such that the TRs in the current target space, i.e., the current subspace, will eventually reach its minimum base length. Recall that in such an event, Bounce increases the target dimension by splitting up the ‘bins’, thus creating a subspace of $(b + 1)$ -times higher dimensionality. Then Bounce creates a new TR that again experiences a sequence of failures that lead to another split, and so on. This series of events repeats until the embedded subspace eventually equals the input space and thus has dimensionality D . See lines 12 – 16 in Algorithm 1 in Sect. 3.

Still supposing that Bounce does not find an optimum in the input space, there must be a sequence of failures such that the side length of the TR again falls below the set minimum base length, now forcing a restart of Bounce. Recall that at every restart, Bounce samples a fresh set of initial points uniformly at random from the input space; see line 18 in Algorithm 1. Therefore, with probability 1, a random sample will eventually be drawn from any subset $\mathcal{Y} \subseteq \mathcal{X}$ with positive Lebesgue measure ($\nu(\mathcal{Y}) > 0$):

$$1 - \lim_{k \rightarrow \infty} (1 - \mu(\mathcal{Y}))^k = 1, \quad (1)$$

where μ is the uniform probability measure of the sampling distribution that Bounce employs for initial data points upon restart [73].

Let

$$\alpha = \inf \{t : \nu[x \in \mathcal{X} \mid f(x) < t] > 0\}$$

denote the essential infimum of f on \mathcal{X} with ν being the Lebesgue measure [73].

Following Solis and Wets [73], we define the optimality region, i.e., the set of points whose function value is larger by at most ε than the essential infimum:

$$R_{\varepsilon, M} = \{x \in \mathcal{X} \mid f(x) < \alpha + \varepsilon\}$$

with $\varepsilon > 0$ and $M < 0$. Because of Ass. 4, at least one optimal point lies in a region of positive measure that is continuous for the continuous variables. Therefore, we have that $\alpha = f(\mathbf{x}^*)$. Note that this is also the case if the domain of f only consists of combinatorial variables (Ass. 5). Then, $R_{\varepsilon, M} = \{x \in \mathcal{X} \mid f(x) < f(\mathbf{x}^*) + \varepsilon\}$.

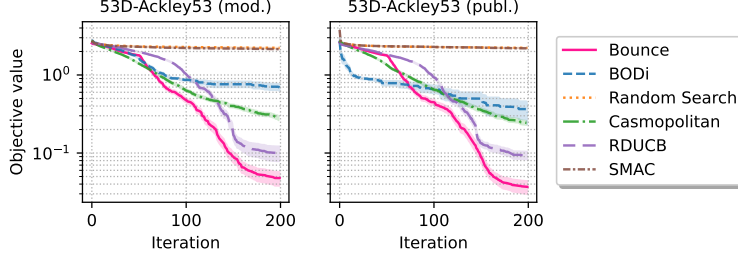


Figure 8: Bounce the other algorithms on the synthetic Ackley53 benchmark function. Bounce outperforms all other algorithms and quickly finds excellent solutions. BODi’s performance degrades upon randomization.

Let $(\mathbf{x}_k^*)_{k=1}^\infty$ denote the sequence of best points that Bounce discovers with \mathbf{x}_k^* being the best point up to iteration k . This sequence satisfies Def. 1 by construction. Note that $\mathbf{x}_k^* \in R_{\varepsilon, M}$ implies that $\mathbf{x}_{k'}^* \in R_{\varepsilon, M}$ for all $k' \geq k + 1$ [73] because observations are noise-free. Then,

$$\begin{aligned} \mathbb{P}[\mathbf{x}_k^* \in R_{\varepsilon, M}] &= 1 - \mathbb{P}[\mathbf{x}_k^* \in \mathcal{X} \setminus R_{\varepsilon, M}] \\ &\geq 1 - (1 - \mu(R_{\varepsilon, M}))^k, \end{aligned}$$

and,

$$1 \geq \lim_{k \rightarrow \infty} \mathbb{P}[\mathbf{x}_k^* \in R_{\varepsilon, M}] \geq 1 - \underbrace{\lim_{k \rightarrow \infty} (1 - \mu(R_{\varepsilon, M}))^k}_{=1, \text{ Eq. (1)}} = 1,$$

i.e., \mathbf{x}_k^* eventually falls into the optimality region [73]. By letting $\varepsilon \rightarrow 0$, \mathbf{x}_k^* converges to the global optimum with probability 1 as $k \rightarrow \infty$. □

B Additional experiments

We compare Bounce to the other algorithms on three additional benchmark problems: Ackley53 and MaxSAT60 [21]. Moreover, we run two additional studies to further investigate the performance of Bounce. First, we run Bounce on a set of continuous problems from Papenmeier et al. [60] to showcase the performance and scalability of Bounce on purely continuous problems. We then present a “low-sequency” version of Bounce to showcase how such a version can outperform its competitors on the original benchmarks by introducing a bias towards low-sequency solutions.

B.1 Bounce and other algorithms on additional benchmarks

B.1.1 The synthetic Ackley53 benchmark function

Ackley53 is a 53-dimensional function with 50 binary and 3 continuous variables. Wan et al. [79] discretized 50 continuous variables of the original Ackley function, requiring these variables to be either zero or one. This benchmark was designed such that the optimal value of 0.0 is at the origin $\mathbf{x} = (0, \dots, 0)$. Here, we perturb the optimal assignment of combinatorial variables by flipping each binary variable with probability $1/2$. Figure 8 summarizes the performances of the algorithms. Bounce outperforms all other algorithms and proves to be robust to the location of the optimum point. Casmopolitan is a distanced runner-up. BODi initially outperforms Casmopolitan on the published benchmark version but falls behind later.

