Abstract—Fitness landscape analysis investigates features with a high influence on the performance of optimization algorithms, aiming to take advantage of the addressed problem characteristics. In this work, a fitness landscape analysis using problem features is performed for a Multi-objective Bayesian Optimization Algorithm (mBOA) on instances of MNK-landscape problem for 2, 3, 5 and 8 objectives. We also compare the results of mBOA with those provided by NSGA-III through the analysis of their estimated runtime necessary to identify an approximation of the Pareto front. Moreover, in order to scrutinize the probabilistic graphic model obtained by mBOA, the Pareto front is examined according to a probabilistic view. The fitness landscape study shows that mBOA is moderately or loosely influenced by some problem features, according to a simple and a multiple linear regression model, which is being proposed to predict the algorithms performance in terms of the estimated runtime. Besides, we conclude that the analysis of the probabilistic graphic model produced at the end of evolution can be useful to understand the convergence and diversity performances of the proposed approach.

I. INTRODUCTION

Population-based metaheuristics and Evolutionary Algorithms (EA) have been applied to solve multi-objective optimization problems, mainly due to their ability to discover multiple solutions in parallel and to handle the complex features of such problems [1]. Besides, probabilistic modeling can also be aggregated to capture and exploit the potential regularities that arise in the promising solutions, which is the basis of an Estimation of Distribution Algorithm (EDA) [2].

The main idea of EDAs is to extract and represent, using a probabilistic model, the regularities shared by a subset of high-valued problem solutions. New solutions are then sampled from the probabilistic model to guide the search toward areas where optimal solutions are more likely to be found. Normally, Multi-objective Estimation of Distribution Algorithm (MOEDA) [3] integrates both model building and sampling techniques into evolutionary multi-objective optimizers using special selection schemes. Probabilistic graphical models, which combine graph and probability theory, have been broadly used to improve EDAs and MOEDAs performance [4]. As reported in [5], most of MOEDAs developed to deal with combinatorial multi-objective optimization problems (MOPs) adopt Bayesian Networks as their PGM.

One of the main challenges in multi-objective optimization is to find the Pareto optimal set, or an approximation of it. The Pareto set plays a central role in the search space structure. The definition and analysis of fitness landscape for MOPs can help to understand the geometry of a combinatorial MOP, for example, and to explain the ability of multi-objective metaheuristics to obtain an approximation of the Pareto set.

The fitness landscape of a problem instance is the topological structure over which a search is being executed [6], defined by the solution candidates, their neighborhood structure and the fitness of the solution candidates.

By addressing the relative importance of features in explaining the metaheuristic performance variance, fitness landscape analysis (FLA) allows one to investigate which features of a combinatorial MOP have the highest influence on the metaheuristic performance. Through the study of these features, one should be able to design metaheuristic algorithms to take advantage of the multi-objective optimization characteristics of a given problem [7].

Several works have addressed combinatorial MOPs from an FLA perspective. Borges and Hansen [8] presented a study of global convexity for a multi-objective travelling salesman problem. The authors investigated features concerning instances solved by scalarizing algorithms (which use weights to aggregate multiple objectives). Garrett and Dasgupta [7] provided a high-level overview of multi-objective search space and FLA. They investigated some features like the distribution of local and Pareto optima, fitness distance correlation, ruggedness and random walk on the multi-objective generalized assignment problem.

This paper addresses a combinatorial MOP - multi-objective NK-landscape (MNK) model which has been recently explored in other works in the literature [9, 10, 11]. In particular, EDAs that use different types of probabilistic models, including Bayesian Networks, have already been applied to the mono-objective NK problem [12, 13, 14].

The objective here is to extend those works to multi and many objective optimization (when the number of objectives
is higher than 3) conducting an FLA to investigate the impact of instance features on the search performance of a MOEDA based on Bayesian Network (BN) as the PGM structure, called Multi-objective Bayesian Optimization Algorithm (mBOA) [15]. The algorithm is compared with NSGA-III [16], a state-of-the-art algorithm applied to solve multi and many-objective optimization problems (MaOPs).

Our main contribution is the use of FLA to explore the relationship between performance measures and relevant problem features for mBOA. As far as we know, this is the first work to consider FLA for MOEDAs. In addition, our work also includes an investigation, from a probabilistic point of view, of the Pareto-front using the probability mass function provided by mBOA at the end of evolution.

