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A Hybrid Metaheuristic for Multiobjective Unconstrained Binary Quadratic Programming

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Abstract

The conventional Unconstrained Binary Quadratic Programming (UBQP) problem is known to be a unified modeling and solution framework for many combinatorial optimization problems. This paper extends the single-objective UBQP to the multiobjective case (mUBQP) where multiple objectives are to be optimized simultaneously. For the purpose of approximating the Pareto set, we propose a hybrid metaheuristic which combines an elitist evolutionary multiobjective optimization algorithm and a state-of-the-art single-objective tabu search procedure by using an achievement scalarizing function. Finally, we define a formal model to generate diverse mUBQP instances and show the interest of the proposed approach in obtaining competitive results on large-size mUBQP instances with two and three objectives.

Key words: Unconstrained binary quadratic programming, Multiobjective combinatorial optimization, Hybrid Metaheuristic, Evolutionary Multiobjective Optimization, Tabu search, Scalarizing function

1. Introduction

The conventional and single-objective unconstrained binary quadratic programming (UBQP) problem is to maximize the function:

$$f(x) = x'Qx = \sum_{i=1}^n \sum_{j=1}^n q_{ij}x_i x_j \quad (1)$$

where $Q = (q_{ij})$ is an n by n matrix of constant values and x is a vector of n binary (zero-one) variables, *i.e.*, $x_i \in \{0, 1\}$, $i \in \{1, \dots, n\}$.

The UBQP is known to be a very general model able to represent a wide range of important problems, including those from financial analysis [1], social psychology [2], computer aided design [3] and cellular radio channel allocation [4]. Moreover, a number of NP-hard problems can be transformed into the UBQP, such as graph coloring problems, maxcut problem, set packing problem, set partitioning problem, maximum clique problem and so on [5, 6]. As a consequence, the UBQP itself is clearly a NP-hard problem [7]. During the past few decades, a large number of algorithms and approaches have been proposed for the single-objective UBQP in the literature. This includes several exact methods based on branch and bound or branch and cut [8, 9, 10] as well as a number of heuristic and metaheuristic methods like simulated annealing [11], tabu

search [12, 13, 14, 15, 16], path-relinking [17], as well as evolutionary and memetic algorithms [18, 19, 20, 21].

In this paper, we extend this conventional single-objective UBQP problem to the multiobjective case, denoted by mUBQP, where multiple objectives are to be optimized simultaneously. Such an extension naturally increases the expressive power of the UBQP and provides a convenient formulation to fit situations where the single-objective UBQP cannot accommodate. For instance, it is known that the UBQP can be used to recast each of two following graph coloring problems: the vertex coloring problem (which is to determine the chromatic number of a graph) [5] and the sum coloring problem (which is to determine the chromatic sum of a graph) [22]. Still, UBQP is not convenient to formulate the bi-objective coloring problem which requires to determine a legal vertex coloring of a graph while minimizing simultaneously the number of colors used and the sum of colors. For this bi-objective coloring problem, the mUBQP formulation can be employed in a straightforward way.

In addition of introducing the mUBQP problem, the paper targets two other goals. First, given that the single-objective UBQP is NP-hard, its generalized mUBQP formulation is also a difficult problem to solve in the general case. For the purpose of approximating the Pareto set of a given mUBQP instance, heuristic approaches will be indispensable. Following the studies on memetic algorithms for the UBQP as well as many other problems, we adopt as our solution approach the memetic framework and propose a hybrid metaheuristic which combines an elitist evolutionary multiobjective optimization algorithm with a state-of-the-art single-objective tabu search procedure based on an achievement scalarizing function. The last goal of the paper is to define a formal and flexible model to

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generate hard mUBQP instances and show the interest of the proposed solution approach in obtaining competitive results on large-size mUBQP instances with two and three objectives.

The paper is organized as follows. In Section 2, our multiobjective formulation of the UBQP problem (mUBQP) is introduced, together with some properties and definitions. The hybrid metaheuristic (HM) proposed for the mUBQP and its main ingredients are presented in Section 3, including the scalarizing evaluation function, the tabu search procedure, the initialization phase and the variation operators. An experimental analysis of our HM algorithm is conducted in Section 4 on a large set of mUBQP instances of different structure and size. Conclusions and further research are discussed in the last section.

2. Multiobjective Unconstrained Binary Quadratic Programming

This section first introduces the multiobjective unconstrained binary quadratic programming problem. Some definitions related to multiobjective combinatorial optimization are then recalled, followed by problem complexity-related properties and a link with similar problem formulations. At last, the construction of problem instances, together with an experimental study on the objective values correlation and the cardinality of the Pareto set, are presented.

2.1. Problem Formulation

The multiobjective unconstrained binary quadratic programming (mUBQP) problem can be stated as follows.

$$\begin{aligned} \max f_k(x) &= \sum_{i=1}^n \sum_{j=1}^n q_{ij}^k x_i x_j & k \in \{1, \dots, m\} \\ \text{subject to } x_i &\in \{0, 1\} & i \in \{1, \dots, n\} \end{aligned} \quad (2)$$

where $f = (f_1, f_2, \dots, f_m)$ is an objective vector function with $m \geq 2$, n is the problem size, and we have m matrices $Q^k = (q_{ij}^k)$ of size n by n with constant values, $k \in \{1, \dots, m\}$. The decision space X is defined on binary strings of size n .

2.2. Definitions

Let $X = \{0, 1\}^n$ be the set of feasible solutions in the *decision space* of Problem (2). We denote by $Z \subseteq \mathbb{R}^m$ the feasible region in the *objective space*, i.e., the image of feasible solutions when using the vector maximizing function f . The Pareto dominance relation is defined as follows. A solution $x \in X$ is dominated by a solution $x' \in X$ (denoted by $x < x'$) if $f_k(x) \leq f_k(x')$ for all $k \in \{1, \dots, m\}$, and $\exists k \in \{1, \dots, m\}$ such that $f_k(x) < f_k(x')$. If neither $x \not< x'$ nor $x' \not< x$ holds, then both are *mutually non-dominated*. A solution $x \in X$ is said to be *Pareto optimal* (or efficient, non-dominated) if there does not exist any other solution $x' \in X$ such that x' dominates x . The set of all Pareto optimal solutions is called the *Pareto set*, denoted by X_{PS} , and its mapping in the objective space is called the *Pareto front*. One of the most challenging issue in multiobjective combinatorial optimization is to identify a minimal complete Pareto set, i.e., one Pareto optimal solution mapping to each point from the Pareto front. Note that such a set may not be unique, since multiple solutions can map to the same non-dominated vector.