B.1.2 Contamination control

The Contamination benchmark models a supply chain with 25 stages [39]. At each stage, a binary decision is made whether to quarantine food that has not yet been contaminated. Each such intervention is costly, and the goal is to minimize the number of contaminated products and prevention cost [6, 56]. Figure 9 shows the performances of the algorithms.

Bounce, Casmopolitan, and BODi all produce solutions of comparable objective value. Bounce and Casmopolitan find better solutions than BODi initially, but after about 100 function evaluations, the solutions obtained by the three algorithms are typically on par.

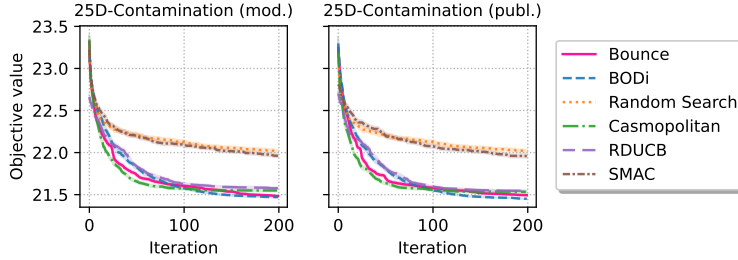


Figure 9: Bounce and the other algorithms on the 25-dimensional contamination problem. Bounce performs on par with Casmopolitan and BODi on both versions of the benchmark.

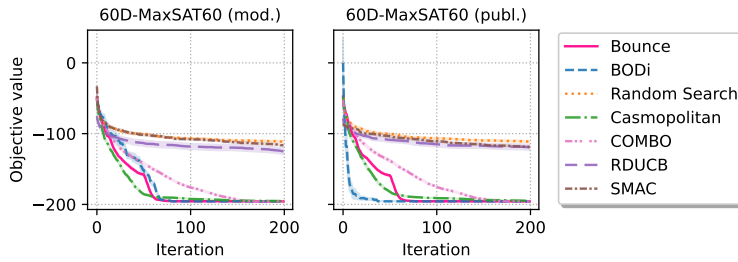


Figure 10: Bounce and other algorithms on the 60-dimensional weighted maximum satisfiability problem. Bounce is the first to find an optimal solution (left). On the published version (right), Bounce comes in second after BODi.

B.1.3 The MaxSAT60 benchmark

MaxSAT60 is a 60-dimensional, weighted instance of the Maximum Satisfiability (MaxSAT) problem. MaxSAT is a notoriously hard combinatorial problem that cannot be solved in polynomial time (unless $\mathbb{P} = \text{NP}$). The goal is to find a binary assignment to the variables that satisfies clauses of maximum total weight. For every i in $\{1, 2, \dots, d\}$, this benchmark has one clause of the form x_i with a weight of 1 and 638 clauses of the form $\neg x_i \vee \neg x_j$ with a weight of 61. Following [21, 56, 79], we normalize these weights to have zero mean and unit standard deviation. This normalization causes the one-variable clauses to have a *negative weight*, i.e., the function value improves if such a clause is not satisfied, which is atypical behavior for a MaxSAT problem. Since the clauses with two variables are satisfied for $x_i = x_j = 0$ and the clauses with one variable of negative weights are never satisfied for $x_i = 0$, the normalized benchmark version has a global optimum at $\mathbf{x}^* = (0, \dots, 0)$ by construction. The problem’s difficulty is finding an assignment for variables such that *all* two-variable clauses are satisfied and *as many* one-variable clauses as possible are not captured by normalized weights.

Figure 10 summarizes the performances of the algorithms. The general version that attains the global optimum for a randomly selected binary assignment is shown on the left. The special case where the global optimum is set to the all-zero assignment is shown on the right.

We observe that Bounce requires the smallest number of samples to find an optimal assignment in general, followed by BODi and Casmopolitan. Only in the special case where the optimum is the all-zero assignment, BODi ranks first, confirming the corresponding result in Deshwal et al. [21].

B.2 Parallel evaluations on continuous problems

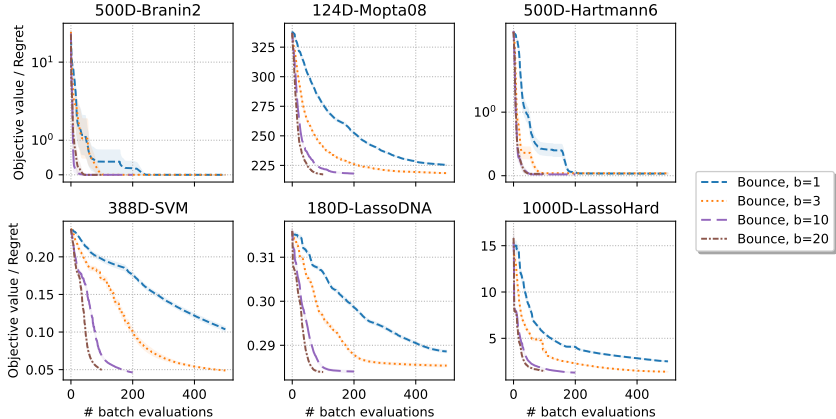


Figure 11: Bounce on continuous problems with different batch sizes (plotted in terms of batch evaluations).