This paper has intersections with other previously published works. It is linked to the work presented by Liefooghe et al. [11] in which some features of the MNK model instances are investigated. It is also related to the work developed by Echegoyen et al. [17] which considers a quantitative analysis to compare the probabilities of sampling the optimum and the most probable solution between successful and failed trials aiming to understand the behaviour of EDAs based on BNs for mono-objective problems. However, differently from [11], we are investigating an EDA approach, and extending the analysis to 8 objectives. Also, in contrast to the research presented in [17], which investigates mono-objective optimization, our work considers a set of non-dominated solutions. Therefore, the probabilities might be calculated according to the distribution of these solutions over the true Pareto front.

This paper is organized as follows. Section II provides a formulation of the MNK-landscape model, and briefly introduces FLA and Bayesian networks as PGM for estimation of distribution algorithms. Section III presents the mBOA framework used in our investigation. Results from numerical experiments are reported and discussed in Section IV. Finally, some conclusions and future directions are presented in Section V.

II. BACKGROUND

A. The MNK-landscape model

The NK fitness landscapes is a family of problems proposed by [18] in order to explore the way in which the neighborhood structure and the strength of the interactions between neighboring variables are linked to the ruggedness of search spaces. The problem consists in finding the maximum of the function for the given parameters [19].

Let \( X = (X_1, \ldots, X_N) \) denote a vector of discrete variables and \( x = (x_1, \ldots, x_N) \) an assignment to the variables.

An NK fitness landscape is defined by the following components [13]:

- Number of variables, \( N \).
- Number of neighbors per variable (ruggedness), \( K \).
- A set of neighbors, \( \Pi(X_n) \in X \), for \( X_n, n \in \{1, \ldots, N\} \) where \( \Pi(X_n) \) contains \( K \) neighbors.
- A subfunction \( f_n \) defining a real value for each combination of values of \( X_n \) and \( \Pi(X_n) \), \( n \in \{1, \ldots, N\} \).

Both the subfunction \( f_n \) for each variable \( X_n \) and the neighborhood structure \( \Pi(X_n) \) are randomly set [13].

The mono-objective function \( z_{NK}(x) \) to be maximized is defined as:

\[
z_{NK}(x) = \sum_{n=1}^{N} f_n(x_n, \Pi(x_n)).
\]

The MNK-landscape [9] is a multi-objective combinatorial optimization problem with 2 or more objectives, where each objective function is determined by a different instance of the NK-landscape model \( z(x) = (z_1(x), z_2(x), \ldots, z_M(x)) : B^N \rightarrow \mathbb{R}^M \), over the same binary string \( x \), where \( N \) is the number of variables, \( M \) is the number of objectives, \( z_m(x) \) is the \( m \)-th objective function, and \( B = \{0, 1\} \). \( K = \{K_1, \ldots, K_M\} \) is a set of integers where \( K_m \) is the size of the neighborhood in the \( m \)-th landscape.

The MNK-landscape problem can be formulated as follows:

\[
\begin{align*}
\max_{x} & \quad z(x) = (z_1(x), \ldots, z_M(x)) \\
\text{subject to} & \quad x \in \{0, 1\}^N, \\
\text{with} & \quad z_m(x) = \frac{1}{N} \sum_{n=1}^{N} f_{m,n}(x_n, \Pi_{m,n}(x_n)), \\
& \quad m \in \{1, \ldots, M\}, \\
& \quad n \in \{1, \ldots, N\},
\end{align*}
\]

where the fitness contribution \( f_{m,n} \) of variable \( x_n \) is a real number in \([0, 1]\) drawn from a uniform distribution.

B. Fitness Landscape

Fitness landscapes illustrate the association between search and fitness space [6]. Given a specific landscape structure, an evolutionary algorithm can be seen as a strategy for navigating this structure in the search for optimal solutions. Therefore, fitness landscapes have been applied to investigate the dynamics of evolutionary and heuristic search algorithms for optimization and design problems [20]. In addition, the study of fitness landscapes can help predicting the performance of those algorithms.

