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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. 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 mUBQP instances and validate the performance of the proposed approach in obtaining competitive results on large-size mUBQP instances with two and three objectives.

1. Introduction

Given a collection of n items such that each pair of items is associated with a profit value that can be positive, negative or zero, unconstrained binary quadratic programming (UBQP) seeks a subset of items that maximizes the sum of their paired values. The value of a pair is accumulated in the sum only if the two corresponding items are selected. A feasible solution to a UBQP instance can be specified by a binary string of size n, such that each variable indicates whether the corresponding item is included in the selection or not. More formally, the conventional and single-objective UBQP problem is to maximize the following objective function.

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

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

The UBQP is known to be a 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 conveniently transformed into the UBQP, such as graph coloring, maxcut, set packing, set partitioning, maximum clique, 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 [8–10] and a number of heuristic and metaheuristic methods like simulated annealing [11], tabu search [12–16], path-relinking [17], evolutionary and memetic algorithms [18–21].

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 ability of the UBQP and provides a convenient formulation to fit situations which the single-objective UBQP cannot accommodate. For instance, UBQP can recast the vertex coloring problem (of determining the chromatic number of a graph) [5] and the sum coloring problem (of

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determining 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 has two contributions. 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 are appealing. Following the studies on memetic algorithms for the UBQP and 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 contribution of this work is to define a formal and flexible model to generate hard mUBQP instances. An experimental analysis validates the effectiveness of the proposed hybrid metaheuristic by achieving a clear improvement over non-hybrid and conventional algorithms on large-size mUBQP instances with two and three objectives.

The paper is organized as follows. Section 2 introduces the multiobjective formulation of the UBQP problem (mUBQP). Section 3 presents the hybrid metaheuristic (HM) proposed for the mUBQP problem and its main ingredients, including the scalarizing evaluation function, the tabu search procedure, the initialization phase and the variation operators. Section 4 gives an experimental analysis of the HM algorithm on a large set of mUBQP instances of different structure and size. The last section concludes the paper and suggests further research lines.

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. Last, the construction of problem instances, together with an experimental study on the correlation of objective values 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:

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

where $f = (f_1, f_2, \ldots, f_m)$ is an objective function vector 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 positive, negative or zero values, $k \in \{1,\ldots,m\}$. The solution 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 *solution 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 maximizing function vector f. The Pareto dominance relation is defined as follows. A solution $x \in X$ is dominated by a solution $x' \in X$, denoted by $x \prec x'$, if $f_k(x) \leq f_k(x')$ for all $k \in \{1,\ldots,m\}$, with at least one strict inequality. If neither $x \nprec x'$ nor $x' \nprec x$ holds, then both solutions are *mutually non-dominated*. A solution $x \in X$ is *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*, denoted by Z_{PF}. One of the most challenging issues 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 computationally prohibitive for two main reasons. First, the question of deciding if a candidate solution is dominated is known to be NP-hard for numerous multiobjective combinatorial optimization problems [23,24]. This is also the case for the mUBQP problem since its single-objective counterpart is NP-hard [7]. Second, the cardinality of the Pareto front 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 prove 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.

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

Let $q_{ij}^2 = -q_{ij}^1$ for all $i, j \in \{1,\ldots,n\}$. It is obvious that all solutions are mutually non-dominated, and that each solution maps to a different vector in the objective space. Therefore, $|Z_{PF}| = |X_{PS}| = |X| = 2^n$.□

The bi-objective mUBQP instance used in the proof is illustrated in Fig. 1 for $n = 3$.

In order to cope with NP-hard and intractable multiobjective combinatorial optimization problems, researchers have developed approximate algorithms that identify a *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

The single-objective UBQP problem is of high interest in practice, since many existing combinatorial optimization problems can be formalized in terms of UBQP [5]. As a consequence, multiobjective versions of such 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 [24,28], multiobjective knapsack problems [29,30], multiobjective maxcut problems [31], or multiobjective set covering and partitioning problems [28], just to mention a few. 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