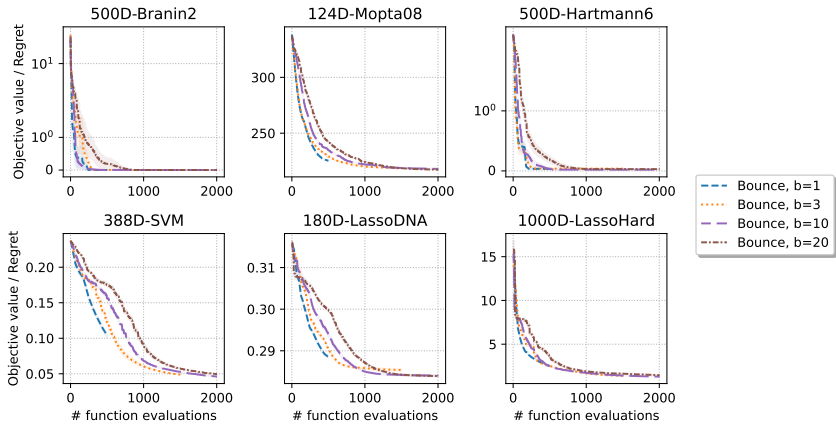


Figure 12: Bounce on continuous problems with different batch sizes (plotted in terms of function evaluations).

To showcase the performance and scalability of Bounce, we run it on a set of continuous problems from Papenmeier et al. [60]. The 124-dimensional Mopta08 benchmark is a constrained vehicle optimization problem. We adopt the soft-constrained version from Eriksson and Jankowiak [23]. The 388-dimensional SVM problem [23] concerns the classification performance with an SVR on the slice localization dataset. The 180-dimensional LassoDNA benchmark [69] is a sparse regression problem on a real-world dataset, and the 1000-dimensional LassoHard benchmark optimizes over a synthetic dataset. The 500-dimensional Branin2 and Hartmann6 problems are versions of the 2- and 6-dimensional benchmark problems where additional dimensions with no effect on the function value were added.

We set the number of function evaluations to $\max(2000, 500B)$ for a batch size of B and configure Bounce such that it reaches the input dimensionality after 500 function evaluations. Figures 11 and 12 show the simple regret for the synthetic Branin2 and Hartmann6 problems, and the best function value obtained after a given number of batch (Figure 11) or function (Figure 12) evaluations for the remaining problems: Mopta08, SVM, LassoDNA, and LassoHard.

We observe that Bounce always benefits from more parallel function evaluations. The difference between smaller batch sizes, such as $B = 1$ and $B = 3$ or $B = 3$ and $B = 10$, is more remarkable

than between larger batch sizes, like $B = 10$ and $B = 20$. Parallel function evaluations prove especially effective on SVM and LassoDNA. Here, the optimization performance improves drastically. We conclude that a small number of parallel function evaluations already helps increase the optimization performance considerably.

On the synthetic Branin2 and Hartmann6 problems, Bounce quickly converges to the global optimum. Here, we see that a larger number of parallel function evaluations also helps in converging to a better solution.

B.3 Parallel evaluations on mixed and combinatorial problems

In addition to Figure 6, which shows the best objective value per batch evaluation, Figure 13 shows the objective value in terms of *function* evaluations.

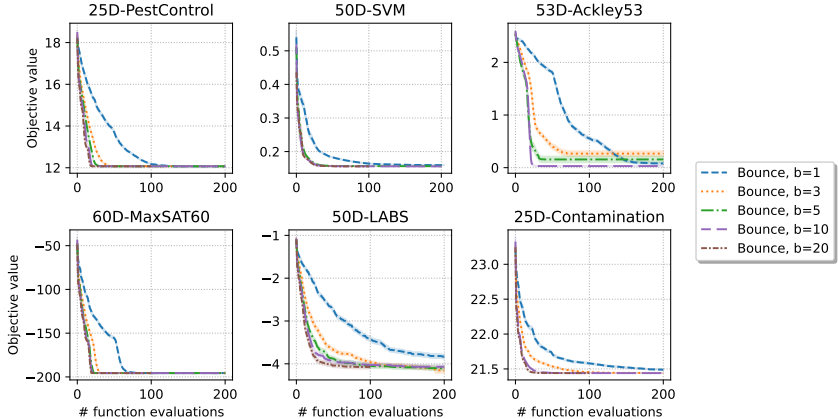


Figure 13: Bounce on mixed and combinatorial problems with different batch sizes (plotted in terms of function evaluations).

The figure confirms that Bounce leverages parallel function values efficiently.

B.4 Low-sequence version of Bounce

We show how we can bias Bounce towards low-sequence solutions. We remove the random signs (for binary and continuous variables) and the random offsets (for categorical and ordinal variables) from the Bounce embedding. We conduct this study to show a) that Bounce can outperform BODi on the unmodified versions of the benchmark problems if we introduce a similar bias towards low-sequence solutions and b) that the random signs empirically show to remove biases towards low-sequence solutions. However, we want to emphasize that the results of this section are not representative of the performance of Bounce on arbitrary real-world problems. Nevertheless, if one knows that the problem has a low-sequence structure, then Bounce can be configured to exploit this structure and outperform BODi.

Figure 14 shows the results of the low-sequence version of Bounce on the original benchmarks from Section 4. We observe that Bounce outperforms BODi and the other algorithms on the unmodified versions of the benchmark problems. This shows that Bounce can outperform BODi on the unmodified version of the benchmarks if we introduce a similar bias towards low-sequence solutions.

Figure 15 shows the results of the low-sequence version of Bounce on the flipped benchmarks from Section 4. The low-sequence version of Bounce is robust towards the randomization of the optimal point.

C Implementation details

We implement Bounce in Python using the BoTorch [5] and GPyTorch [29] libraries.

We employ a $\Gamma(1.5, 0.1)$ prior on the lengthscales of both kernels and a $\Gamma(1.5, 0.5)$ prior on the signal variance. We further use a $\Gamma(1.1, 0.1)$ prior on the noise variance.

