



Bayesian optimization for mixed-variable, multi-objective problems

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Abstract

Optimizing multiple, non-preferential objectives for mixed variable, expensive black-box problems is important in many areas of engineering and science. The expensive, noisy, black-box nature of these problems makes them ideal candidates for Bayesian optimization (BO). mixed variable and multi-objective problems, however, are a challenge due to BO's underlying smooth Gaussian process surrogate model. Current multi-objective BO algorithms cannot deal with mixed variable problems. We present MixMOBO, the first mixed variable, multi-objective Bayesian optimization framework for such problems. Using MixMOBO, optimal Pareto-fronts for multi-objective, mixed variable design spaces can be found efficiently while ensuring diverse solutions. The method is sufficiently flexible to incorporate different kernels and acquisition functions, including those that were developed for mixed variable or multi-objective problems by other authors. We also present HedgeMO, a modified Hedge strategy that uses a portfolio of acquisition functions for multi-objective problems. We present a new acquisition function, SMC. Our results show that MixMOBO performs well against other mixed variable algorithms on synthetic problems. We apply MixMOBO to the real-world design of an architected material and show that our optimal design, which was experimentally fabricated and validated, has a normalized strain energy density 10^4 times greater than existing structures.

Keywords Bayesian optimization · Mixed variables · Multi-objective · MixMOBO · HedgeMO · Architected meta-materials

1 Introduction

Optimization is an inherent part of design for complex physical systems. Often optimization problems are posed as noisy black-box problems subject to constraints, where each function call requires an extremely expensive computation or a physical experiment. Many of these problems require optimizing a mixed variable design space (combinatorial, discrete, and continuous) for multiple non-preferential objectives. Architected material design (Frazier and Wang 2015; Chen et al. 2018a, 2019; Shaw et al. 2019; Song et al. 2019a; Vangelatos et al. 2021), hyper-parameter tuning for machine learning algorithms (Snoek et al. 2012; Chen et al. 2018b; Oh et al. 2018), drug design (Pyzer-Knapp 2018; Korovina et al. 2020), fluid machinery (Sheikh et al. 2021, 2022a, b)

and, controller sensor placement (Krause et al. 2008) pose such problems. Due to their cost of evaluation, Bayesian optimization is a natural candidate for their optimization.

Much research has gone into Bayesian optimization for continuous design spaces using Gaussian processes (GP) as a surrogate model and efficiently optimizing this design space with a minimum number of expensive function calls (Mockus 1994; Rasmussen and Williams 2006; Brochu et al. 2010). Despite the success of continuous variable Bayesian optimization strategies, multi-objective and mixed variable problems remain an area of open research. The inherent continuous nature of GP makes dealing with mixed variable problems challenging. Finding a Pareto-front for multi-objective problems, and parallelizing function calls for batch updates, Q-batch, also remain challenges in the sequential setting of the BO algorithm. Hedge strategies, which use a portfolio of acquisition functions to reduce the effect of choosing a particular acquisition function, have not been formulated for multi-objective problems.

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1.1 Mixed variable BO algorithms

We provide a brief description of the current approaches in recent studies for dealing with mixed variables.

One Hot Encoding Approach Most BO schemes use Gaussian processes as surrogate models. When dealing with categorical variables, a common method is ‘one-hot encoding’ (Golovin et al. 2017). Popular BO packages, such as GPyOpt and Spearmint (Snoek et al. 2012), use this strategy. However, this can result in inefficiency when searching the parameter space because the surrogate model is continuous. For categorical variables, this approach also leads to a quick explosion in dimensional space (Ru et al. 2020).

Multi-Armed Bandit (MAB) Approach Some studies use the MAB approach when dealing with categorical variables where a surrogate surface for continuous variables is defined for each bandit arm. These strategies can be expensive in terms of the number of samples required (Gopakumar et al. 2018; Nguyen et al. 2019), and they do not share information across categories. An interesting approach, where coupling is introduced between continuous and categorical variables, is presented in the CoCaBO algorithm (Ru et al. 2020), and it is one of the baselines that we test MixMOBO against.

Latent Space Approach A latent variable approach has also been proposed to model categorical variables (Qian et al. 2008; Zhou et al. 2011; Zhang et al. 2020; Deshwal and Doppa 2021). This approach embeds each categorical variable in a Z latent variable space. However, the embedding is dependent on the kernel chosen, and for small-data settings can be inefficient.

Modified Kernel Approach There is a rich collection of studies in which the underlying kernel is modified to work with ordinal or categorical variables. For example, (Ru et al. 2020) considers the sum + product kernel; (Deshwal et al. 2021) proposes hybrid diffusion kernels, HyBO; and (Oh et al. 2021) proposes frequency modulated kernels. The BOCS algorithm (Baptista and Poloczek 2018) for categorical variables uses a scalable modified acquisition function. (Pelamatti et al. 2018; Oh et al. 2019; Nguyen et al. 2019; Garrido-Merchán and Hernández-Lobato 2020) all use modified kernels to adapt the underlying surrogate surface. Our approach is unique in that any modified kernel can be incorporated into our framework. Currently we use the modified radial basis function (RBF) kernel for modelling the surrogate surface, with our future research focused on using different kernels in our framework.

Other Surrogate Models Other surrogate models can be used in place of the GP to model mixed variable problems such as random forests, an approach used by SMAC3 (Lindauer et al. 2021) or tree-based estimators, used in

the Tree-Parzen Estimator (TPE) (Bergstra et al. 2013). Daxberger et al. (2020) considers a linear model with cross-product features. BORE (Tiao et al. 2021) leverages the connection to density ratio estimation.

1.2 Multi-objective BO algorithms

Multi-objective Bayesian optimization (MOBO) has been the subject of some recent studies. BoTorch (Balandat et al. 2020), the popular BO framework, uses the EHVI and ParEGO based on the works of Fonseca et al. (2006) and (Daulton et al. 2020, 2021). Hyper-volume improvement is the main mechanism used to ensure diversity in generations. ‘ Q -batch’ parallel settings of the above two acquisition functions use hyper-volume improvement and the previously selected point in the same batch to choose the next set of points. For most single-objective BO algorithms with parallel batch selection, the next batch of test points is selected by adding the ‘fantasy’ cost function evaluation, usually the predicted mean, to the previously selected test point within that batch. However, this commonly used method often leads to overly confident test point selection, and the surrogate surface then needs to be optimized, and sometimes refitted Q times. Using a genetic algorithm (GA), we can select a ‘ Q -batch’ of points with a single optimization of the surrogate surface from the GA generation.

Suzuki et al. (2020) provide an interesting Pareto-frontier entropy method as an acquisition function, and (Shu et al. 2020) use Pareto-frontier heuristics to formulate new acquisition functions. Their approaches were not extended to mixed variable problems.

1.3 Hedge strategies

Hedge algorithms have proven to be efficient in dealing with a diverse set of problems using a portfolio of acquisition functions. ‘GP-Hedge’, introduced by Brochu et al. (2011) is a well-known and efficient algorithm. However, current Hedge algorithms have not been extended for multi-objective problems and, to the authors’ knowledge, there is no existing Hedge strategy implementation that solves such problems.

2 MixMOBO

In this paper, we present a mixed variable, Multi-Objective Bayesian Optimization (MixMOBO) algorithm, the first generalized framework that can deal with mixed variable, multi-objective problems in small-data setting and can optimize a noisy black-box function with a small number of function calls.

Genetic algorithms, such as NSGA-II (Deb et al. 2002), are well-known for dealing with mixed variable spaces and finding an optimal Pareto-frontier. However, these algorithms require a large number of black-box function calls and are not well-suited to expensive small-data problems. Our approach is to use a GA to optimize the surrogate model itself and find a Pareto-frontier. Diversification is ensured by the distance metrics used while optimizing the surrogate model. This method allows cheap Q-batch samples from within the GA generation, and also allows the use of commonly used acquisition functions such as Expected Improvement (EI), Probability of Improvement (PI) and Upper Confidence Bound (UCB) (Brochu et al. 2011), which work well for single-objective problems. We note here that other metrics can easily be incorporated instead of a distance metric within the GA setting and is one of the areas of our future work. Using a GA on a mixed variable surrogate model in a multi-objective setting allows us to work with modified kernels that were developed for mixed variable problems in literature. We also present a new acquisition function, ‘Stochastic Monte-Carlo’ (SMC), which performs well for multi-objective categorical variable problems (Vangelatos et al. 2021).

Hedge strategies for Bayesian optimization are efficient for single-objective algorithms. We present here our Hedge Multi-Objective (HedgeMO) algorithm, which uses a portfolio of acquisition functions for multi-objective problems and can work with Q-batch updates. It is an extension of GP-Hedge (Brochu et al. 2011), which has regret bounds, and the same bounds hold for HedgeMO.