Cost models have been used to make specific predictions regarding the behavior of evolutionary algorithms identifying the fitness landscape features that make a problem more or less difficult to solve [6]. Cost models are expressed as linear or multiple regression models of features and search cost.

There are several problem features that define the structure of fitness landscapes and can influence the difficulty level during the search. In this paper we are interested in the MNK-landscape problem, which has been explored by [9, 10], for example, in order to study algorithm’s behavior with respect to a set of relevant problem features. The features examined in our work are based on [11] and will be presented in Table II of Section IV.

C. Bayesian Network

A Bayesian Network (BN) is a probabilistic model that consists of a directed acyclic graph (DAG) whose nodes
represent variables, and whose edges express the probabilistic dependency between them [21].

Let us assume $Y = (Y_1, \ldots, Y_M)$ as a vector of random variables, where $y_m$ is a value of the $m$-th component ($Y_m$) of the vector $Y$. The set of conditional dependencies of all variables in $Y$ is described by the DAG structure $B$. $P_{mjk}$ represents the set of parents of the variable $Y_m$ given by $B$, and the set of local parameters $\theta$ contains, for each variable, the conditional probability distribution of its values given different value settings for its parents, according to structure from its parents and $Y$. It has been taken their $j$-th combination of values ($y_m^j$) can be defined as:

$$p(y_m^j | Pa_m^B) = \theta_{y_m^j | Pa_m^B} = \theta_{mjk} \quad (4)$$

We can assume, in discrete domains, that $Y_m$ has $s_m$ possible values, $y_m^1, \ldots, y_m^{s_m}$, therefore the particular conditional probability, $p(y_m^j | Pa_m^B)$ can be defined as:

$$p(y_m^j | Pa_m^B) = \theta_{y_m^j | Pa_m^B} = \theta_{mjk} \quad (4)$$

where $Pa_m^B \in \{Pa_m^1, \ldots, Pa_m^{s_m} \}$ denotes a particular combination of values for $Pa_m^B$ and $t_m$ is the total number of possible instantiations of the parent variables of $Y_m$ given by $t_m = \prod_{v \in Pa_m} s_v$, where $s_v$ is the total number of possible values (states) that $Y_v$ can assign. The parameter $\theta_{mjk}$ represents the conditional probability that variable $Y_m$ takes its $k$-th value ($y_m^k$), knowing that its parent variables have taken their $j$-th combination of values ($Pa_m^B$).

The parameters $\theta_{mjk}$ can be estimated based on the current data $D$ with $N$ observations (instantiations) of $Y$ using Bayesian Estimate, where the expected value $E(\theta_{mjk} | N_{mj}, B)$ of $\theta_{mjk}$ is given by Equation 5:

$$\hat{\theta}_{mjk} = (1 + N_{mjk})/(s_m + N_{mj}) \quad (5)$$

where $N_{mj}$ is the number of observations in $D$ for which $Y_m$ assumes the $k$-th value given the $j$-th combination of values from its parents and $N_{mj} = \{N_{mj1}, \ldots, N_{mjs_m}\}$.

To learn the BN parameters and the structure, the Bayesian Estimate and the K2 [22] algorithm is used, respectively. K2 is a greedy local based procedure that optimizes a score that measures the quality of the network structure.

A BN is used as the PGM for mBOA, whose performance is examined here using FLA concepts associated with the exploration of the final PGM model.

III. MULTI-OBJECTIVE ESTIMATION OF DISTRIBUTION ALGORITHM

In this paper, we consider a MOEDA called mBOA [15] based on Bayesian Network as the probabilistic model and Pareto dominance as the selection scheme.

Algorithm 1 MOEDA framework

| INPUT: Instance: problem instance |
| $P$: population size |
| $P_{GM}$: number of solutions selected to support the probabilistic model estimation |
| $P_{POP}$: number of solutions sampled from the probabilistic model |
| $T_{MAX}$: maximum number of evaluations |