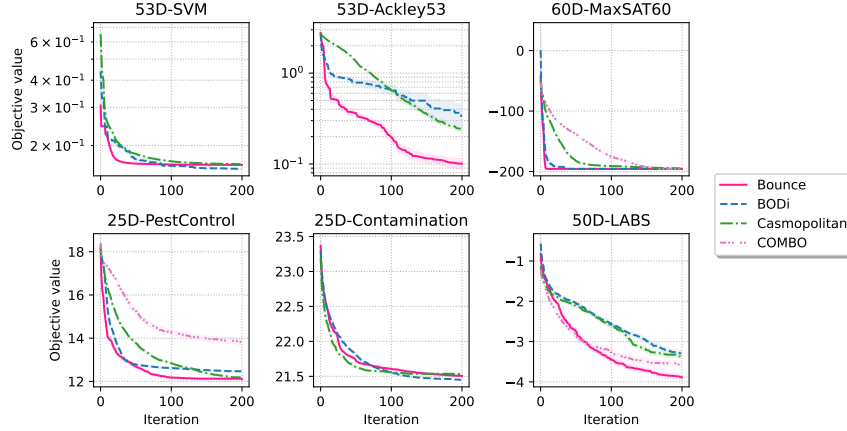


Figure 14: ‘Low-sequence’ version of Bounce on the **original** benchmarks from Section 4: with a bias towards low-sequence solutions, Bounce outperforms BODi on the original versions of the benchmark problems.

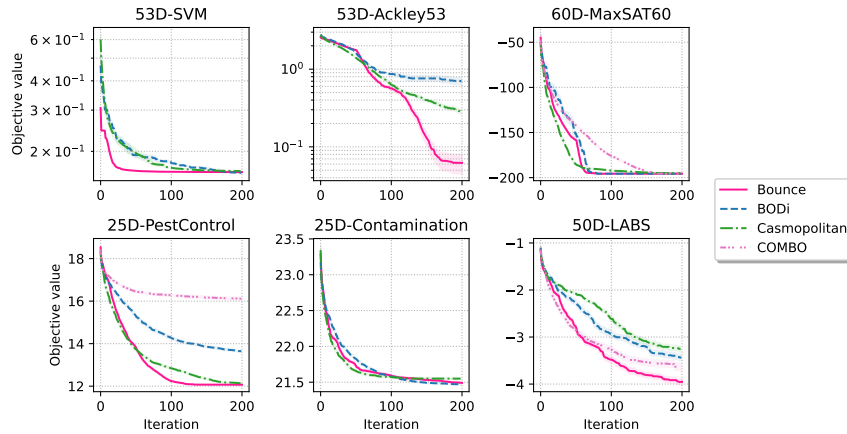


Figure 15: “Low-sequence” version of Bounce on the **modified** benchmarks from Section 4.

Motivated by Wan et al. [79] and Eriksson et al. [25], we use an initial trust region baselength of 40 for the combinatorial variables, and 0.8 for the continuous variables. We maintain two separate TR shrinkage and expansion parameters (γ_{cmb} and γ_{cnt}) for the combinatorial and continuous variables, respectively such that each TR base length reaches its respective minimum of 1 and 2^{-7} after a given number of function evaluations. When Bounce finds a better or worse solution, we increase or decrease both TR base lengths.

We use the author’s implementations for COMBO², BODi³, RDUCEB⁴, SMAC⁵, and Casmopolitan⁶. We use the same settings as the authors for COMBO, RDUCEB, SMAC, and BODi. For Casmopolitan, we use the same settings as the authors for benchmarks reported in Wan et al. [79] and set the initial trust region base length to 40 otherwise.

Due to its high-memory footprint, we ran BODi on NVidia A100 80GB GPUs for 300 GPU/h. We ran Bounce on NVidia A40 GPUs for 2,000 GPU/h. We ran the remaining methods for 20,000 GPU/h on one core of Intel Xeon Gold 6130 CPUs with 60GB of memory.

²<https://github.com/QUVA-Lab/combo>, unspecified license, last access: 2023-05-04

³<https://github.com/aryandeshwal/bodi>, no license provided, last access: 2023-05-04

⁴<https://github.com/huawei-noah/HEBO/tree/master/RDUCEB>, MIT license, last access: 2023-10-20

⁵<https://github.com/automl/pysmac>, AGPL-3.0 license, last access 2023-10-20

⁶<https://github.com/xingchenwan/casmo>, MIT license, last access: 2023-05-04

C.1 Optimization of the acquisition function

We use different strategies to optimize the acquisition function depending on the type of variables present in a problem.

Continuous problems. For purely continuous problems, we follow a similar approach as TuRBO [25]. In particular, we use the lengthscales of the GP posterior to shape the TR. We use gradient descent to optimize the acquisition function within the TR bounds with 10 random restarts and 512 raw samples. For a batch size of 1, we use analytical EI. For larger batch sizes, we use the BoTorch implementation of qEI [5, 66, 86].

Binary problems. Similar to Wan et al. [79], we use discrete TRs centered on the current best solution. A discrete TR describes all solutions with a certain Hamming distance to the current best solution.