We note here that MixMOBO is designed for mixed variable, multi-objective problems. Although there are algorithms in the literature that can solve problems with a *subset* of these attributes (e.g., mixed variable single-objective or multi-objective continuous variable problems), no algorithm, to our knowledge, can deal with all of these attributes. In addition, MixMOBO outputs a batch of query points and uses HedgeMO, the first multi-objective hedging strategy. To the authors’ knowledge, no existing approaches can achieve all this within a single framework.

In summary, the main contributions of our work are as follows:

- We present mixed variable, Multi-Objective Bayesian Optimization (MixMOBO), the first algorithm that can deal with mixed variable, multi-objective problems. The framework uses GA to optimize the acquisition function on a surrogate surface, so it can use modified kernels or surrogate surfaces developed to deal with mixed variable problems in previous studies. This extends the capabilities of previous approaches in literature to handle mixed variable and multi-objective problems as well if adopted within our framework, since our framework is agnostic to the underlying GP kernel over mixed variables.

- GA is used to optimize surrogate models, which allows the optimization of multi-objective problems. ‘Q-batch’ samples can be extracted in parallel from within the GA generation without sacrificing diversification.
- We present a Hedge Multi-Objective (HedgeMO) strategy for multiple objectives for which regret bounds hold. We also present an acquisition function, Stochastic Monte-Carlo (SMC), which performs well for combinatorial multi-objective problems, and use it as part of our HedgeMO portfolio.
- We benchmark our algorithm against other mixed variable algorithms and prove that MixMOBO performs well on test functions. We applied MixMOBO to a practical engineering problem: the design of a new architected meta-material that was optimized to have the maximum possible strain energy density within the constraints of a design space. The fabrication and testing of this new material showed that it has a normalized strain energy density that is 10^4 times greater than existing unblemished microlattice structures in literature.

The rest of the paper is organized in the following manner: Sect. 3 defines the optimization problem to be solved with MixMOBO. The detailed workings of MixMOBO and HedgeMO are presented in Sect. 4. Section 5 details the validation tests performed on our framework to test its efficiency and comparison to existing algorithms. Our application of MixMOBO for design of architected materials and its results are presented in Sect. 6.

3 MixMOBO problem statement

We pose the multi-objective and mixed variable problem as:

$$\vec{w}_{opt} = \operatorname{argmax}_{\vec{w} \in \mathcal{W}} (\vec{f}(\vec{w})) \quad (1)$$

for maximizing the objective. Here $\vec{f}(\vec{w}) = [f_1(\vec{w}), f_2(\vec{w}), \dots, f_K(\vec{w})]$ are the K non-preferential objectives to be maximized, and \vec{w} is a mixed variable vector, defined as $\{\vec{w} \in \mathcal{W}\} = \{\vec{x} \in \mathcal{X}, \vec{y} \in \mathcal{Y}, \vec{z} \in \mathcal{Z}\}$. \vec{x} is an m -dimensional vector defined over a bounded set $\mathcal{X} \subset \mathbb{R}^m$ representing m continuous variables. Ordinal and categorical variables are defined as $\vec{y} = [y_1, \dots, y_n]$ and $\vec{z} = [z_1, \dots, z_o]$, respectively. Each variable $y_j \in \{O_1, \dots, O_j\}$ takes one of O_j ordinal ‘levels’ (discrete numbers on the real-number line) and each categorical variable takes a value $z_j \in \{C_1, \dots, C_j\}$ from C_j unordered categories (that cannot, by definition, be ordered on the real-number line). \mathcal{Y} and \mathcal{Z} are the ordinal and combinatorial spaces, respectively.

Generally, $\{\vec{w}_{opt}\}$ is a set of Pareto-optimal solution vectors i.e., vectors that are not Pareto-dominated by any

other vector. A vector \vec{w} is Pareto-dominated by \vec{w}' , iff $f_k(\vec{w}) \leq f_k(\vec{w}') \forall k = 1, \dots, K$. This $\{\vec{w}_{opt}\}$ is the optimal set found by MixMOBO, details of which are presented in the following section.

4 Methodology

4.1 Preliminaries

Single-objective Bayesian optimization is a sequential optimization technique, aimed at finding the global optimum of a single-objective noisy black-box function f with minimum number of evaluations of f . For every i th iteration, a surrogate model, g , is fit over the existing data set $\mathcal{D} = \{(w_1, f(w_1)), \dots, (w_i, f(w_i))\}$. An acquisition function then determines the next point \vec{w}_{i+1} for evaluation with f , balancing exploration and exploitation. Data are appended for the next iteration, $\mathcal{D} = \mathcal{D} \cup (w_{i+1}, f(w_{i+1}))$, and the process is repeated until the evaluation budget for f or the global optimum is reached.

Gaussian processes are often used as surrogate models for BO (Rasmussen and Williams 2006; Murphy 2012). A GP is defined as a stochastic process such that a linear combination of a finite set of the random variables is a multivariate Gaussian distribution. A GP is uniquely specified by its mean $\mu(\vec{w})$ and covariance function $ker(\vec{w}, \vec{w}')$. The GP is a distribution over functions, and $g(\vec{w})$ is a function sampled from this GP:

$$\vec{g}(\vec{w}) \sim GP(\mu(\vec{w}), ker(\vec{w}, \vec{w}')). \quad (2)$$

Here, $ker(\vec{w}, \vec{w}')$ is the covariance between input variables \vec{w} and \vec{w}' . Once a GP has been defined, at any \vec{w} the GP returns the mean $\mu(\vec{w})$ and variance $\sigma(\vec{w})$. The acquisition function $\mathcal{A}(\vec{g})$, balances exploration and exploitation, and is optimized to find the next optimal point \vec{w}_{i+1} . The success of BO comes from the fact that evaluating \vec{g} is much cheaper than evaluating \vec{f} .

4.2 MixMOBO approach

Our mixed variable Multi-Objective Bayesian Optimization (MixMOBO) algorithm extends the single-objective, continuous variable BO approach presented in the preceding section, to more generalized optimization problems and is detailed in Algorithm 1.

A single noisy GP surrogate surface is fit for multiple objectives, $\vec{g}(\vec{w}) \sim GP(\vec{\mu}(\vec{w}), ker(\vec{w}, \vec{w}'))$. Note that this is different from Eq. 2, since the GP would predict mean for multiple objectives. For details on fitting a single GP to multi-objective data, we refer the reader to (Rasmussen and Williams 2006, Eq. 2.25–2.26). For multiple objectives, the response vector, with n -data points, is of size $k \times n$. The predicted

variance remains the same, but the predicted mean is a $k \times 1$ vector. This is equivalent to fitting K GP surfaces with the same kernel for all of the surfaces, where K is the total number of objectives. All K objectives are assumed to have equal noise levels. Only one set of hyper-parameters needs to be fit over this single surface, rather than fitting K sets of hyper-parameters for K different surfaces; thus, when K is large, the overall computational cost for the algorithm is reduced. Note that we could fit K different GP surfaces, particularly if different noise levels for different objectives is to be considered, with different hyper-parameters to the data to add further flexibility to the fitted surfaces. This idea will be investigated in our future work. We use LOOCV (Murphy 2012) for estimating hyper-parameters since we are dealing with small-data problems.

Algorithm 1 Mixed-variable Multi-Objective Bayesian Optimization (MixMOBO) Algorithm

-
- 1: **Input:** Black-box function $\vec{f}(\vec{w}) : \vec{w} \in \mathcal{W}$, initial data set size N_i , batch points per epoch Q , total epochs N , mutation rate $\beta \in [0, 1]$
 - 2: **Initialize:** Sample black-box function \vec{f} for $\mathcal{D} = \left\{ \left(\vec{w}_j, \vec{f}(\vec{w}_j) \right) \right\}_{j=1:N_i}$
 - 3: **for** $n = 1$ **to** N **do**
 - 4: Fit a noisy Gaussian process surrogate function $\vec{g}(\vec{w}) \sim GP(\vec{\mu}(\vec{w}), ker(\vec{w}, \vec{w}'))$
 - 5: For L total acquisition functions, from each \mathcal{A}^l acquisition function, propose Q -batch test-points, $\{(\vec{u}_n^l)_{1:Q} = \{argmax_{\vec{u} \in \mathcal{W}, \mathcal{A}^l(\vec{g})\}_{1:Q}}\}$ within the constrained search space \mathcal{W} using multi-objective GA
 - 6: Mutate point $\{(\vec{u}_n^l)_{1:Q}\}$ within the search space \mathcal{W} with probability rate β if L_2 -norm of its difference with any other member in set $\{(\vec{u}_n^l)_{1:Q}\}$ is below tolerance
 - 7: Select batch of Q points using HedgeMO, $\{\vec{w}_n\}_{1:Q} = HedgeMO(\vec{g}, \{(\vec{u}_n^l)_{1:Q}\}_{1:Q}, \mathcal{D})$
 - 8: Evaluate the selected points from the black-box function, $\{\vec{f}(\vec{w}_n)\}_{1:Q}$
 - 9: Update $\mathcal{D} = \mathcal{D} \cup \left\{ \left(\vec{w}_n, \vec{f}(\vec{w}_n) \right) \right\}_{1:Q}$
 - 10: **end for**
 - 11: **return** Pareto-optimal solution set $\left\{ \left(\vec{w}_{opt}, \vec{f}(\vec{w}_{opt}) \right) \right\}$
-