| OUTPUT: $Pop_{ND}$: the set of non-dominated solutions |

1. $I \leftarrow $ LoadInstance(Instance) |
2. $Pop^0 \leftarrow $ RandomGenerate($P$, $I$) (initial population) |
3. $g \leftarrow 1$ |
4. Main loop |
5. for each solution $x \in Pop^g$ do |
6. $fitness(x) \leftarrow $ EvaluateFitness($x, I$) |
7. end for |
8. $F_1, \ldots, F_{P_{OF}} \leftarrow $ ParetoDominance($Pop^g$); |
9. $Pop^g = (F_1 \cup \ldots \cup F_{P_{OF}})$; |
10. $Pop^g_{GM} \leftarrow $ Selection($Pop^g$, $P_{GM}$) (binary tournament) |
11. $PGM \leftarrow $ ProbabilisticModelEstimation($Pop^g_{GM}$) |
12. $Pop_{smp} \leftarrow $ Sampling($PGM$, $P_{POP}$) |
13. for each solution $x \in Pop_{smp}$ do |
14. $fitness(x) \leftarrow $ EvaluateFitness($x, I$) |
15. end for |
16. $Pop_{ND} \leftarrow $ ParetoDominance($Pop_{smp}$); |
17. $Pop^g_{GM} \leftarrow $ Selection($Pop^g \cup Pop_{smp}$), $P$ (truncation selection) |
18. $g \leftarrow g + 1$ |
19. until no success and $T_{MAX}$ is not exceeded |
20. $Pop_{ND} \leftarrow $ Pop$^{g-1}_{ND}(x)$ |

A. The Multi-objective Bayesian Optimization Algorithm

The framework for the MOEDA considered here is presented in Algorithm 1.

In the context of the addressed MNK-landscape problem, the Initialization phase loads the problem instance for a given $M$, $N$ and $K$ (both the subfunctions and the neighborhood structure are obtained from a uniform distribution) and randomly generates an initial population $Pop^1$ of $P$ solutions. Each solution $x$ is a binary string of size $N$.

The EvaluateFitness phase, Step 6 in Algorithm 1, calculates the fitness based on the MNK-landscape model objective functions.

In the ParetoDominance phase, the individuals are sorted using Non-dominated Sorting [23] and a binary tournament selects $N_{PGM}$ individuals from $Pop^g$ in the Selection phase. The procedure randomly selects two solutions and the one positioned in the best front is chosen. If they lie in the same front, it chooses that solution with the greatest crowding distance. Then, $Pop^g_{PGM}$ is obtained encompassing $N_{PGM}$ good individuals.

Afterward, at Step 9, the PGM construction phase in ProbabilisticModelEstimation starts, according to $Pop^g_{PGM}$ population.

Aiming to learn the PGM, the network is modeled using the Bayesian estimate (Equation 5) associated with the K2 algorithm.

1In Section III D is the population set $Pop$ with $P$ observations.
The PGM is used to sample the set of new solutions ($Pop_{smp}$) in Step 10. New solutions (a total of $N_{smp}$), are generated from the joint distribution encoded by the network using the probabilistic logic sampling.

Solutions from $Pop_{smp}$ are then evaluated (Step 14) and sorted according to the Pareto Dominance. The sampled population ($Pop_{smp}$) is joined with $Pop^g$ to create the new population for the next generation. However, only the $T$ best solutions are selected (truncation selection) in the Survival process to proceed in the evolutionary process as a new population $Pop^{g+1}$.

This process is iteratively performed until a termination criterion is satisfied. In this paper, such as in [11], we are interested in the runtime, in terms of a number of function evaluations, until a $(1+\epsilon)$-approximation of the Pareto set is identified (success), subject to a maximum budget of function evaluations ($T_{max}$) for each run.

B. Estimation of the Expected Runtime (crt)

Consider $\epsilon$ as a constant value where $\epsilon \geq 0$. For $x, x' \in X$, $x$ is $\epsilon$-dominated by $x' (x \preceq_\epsilon x')$ if $f_m(x) \leq (1+\epsilon) f_m(x')$, $\forall m \in \{1, \ldots, M\}$. A set $X' \subseteq X$ is an $(1+\epsilon)$-approximation of the Pareto set if for any solution $x \in X$, there is one solution $x' \in X'$ such that $x \preceq_\epsilon x'$. This is equivalent to finding an approximation set whose multiplicative epsilon quality indicator value with respect to the (exact) Pareto set is lower than $(1+\epsilon)$ [11, 24], meaning that if all objective values of all solutions in this approximation set can be improved by a factor $(1+\epsilon)$, then this approximation set dominates the exact Pareto set.