We use a local search approach to optimize the acquisition function for all problems with a combinatorial search space of only binary variables: When starting the optimization, we first create a set of $\min(5000, \max(2000, 200 \cdot d_i))$ random solutions. The choice of the number of random solutions is based on TuRBO [25]. For each candidate, we first draw L_i indices uniformly at random from $\{1, \dots, d_i\}$ without replacement, where L_i is the TR length at the i -th iteration. We then sample d_i values in $\{0, 1\}$ and set the candidate at the sampled indices to the sampled values. All other values are set to the values of the current best solution. Note that this construction ensures that each candidate solution lies in the TR bounds of the current best solution. We add all neighbors (i.e., points with a Hamming distance of 1) of the current best solution to the set of candidates. This is inspired by BODi [21]. We find the 20 candidates with the highest acquisition function value and use local search to optimize the acquisition function within the TR bounds: At each local search step, we create all direct neighbors that do not coincide with the current best solution or would violate the TR bounds. We then move the current best solution to the neighbor with the highest acquisition function value. We repeat this process until the acquisition function value does not increase anymore. Finally, we return the best solution found during local search.

Categorical problems. We adopt the approach for binary problems, i.e., we first create a set of random solutions with the same size as for purely binary problems and start the local search on the 20 best initial candidates.

Suppose the number of categorical variables of the problem is smaller or equal to the current TR length. In that case, we sample, for each candidate and each categorical variable, an index uniformly at random from $\{1, 2, \dots, |v_i|\}$ where $|v_i|$ is the number of values of the i -th categorical variable. We then set the candidate at the sampled index to 1 and all other values to 0.

If the number of categorical variables of the problem is larger than the current TR length L_i , we first sample L_i categorical variables uniformly at random from $[d_i]$ without replacement. For each initial candidate and each sampled categorical variable, we sample an index uniformly at random, for which we set the categorical variable to 1 and all other values to 0. The values for the variables that were not sampled are set to the values of the current best solution.

As for the binary case, we add all neighbors of the current best solution to the set of candidates, and we sample the 20 candidates with the highest acquisition function value.

We then use multi-start local search to optimize the acquisition function within the TR bounds while neighbors are created by changing the index of one categorical variable. Again, we repeat until convergence and return the best solution found during the local search.

Ordinal problems. The construction for ordinal problems is similar to the one for categorical problems.

Suppose the number of ordinal variables of the problem is smaller or equal to the current TR length. In that case, we sample an ordinal value uniformly at random to set the ordinal variable for each candidate and each ordinal variable. Otherwise, we choose as many ordinal variables as each candidate's current TR length and sample an ordinal value uniformly at random to set the ordinal variable. We add all neighbors of the current best solution, all solutions where the distance to the current best solution is 1 for one ordinal variable, to the set of candidates. We then sample the 20 candidates with the highest acquisition function value and use local search to optimize the acquisition function within the TR bounds. In the local search, we increment or decrement the value of a single ordinal variable.

Mixed problems. Mixed problems are effectively handled by treating every variable type separately. Again, we create a set of initial random solutions where the values for the different variable types are sampled according to the abovementioned approaches. This can lead to solutions outside the TR bounds. We remove these solutions and find the 20 best candidates only across the solutions within the TR bounds.

When optimizing the acquisition function, we differentiate between continuous and combinatorial variables. We optimize the continuous variables by gradient descent with the same settings as purely continuous problems. When optimizing, we fix the values for the combinatorial values.

We use local search to optimize the acquisition function for the combinatorial variables. In this step, we fix the values for the continuous variables and only optimize the combinatorial variables. We create the neighbors by creating neighbors within Hamming distance of 1 for each combinatorial variable type and then combining these neighbors. Again, we run a local search until convergence.

We do five interleaved steps, starting with the continuous variables and ending with the combinatorial variables.

C.2 Kernel choice

We use the CoCaBo kernel [67] with one global lengthscale for the combinatorial and ARD for the continuous variables:

$$\begin{aligned}
 k(\mathbf{x}, \mathbf{x}') &= \sigma_f^2 (\rho k_{\text{cmb}}(\mathbf{x}_{\text{cmb}}, \mathbf{x}'_{\text{cmb}}) k_{\text{cnt}}(\mathbf{x}_{\text{cnt}}, \mathbf{x}'_{\text{cnt}}) \\
 &\quad + (1 - \rho)(k_{\text{cmb}}(\mathbf{x}_{\text{cmb}}, \mathbf{x}'_{\text{cmb}}) + k_{\text{cnt}}(\mathbf{x}_{\text{cnt}}, \mathbf{x}'_{\text{cnt}}))) \\
 k_{\text{cmb}}(\mathbf{x}_{\text{cmb}}, \mathbf{x}'_{\text{cmb}}) &= \left(1 + \frac{\sqrt{5}r_{\text{cmb}}}{\ell_{\text{cmb}}} + \frac{5r_{\text{cmb}}^2}{3\ell_{\text{cmb}}^2} \right) \exp\left(-\frac{\sqrt{5}r_{\text{cmb}}}{\ell_{\text{cmb}}}\right) \\
 r_{\text{cmb}} &= \|\mathbf{x}_{\text{cmb}} - \mathbf{x}'_{\text{cmb}}\| \\
 k_{\text{cnt}}(\mathbf{x}_{\text{cnt}}, \mathbf{x}'_{\text{cnt}}) &= \left(1 + \sqrt{5}r_{\text{cnt}} + 5r_{\text{cnt}}^2 \right) \exp\left(-\sqrt{5}r_{\text{cnt}}\right) \\
 r_{\text{cnt}} &= \sqrt{\sum_{i \in [d]; d_i \text{ continuous}} \frac{(x_i - x'_i)^2}{\ell_{\text{cnt},i}^2}}
 \end{aligned}$$

where \mathbf{x}_{cnt} and \mathbf{x}_{cmb} are the continuous and combinatorial variables in \mathbf{x} , respectively, i.e.,

$$\begin{aligned}
 \mathbf{x}_{\text{cmb}} &= (x_i : d_i \text{ is combinatorial}) \\
 \mathbf{x}_{\text{cnt}} &= (x_i : d_i \text{ is continuous})
 \end{aligned}$$

and $\rho \in [0, 1]$ is a tradeoff parameter learned jointly with the other hyperparameters during the likelihood maximization. Here, ℓ_{cmb} and $\ell_{\text{cnt},i}$ are the lengthscale hyperparameters.