Gaussian processes are defined for continuous variables. For mixed variables, we need to adapt the kernel so that a GP can be fit over these variables. Cited works in Sect. 1 dealt with modified kernels that were designed to model mixed variables. Those kernels can be used in the MixMOBO algorithm. For the current study, we use a simple modified squared exponential kernel:

$$ker(\vec{w}, \vec{w}') \equiv e_f^2 \exp \left[-\frac{1}{2} |\vec{w}, \vec{w}'|_C^T M |\vec{w}, \vec{w}'|_C \right], \quad (3)$$

where $\vec{\theta} = (\{M\}, \epsilon_f)$ is a vector containing all the hyperparameters, $\{M\} = \text{diag}(\vec{h})^{-2}$ is the covariance hyperparameter matrix and \vec{h} is the vector of covariance lengths. The distance metric, $|\vec{w}, \vec{w}'|_C$, is an concatenated vector, with the distance between categorical variables defined to be the Hamming distance, and the distance between continuous variables and the distance between ordinal variables defined to be their Euclidean distances. Noise is added to the diagonal of the covariance matrix. We emphasize that *any* modified kernel discussed in the citations of Sect. 1 can be used within our framework and is a focus of our future work.

Once the GP is fit over multi-objective data, acquisition functions, \mathcal{A}^l , explore the surrogate model to maximize reward by balancing exploration and exploitation. Using a standard optimization scheme is problematic when dealing with mixed variable and multi-objective problems due to non-smooth surrogate surface and conflicting objectives. We propose using a constrained, multi-objective GA to optimize the acquisition functions, which, although expensive to use on an actual black-box function, is an ideal candidate for optimizing the acquisition function working on the surrogate surface. For multi-objective problems, multi-objective GA algorithms, such as Deb et al. (2002), are ideal candidates for obtaining a Pareto-front of optimal solutions.

Within a GA generation, for multi-objectives, diversification is ensured by a ‘distance crowding function’ which ranks the members of a non-dominated Pareto-front. The ‘distance crowding function’ can be computed in decision variable space, in function space or a hybrid of the two, and ensures that the generations are distinct and diverse. This inherent feature of GA is exploited to ensure diversity in the ‘ Q -batch’ of points. The ranking takes place when choosing the test points from an acquisition function for a multi-objective problem because the choice must take into account the diversity of the solution and propagate the Pareto-front. Because the members of the population are ranked by the GA, we can easily extract a ‘ Q -batch’ of points from each of the acquisition functions without needing to add any ‘fantasy’ cost function evaluations or optimizing the acquisition functions again. This is a great advantage of using GA as our optimizer since we can output a ‘ Q -batch’ of diverse query points using the inherent GA features.

For dealing with mixed variable problems, GA are again ideal candidates. Genetic algorithms (GA) can be easily be constrained to work in mixed variable spaces. These variables can be dealt with using probabilistic mutation rates. The genes are allowed to mutate within their prescribed categories, thereby constraining the proposed test points to the \mathcal{W} space.

Common acquisition functions, such as EI, PI, and UCB, can be used within this framework and can be used to nominate a ‘ Q -batch’ of points. If a candidate in a Q -batch is within the tolerance limit of another candidate in the same batch or a previous data point (for convex

functions), we mutate the proposed point within \mathcal{W} to avoid sampling the same data point again.

Test points are selected from \mathcal{W} to evaluate their \vec{f} using HedgeMO algorithm which is detailed in the next section. HedgeMO selects a ‘ Q -batch’ of test points from the candidates proposed by each of the acquisition functions. These points are then, along with their function evaluations \vec{f} s, appended to the data set.

4.3 HedgeMO Algorithm

Hedge strategies use a portfolio of acquisition functions, rather than a single acquisition function. It is an extension to multi-objective problems of GP-Hedge algorithm proposed by Brochu et al. (2011). HedgeMO is part of our MixMOBO algorithm that not only extends the Hedge strategy to multi-objective problems, but also allows ‘ Q -batches’. Our algorithm is shown in Algorithm 2.

Algorithm 2 HedgeMO Algorithm

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- 1: **Input:** Surrogate function $\vec{g}(\vec{w}) : \vec{w} \in \mathcal{W}$, proposed test points by AFs $(\{(\vec{u})_{1:L}^{1:n}\}_{1:Q})$, batch points per epoch Q , current epoch n , total objective K , parameter $\eta \in \mathcal{R}^+$
 - 2: **for** $l = 1$ **to** L **do**
 - 3: For l^{th} acquisition function, find rewards for Q -batch points nominated by that AF from epochs $1:n-1$, by sampling from \vec{g} ,

$$\left\{ \vec{\theta}_{1:n-1}^l \right\}_{1:Q} = \vec{\mu}(\{(\vec{u})_{1:L}^{1:n-1}\}_{1:Q}), \text{ where } \vec{\theta} = \{\theta\}^k \text{ for each objective } k$$
 - 4: **end for**
 - 5: Normalize rewards for each l^{th} AF and k^{th} objective,

$$\phi_l^k = \sum_{j=1}^{n-1} \sum_{q=1}^Q \frac{\{\theta_j^l\}_q^k - \min(\Theta)}{\max(\Theta) - \min(\Theta)}, \text{ where } \Theta \text{ is defined as}$$

$$\Theta = \{\theta_{1:n-1}^{1:L}\}_{1:Q}^k$$
 - 6: Calculate probability for selecting nominees from l^{th} acquisition function, $p^l = \frac{\exp(\eta \sum_{k=1}^K \phi_l^k)}{\sum_{i=1}^L \exp(\eta \sum_{k=1}^K \phi_i^k)}$
 - 7: **for** $q = 1$ **to** Q **do**
 - 8: Select q^{th} nominee as test-point \vec{w}_n^q from l^{th} AF with probability p^l
 - 9: **end for**
 - 10: **return** Batch of test points $\{\vec{w}_n\}_{1:Q}$
-

Extending the methodology presented by Brochu et al. (2011), HedgeMO chooses the next ‘ Q -batch’ of test points from the history of the candidates nominated by all of the acquisition functions. Rewards are calculated for each acquisition function from the surrogate surface for the entire history of the nominated points by the L acquisition functions. The rewards are then normalized to scale them to the same range for each objective. This step is fundamentally

important because it prevents biasing the probability of any objective. This type of bias, of course, cannot occur in single-objective problems. The rewards for different objectives k are then summed and the probability, p^l , of choosing a nominee from a specific acquisition function is calculated using step 6 in Algorithm 2. For a ‘ Q -batch’ of test points, the test points are chosen Q times.

Regret Bounds The regret bounds derived by Brochu et al. (2011) hold for HedgeMO if and only if the Upper Confidence Bound (UCB) acquisition function is a part of the portfolio of acquisition functions. The regret bounds follow from the work of Srinivas et al. (2012) who derived cumulative regret bounds for UCB. In essence, the cumulative regret in our case is bounded by two sublinear terms as for UCB and an additional term which depends on proximity of the chosen point with the test point proposed by UCB. The interested reader is directed to Srinivas et al. (2012) and Brochu et al. (2011) for a description of the exact regret bounds and their derivation.

4.4 SMC acquisition function

We introduce a new acquisition function, Stochastic Monte-Carlo (SMC), which for the maximization of an objective, is defined as:

$$SMC \equiv \operatorname{argmax}_{\vec{w} \in \mathcal{W}} [\tilde{\mu}(\vec{w}) + r(\vec{w})], \quad (4)$$

where $r(\vec{w})$ is sampled from $U(0, 2\sigma(\vec{w}))$, and $\tilde{\mu}(\vec{w})$ and $\sigma(\vec{w})$ are the mean and standard deviation returned by the GP at \vec{w} , respectively. This is equivalent to taking Monte-Carlo samples from a truncated distribution. For categorical and ordinal variable problems, this acquisition function performs well across a range of benchmark tests (Vangelatos et al. 2021). We use this acquisition function as part of our portfolio of HedgeMO in the MixMOBO algorithm.