2.3. Properties

For many multiobjective combinatorial optimization problems, computing the Pareto set is infeasible for two main reasons. First, deciding if a candidate solution is Pareto optimal is known to be NP-complete for numerous multiobjective combinatorial optimization problems [23, 24]. This is also the case for the mUBQP problem since its single-objective counterpart is known to be NP-hard [7]. Second, the number of Pareto optimal solutions typically grows exponentially with the size of the problem instance [24]. In that sense, most multiobjective combinatorial optimization problems are said to be *intractable*. In the following, we show that the mUBQP problem is intractable.

Proposition 1. *The multiobjective unconstrained binary quadratic programming problem (2) is intractable, even for $m = 2$.*

Proof. Consider the following bi-objective mUBQP instance.

$$q_{ij}^1 = \begin{cases} 2^{n(i-1) - \frac{i(i-1)}{2} + j - 1} & \text{if } i \geq j \\ 0 & \text{if } i < j \end{cases} \quad i, j \in \{1, \dots, n\}$$

Let $q_{ij}^2 = -q_{ij}^1$ for all $i, j \in \{1, \dots, n\}$. As illustrated in Figure 1 for $n = 3$, it is obvious to see that all solutions are mutually non-dominated. Therefore, all feasible solutions are Pareto optimal, and $|X_{PS}| = |X| = 2^n$. \square

To cope with NP-hard and intractable multiobjective combinatorial optimization problems, researchers have been interested in developing approximate algorithms. As a consequence, the goal is often to identify a good *Pareto set approximation*, having both good convergence and distribution properties [25, 26]. To this end, metaheuristics in general, and evolutionary algorithms in particular, have received a growing interest since the late eighties [27].

2.4. Links with Existing Problem Formulations

In its single-objective form, the UBQP problem is of high interest in practice, since many existing combinatorial optimization problems can be formalized in terms of UBQP. This definition includes linear assignment, knapsack, set covering, set partitioning, set packing, graph coloring, maxcut, and maximum clique problems, just to mention a few [5, 6]. As a consequence, multiobjective versions of these problems can potentially be defined in terms of mUBQP. However, to the best of our knowledge, the UBQP problem has never been explicitly defined in the multiobjective formulation given in Eq. (2).

Existing multiobjective formulations of classical combinatorial optimization problems with binary variables include multiobjective linear assignment problems, multiobjective knapsack problems, or multiobjective set covering and partitioning problems [24, 28, 29]. Nevertheless, the objective functions of such formulations are linear, and not quadratic as in mUBQP. Still, they often contain additional constraints; typically the unimodularity of the constraint matrix for linear assignment, or the capacity constraint for knapsack. This means that existing binary multiobjective combinatorial optimization problems can be formalized in terms of mUBQP by adapting and generalizing the

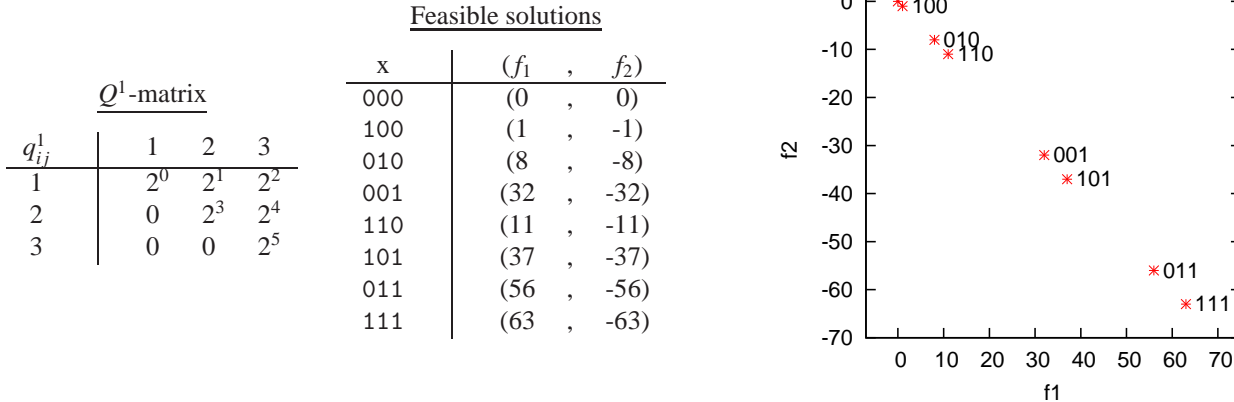


Figure 1: Enumeration of all feasible solutions for the mUBQP problem instance considered in the proof of Proposition 1: The input data of the Q^1 -matrix (left), the enumeration of feasible solutions (middle), and their representation in the objective space (right). The problem size is $n = 3$.

techniques from [5] to the multiobjective case, whereas the opposite does not hold in general due to the quadratic nature of mUBQP.

2.5. Problem Instances

mUBQP problem instances could be designed in multiple ways. For instance, each objective function could be independent, or could be defined as well-known problem objective functions like in knapsack, linear assignment, set partitioning, and so on.

In this work, we propose to define correlated mUBQP problem instances as follows. Each objective function is defined by means of a matrix Q^k , $k \in \{1, \dots, m\}$. Based on the single-objective UBQP instances available in the OR-lib [30], non-null matrix integer values are randomly generated according to a uniform distribution in $[-100, +100]$. As in the single-objective case, the density d gives the proportion of non-null numbers in the matrix. In order to define matrices of a given density d , we set $q_{ij}^k = 0$ for all $k \in \{1, \dots, m\}$ at the same time, following a Bernoulli distribution of parameter d .

Moreover, we define a correlation between the data contained in the m matrices Q^k , $k \in \{1, \dots, m\}$. The positive (respectively negative) data correlation decreases (respectively increases) the degree of conflict between the objective function values. For the sake of simplicity, we here consider the same correlation between all pairs of objective functions, given by a correlation coefficient $\rho \geq \frac{-1}{m-1}$. The generation of correlated data follows the procedure given in [31], based on a multivariate uniform law of dimension m . In order to validate the behavior of the objective correlation coefficient experimentally, we conduct an empirical study for $n = 18$ in order to enumerate the decision space exhaustively. Figure 2 reports the average value of the Spearman correlation coefficient over 30 different and independent instances for different parameter combinations: ρ , m , and d . The correlation coefficient ρ clearly allows to tune the objective correlation very precisely.

To summarize, the four parameters used to define a mUBQP instance are (i) the problem size n , (ii) the matrix density d ,

(iii) the number of objective functions m , and (iv) the objective correlation coefficient ρ . We make the mUBQP problem instances investigated in the paper as well as an instance generator available at the following URL: <http://mocobench.sf.net/>.