D Additional analysis of BODi and COMBO

D.1 Analysis of BODi

Binary problems. BODi by Deshwal et al. [21] uses a dictionary of anchor points $\mathbf{A} = (\mathbf{a}_1, \dots, \mathbf{a}_m)$ to encode a candidate point \mathbf{z} . In particular, the i -th entry of the m -dimensional embedding $\phi_{\mathbf{A}}(\mathbf{z})$ is obtained by computing the Hamming-distance between \mathbf{z} and \mathbf{a}_i . Notably, Deshwal et al. [21] choose the dimensionality of the embedding m is chosen to be 128, which is larger than the dimensionality of the benchmark functions themselves.

The sampling procedure for dictionary elements \mathbf{a}_i is chosen to yield a wide range of *sequences*. The sequence of a binary string is defined as the number of times the string changes from 0 to 1 and vice versa. Deshwal et al. [21] propose two approaches to generate the dictionary elements: (i) using binary wavelets, and (ii) by first drawing a Bernoulli parameter $\theta_i \sim \mathcal{U}(0, 1)$ for each $i \in [m]$ and then drawing a binary string \mathbf{a}_i from the distribution $\mathcal{B}(\theta_i)$. The latter approach is their default method.

We will now show that the probability of sampling a point of sequence zero (i.e., $\mathbf{a}_i = \mathbf{0}$ or $\mathbf{a}_i = \mathbf{1}$) is higher than the probability to sample an arbitrary point. We hypothesize that it is beneficial for BODi's dictionary to contain such a point with high probability if the optimal point is also of

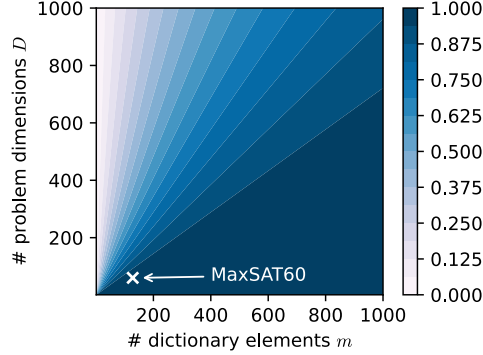


Figure 16: Probabilities of BODi to contain a zero-sequence solution for different choices of the dictionary size m and the function dimensionality D .

sequence zero (cf. Section 4.6). Since BODi’s performance degrades when randomizing the optimal point, we further hypothesize that BODi’s performance on problems with a zero- or low-sequence solution is not representative of problems with an arbitrary solution.

Deshwal et al. [21] choose the dictionary to have $m = 128$ dictionary elements. Given a Bernoulli parameter θ_i , the probability that the i -th dictionary point \mathbf{a}_i is a point of sequence zero is given by $\theta_i^D + (1 - \theta_i)^D$:

$$\mathbb{P}(\text{“zero sequence”} \mid \theta_i) = \prod_{i=1}^m \theta_i^D + (1 - \theta_i)^D$$

Then, since θ_i follows a uniform distribution, the overall probability for a point of zero sequence is given by

$$\begin{aligned} \mathbb{P}(\text{“zero sequence”}) &= 1 - \underbrace{\prod_{i=1}^m \int_0^1 (1 - \theta_i^D - (1 - \theta_i)^D) \underbrace{p(\theta_i)}_{=1} d\theta_i}_{\text{prob. of } m \text{ times not zero sequence}} \\ &= 1 - \prod_{i=1}^m \left(\theta_i - \frac{\theta_i^{D+1}}{D+1} + \frac{(1 - \theta_i)^{D+1}}{D+1} \right) \Big|_{\theta_i=1} \\ &= 1 - \left(1 - \frac{2}{D+1} \right)^m, \end{aligned}$$

i.e., the probability of at least one dictionary element being of sequence zero is $1 - \left(1 - \frac{2}{D+1} \right)^m$. The probability of BODi’s dictionary to contain a zero-sequence point increases with the number of dictionary elements m and decreases with the function dimensionality D (see Figure 16).

For instance, for the 60-dimensional MaxSAT60 benchmark, the probability that at least one dictionary element is of sequence zero is $1 - \left(1 - \frac{2}{60+1} \right)^{128} \approx 0.986$ (see Figure 16).

Note that at least one point \mathbf{z}^* has a probability of $\leq 1/2^d$ to be drawn. The probability of the dictionary containing that \mathbf{z}^* is less than or equal to $1 - (1 - 1/2^d)^m$ which is already less than 0.01 for $d = 14$ and $m = 128$. In Section 4, we show that randomizing the optimal point structure leads to performance degradation for BODi. We hypothesize this is due to the reduced probability of the dictionary containing the optimal point after randomization.