In this work we use the expected number of function evaluations necessary to achieve a $(1+\epsilon)$-approximation to measure algorithm performance (search cost) assuming that we have the exact Pareto set. We apply the same approach presented in [11, 24]: we record the number of function evaluations until a $(1+\epsilon)$-approximation is found which characterizes success. Otherwise, the search cost is set to $T_{max}$.

We consider that the algorithm has a probability of success $p_s \in (0;1)$ and define $T_f$ as the random variable measuring the "simulated runtime" (number of function evaluations) for unsuccessful runs (failures). Precisely, after $(t-1)$ failures, each one requiring $T_f$ evaluations, and the final successful run of $T_s$ evaluations, the total runtime is $T = \sum_{i=1}^{t-1} T_f + T_s$, where $t$ is the random variable measuring the number of runs. The random variable $t$ follows a geometric distribution with parameter $p_s$.

By taking the expectation and by considering independent runs for each instance, stopping at the first success, we have:

$$E[T] = (E[t] - 1)E[T_f] + E[T_s]$$

(6)

In our case, the estimated success rate ($\hat{p}_s$) is computed by the ratio of successful runs over the total number of executions, considering the property that the expectation of a geometric distribution for $t$ with parameter $p_s$ is equal to $1/p_s$. The expected runtime for unsuccessful runs $E[T_f]$ is set as a constant limit ($T_{max}$) on the number of function evaluation calls, and the expected runtime for successful runs $E[T_s]$ is estimated as the average number of function evaluations performed by successful runs. Therefore $crt$ can be expressed as an estimation of the expected runtime $E[T]$ [11, 24]:

$$crt = \frac{1-\hat{p}_s T_{max} + \frac{1}{t_s} \sum_{i=1}^{t_s} T_i}{t_s} \sum_{i=1}^{t_s} T_i$$

(7)

where $t_s$ is the number of successful runs, $T_i$ is the number of evaluations for successful run $i$.

IV. EXPERIMENTS AND RESULTS

In this section, we are interested in the ability of the mBOA, presented in Section III, to find a Pareto set approximation for multi and many-objective combinatorial optimization problems in comparison with NSGA-III [16], a state-of-the-art algorithm applied to solve MOPs. In particular, we investigate the (estimated) runtime of mBOA and NSGA-III necessary to identify a $(1+\epsilon)$-approximation of the Pareto set over enumerable MNK-landscapes instances.

We consider a population size of $P = 100$ for both algorithms. For mBOA the number of solutions selected to support the probabilistic model estimation is $P_{PGM} = P/2$, and the number of solutions sampled from the probabilistic model is $P_{smp} = 10 \times P$.

NSGA-III was adapted from PlatEmo platform [25] considering Uniform Crossover Probability of 0.8 and Bit Flip Mutation Probability of 1/500, as well the same method for the number of reference points used by [16].

We consider MNK-landscapes with an epistatic degree $K \in \{2, 4, 6, 8, 10\}$, an objective space dimension $M \in \{2, 3, 5, 8\}$. The problem size is set to $N = 18$ in order to enumerate the solution space exhaustively - we used the largest value of $N$ that can still be analyzed with reasonable computational resources. A set of 30 different landscapes are independently generated at random for each parameter combination $M$ and $K$. The time limit is set to $T_{max} = 2^N \times 10^{-1} < 26215$ function evaluations [11] without identifying a $(1+\epsilon)$-approximation. Each algorithm is executed 100 times per instance, with $\epsilon = 0.1$. The number of neighbors per variable is the same for all functions $f_m$, i.e. $K_m = K$ for all $m \in \{1, \ldots, M\}$, as proposed in [9, 19].

For each landscape, we enumerate the search space classifying solutions into non-dominated fronts. The first front is the Pareto front and corresponds to the Pareto optimal set that contains the best non-dominated solutions.

A. Fitness Landscape Analysis

In this paper we consider some features extracted from the problem instance (low-level features), or computed from the enumerated Pareto set and solution space (high-level features) [11], as presented in Table I. For more details and a comprehensive explanation of these features, the reader is referred to [20]. We addressed these features in order to examine their impact on the algorithm’s performance. Note
that for the hypervolume computation, the reference point is set to the origin.