5 Validation tests

MixMOBO is designed to deal with mixed variable, multi-objective problems. However, no other small-data algorithm, to the authors’ knowledge, can similarly deal with all the attributes of such problems to provide an honest comparison. In the absence of such competition, we use the specific case of mixed variable, single-objective problems to provide a comparison to state-of-the-art algorithms present for such problems and prove that even for this subset case, MixMOBO is able to perform better than existing algorithms in the literature. We then perform further experiments in both single and multi-objective settings to show the efficacy of the HedgeMO algorithm compared to stand-alone acquisition functions and the performance of SMC in the multi-objective setting.

We benchmarked MixMOBO against a range of existing state-of-the-art optimization strategies that are commonly used for optimizing expensive black-box functions with mixed variable design spaces. We chose the following single-objective optimization algorithms for comparison: **CoCaBO** (Ru et al. 2020), which combines the multi-armed bandit (MAB) and Bayesian optimization approaches using a mixing kernel. CoCaBO has been shown to be more efficient than GPyOpt (one-hot encoding approach (GPyOptAuthors 2016)) and EXP3BO (multi-armed bandit (MAB approach (Gopakumar et al. 2018))). We used CoCaBO with a mixing parameter of 0.5. We also tested MixMOBO against **GBRT**, a sequential optimization technique using gradient boosted regression trees (Scikit-learn 2021). **TPE_Hyperopt** (Tree-structured Parzen Estimator) is a sequential method for optimizing expensive black-box functions, introduced by Bergstra et al. (2011). **SMAC3** is a popular Bayesian optimization algorithm in combination with an aggressive racing mechanism (Hutter et al. 2011). Both of these algorithms, in addition to **Random Sampling**, were used as baselines. Publicly available libraries for these algorithms were used.

Six different test functions for mixed variables were chosen as benchmarks. A brief description of these test functions and their properties is given below with further details in Appendix A:

Contamination problem This problem, introduced by Hu et al. (2011), considers a food supply chain with various stages in the chain where food may be contaminated with pathogens. The objective is to maximize the reward of prevention efforts while making sure the chain does not get contaminated. It is widely used as a benchmark for binary categorical variables. We use the problem as a benchmark with 21 binary categorical variables.

Encrypted Amalgamated An anisotropic, mixed variable function created using a combination of other commonly used test functions (Tušar et al. 2019). We modify the combined function so that it can be used with mixed variables. In particular, it is adapted for categorical variables by encrypting the input space with a random vector, which produces a random landscape mimicking categorical variables (Vangelatos et al. 2021). Our Encrypted Amalgamated function has 13 inputs: 8 categorical, 3 ordinal variables (with 5 categories or states each) and 2 continuous.

NK Landscapes This is a popular benchmark for simulating categorical variable problems using randomly rugged, interconnected landscapes (Kauffman and Levin 1987; Li et al. 2006). The fitness landscape can be produced with random connectivity and number of optima. The problem is widely used in evolutionary biology and control optimization and is *NP*-complete. The probability of connectivity between *NK* is controlled by a ‘ruggedness’ parameter, which we set at 20%. We test the Li et al. (2006) variant with 8 categorical variables with 4 categories each.

Rastrigin This is an isotropic test function, commonly used for continuous design spaces (Tušar et al. 2019). We use a 9-D Rastrigin function for testing a design space of 3 continuous and 6 ordinal variables with 5 discrete states.

Encrypted Syblinski-Tang This function is isotropic (Tušar et al. 2019), and we have modified it as we did with the Encrypted Amalgamated test function so that it can work with categorical variables and was used as a representative benchmark for N -categorical variable problems. The 10-D variant tested here consists only of categorical variables with 5 categories each.

Encrypted ZDT6 This is a multi-objective test function introduced by Zitzler et al. (2000) that we modified with encryption so that it can deal with mixed variables. The test function is non-convex and non-uniform in the parameter space. We test ZDT6 with 10 categorical variables with 5 states each. ZDT6 was only used for testing HedgeMO.

To the extent of our knowledge, no other optimization algorithm is capable of handling mixed variable, multi-objective problems in small-data settings. Thus, we have no direct comparisons between MixMOBO and other published algorithms. Therefore, we tested MixMOBO against a variant of NSGA-II (Deb et al. 2002) with the ZDT4 and ZDT6 test functions with mixed variables. However, we found that using a GA required more than 10^2 more function calls to find the Pareto-front to a similar tolerance. For visualization purposes, we do not plot the GA results.

All of the optimization algorithms were run as maximizers, with a 0.005 noise variance built into all the benchmarks. The budget for each benchmark test was fixed at 250 function calls including the evaluations of 50 initial randomly sampled data points for all algorithms, except for SMAC3 which determines its own initial sample size. The algorithms were run in single output setting (GBRT, CoCaBO and MixMOBO's batch mode

was not used for fair comparison). Each algorithm was run 10 times for every benchmark. Our metric for optimization is the 'Normalized Reward', defined as $(\text{current optimum} - \text{random sampling optimum})/(\text{global optimum} - \text{random sampling optimum})$. Figure 1 shows the Normalized Rewards versus the number of black-box function evaluations for MixMOBO and five other algorithms. The mean and standard deviation of the Normalized Rewards of the 10 runs for each algorithm, along with their standard deviations (S.D.), are plotted. The width of each of the translucent colored bands is equal to 1/5 of their S.D.

MixMOBO outperforms all of the other baselines and is significantly better in dealing with mixed variable problems. GBRT is the next best algorithm and performs better than MixMOBO on the Rastrigin function; however, note that the Rastrigin function does not include any categorical variables. For problems involving categorical variables, MixMOBO clearly outperforms the others. TPE and CoCaBO have similar performances, and SMAC3 has the poorest performance. All three are outdistanced by MixMOBO.

We then perform experiments to test the performance of our HedgeMO algorithm by comparing it to four different acquisition functions which make up the entirety of its portfolio. These acquisition functions, namely, EI, PI, UCB, and SMC, along with HedgeMO are tested on three different test functions: the Encrypted Amalgamated, Encrypted Syblinski-Tang, and Encrypted ZDT6. The latter is used as the multi-objective test function. The Normalized Reward for the multi-objective Encrypted ZDT6 is defined as $(\text{current } P\text{-optimum} - \text{random sampling } P\text{-optimum})/(\text{global } P\text{-optimum} - \text{random sampling } P\text{-optimum})$. Here, $P\text{-optimum} = \frac{1}{N} \sum_{i=1}^N \exp(-\text{minimum Hamming distance in parameter space between } i\text{th global Pareto-optimal point and any point in the current Pareto-optimal set})$, where N is the number of global Pareto-optimal points.