Categorical problems. We calculate the probability that BODi contains a vector in its dictionary where all elements are the same. For categorical problems, BODi first samples a vector $\boldsymbol{\theta}$ from the τ_{\max} -simplex $\Delta^{\tau_{\max}}$ for each vector \mathbf{a}_i in the dictionary, with τ_{\max} being the maximum number of categories across all categorical variables of a problem. We assume that all variables have the same

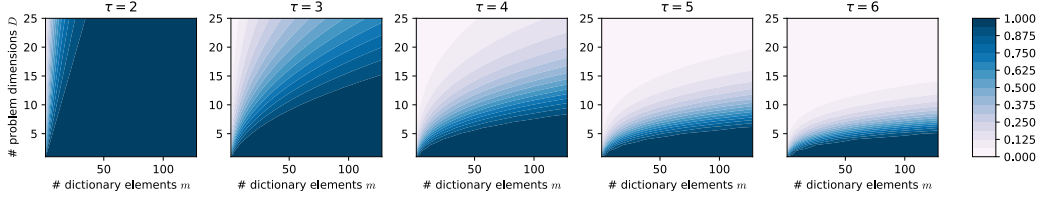


Figure 17: Probabilities of BODi’s dictionary to contain at least one categorical point where each category has the same value. The probability increases with the number of dictionary elements m but decreases with the number of categories τ and the number of problem dimensions D .

number of categories as is the case for the benchmarks in Deshwal et al. [21]. Let τ be the number of categories of the variables. For each element in \mathbf{a}_i , BODi draws a value from the categorical distribution with probabilities θ . While line 7 in Algorithm 5 in Deshwal et al. [21] might suggest that the elements in θ are shuffled for every element in \mathbf{a}_i , we observe that θ remains fixed based on the implementation provided by the authors⁷. The random resampling of elements from θ is probably only used for benchmarks where the number of realizations differs between categorical variables.

Then, for a fixed θ , the probability that all D elements in \mathbf{a}_i for any i are equal to some fixed value $t \in \{1, 2, \dots, \tau\}$ is given by θ_t^D . The probability that, for any of the m dictionary elements, all D elements in \mathbf{a}_i are equal to some fixed value $t \in \{1, 2, \dots, \tau\}$ is given by

$$\mathbb{P}(\text{“all one specific category”}) = 1 - \prod_{i=1}^m \int (1 - \theta_t^D) p(\theta_t) d\theta_t. \quad (2)$$

We note that θ follows a Dirichlet distribution with $\alpha = \mathbf{1}$ [54]. Then, θ_t is marginally Beta($1, \tau-1$)-distributed [54]. With that, Eq. (2) becomes

$$\begin{aligned} \mathbb{P}(\text{“all one specific category”}) &= 1 - \prod_{i=1}^m \mathbb{E}_{\theta_t \sim \text{Beta}(1, \tau-1)} [1 - \theta_t^D] \\ &= 1 - \prod_{i=1}^m 1 - \mathbb{E}_{\theta_t \sim \text{Beta}(1, \tau-1)} [\theta_t^D] \end{aligned}$$

now, by using the equality $\mathbb{E}[x^D] = \prod_{r=0}^{D-1} \frac{\alpha+r}{\alpha+\beta+r}$ for the D -th raw moment of a Beta(α, β) distribution [54]

$$\begin{aligned} &= 1 - \left(1 - \prod_{r=0}^{D-1} \frac{1+r}{\tau+r} \right)^m \\ &= 1 - \left(1 - \frac{1}{\tau} \cdot \frac{2}{\tau+1} \cdot \dots \cdot \frac{D}{\tau+D-1} \right)^m \\ &= 1 - \left(1 - \frac{D! \tau!}{(\tau+D-1)!} \right)^m \end{aligned}$$

We discussed in Section 4.3 that the PestControl benchmark obtains a good solution at $\mathbf{x} = \mathbf{5}$. One could assume that BODi performs well on this benchmark because its dictionary will likely contain this point. However, we observe that the probability is effectively zero for $\tau = 5$, $m = 128$, and $D = 25$ (see Figure 17), which are the choices for the PestControl benchmark in Deshwal et al. [21]. This raises the question of (i) whether our hypothesis is wrong and (ii) what the reason for BODi’s performance degradation on the PestControl benchmark is.

We show that BODi’s reference implementation differs from the algorithmic description in an important detail, causing BODi to be considerably more likely to sample category five on PestControl (or the “last” category for arbitrary benchmarks) than any other category.

⁷See https://github.com/aryandeshwal/bodi/blob/aa507d34a96407b647bf808375b5e162ddf10664/bodi/categorical_dictionary_kernel.py#L18

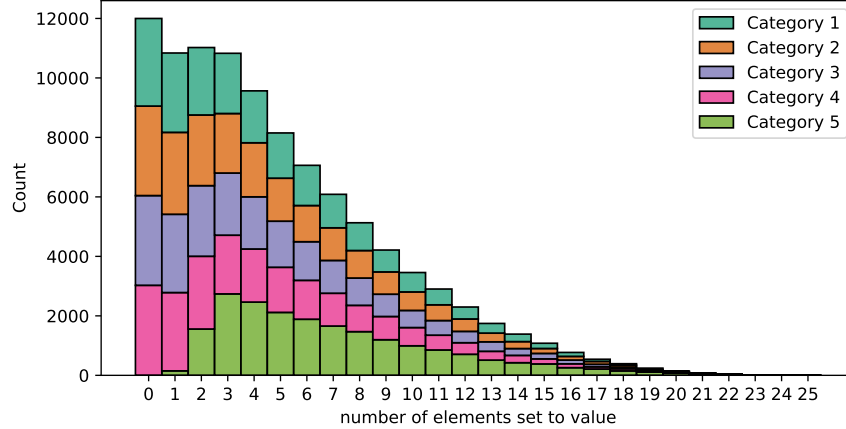


Figure 18: Histograms over the number of dictionary element entries set to each category for 20,000 repetitions of the sampling of dictionary elements for the `PestControl` benchmark. For each of the five categories and each value on the x -axis, the figure shows how often the number of entries in a dictionary element equals the value on the x -axis for the given category. For example, the count for $x = 0$ and category 5 is zero, indicating that all 20,000 dictionary points had at least one entry ‘5’. There is a considerably higher chance for a dictionary element entry to be set to category five than to any of the other categories.