As an attempt to understand the impact of problem features on both mBOA and NSGA-III performances, we conduct a linear regression analysis on the correlation between the problem features presented in Table I and the estimated runtime (ert).

To measure the accuracy of the linear regression model, the following statistics are analyzed in the experiments [11]:

- The absolute correlation coefficient \( r \) measures the linear association between the predicted and the actually observed values (the Pearson correlation coefficient is used here). Its absolute value ranges from 0 to 1. Values closer to 1.0 mean better fittings.
- The mean absolute error \( MAE \) corresponds to the average value of the absolute difference between the values predicted by the regression model and the values actually observed (i.e. the residuals), therefore, the lower the \( MAE \), the better the regression model.
- The root mean-square error \( RMSE \) measures the square root of the average squared difference between the values predicted by the regression model and the actual value observed, the lower the \( RMSE \), the better the regression model.

The corresponding regression model statistics are reported in Table II. Aiming at approaching linearity, we also use a log-log scale for the features \( m, k, npo, nconnect, \) and \( lconnect \). Note that the amount of bias in the set of results is negligible according to the equivalent statistics obtained using 10-fold cross validation.

The average ert values for mBOA and NSGA-III are respectively 5922 and 21498 with respective standard deviations of 5682 and 11696. The statistics presented in Table II show that the feature that has the most significant impact is the ruggedness. This can be clearly seen in NSGA-III for which we obtained a high correlation of 0.85 between \( log(k) \) and \( log(ert) \). On the other hand, most features seem to have a moderate or low impact on the mBOA performance. The correlation of features and ert is bounded between 0.30 and 0.53, with the low-level features \( k \) and \( m \) being those with the highest impact.

Given the above-mentioned remarks, it is hard to use a linear regression model to predict an algorithm performance based on the individual problem features. However, it is possible to obtain reasonable precision of runtime prediction using the ruggedness or the number of objectives. In fact, the \( MAE \) values of mBOA for \( k \) and \( m \) are respectively 0.55 and 0.56, which are slightly better than the precisions of the other models. The fact that the \( RMSE \) values (0.70 and 0.69 respectively) are larger than the corresponding \( MAE \) values suggests that there is error variation. However, the gap between \( RMSE \) and \( MAE \) is not large enough, indicating that large errors are unlikely to happen.

As the linear model for mBOA does not provide a precise runtime prediction given the individual features, we decided to take our work a step forward by studying the impact of combined problem features using a multiple linear model. To do so, we start by considering the impact of all the problem features on the algorithms ert. Since some features may have a negligible or noisy impact, they should be removed from the

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**TABLE I: Low-level and high-level features used in the study**

| Feature | Description |
|---------|-------------|
| \( k \) | Number of variable interactions |
| \( m \) | Number of objective functions |
| \( npo \) | Number of Pareto optimal solutions |
| \( hv \) | Hypervolume value of a the Pareto set |
| \( avgd \) | Average distance between Pareto optimal solutions |
| \( maxd \) | Maximum distance between Pareto optimal solutions |
| \( nconnect \) | Number of connected components in the Pareto set |
| \( lconnect \) | Proportion of the largest connected component of the Pareto set |
| \( lconnect \) | Minimal Hamming distance to connect the Pareto set |

**TABLE II: Statistics of the simple linear regression models.**

| Linear Regression - mBOA | 10-fold cross validation |
|--------------------------|-------------------------|
| \( r \) | MAE | RMSE | \( r \) | MAE | RMSE |
| none | 0.00 | 0.68 | 0.82 | 0.00 | 0.68 | 0.82 |
| \( log(lconnect) \) | 0.30 | 0.65 | 0.78 | 0.30 | 0.65 | 0.79 |
| \( hv \) | 0.35 | 0.62 | 0.77 | 0.30 | 0.64 | 0.79 |
| \( log(nconnect) \) | 0.40 | 0.61 | 0.75 | 0.40 | 0.62 | 0.76 |
| \( kconnect \) | 0.41 | 0.60 | 0.75 | 0.40 | 0.60 | 0.75 |
| \( maxd \) | 0.48 | 0.68 | 0.82 | 0.46 | 0.68 | 0.83 |
| \( avgd \) | 0.48 | 0.58 | 0.72 | 0.48 | 0.59 | 0.73 |
| \( log(npv) \) | 0.50 | 0.57 | 0.71 | 0.50 | 0.57 | 0.72 |
| \( log(m) \) | 0.52 | 0.56 | 0.70 | 0.53 | 0.56 | 0.71 |
| \( log(k) \) | 0.53 | 0.55 | 0.69 | 0.54 | 0.56 | 0.70 |