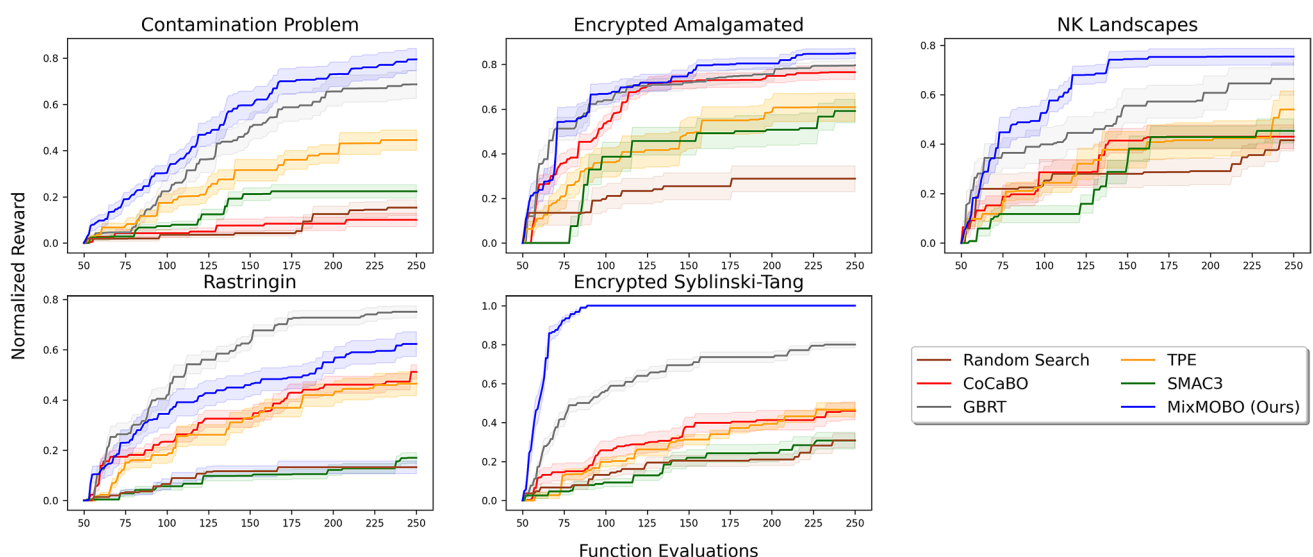


Fig. 1 Performance comparison of MixMOBO against other mixed variable algorithms

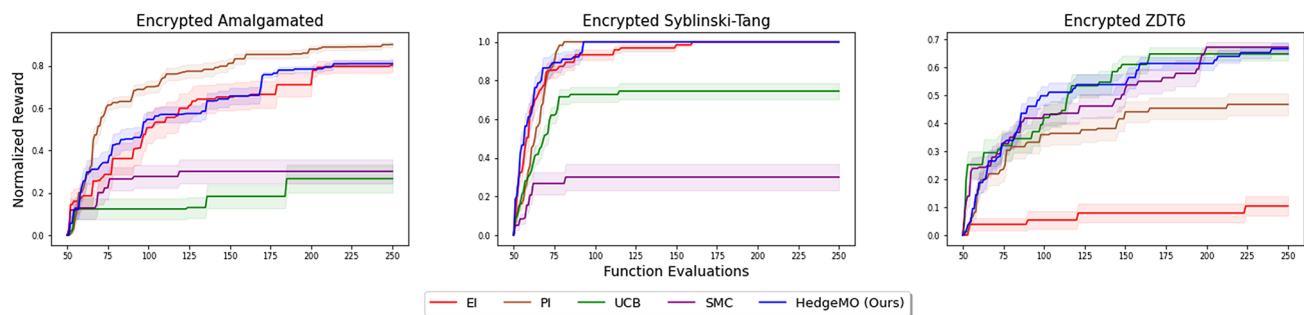


Fig. 2 Performance comparison of HedgeMO against other acquisition functions

The results of our acquisition function comparisons are shown in Figure 2, which shows that HedgeMO performs well across all three test functions. For single-objective test functions, PI outperforms HedgeMO for Encrypted Amalgamated test function. However, for the multi-objective Encrypted ZDT6 test function, PI performs significantly worse and is outperformed by both SMC and UCB. SMC performs well on multi-objective problems combinatorial problems and hence should be a part of portfolio for a hedging algorithm.

These results prove that for a range of different problems, acquisition function choice can play a huge role in the performance of the algorithm. For a black-box function, this information can not be known a priori, making hedging necessary. HedgeMO consistently performs well in all scenarios and ensures efficiency across a range of different problems. Thus, for unknown black-box functions, HedgeMO should be the hedge strategy of choice for multi-objective problems.

6 Application to architected materials

We applied our MixMOBO framework to the optimization of the design of architected, microlattice structures. Advances in modeling, fabrication, and testing of architected materials have promulgated their utility in engineering applications, such as ultralight (Zheng et al. 2014; Pham et al. 2019; Zhang et al. 2019), reconfigurable (Xia et al. 2019), and high-energy-absorption materials (Song et al. 2019b), and in bio-implants (Song et al. 2020). The optimization of architected materials (Bauer et al. 2016; Pham et al. 2019; Xia et al. 2019; Zhang et al. 2019) often requires searching huge combinatorial design spaces, where the

evaluation of each design is expensive. (Meza et al. 2014; Berger et al. 2017; Tancogne-Dejean et al. 2018).

The design space for the architected material we optimize here has ~ 8.5 billion possible combinations of its 17 categorical inputs (one with 2 possible states, and the other 16 with 4 possible states). Our goal is to maximize the strain energy density of a microlattice structure. We maximize the strain energy density (which is extremely expensive to compute, even for one design) by minimizing the buckling load P_c , while maintaining the lattice's structural integrity and stiffness before fracturing. Minimizing P_c (a proxy for maximizing the strain energy density by instigating buckling which leads to the densification of the deformed lattice members) is a more computationally tractable cost function to evaluate (but, it is still expensive and involves solving a numerical finite element code for each evaluation of the cost function.) The manufacturing and testing details of our methodology are included in Vangelatos et al. (2021), which focuses on the material aspects of the problem.

The design space consists of choosing one of four possible unit cells (shown in the upper left of Fig. 3, each with one or more defects (shown in color) in them, at each of the 16 independent lattice sites) creating 16 of the categorical inputs with 4 possible values; and the choice of whether the cells are connected along their faces or along their edges on 45° -diagonals (shown in the upper right panel of Fig. 3) creating the 17th categorical input with 2 possible values.

The minimization of P_c using MixMOBO was initialized with 50 random structures and the evaluation budget, including initial samples, was set at 250. The algorithm achieved a 42% improvement in the P_c of the lattice structure over the best structure obtained with the first 50 random samples (Figure 3).

Table 1 Experimental values of the critical buckling P_c (minimization objective for MixMOBO), strain energy density at buckling and fracture, u_b and u_f , respectively, elastic stiffness S , and ratio of normalized strain energy density compared to the Unblemished structure

Structure	$P_c [\mu N]$	$u_b [MJm^{-3}]$	$u_f [MJm^{-3}]$	$S [MPa]$	$(u_f/u_b)/(u_{f1}/u_{b1})$
Unblemished	3814.5	1.08	0.071	388.21	1
Random Sampling Optimal	996.2	0.08	2.85	347.19	526
MixMOBO Optimal	545.1	0.02	14.71	460.35	12030

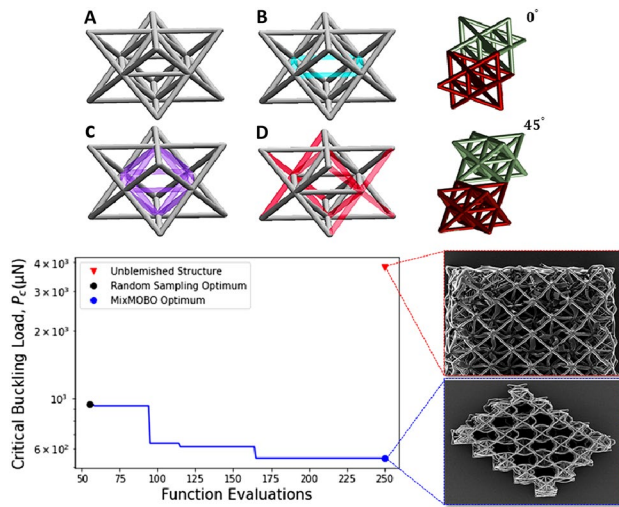


Fig. 3 Top Left: The 4 unit cells, labelled A–D. Top Right: The 2 orientations in which they can be joined. Bottom Left: Optimization results using MixMOBO. Bottom Right: SEM images of Unblemished and Optimum structures

The optimal microlattice obtained using P_c as a proxy with MixMOBO has an experimentally measured normalized strain energy density that is 12,030 times greater than that of the unblemished microlattice structure with no defects that is cited in the literature to have the best strain energy density (Vangelatos et al. 2020), a 4 orders of magnitude improvement. Table 1 shows the properties of the fabricated and experimentally measured design created with MixMOBO. The choices of the units cells in the optimally designed lattice that were determined by MixMOBO are not intuitive and have no obvious pattern or structure. Images of our optimized structures using Helium Ion Microscopy (HIM) 4, shows the comparison of the Unblemished structure from literature with our MixMOBO Optimal structure, before and after loading. It is evident that the MixMOBO Optimal structure due to its densification mechanism, can handle much higher loads without breaking (Vangelatos et al. 2021).

7 Conclusions

The existing optimization literature does not offer an algorithm for optimizing multi-objective, mixed variable problems with expensive black-box functions. We have introduced mixed variable Multi-Objective Bayesian Optimization (MixMOBO), the first BO-based algorithm for optimizing such problems. MixMOBO is agnostic to the underlying kernel. It is compatible with modified kernels and other surrogate methods developed in previous studies for mixed variable problems. MixMOBO allows for parallel batch updates without repeated evaluations of the surrogate surface, while maintaining diversification within the solution set. We presented the Hedge Multi-Objective

(HedgeMO) algorithm, a novel Hedge strategy for which regret bounds hold for multi-objective problems. A new acquisition function, Stochastic Monte-Carlo (SMC) was also proposed as part of the HedgeMO portfolio. MixMOBO and HedgeMO were benchmarked and shown to be significantly better on a variety of test problems compared to existing mixed variable optimization algorithms. MixMOBO was then applied to the real-world optimization of an architected micro-lattice, and we increased the structure's strain energy density by 10^4 compared to existing Unblemished structures in the literature reported to have highest strain energy density. Our future work entails further testing multi-objective and 'Q-batch' settings. We have also applied MixMOBO for optimization of draft-tubes for hydrokinetic turbines (Sheikh et al. 2022b) and Cauchy symmetric meta-material structures and are currently applying it for optimization of vertical-axis wind turbines.

Appendix A: Benchmark Test Functions

In this section, we define the benchmark test functions, all of which are set to be maximized during our optimizations.