2.6. Cardinality of the Pareto Set

In this section, we analyze the impact of the mUBQP problem instance features (in particular, d , m and ρ) on the number of Pareto optimal solutions. The Pareto set cardinality plays an important role on the problem complexity (in terms of intractability), and then on the behavior and the performance of solution approaches. Indeed, the higher the number of Pareto optimal solutions, the more computational resources required to identify a minimal complete Pareto set.

We set $n = 18$ in order to enumerate the decision space exhaustively. The measures reported are the average values over 30 different and independent mUBQP instances of same structure. Figure 3 gives the proportion of Pareto optimal solutions. The matrix density d has a low influence on the results. However, the number of objective functions m and the objective correlation ρ both modifies the proportion of Pareto optimal solutions to several orders of magnitude. Indeed, this proportion decreases from 10^{-4} for $\rho = -0.9$ to 10^{-5} for $\rho = +0.9$ for two- and three-objective mUBQP problem instances. As well, for a negative objective correlation $\rho = -0.2$, this proportion goes from 10^{-4} up to 10^{-1} , whereas it goes from 10^{-5} up to 10^{-3} for a positive objective correlation $\rho = +0.9$, for $m = 2$ and $m = 5$, respectively. Figure 4 shows three examples of mUBQP problem instances represented in a two-objective space. When the objective correlation is negative, the objective functions are in conflict, and the Pareto set is large (left). When the objective correlation is null, the objective space can be embedded in a multidimensional ball (middle). At last, when the objective correlation is positive, there exists few solutions in the Pareto set (right).

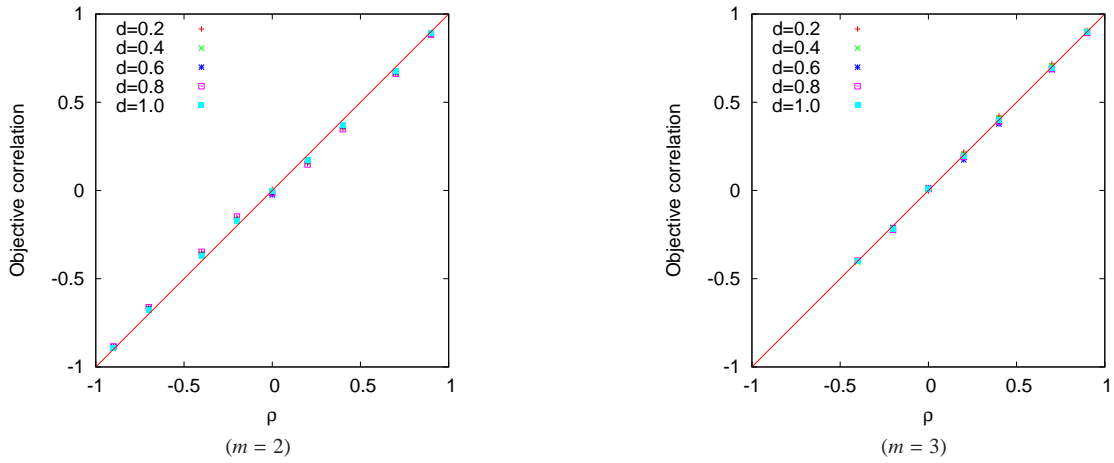


Figure 2: Correlation between the objective function values according to the correlation coefficient ρ . The average value of the Spearman correlation coefficient is reported. The decision space is enumerated exhaustively for $n = 18$ on a set of 30 independent random instances. The number of objectives is $m = 2$ (left) and $m = 3$ (right).