| Linear Regression - NSGA-III | 10-fold cross validation |
|-----------------------------|-------------------------|
| \( r \) | MAE | RMSE | \( r \) | MAE | RMSE |
| none | 0.00 | 0.48 | 0.58 | 0.00 | 0.49 | 0.58 |
| \( log(lconnect) \) | 0.12 | 0.48 | 0.57 | 0.12 | 0.45 | 0.57 |
| \( hv \) | 0.21 | 0.48 | 0.57 | 0.22 | 0.48 | 0.58 |
| \( log(nconnect) \) | 0.25 | 0.48 | 0.56 | 0.24 | 0.48 | 0.56 |
| \( kconnect \) | 0.33 | 0.46 | 0.55 | 0.32 | 0.47 | 0.56 |
| \( maxd \) | 0.40 | 0.48 | 0.58 | 0.40 | 0.48 | 0.59 |
| \( avgd \) | 0.40 | 0.46 | 0.53 | 0.41 | 0.47 | 0.53 |
| \( log(m) \) | 0.43 | 0.45 | 0.52 | 0.44 | 0.45 | 0.53 |
| \( log(k) \) | 0.57 | 0.38 | 0.48 | 0.56 | 0.39 | 0.48 |
| \( log(k) \) | 0.85 | 0.25 | 0.31 | 0.86 | 0.25 | 0.31 |

Fig. 1: log(ert) vs. fitted values for the model with joint features \( k \) and \( m \) for a) mBOA and b) NSGA-III.
model. Therefore, we proceed by eliminating the least impact feature at each step, until no feature is left. This process is summarized in Table III, and the corresponding scatter plots are illustrated in Figure 1.

The models’ statistics presented in Table III show that using combined features provides a significantly more precise model for both algorithms — specially in mBOA’s case. In fact, the multiple linear model provides a correlation coefficient of 0.89 instead of the ruggedness-based model, which has a correlation coefficient of 0.53 for mBOA. We can clearly see that the most influencing features are \(k\) and \(m\). Indeed, by using two feature the runtime of mBOA can be estimated with a relatively small error (\(MAE = 0.23\) and \(RMSE = 0.24\)).

Interestingly, when removing some features using backward elimination, the correlation coefficient increases. Indeed, the correlation coefficient starts with 0.86 when using all the features, and increases to 0.89 after eliminating 6 features (the first 6 lines in Table III). Although the impact seems too small, it tells us that these features have a negative impact on the efficiency of the model (acting like noisy features).

### B. Probabilistic Analysis of Pareto Front

In the previous section we have analyzed the influence of selected features on the estimated runtime for \((1 + \epsilon)\) approximations. However, the \((1 + \epsilon)\) approximation purely might not reveal some important aspects of non-dominated solutions of the Pareto front as convergence and distribution. These aspects are investigated in this section by analyzing the probabilistic information of the final PGM (BN structure and parameters) for mBOA when the \((1 + \epsilon)\)—approximation is found. We calculate the pmf \(P(y)\), defined in Equation 3, for each solution in the Pareto set, based on the PGM learned at the end of each execution of each landscape.

Afterwards, the mean of the pmf values along all executions is obtained in order to calculate the marginal distribution \(P(Z_1 = z_1, ..., Z_M = z_M)\). Each non-dominated solution is represented by a circle in its corresponding point in the PF, which is proportional to the marginal probability \(P(Z_1 = z_1, ..., Z_M = z_M)\) [27]. Due to the space limitation, we present, in Figures 2 and 3, the PF probability view of mBOA for one specific landscape with \(K = 6\). Since it is not practical to visualize the Pareto front for more than two objectives, we illustrate the ordered Euclidean distance (from the nearest to the farthest) between each point from the Pareto front and the ideal point \(^2\) for 3, 5, and 8 objectives.