Contamination Problem

The contamination problem was introduced by Hu et al. (2011) and is used to test categorical variables with binary categories. The problem aims to maximize the reward function for applying a preventative measure to stop contamination in a food supply chain with D stages. At each i^{th} stage, where $i \in [1, D]$, decontamination efforts can be applied. However, this effort comes at a cost c and will decrease the contamination by a random rate Γ_i . If no prevention effort is taken, the contamination spreads with a rate of Ω_i . At each stage i , the fraction of contaminated food is given by the recursive relation:

$$Z_i = \Omega_i(1 - w_i)(1 - Z_{i-1}) + (1 - \Sigma_i w_i)Z_{i-1} \quad (A1)$$

here $w_i \in 0, 1$ and is the decision variable to determine if preventative measures are taken at i^{th} stage or not. The goal is to decide which stages i action should be taken to make sure Z_i does not exceed an upper limit U_i . Ω_i and Σ_i are determined by a uniform distribution. We consider the problem setup with Lagrangian relaxation (Baptista and Poloczec 2018):

$$f(\vec{w}) = - \sum_{i=1}^D \left(cw_i + \frac{\rho}{T} \sum_{k=1}^T 1_{\{Z_k > U_i\}} \right) - \lambda \|\vec{w}\|_1 \quad (A2)$$

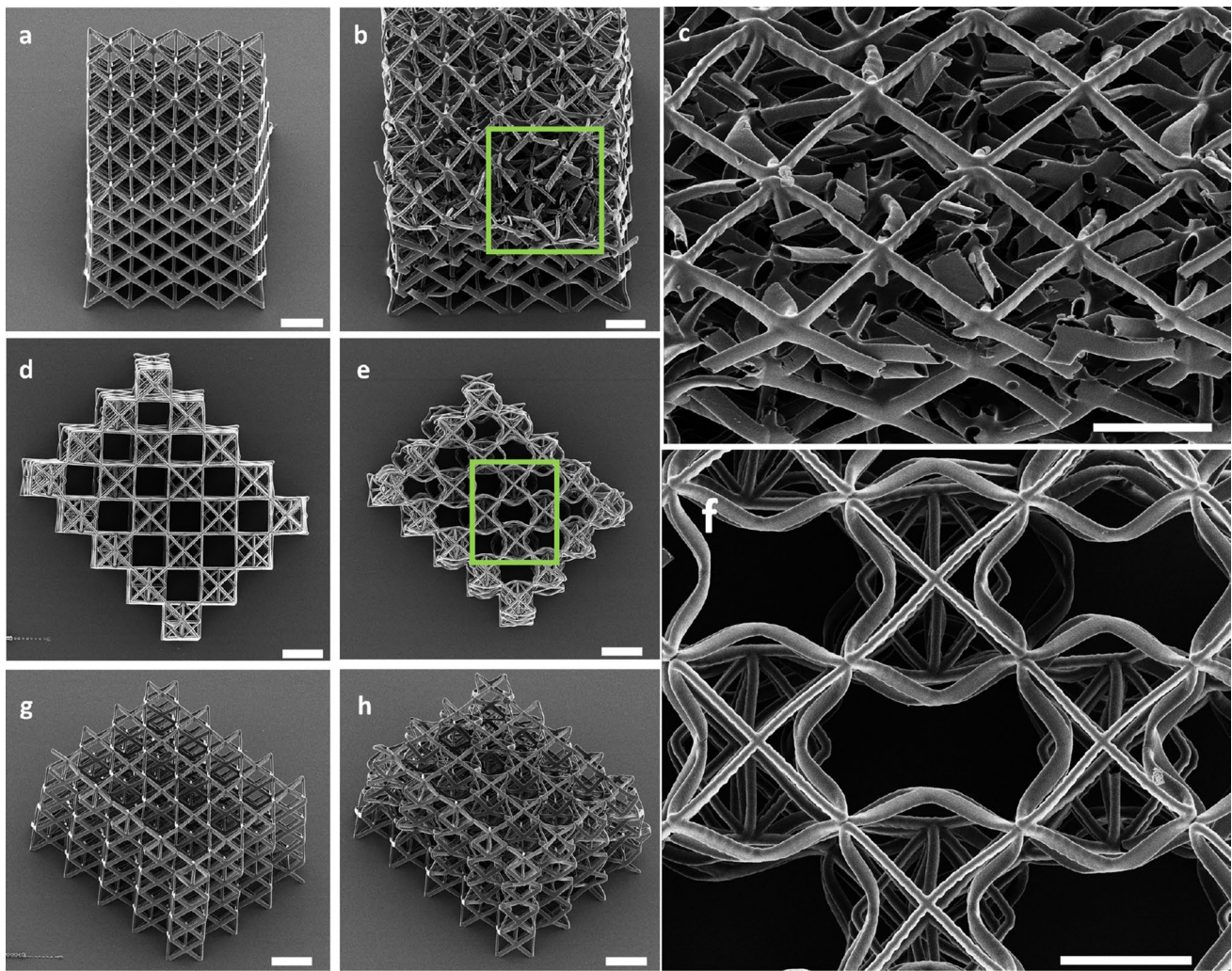


Fig. 4 HIM images of the loaded and unloaded unblemished and optimum structures. (a) Unloaded Unblemished structure (b) Unblemished structure after loading, showing severe fracture and collapse of many beam members. (c) Focused image revealing several fractured beams and the internal collapse of the upper layer that subsequently instigated the accumulation of damage in the underlying layers. (d) Unloaded MixMOBO Optimum structure. (e) MixMOBO Optimum structure after the structure was subjected to the same maximum compressive load as the structure shown in (b). Unload-

ing of the optimum structure showed only excessive plastic deformation without catastrophic collapse and the manifestation of the buckling mode. (f) Focused revealing the effect of buckling that led to deformation but no fracture due to the occurrence of densification. (g) Side view of the unloaded optimum structure. (h) Side view of the unloaded optimum structure revealing that fracture was inhibited throughout the structure due to the densification precipitated by the low critical buckling load. **Scale:** Each scale bar is equal to 10 μm

Here violation of $Z_k < U_i$ is penalized by $\rho = 1$ and summing the contaminated stages if the limit is violated and our total stages or dimensions are $D = 21$. The cost c is set to be 0.2 and $Z_1 = 0.01$. As in the setup for Baptista and Poloczek (2018), we use $T = 100$ stages, $U_i = 0.1$, $\lambda = 0.01$ and $\epsilon = 0.05$.

Encrypted Amalgamated

Analytic test functions generally cannot mimic mixed variables. To map the continuous output of a function into N discrete ordinal or categorical variables, the continuous range of the test function's

output is first discretized into N discrete subranges by selecting $(N - 1)$ break points, often equally spaced, within the bounds of the range. Then, the continuous output variable is assigned the integer round-off value of the subrange defined by its surrounding pair of break points. If necessary, the domain of the test function's output is first mapped into a larger domain so that each subrange has a unique integer value. To mimic ordinal variables, we are done, but for categorical variables, a random vector for each categorical variable is then generated which scrambles or 'encrypts' the indices of these values, thus creating random landscapes as is the case for categorical variables with a latent

space. The optimization algorithm only sees the encrypted space and the random vector is only used when evaluating the black-box function.

We also define a new test function that we call the *Amalgamated function*, a piece-wise function formed from commonly used analytical test functions with different features (for more details on these functions we refer to Tušar et al. (2019)). The Amalgamated function is non-convex and anisotropic, unlike conventional test functions where isotropy can be exploited.

For $i = 1 \dots n$, $k = \text{mod}(i - 1, 7)$:

$$f(\vec{w}) = \sum_{i=1}^D g(w_i) \quad (\text{A3})$$

where

$$g(w_i) = \begin{cases} \sin(w_i) & \text{if } k = 0, w_i \in (0, \pi) \\ -\frac{w_i^4 - 16w_i^2 + 5w_i}{2} & \text{if } k = 1, w_i \in (-5, 5) \\ -(w_i^2) & \text{if } k = 2, w_i \in (-10, 10) \\ -[10 + w_i^2 - 10\cos(2\pi w_i)] & \text{if } k = 3, w_i \in (-5, 5) \\ -[100(w_i - w_{i-1}^2)^2 + (1 - w_i)^2] & \text{if } k = 4, w_i \in (-2, 2) \\ \text{abs}(\cos(w_i)) & \text{if } k = 5, w_i \in (-\pi/2, \pi/2) \\ -w_i & \text{if } k = 6, w_i \in (-30, 30) \end{cases} \quad (\text{A4})$$

To create the Encrypted Amalgamated function, for categorical and ordinal variables, equally spaced points are taken within the bounds defined above. For our current work, we use a $D = 13$ with 8 categorical and 3 ordinal variables with 5 states each, and 2 continuous variables.