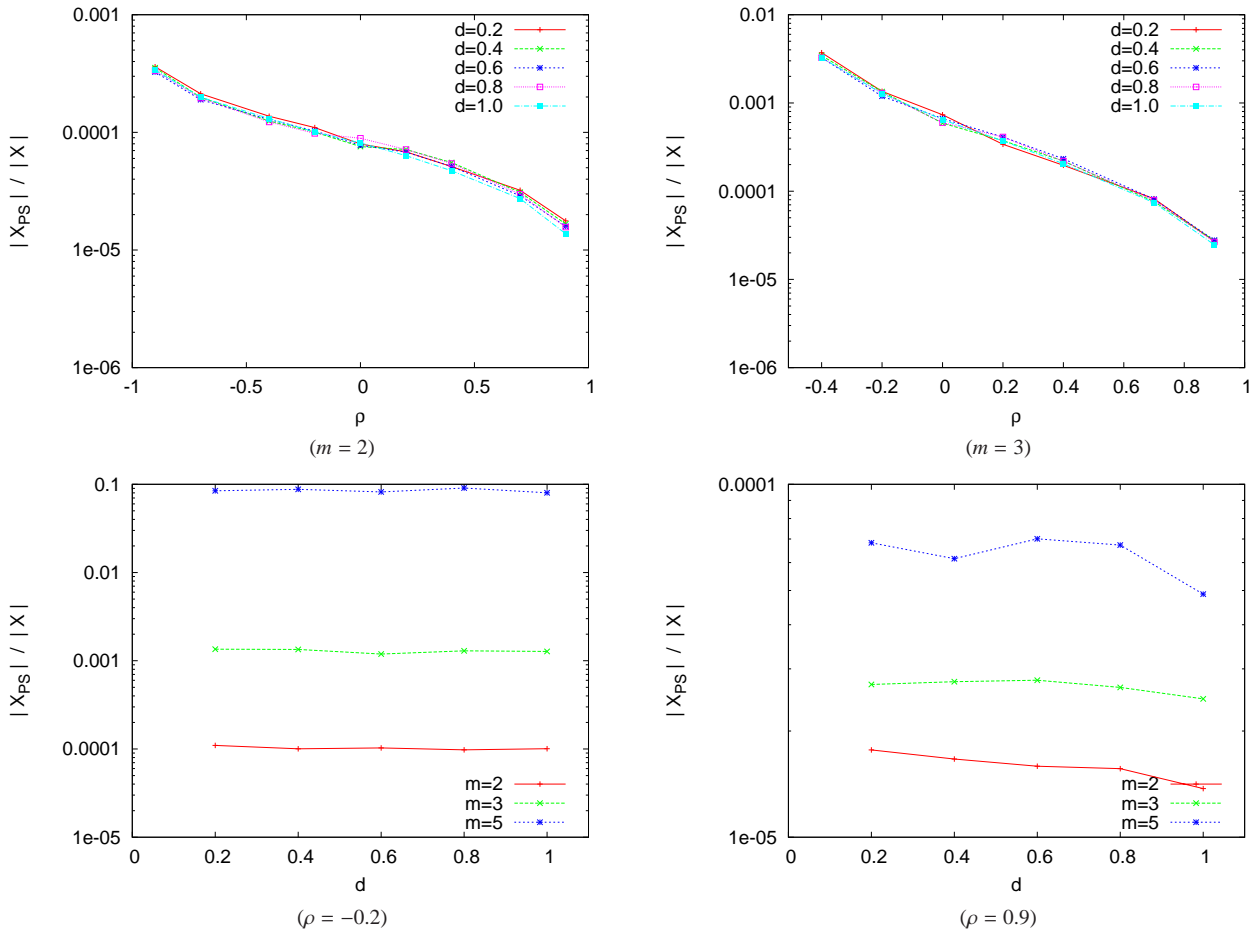


Figure 3: Average ratio of the minimal complete Pareto set cardinality ($|X_{PS}|$) to the decision space size ($|X| = 2^{18}$) according to the objective correlation ρ (top left $m = 2$, right $m = 3$), and according to the Q-matrix density d (bottom left $\rho = -0.2$, right $\rho = 0.9$). The problem size is $n = 18$. Notice the log-scale.

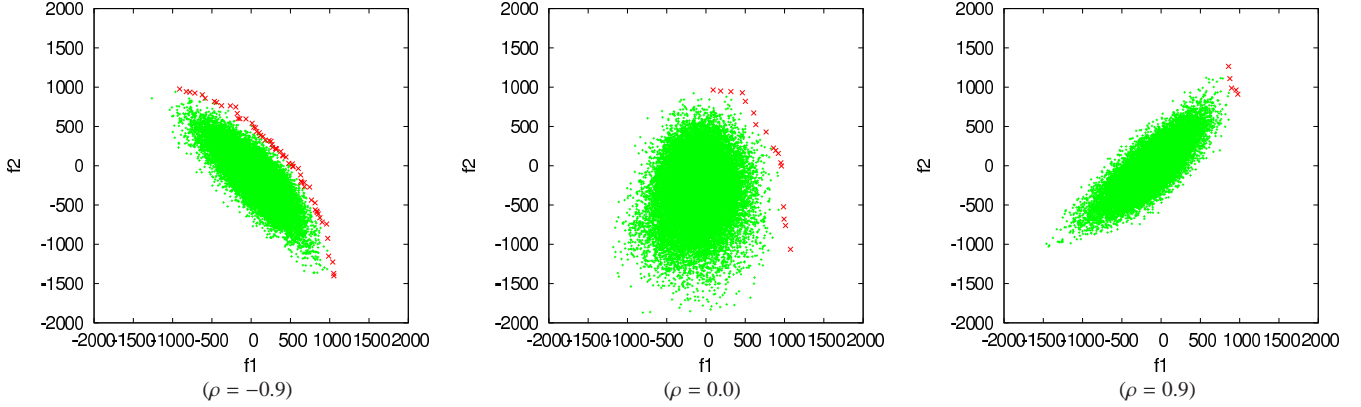


Figure 4: Representation of feasible solutions of a mUBQP problem instance in a two-objective space. The problem size is $n = 18$, the Q-matrix density is $d = 0.8$, the number of objective functions is $m = 2$, and the objective correlation is $\rho = -0.9$ (left), $\rho = 0.0$ (middle) and $\rho = 0.9$ (right). Green points are the objective vectors of random solutions (10% of the decision space size), and red points corresponds to non-dominated objective vectors.

3. A Hybrid Metaheuristic for mUBQP

The hybrid metaheuristic proposed for the mUBQP problem is based on a memetic algorithm framework [32], which is known to be an effective approach for discrete optimization [33]. Our approach uses one of the best performing single-objective local search algorithm as one of its main components [12, 13].

3.1. General Principles

Memetic algorithms constitute a whole class of hybrid metaheuristics combining an evolutionary algorithm and a local search algorithm. In particular, this class includes genetic and tabu search hybrid approaches [34]. We focus on multiobjective memetic algorithms [35] whose goal is to find an approximation of the whole Pareto set (not only a subpart of it). A simple elitist multiobjective population-based evolutionary algorithm operates as the main metaheuristic, whereas an advanced single solution-based local search is used as an improvement operator in place of the mutation step. Keeping the exploration vs. exploitation trade-off in mind, the idea behind such an approach is that the evolutionary algorithm will offer more facilities for diversification, while the local search algorithm will provide more capabilities for intensification.

An outline of our hybrid metaheuristic (HM) is given in Algorithm 1. The search space under consideration is composed of all binary vectors of size n , *i.e.*, the decision space $X = \{0, 1\}^n$. The size of the search space is then equal to 2^n . The evaluation function is the canonical objective function given in Eq. (2). An unbounded *archive*, or population, of mutually non-dominated solutions found so far is maintained with respect to the Pareto dominance relation defined in Section 2.2. In other words, throughout the search process, solutions are discarded as soon as they are detected to be dominated by at least one other solution from the archive. Equivalent solutions are also eliminated. At each iteration, two parents are selected at random from the archive and then recombined to produce a single offspring solution (Section 3.5). The newly generated solution

Algorithm 1 Pseudo-code of our hybrid metaheuristic (HM) for mUBQP

Input: matrix Q (dimension $m \times n \times n$)

Output: Pareto set approximation A

- 1: initialize the archive A /* see Section 3.4 */
 - 2: **repeat**
 - 3: randomly select two individuals x_i, x_j from A
 - 4: $x \leftarrow \text{recombine}(x_i, x_j)$ /* see Section 3.5 */
 - 5: $x^* \leftarrow \text{tabu_search}(x)$ /* see Section 3.3 */
 - 6: $A \leftarrow \text{non-dominated solutions from } (A \cup \{x^*\})$
 - 7: **until** a stopping condition is satisfied
-

is further improved by means of a tabu search algorithm (Section 3.3). The evaluation function used by tabu search is based on an scalarizing technique of the initial objective function values (Section 3.2). The corresponding achievement scalarizing function is defined in such a way that the tabu search procedure focuses its search within the objective space area enclosed by the positions of parent solutions. Another crucial component of our HM algorithm appears at the initial phase (Section 3.4), where a computational effort is made in order to identify close-to-optimal solutions located at the extreme regions of the objective space. The algorithm is iterated until a user-given stopping condition is satisfied. The main components of our HM algorithm are detailed below.