Figure 18 shows five histograms over the number of dictionary elements set to each category. The values on the x -axis give the number of elements in a 25-dimensional categorical vector being set to a specific category. One would expect that the histograms have a similar shape regardless of the category. However, for category 5, we see that more elements are set to this category than for the other categories: The probability of k elements being set to category 5 is almost twice as high as the probability of being set to another category for $k \geq 3$. In contrast, the probability that no element in the vector belongs to category 5 is virtually zero. This behavior is beneficial for the `PestControl` benchmark, which obtained the best value found during our experiments for $x^* = (5, 5, \dots, 5, 1)$ (see Section 4). While we see that the probability of each dictionary entry being set to category 5 is very low, we assume that we sample sufficiently many dictionary elements within a small Hamming distance to the optimizer such that BODi’s GP can use this information to find the optimizer.

The reason for oversampling of the last category lies in a rounding issue in sampling dictionary elements. In particular, for a given dictionary element a_i and a corresponding vector θ with $|\theta| = \tau$, for each $i \in \{1, 2, \dots, \tau - 1\}$, Deshwal et al. [21] set $\lfloor D\theta_i \rfloor$ elements to category i . The remaining $D - \sum_{i=1}^{\tau-1} \lfloor D\theta_i \rfloor$ elements are then set to category τ . This causes the last category to be overrepresented in the dictionary elements. For the choices of the `PestControl` benchmark, $D = 25$ and $\tau = 5$, the first four categories had a probability of ≈ 0.1805 . In contrast, the last one had a probability of ≈ 0.278 for 10^8 simulations⁸. We assume that the higher probability of the last category is the reason for the performance difference between the modified and the unmodified version of the `PestControl` benchmark.

D.2 COMBO on categorical problems

On the categorical `PestControl` benchmark, we could observe a similar behavior for COMBO [56] as for BODi.

⁸The 95% confidence intervals for categories 1–5 are (0.1799, 0.1807), (0.1802, 0.1810), (0.1803, 0.1811), (0.1801, 0.1809), (0.2775, 0.2783). Pairwise Wilcoxon signed-rank tests between categories 1–4 and category 5 gives p values of 0 ($W \approx 4.7 \cdot 10^{10}$ each).

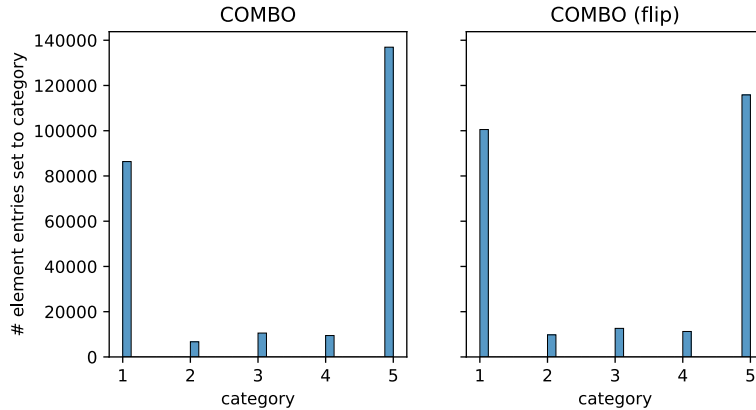


Figure 19: Histograms over the number of dictionary element entries set to each category for 20,000 repetitions of the sampling of dictionary elements for the `PestControl` benchmark. The histogram shows how many element entries of a 25-dimensional dictionary element are set to each of the five categories. There is a considerably higher chance for a dictionary element entry to be set to category 1 or 5 than to one of the other categories.

Figure 19 shows the histograms over the number of dictionary elements set to each category for both the modified and the unmodified version of the `PestControl` benchmark. We see that the first and the last categories are over-represented on both benchmark versions. As discussed in Section 4, this benchmark attains its best value for $\mathbf{x}^* = (5, 5, \dots, 5, 1)$. Therefore, it seems unexpected that COMBO sets so many entries to category 1 for the unmodified benchmark version. For the modified benchmark version, this is entirely unexpected as the optimizer has a random structure. Here, one would expect the histogram to be uniform.

We argue that this behavior is at least partially caused by implementation error in the construction of the adjacency matrix and the Laplacian for categorical problems⁹. This error causes categorical variables to be modeled like ordinal variables. According to Oh et al. [56], categorical variables are modeled as a complete graph (see Figure 20).

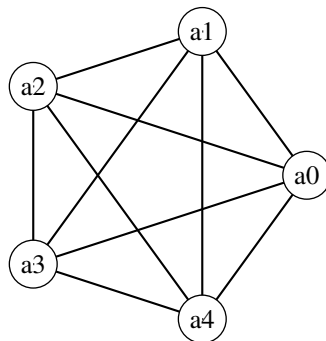


Figure 20: A categorical variable with five categories is modeled as a complete graph.

However, we find the adjacency matrix for the first category of a categorical variable with five categories is constructed as

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix},$$

⁹https://github.com/QUVA-Lab/COMBO/blob/9529eabb86365ce3a2ca44fff08291a09a853ca2/COMBO/experiments/test_functions/multiple_categorical.py#L137, last access: 2023-04-26

which is the adjacency matrix for a five-vertex path graph. We assume the search space has boundaries due to treating categorical variables as ordinal variables. Due to the high dimensionality of the search space, COMBO visits the boundaries of the search space more often than the interior.