![Fig. 2: A probabilistic view for a) the Pareto front for 2 objectives and b) the Euclidean distance between the ideal point for 3 objectives. \(k = 6\) in all cases.](image)

![Fig. 3: A probabilistic view for the Euclidean distance between the ideal point for a) 5 objectives and b) 8 objectives. \(k = 6\) in all cases.](image)
circles) distributed along the entire front (many in the extreme regions instead of being concentrated in the knee). This is also observed in the Figure 2b, however here, some solutions nearby ideal and extreme points present high probabilities.

In the plots for 5 and 8 objectives in Figure 3, we note that the solutions present similar probabilities, since there are few large points plotted in the Pareto front.

The results show that, for smaller number of objectives, solutions around Pareto front knee and extreme points are better represented because they have higher probabilities of occurrence as depicted in Figure 2. This does not happen for 5 and 8 objectives. These observations can be useful to understand the convergence and diversity performance of a given approach. As shown in Figures 2 and 3, some fronts can present solutions concentrated around specific regions and gaps in other regions. We believe that these characteristics might be caused by non-uniform distributed probabilities codified by the BN which provide more solutions in some regions than in others.

With the aim of verifying this conjecture in our experiments, we performed a rigorous study on the probability distributions codified by the BN by using the Kolmogorov-Smirnov test to investigate the adequacy of a uniform model. The test is performed on all 30 landscapes for each combination of $K$ and $M$, and the rates at which the test fails to reject the null hypothesis (that the data come from the considered distribution model) are shown in Table IV, organized by the number of objectives.

![Table IV](https://example.com/table.png)

| $M = 2$ | $M = 3$ | $M = 5$ | $M = 8$ |
|--------|--------|--------|--------|
| Uniform distribution | 0.03 | 0.18 | 1 | 1 |

Although the probability distributions fit uniform models for all landscapes with $M = 5$ and $M = 8$, (see a representative landscape for $K = 6$ in Figure 3), a uniform model can not be generalized to describe the probability distributions for landscapes with $M = 2$ and $M = 3$, i.e., for 97% of landscapes with 2 objectives the uniform model can be rejected with a significance level of 0.1. It is important to point out that although the Kolmogorov-Smirnov test indicates that non-uniform distributions encoded by the BN model can be associated with non-well spread frontiers, these results are not sufficient to define uniform distributions as a unique metric for the BN model since gaps might occur even with uniform distributions.

In fact, the experiments we performed show that examining the PGM structures according to the marginal distribution of the corresponding objectives values from the Pareto front can be very useful to analyze the performance of mBOA and in the future we can use this information associated with Kolmogorov-Smirnov tests to guide the search process through specific regions of the Pareto front using the current state of the Bayesian Network.

V. CONCLUSION

In this paper we have analyzed a PGM-based MOEDA named Multi-objective Bayesian Optimization Algorithm (mBOA) in the context of multi and many objective combinatorial optimization. The main issues investigated in this paper concern a fitness landscape analysis of general-purpose problem features and the analysis of the final PGM structure obtained by mBOA.

We have extracted some features enumerating MNK-landscape problem instances for 2, 3, 5 and 8 objectives. We aimed to explore the correlation between the problem features and the estimated runtime for mBOA in comparison with NSGA-III, a state-of-the-art algorithm applied to multi and many optimization. In addition, we have evaluated mBOA through the analysis of the final achieved PGM in order to explore one of the main advantages of using EDAs: the possibility of scrutinizing its probabilistic model.

Based on experiments with the MNK instances addressed in this paper, we can conclude that mBOA has a significantly lower estimated runtime compared to NSGA-III, and as expected the feature that has the most significant impact on the estimated runtime is the ruggedness. We observed nevertheless that there are features with a negative impact on the efficiency of the model (acting like noisy features).

Furthermore, examining the Pareto front according to a probabilistic view based on the PGM structures, enables the analysis of how the BN can guide the search through specific regions of the Pareto front, being useful to understand the convergence and diversity performance of a given approach.

In the future, other relevant features can be investigated, as those associated with statistics of the probability distribution of points on the Pareto Front. The approaches will be investigated considering more than eight objectives and other problems. Additionally, another interesting research direction is the application of other types of PGM that can learn and explore dependencies between variables and objectives.

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