3.2. Achievement Scalarizing Function

The tabu search procedure, that will be presented later in the paper, is known to be very well-performing for solving single-objective UBQP instances of different structures and sizes [12, 13, 14, 15, 16]. Of course, given that it manipulates a single solution only, a scalarization of the multiple objective functions is required due to the multiobjective nature of the mUBQP. The goal here is to temporarily transform the mUBQP problem into a single-objective one so that the tabu search algorithm can be used in a straightforward way. Many general-

purpose scalarizing functions have been proposed for multiobjective optimization [36], generally with the aim of incorporating preference information coming from a decision-maker. Here, the matter is somehow different since we are interested in approximating the whole Pareto set. Hence, the parameters required by the scalarizing function under consideration are dynamically set according to the current state of the search process. This will be discussed in Section 3.5.

In multiobjective memetic algorithms, the most popular scalarizing function is the weighted-sum aggregation [35, 37], where a weighting coefficient vector represents the relative importance of each objective function. However, despite its relative simplicity, this approach does not allow to identify a number of Pareto optimal solutions, whose corresponding non-dominated objective vectors are located on the convex hull of the Pareto front [24, 36]. Another example is the *achievement scalarizing function*, proposed by Wierzbicki [38]. This technique is particularly well-suited to work with reference points. A reference point gives desirable or acceptable values for each objective function. These objective values are called *aspiration levels* and the resulting objective vector is called a *reference point* and can be defined either in the feasible or in the infeasible region of the objective space. One of the families of achievement scalarizing functions can be stated as follows. Let us recall that the maximization of the objective functions are here assumed.

$$\sigma_{(z^r, \lambda, \epsilon)}(x) = \max_{k \in \{1, \dots, m\}} \left\{ \lambda_k (z_k^r - f_k(x)) \right\} + \epsilon \sum_{k=1}^m \lambda_k (z_k^r - f_k(x)) \quad (3)$$

where σ is a mapping function from X to \mathbb{R} , $x \in X$ is a feasible solution, $z^r \in \mathbb{R}^m$ is a reference point vector, $\lambda \in \mathbb{R}^m$ is a weighting coefficient vector, and ϵ is an arbitrary small positive number ($0 < \epsilon \ll 1$). Notice that we keep the ϵ parameter constant throughout the search process. The following achievement scalarizing optimization problem can be formalized.

$$\begin{aligned} \min \quad & \sigma_{(z^r, \lambda, \epsilon)}(x) \\ \text{subject to} \quad & x \in X \end{aligned} \quad (4)$$

Interestingly, two properties are ensured [39]:

- (i) if $x^* = \arg \min_{x \in X} \sigma_{(z^r, \lambda, \epsilon)}(x)$, then x^* is a Pareto optimal solution;
- (ii) if x^* is a Pareto optimal solution, then there exists a function $\sigma_{(z^r, \lambda, \epsilon)}$ such that x^* is a (global) optimum of Problem (4).

This makes the achievement function very attractive compared to simpler forms of scalarizing functions. Indeed, as noticed earlier, only a subset of Pareto optimal solutions, known as supported solutions [24], can be found within a weighted-sum aggregation function, since the second property (ii) is not satisfied. Those solutions are known as supported Pareto optimal solutions, and their corresponding non-dominated objective vectors

are located on the convex hull of the Pareto front. On the contrary, the achievement scalarizing function potentially allows to identify both supported and non-supported Pareto optimal solutions [36]. Successful integrations of the achievement scalarizing function into evolutionary multiobjective optimization algorithms can be found in [40, 41, 42].

3.3. Tabu Search

The following tabu search algorithm, used as a subroutine of our HM, is reported to be one of the best-performing approaches for the single-objective UBQP problem [13]. In order to extend it to the multiobjective case, we consider the achievement scalarizing function, so that the initial objective vector values are transformed into a single scalar value. Notice, however, that the nature of the evaluation function considered in the paper has a different structure than the classical evaluation function of single-objective UBQP. We describe the main principles of the tabu search below.

The neighborhood structure is based on the 1-flip operator. Two feasible solutions are neighbors if they differ exactly on one variable. In other words, a given neighbor can be reached by changing the value of a binary variable to its complement from the current solution. The size of the 1-flip neighborhood structure is linear with the problem size n . As in the single-objective UBQP, each mUBQP objective function can be evaluated incrementally. We follow the fast incremental evaluation procedure presented in [43] to calculate the move gain of a given neighboring solution. For a given objective function, the whole set of neighbors can be evaluated in linear time. As a consequence, the objective values of all neighboring solutions are evaluated in $O(m \cdot n)$ in the multiobjective case. Once the objective values of a given neighboring solution have been (incrementally) evaluated, we compute its scalar fitness value with respect to Eq. (3).

As a short-term memory, we maintain the tabu list as follows. Revisiting solutions is avoided within a certain number of iterations, called the tabu tenure. The *tabu tenure* of a given variable x_i is denoted by $tenure(i)$. Hence, variable x_i will *not* be flipped again for a number of $tenure(i)$ iterations. Following [20], we set the tabu tenure of a given variable x_i after it has been flipped as follows.

$$tenure(i) = tt + rand(10) \quad (5)$$

where tt is a user-given parameter and $rand(10)$ gives a random integer value between 1 and 10. From the set of neighboring solutions produced by all non-tabu moves, we select the one with the best (smallest) fitness value according to Eq. (3). Indeed, let us recall at this point that the aim of the tabu search algorithm is to find a good approximate solution for Problem (4), for a given definition of z^r and λ . However, notice that all neighboring solutions are always evaluated, and that a tabu move can still be selected if it produces a better solution than the current global best. This is called an aspiration criterion in tabu search. The stopping condition of the tabu search algorithm is met when no improvement has been performed within a given number of moves α . The parameter α is called the *improvement*

cutoff. For more details on the tabu search algorithm for the single-objective UBQP, the reader is referred to [13, 20].

3.4. Initial Phase

The goal of the initial phase is to identify good-quality solutions with respect to each objective function of the mUBQP, *i.e.*, solutions mapping to the extreme points of the Pareto front in the objective space. This set of solutions initializes the search process in order to ensure that our HM provides a good covering of the Pareto front. To this end, we define the following achievement scalarizing function parameter setting. We set the reference point $z^r = \{z_1^{max}, \dots, z_m^{max}\}$ such that z_k^{max} is higher than any possible f_k -value. This (unfeasible) objective vector can be seen as a rough approximation of the utopia point [24, 36]. Now, let us consider a particular objective function $k \in \{1, \dots, m\}$. We set $\lambda_k = 1$, and $\lambda_l = 0$ for all $l \in \{1, \dots, m\} \setminus \{k\}$.