NK Landscapes

NK Landscapes were introduced by Kauffman and Levin (1987) as a way of creating optimization problems with categorical variables. N describes the number of genes or number of dimensions D and K is the number of epistatic links of each gene to other genes, which describes the ‘ruggedness’ of the landscape. A large number of random landscapes can be created for given N and K values. The global optimum of a generated landscape for experimentation can only be computed through complete enumeration. The landscape cost for any vector is calculated as an average of each component cost. Each component cost is based on the random values generated for the categories, not only by its own alleles, but also by the alleles in the other genes connected through the random epistasis matrix, with K probability or ruggedness. A $K = 1$ ruggedness translates to a fully connected genome.

The NK Landscapes from Kauffman and Levin (1987) were formulated only for binary variables. They were extended by Li et al. (2006) for multi-categorical problems, which is the formulation we use. Details of the NK Landscape

test-functions we use can be found in Li et al. (2006). For the current study, we use $N = 8$ with 4 categories each and ruggedness $K = 0.2$.

Rastrigin

Rastrigin function is a commonly used non-convex optimization function (Tušar et al. 2019) with a large number of local optima. It is defined as:

$$f(\vec{w}) = -[10 + w_i^2 - 10\cos(2\pi w_i)], w_i \in (-5, 5) \quad (\text{A5})$$

We use $D = 9$ for testing with 6 ordinal with 5 discrete states and 3 continuous variables. The ordinal variables are equally spaced within the bounds.

Encrypted Syblinski-Tang

We use the *Syblinski-Tang function* (Tušar et al. 2019), an isotropic non-convex function. The function is considered difficult to optimize because many search algorithms get ‘stuck’ at a local optimum. For use with categorical variables, we encrypt it as described previously. The Syblinski-Tang function, in terms of input vector \vec{w} , is defined as:

$$f(\vec{w}) = -\frac{\sum_{i=1}^D w_i^4 - 16w_i^2 + 5w_i}{2}, w_i \in (-5, 2.5) \quad (\text{A6})$$

For the current study, this function was tested with $D = 10$ categorical variables and 5 categories for each variable.

Encrypted ZDT6

ZDT benchmarks are a suite of multi-objective problems, suggested by Zitzler et al. (2000), and most commonly used for testing such problems. We use ZDT6, which is non-convex and non-uniform in its parameter space. We again modify the function by encrypting it to work with categorical problems. ZDT6 is defined as:

$$\begin{aligned} f_1(\vec{w}) &= \exp(-4w_1)\sin^6(6\pi w_1) - 1 \\ f_2(\vec{w}) &= -g(\vec{w})[1 - (f_1(\vec{w})/g(\vec{w}))^2] \\ g(\vec{w}) &= 1 + 9 \left[\left(\sum_{i=2}^D w_i \right) / (n - 1) \right]^{1/4} \end{aligned} \quad (\text{A7})$$

Here $w_1 \in [0, 1]$ and $w_i = 0$ for $i = 2, \dots, D$. The function was tested for $D = 10$ with 5 categories each. We note that to evaluate the performance of MixMOBO, we compared it against the NSGA-II variant Deb et al. (2002) that can deal

with mixed variables (by running *ZDT4* in a mixed variable setting and *ZDT6* with categorical variables). No encryption is necessary for GAs. GAs required, on average, 10^2 more function calls compared to MixMOBO.

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Author contributions H.M.S conceptualized the algorithm, designed the methodology and performed experiments under the supervision of P.S.M. H.M.S and P.S.M then wrote and edited the manuscript.

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Data availability Complete data sets to reproduce any and all experiments which were generated during and analysed during the current study and MixMOBO code are available from the corresponding author on reasonable request.

Declarations

Conflict of interest The authors declare conflicts or competing interests that need to be disclosed.

Replication of Results All the results in this manuscript can be replicated. The complete data sets, MixMOBO algorithm or any other supplementary material and information required for replication are available from the corresponding author on reasonable request.

References

- Balandat M, Karrer B, Jiang DR, Daulton S, Letham B, Wilson AG, Bakshy E (2020) A framework for efficient monte-carlo Bayesian optimization, Botorch
- Baptista R, Poloczek M (2018) Bayesian optimization of combinatorial structures
- Bauer J, Schroer A, Schwaiger R, Kraft O (2016) Approaching theoretical strength in glassy carbon nanolattices. *Nat Mater* 15(4):438–443
- Berger JB, Wadley HNG, McMeeking RM (2017) Mechanical metamaterials at the theoretical limit of isotropic elastic stiffness. *Nature* 543(7646):533–537
- Bergstra J, Bardenet R, Bengio Y, Kégl B (2011) Algorithms for hyper-parameter optimization. In: *Proceedings of the 24th international conference on neural information processing systems, NIPS’11*, PP 2546–2554, Red Hook, NY, USA. Curran Associates Inc
- Bergstra J, Yamini D, Cox D (2013) Making a science of model search: Hyperparameter optimization in hundreds of dimensions for vision architectures. In: *Proceedings of the 30th international conference on machine learning*, volume 28 of *Proceedings of Machine Learning Research*, pp 115–123, Atlanta, Georgia, USA, 17–19 Jun 2013. PMLR
- Brochu E, Cora VM, de Freitas N (2010) A tutorial on bayesian optimization of expensive cost functions, with application to active user modeling and hierarchical reinforcement learning
- Brochu E, Hoffman MW, de Freitas N (2011) Portfolio allocation for Bayesian optimization
- Chen D, Skouras M, Zhu B, Matusik W (2018a) Computational discovery of extremal microstructure families. *Sci Adv* 4(1):eaao7005
- Chen Y, Huang A, Wang Z, Antonoglou I, Schrittwieser J, Silver D, de Freitas N (2018b) Bayesian optimization in alphago. *CoRR*. [arXiv:abs/1812.06855](https://arxiv.org/abs/1812.06855)
- Chen W, Watts S, Jackson JA, Smith WL, Tortorelli DA, Spadaccini CM (2019) Stiff isotropic lattices beyond the Maxwell criterion. *Sci Adv* 5(9):eaaw1937
- Daulton S, Balandat M, Bakshy E (2020) Differentiable expected hypervolume improvement for parallel multi-objective Bayesian optimization, 2020
- Daulton S, Eriksson D, Balandat M, Bakshy E (2021) Multi-objective Bayesian optimization over high-dimensional search spaces, 2021
- Daxberger E, Makarova A, Turchetta M, Krause A (2020) Mixed-variable Bayesian optimization. In: *Proceedings of the twenty-ninth international joint conference on artificial intelligence*, July. <https://doi.org/10.24963/ijcai.2020/365>
- Deb K, Pratap A, Agarwal S, Meyarivan T (2002) A fast and elitist multiobjective genetic algorithm: Nsga-ii. *IEEE Trans Evol Comput* 6(2):182–197. <https://doi.org/10.1109/4235.996017>
- Deshwal A, Doppa JR (2021) Combining latent space and structured kernels for bayesian optimization over combinatorial spaces. *CoRR*, abs/2111.01186
- Deshwal A, Belakaria S, Doppa JR (2021) Bayesian optimization over hybrid spaces
- Fonseca CM, Paquete L, Lopez-Ibanez M (2006) An improved dimension-sweep algorithm for the hypervolume indicator. In: *2006 IEEE international conference on evolutionary computation*, PP 1157–1163. <https://doi.org/10.1109/CEC.2006.1688440>
- Frazier PI, Wang J (2015) Bayesian optimization for materials design, *Springer Series in Materials Science*. Springer, Berlin. pp 45–75. https://doi.org/10.1007/978-3-319-23871-5_3
- GPyOptAuthors (2016) GPyOpt: a Bayesian optimization framework in python. <http://github.com/SheffieldML/GPyOpt>
- Garrido-Merchán EC, Hernández-Lobato D (2020) Dealing with categorical and integer-valued variables in Bayesian optimization with Gaussian processes. *Neurocomputing* 380:20–35. <https://doi.org/10.1016/j.neucom.2019.11.004>
- Golovin D, Solnik B, Moitra S, Kochanski G, Karro J, Sculley D (2017) Google vizier: a service for black-box optimization. In: *Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, KDD ’17*, pp 1487–1495, New York, NY, USA. Association for Computing Machinery. ISBN 9781450348874. <https://doi.org/10.1145/3097983.3098043>
- Gopakumar S, Gupta S, Rana S, Nguyen V, Venkatesh S (2018) Algorithmic assurance: An active approach to algorithmic testing using Bayesian optimisation. In: Bengio S, Wallach H, Larochelle H, Grauman K, Cesa-Bianchi N, Garnett R (eds) *Advances in Neural Information Processing Systems*, vol 31. Curran Associates, New York
- Hutter F, Hoos HH, Leyton-Brown K (2011) Sequential model-based optimization for general algorithm configuration. In:

- Coello Coello CC (ed) Learning and Intelligent Optimization, pp 507–523. Springer, Berlin
- Korovina K, Xu S, Kandasamy K, Neiswanger W, Poczos B, Schneider J, Chembo EX (2020) Bayesian optimization of small organic molecules with synthesizable recommendations. In: Proceedings of the twenty third international conference on artificial intelligence and statistics, volume 108 of Proceedings of Machine Learning Research, pp 3393–3403. PMLR, 26–28 Aug
- Krause A, Singh A, Guestrin C (2008) Near-optimal sensor placements in Gaussian processes: Theory, efficient algorithms and empirical studies. *J Mach Learn Res* 9(8):235–284
- Li R, Emmerich M, Eggermont J, Bovenkamp E, Bäck T, Dijkstra J, Reiber J (2006) Mixed-integer nk landscapes. 4193:42–51. https://doi.org/10.1007/11844297_5
- Lindauer M, Eggenberger K, Feurer M, Biedenkapp A, Deng D, Benjamins C, Sass R, Hutter F (2021) Smac3: a versatile Bayesian optimization package for hyperparameter optimization, 2021
- Meza Lucas R, Das S, Greer Julia R (2014) Strong, lightweight, and recoverable three-dimensional ceramic nanolattices. *Science* 345(6202):1322–1326
- Mockus J (1994) Application of Bayesian approach to numerical methods of global and stochastic optimization. *J Glob Optim* 4:347–365
- Murphy KP (2012) Machine learning: a probabilistic perspective. MIT Press, New York
- Nguyen D, Gupta S, Rana S, Shilton A, Venkatesh S (2019) Bayesian optimization for categorical and category-specific continuous inputs
- Oh C, Gavves E, Welling M (2018) BOCK : Bayesian optimization with cylindrical kernels. In: Proceedings of the 35th International Conference on Machine Learning, vol. 80 of Proceedings of Machine Learning Research, pp 3868–3877. PMLR, 10–15 Jul
- Oh C, Tomczak JM, Gavves E, Welling M (2019) Combinatorial Bayesian optimization using the graph Cartesian product, 2019
- Oh C, Gavves E, Welling M (2021) Mixed variable bayesian optimization with frequency modulated kernels
- Pelamatti J, Brevault L, Balesdent M, Talbi E-G, Guerin Y (2018) Efficient global optimization of constrained mixed variable problems
- Pham M-S, Liu C, Todd I, Lertthanasarn J (2019) Damage-tolerant architected materials inspired by crystal microstructure. *Nature* 565(7739):305–311
- Pyzer-Knapp E (2018) Bayesian optimization for accelerated drug discovery. *IBM J Res Dev* 11:1–1. <https://doi.org/10.1147/JRD.2018.2881731>
- Qian PZG, Wu H, Jeff Wu CF (2008) Gaussian process models for computer experiments with qualitative and quantitative factors. *Technometrics* 50(3):383–396
- Rasmussen CE, Williams CKI (2006) Gaussian processes for machine learning, Adaptive computation and machine learning. MIT Press, New York
- Ru B, Alvi AS, Nguyen V, Osborne MA, Roberts SJ (2020) Bayesian optimisation over multiple continuous and categorical inputs
- Scikit-learn (2021) scikit-optimize. <https://scikit-optimize.github.io/stable/>
- Shaw LA, Sun F, Portela CM, Barranco RI, Greer JR, Hopkins JB (2019) Computationally efficient design of directionally compliant metamaterials. *Nat Commun* 10(1):1–13
- Sheikh HM, Callan T, Hennessy K, Marcus P (2021) Shape optimization methodology for fluid flows using mixed variable Bayesian optimization and design-by-morphing. In: APS division of fluid dynamics meeting abstracts, APS Meeting Abstracts, page A15.004
- Sheikh HM, Lee S, Wang J, Marcus PS (2022a) Airfoil optimization using design-by-morphing. <https://arxiv.org/abs/2207.11448>
- Sheikh HM, Callan TA, Hennessy KJ, Marcus PS (2022b) Optimization of the shape of a hydrokinetic turbine's draft tube and hub assembly using design-by-morphing with Bayesian optimization. [arXiv: abs/2207.11451](https://arxiv.org/abs/2207.11451)
- Shu L, Jiang P, Shao X, Wang Y (2020) A new multi-objective bayesian optimization formulation with the acquisition function for convergence and diversity. *J Mech Des* 142(9):032020. <https://doi.org/10.1115/1.4046508.091703>
- Snoek J, Larochelle H, Adams RP (2012) Practical Bayesian optimization of machine learning algorithms
- Song J, Wang Y, Zhou W, Fan R, Bin Y, Yang L, Li L (2019) Topology optimization-guided lattice composites and their mechanical characterizations. *Compos Part B* 160:402–411
- Song J, Zhou W, Wang Y, Fan R, Wang Y, Chen J, Yang L, Li L (2019) Octet-truss cellular materials for improved mechanical properties and specific energy absorption. *Mater Des* 173:107773
- Song J, Michas C, Chen Christopher S, White Alice E, Grinstaff Mark W (2020) From simple to architecturally complex hydrogel scaffolds for cell and tissue engineering applications: Opportunities presented by two-photon polymerization. *Adv Healthc Mater* 9(1):1901217
- Srinivas N, Krause A, Kakade SM, Seeger MW (2012) Information-theoretic regret bounds for gaussian process optimization in the bandit setting. *IEEE Trans Inf Theory* 58(5):3250–3265. <https://doi.org/10.1109/tit.2011.2182033>
- Stuart K, Simon L (1987) Towards a general theory of adaptive walks on rugged landscapes. *J Theoret Biol* 128(1):11–45. [https://doi.org/10.1016/S0022-5193\(87\)80029-2](https://doi.org/10.1016/S0022-5193(87)80029-2)
- Suzuki S, Shion T, Kazuki S, Masayuki K (2020) Multi-objective Bayesian optimization using pareto-frontier entropy, Tomoyuki Tamura
- Tancogne-Dejean T, Diamantopoulou M, Gorji MB, Bonatti C, Mohr D (2018) 3d plate-lattices: an emerging class of low-density metamaterial exhibiting optimal isotropic stiffness. *Adv Mater* 30(45):1803334
- Tea T, Dimo B, Nikolaus H (2019) Mixed-integer benchmark problems for single- and bi-objective optimization. In: Proceedings of the Genetic and Evolutionary Computation Conference, GECCO '19, pp 718–726, New York, NY, USA. Association for Computing Machinery. <https://doi.org/10.1145/3321707.3321868>
- Tiao LC, Klein A, Seeger M, Bonilla EV, Archambeau C, Fabio R (2021) Bayesian optimization by density-ratio estimation, Bore
- Vangelatos Z, Komvopoulos K, Grigoropoulos C (2020) Regulating the mechanical behavior of metamaterial microlattices by tactical structure modification. *J Mech Phys Solids* 1:104112
- Vangelatos Z, Sheikh HM, Marcus PS, Grigoropoulos CP, Lopez VZ, Flamourakis G, Farsari M (2021) Strength through defects: a novel Bayesian approach for the optimization of architected materials. *Sci Adv* 7:41. <https://doi.org/10.1126/sciadv.abk2218>
- Xia X, Afshar A, Yang H, Carlos MP, Dennis MK, Claudio VDL, Julia R (2019) Electrochemically reconfigurable architected materials. *Nature* 573(7773):205–213
- Yingjie H, Jianqiang H, Yifan X, Fengchun W, Rong C (2011) Contamination control in food supply chain. pp 2678–2681. <https://doi.org/10.1109/WSC.2010.5678963>
- Zhang X, Vyatskikh A, Gao H, Greer JR, Li X (2019) Lightweight, flaw-tolerant, and ultrastrong nanoarchitected carbon. *Proc Natl Acad Sci USA* 116(14):6665–6672
- Zhang Y, Apley DW, Chen W (2020) Bayesian optimization for materials design with mixed quantitative and qualitative variables. *Sci Rep* 10(1):1–13
- Zheng X, Lee H, Weisgraber TH, Shusteff M, DeOtte J, Duoss EB, Kuntz JD, Biener MM, Ge Q, Jackson JA et al (2014)

- Ultralight, ultrastiff mechanical metamaterials. *Science* 344(6190):1373–1377
- Zhou Q, Qian PZG, Zhou S (2011) A simple approach to emulation for computer models with qualitative and quantitative factors. *Technometrics* 53(3):266–273
- Zitzler E, Deb K, Thiele L (2000) Comparison of multiobjective evolutionary algorithms: empirical results. *Evol Comput* 8(2):173–195. <https://doi.org/10.1162/106365600568202>

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