The tabu search algorithm, seeded with a random solution, is then considered with the corresponding achievement scalarizing function as an evaluation function. Those initial solutions have a high impact on the performance of our HM, particularly in terms of diversification. As a consequence, we perform γ independent restarts of the tabu search *per* objective function in order to increase the chance of getting very high-performing solutions in all extreme regions of the Pareto front. This process is iterated for every objective function of the mUBQP problem instance under consideration.

3.5. Variation Operator

At each iteration of our HM algorithm, a single offspring solution is created by a recombination operator. First, we select two mutually non-dominated parent solutions at random from the current archive $x_i, x_j \in A$ such that $x_i \neq x_j$. Then, an offspring solution is created with uniform crossover. Common variables between both parents are thus assigned to the offspring solution, while the remaining ones are assigned at random. The offspring solution is further improved by means of the tabu search procedure presented in Section 3.3. Here, we aim at obtaining a new solution in an unexplored region of the Pareto front by defining the parameters of the achievement scalarizing function properly. The procedure attempts to find a non-dominated point that “fills the gap” between the objective vectors associated with x_i and x_j . The region of the objective space where the tabu search algorithm operates is then delimited by the position of parent solutions, given by the following definition of the achievement scalarizing function.

$$z_k^r = \max\{f_k(x_i), f_k(x_j)\} \quad k \in \{1, \dots, m\} \quad (6)$$

$$\lambda_k = \frac{1}{|f_k(x_i) - f_k(x_j)|} \quad k \in \{1, \dots, m\} \quad (7)$$

This procedure allows our HM to improve, at each iteration, a particular part of the Pareto front, dynamically chosen with respect to the pair of parent solutions under selection. The overall variation procedure is illustrated in Figure 5.

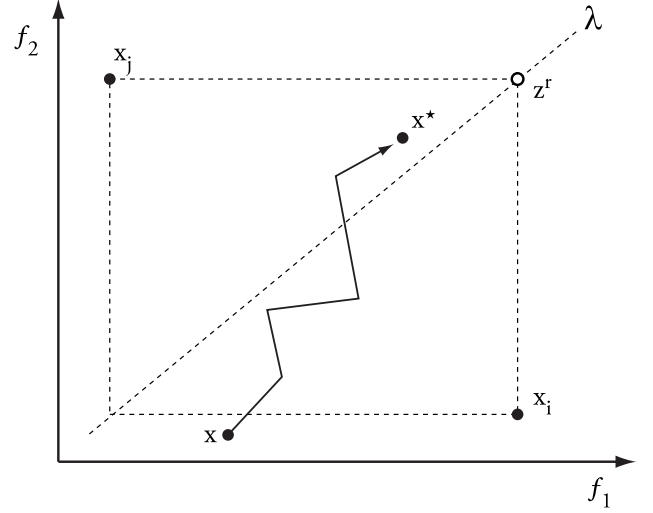


Figure 5: Graphical representation of the improvement phase in a two-objective space, where x_i and x_j are the parent solutions, x is the offspring solution and x^* is the solution improved by means of the tabu search procedure through the achievement scalarizing evaluation function defined by the reference point z^r and the weighting coefficient vector λ .

4. Experimental Analysis

This section presents an experimental analysis of the proposed approach on a broad range of mUBQP problem instances.

4.1. Experimental Design

In the following, we conduct an experimental study on the influence of the problem size (n), the number of objectives (m), and the objective correlation (ρ) of the mUBQP problem on the performance of the HM algorithm proposed in the paper. In particular, we investigate the following parameter setting: $n \in \{1000, 2000, 3000, 4000, 5000\}$, $m \in \{2, 3\}$, and $\rho \in \{-0.5, -0.2, 0.0, +0.2, +0.5\}$. The density of the matrix is set to $d = 0.8$. One instance, generated at random, is considered *per* parameter combination. This leads to a total of 50 problem instances.

We compare the performance of our algorithm against a steady-state evolutionary algorithm that follows the same structure as the HM, but where the tabu search is replaced by a random mutation. This allows us to appreciate the impact of the tabu search and scalarizing procedure on the performance of the proposed approach. The same initialization phase is applied. Then, at each iteration, an offspring solution is created by uniform crossover and an independent bit-flip operator is applied, *i.e.*, each variable is randomly flipped with a probability $1/n$. We refer to this algorithm as SS-EA, for steady-state evolutionary algorithm. We also compare the results of the algorithms to a baseline algorithm, the well-known NSGA-II [44]. NSGA-II maintains a population of constant size, initialized at random, and produces the same number of offspring solutions at every iteration. Selection for reproduction and replacement is based on dominance-depth ranking first, and on crowding distance at second-level. A binary tournament is used for selection, and

Table 1: Parameter setting used in the paper for the experimental analysis.

Description	Parameter	Value(s)
Instances		
Problem size	n	{1000, 2000, 3000, 4000, 5000}
Matrix density	d	0.8
Number of objectives	m	{2, 3}
Objective correlation	ρ	{-0.5, -0.2, 0.0, +0.2, +0.5}
Algorithms		
Crossover rate		1.0
Mutation rate (SS-EA, NSGA-II)		$1.0/n$
Population size (NSGA-II)		100
Tabu tenure	tt	$n/150$
Tabu improvement cutoff	α	$5n$
Number of restarts (initialization)	γ	5
ϵ -parameter (achievement scalarizing function)	ϵ	10^{-8}
Stopping condition (CPU time)		$(n \cdot m \cdot 10^{-3})$ minutes

an elitist strategy is used for replacement. The same crossover and mutation operators as for SS-EA are considered. In other words, the main differences between SS-EA and NSGA-II are: (i) SS-EA uses an unbounded population whereas NSGA-II maintains a fixed-size population, (ii) selection for reproduction is performed at random within SS-EA whereas it is based on dominance-depth and crowding distance within NSGA-II, and (iii) the archive is initialized as detailed in Section 3.4 for SS-EA whereas the NSGA-II initial population is generated at random. However, notice that an external unbounded archive has been added to the canonical NSGA-II in order to prevent the loss of non-dominated solutions.

All the algorithms stop after $(n \cdot m \cdot 10^{-3})$ minutes of CPU time, *i.e.*, from 2 minutes *per* run for smaller instances up to 15 minutes for large-size instances. Since neighboring solutions are evaluated incrementally within HM during the tabu search phases, a maximum number of evaluations cannot be used as a stopping condition. Following [20], the tabu tenure constant is set to $tt = n/150$, and the improvement cutoff to $\alpha = 5n$. During the initialization phase, the number of random restarts *per* objective function is set to $\gamma = 5$. At last, the ϵ -parameter of the achievement scalarizing function is set to $\epsilon = 10^{-8}$. The population size of NSGA-II is set to 100 solutions. A summary of all the parameters used in the paper is given in Table 1.

HM, SS-EA and NSGA-II have been implemented within the ParadisEO software framework [45, 46]. All the algorithms have been executed under comparable conditions and share the same base components for a fair comparison between them. The experiments have been conducted on an Intel Core 2 quad-core processor (2.40 GHZ, 4GB RAM) running under Ubuntu 10.04. All codes were compiled with g++ 4.4.3 using the -O3 compilation option.

4.2. Performance Assessment

A set of 30 runs *per* instance has been performed for each algorithm. In order to evaluate the quality of the approximations found for each instance, we follow the performance assessment protocol given in [26]. Such a way of comparing multiple stochastic multiobjective optimizers is a common practice in the specialized literature. Let us consider a given mUBQP

problem instance. Let Z^{all} be the set of objective vectors from all the Pareto set approximations we obtained during all our experiments. Note that Z^{all} may contain both dominated and non-dominated objective vectors, since a given approximation may contain points dominating the ones of another approximation, and *vice versa*. We define $z^{min} = (z_1^{min}, \dots, z_m^{min})$ and $z^{max} = (z_1^{max}, \dots, z_m^{max})$, where z_k^{min} (respectively z_k^{max}) denotes the lower (respectively upper) bound of the k^{th} objective for all the points contained in Z^{all} , $\forall k \in \{1, \dots, m\}$. In order to give a roughly equal range to the objective functions, values are normalized between 1 and 2 with respect to z^{min} and z^{max} . Then, we compute a reference set Z^* containing the non-dominated points of Z^{all} . In order to measure the quality of Pareto front approximations, we use both the Pareto dominance relation extended to sets, as well as the difference hypervolume indicator (I_H^-) [25]. They are illustrated in Figure 6 and Figure 7, respectively. The Pareto dominance relation over sets can be defined as follows. A given Pareto front approximation A^1 is dominated by another approximation A^2 , if for all objective vector $z^1 \in A^1$, there exists an objective vector $z^2 \in A^2$ such that z^1 is dominated by z^2 . The I_H^- -indicator value of a given approximation A gives the portion of the objective space that is dominated by Z^* and not by A , $z^l = (0.9, \dots, 0.9)$ being the reference point. Note that I_H^- -values are to be minimized. The experimental results report average I_H^- -values as well as a Wilcoxon signed rank statistical test with a p -value of 0.05. Notice that this procedure has been achieved using the performance assessment tools provided in PISA [26].

4.3. Computational Results and Discussion

Computational results are presented in Table 2. Let us start with an example. The left part of the first line corresponds to the following mUBQP problem instance: $n = 1000$, $\rho = -0.5$ and $m = 2$. The average I_H^- -value obtained by HM, NSGA-II and SS-EA over the 30 executions is 0.042, 0.325 and 0.085, respectively. According to the I_H^- indicator, the ranking deduced from the statistical test is as follows: (i) HM, (ii) SS-EA, and (iii) NSGA-II. The Pareto set approximations obtained by NSGA-II are reported to be statistically outperformed by the

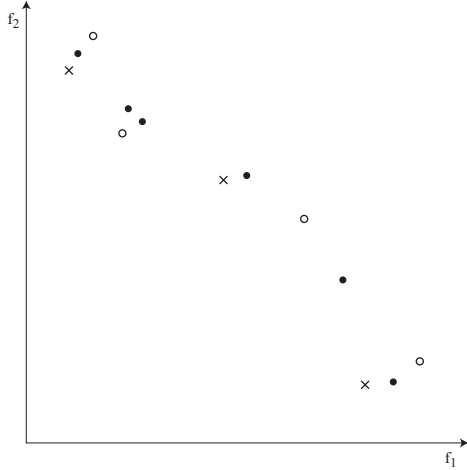


Figure 6: Illustration of the Pareto dominance relation over Pareto front approximations: (i) the approximation (•) dominates the approximation (×), (ii) the approximations (•) and (◦) are incomparable, and (iii) the approximations (×) and (◦) are incomparable.

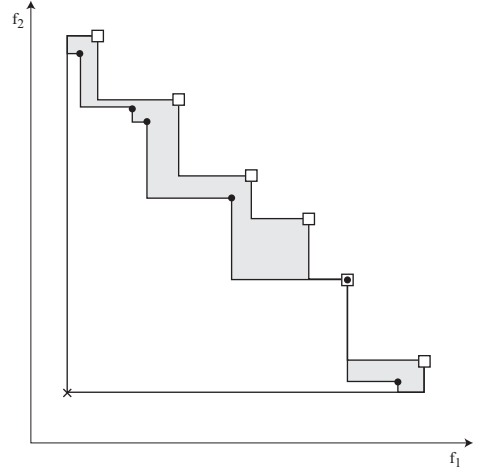


Figure 7: Illustration of the hypervolume-difference quality indicator (I_H^-). The reference set is represented by boxes (◻), the Pareto front approximation by bullets (•) and the reference point z^l by a cross (×). The shaded area represents the hypervolume difference $I_H^-(•, ◻)$.

ones from HM in terms of Pareto dominance. Similarly, SS-EA is outperformed by HM in terms of hypervolume indicator-values.

First, compared against NSGA-II, our HM algorithm clearly performs better. Indeed, the Pareto set approximation found by NSGA-II is always dominated by the one obtained by HM. That is, every solution found by NSGA-II is dominated by at least one solution found by HM for all the runs over all the instances we experimented. The only cases where this does not happen is for $m = 3$ and $\rho = -0.5$ as well as the following instance: $n = 1000$, $m = 3$ and $\rho = -0.2$. Still, HM outperforms NSGA-II in terms of hypervolume for the corresponding instances.

With respect to SS-EA, the hypervolume indicator is always required to differentiate approximation sets. For all the instances with $n \leq 3000$, HM is reported to give better results, except for $m = 3$ and $\rho = -0.5$. However, for large-size instances ($n \geq 4000$), HM seems to have more troubles in finding a better approximation set than SS-EA in some cases, particularly when the objective functions are in conflict. Indeed, HM performs better than SS-EA on nine out of the twenty largest instances while the reverse holds for eight cases. For such problem instances, the number of non-dominated solutions can become very large, such that there is probably a lack of diversity for the HM algorithm compared to its non-hybrid counterpart.

Overall, we can conclude that the HM algorithm gives significantly better results on most mUBQP problem instances. It clearly outperforms the state-of-the-art NSGA-II algorithm on the whole set of instances, whereas it is outperformed by SS-EA on only ten out of fifty mUBQP instances.

5. Conclusions

The contributions of the paper are three-fold. First, the unconstrained binary quadratic programming (UBQP) problem has been extended to the multiobjective case (mUBQP) which

involves an arbitrary number of UBQP objective functions to be maximized simultaneously over the same decision space of binary strings of size n . In the single-objective case, the UBQP problem is one of the most challenging problem from combinatorial optimization, and is known to enable the formulation of a large number of practical applications in many areas. The multiobjective UBQP problem introduced in this paper will allow more practical applications to be formulated and solved.

Second, multiobjective UBQP problem instances, together with an instance generator, have been made available at the following URL: <http://mocobench.sf.net>. These problem instances are characterized by a problem size, a matrix density, a number of objective functions, and a correlation coefficient between the objective values. In particular, the objective correlation can be tuned very precisely, allowing one to study the impact of this feature on the size of the Pareto front, and then on the performance of solution approaches. These instances are useful for performance assessment and comparison of new algorithms for the general mUBQP problem.

Third, we have presented a hybrid evolutionary-tabu search algorithm for the multiobjective UBQP. The proposed approach integrates a state-of-the-art tabu search algorithm for the single-objective UBQP, together with Pareto-based evolutionary optimization principles. Based on the achievement scalarizing function, our algorithm is able to generate both supported and unsupported solutions, with the aim of finding a well-converged and well-diversified Pareto set approximation. We have showed that this hybrid metaheuristic obtains significantly better results than two conventional evolutionary multiobjective optimization techniques for large-size multiobjective UBQP problem instances of different structure and size.

A better understanding of the main problem characteristics would allow us to improve the design of heuristic search algorithms by incorporating a deeper problem knowledge. To this end, we plan to study the correlation between the main

Table 2: Comparison of the proposed HM against NSGA-II and SS-EA. The symbol ‘>’ (resp. ‘<’) means that HM significantly outperforms (resp. is significantly outperformed by) the algorithm under consideration with respect to the set-based Pareto dominance relation. The symbol ‘ \succeq ’ (resp. ‘ \preceq ’) means that HM significantly outperforms (resp. is significantly outperformed by) the algorithm under consideration with respect to the difference hypervolume indicator (I_H^-). The symbol ‘ \equiv ’ means that no algorithm outperforms the other in terms of Pareto dominance nor I_H^- -values. The average I_H^- -value is reported in brackets for HM, NSGA-II and SS-EA, respectively (lower is better).

n	ρ	$m = 2$			$m = 3$						
		NSGA-II		SS-EA	NSGA-II		SS-EA				
1000	-0.5	(0.042)	>	(0.325)	\succeq	(0.085)	(0.104)	\succeq	(0.273)	\succeq	(0.113)
	-0.2	(0.052)	>	(0.336)	\succeq	(0.094)	(0.120)	\succeq	(0.410)	\succeq	(0.339)
	0.0	(0.037)	>	(0.336)	\succeq	(0.109)	(0.127)	>	(0.449)	\succeq	(0.405)
	+0.2	(0.037)	>	(0.348)	\succeq	(0.120)	(0.096)	>	(0.471)	\succeq	(0.420)
	+0.5	(0.032)	>	(0.385)	\succeq	(0.132)	(0.092)	>	(0.508)	\succeq	(0.409)
2000	-0.5	(0.099)	>	(0.416)	\succeq	(0.176)	(0.140)	\succeq	(0.248)	\preceq	(0.080)
	-0.2	(0.112)	>	(0.473)	\succeq	(0.188)	(0.221)	>	(0.434)	\succeq	(0.335)
	0.0	(0.070)	>	(0.520)	\succeq	(0.177)	(0.208)	>	(0.518)	\succeq	(0.427)
	+0.2	(0.097)	>	(0.587)	\succeq	(0.215)	(0.193)	>	(0.577)	\succeq	(0.477)
	+0.5	(0.054)	>	(0.757)	\succeq	(0.229)	(0.171)	>	(0.738)	\succeq	(0.556)
3000	-0.5	(0.136)	>	(0.471)	\succeq	(0.153)	(0.159)	\succeq	(0.239)	\preceq	(0.071)
	-0.2	(0.125)	>	(0.566)	\succeq	(0.192)	(0.262)	>	(0.417)	\succeq	(0.288)
	0.0	(0.111)	>	(0.640)	\succeq	(0.223)	(0.321)	>	(0.529)	\succeq	(0.394)
	+0.2	(0.177)	>	(0.728)	\succeq	(0.303)	(0.282)	>	(0.639)	\succeq	(0.470)
	+0.5	(0.131)	>	(0.931)	\succeq	(0.341)	(0.254)	>	(0.845)	\succeq	(0.572)
4000	-0.5	(0.216)	>	(0.497)	\preceq	(0.178)	(0.188)	\succeq	(0.235)	\preceq	(0.051)
	-0.2	(0.195)	>	(0.607)	\succeq	(0.238)	(0.311)	>	(0.405)	\preceq	(0.267)
	0.0	(0.157)	>	(0.687)	\succeq	(0.233)	(0.325)	>	(0.441)	\preceq	(0.280)
	+0.2	(0.147)	>	(0.813)	\succeq	(0.271)	(0.349)	>	(0.647)	\succeq	(0.450)
	+0.5	(0.089)	>	(1.001)	\succeq	(0.263)	(0.299)	>	(0.860)	\succeq	(0.568)
5000	-0.5	(0.267)	>	(0.500)	\preceq	(0.153)	(0.201)	\succeq	(0.231)	\preceq	(0.056)
	-0.2	(0.250)	>	(0.624)	\equiv	(0.204)	(0.283)	>	(0.319)	\preceq	(0.156)
	0.0	(0.219)	>	(0.725)	\equiv	(0.235)	(0.305)	>	(0.403)	\preceq	(0.238)
	+0.2	(0.192)	>	(0.802)	\succeq	(0.253)	(0.359)	>	(0.576)	\equiv	(0.393)
	+0.5	(0.125)	>	(1.023)	\succeq	(0.236)	(0.359)	>	(0.859)	\succeq	(0.518)

problem features and the algorithm performance through fitness landscapes analysis in multiobjective combinatorial optimization [31, 47]. At last, we hope that the challenge proposed by multiobjective UBQP will gain the attention of other researchers. In particular, a stronger link is required between multiobjective UBQP formulations and existing academic or real-world applications, including the multi-objective variants of assignment, covering, partitioning, packing and quadratic knapsack problems. This would enable the identification of a Pareto front approximation for many problems from multi-objective combinatorial optimization under a unified modeling, even to enhance the performance of exact approaches by allowing a fast computation of a lower bound set.

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