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A multi-objective tabu search algorithm based on decomposition for multi-objective unconstrained binary quadratic programming problem

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ABSTRACT

Unconstrained binary quadratic programming problem (UBQP) is a well-known NP-hard problem. In this problem, a quadratic 0–1 function is maximized. Numerous single-objective combinatorial optimization problems can be expressed as UBQP. To enhance the expressive ability of UBQP, a multi-objective extension of UBQP and a set of benchmark instances have been introduced recently. A decomposition-based multi-objective tabu search algorithm for multi-objective UBQP is proposed in this paper. In order to obtain a good Pareto set approximation, a novel weight vector generation method is first introduced. Then, the problem is decomposed into a number of subproblems by means of scalarizing approaches. The choice of different types of scalarizing approaches can greatly affect the performance of an algorithm. Therefore, to take advantages of different scalarizing approaches, both the weighted sum approach and the Tchebycheff approach are utilized adaptively in the proposed algorithm. Finally, in order to better utilize the problem-specific knowledge, a tabu search procedure is designed to further optimize these subproblems simultaneously. Experimental results on 50 benchmark instances indicate that the proposed algorithm performs better than current state-of-the-art algorithms.

1. Introduction

Unconstrained binary quadratic programming (UBQP) problem is a hard single-objective combinatorial optimization problem [1]. In UBQP, given a symmetric rational $n \times n$ matrix $Q = (q_{ij})$, a binary vector $\boldsymbol{x} = \{x_1, \ldots, x_n\},\ x_i \in \{0,\ 1\}$ is searched, such that the objective function

$$f(\boldsymbol{x}) = \sum_{i=1}^{n} \sum_{j=1}^{n} q_{ij} x_i x_j \tag{1}$$

is maximized [2].

UBQP is a unified model for combinatorial optimization problems [3]. In many application fields, such as finance, project selection, cluster analysis, economic analysis, computer aided design, traffic management and so on [4], various difficult problems can be expressed as UBQP. In addition, a variety of graph problems, e.g., max-2sat problem, max-cut problem, number partitioning problem and maximum clique problem [4], can also be converted to UBQP. Exact methods (see the most recent review [4]) can solve UBQP only with small or moderate-scale problem instances due to the NP-hard nature of UBQP [5]. On the other hand, metaheuristic algorithms are very powerful in solving hard combinatorial optimization problems. Hence, UBQP has been solved by several metaheuristic approaches, including tabu search (TS) [6–8], neural network [3,9,10], path relinking [11], global equilibrium search [12] and f-flip strategies [13].

Only one objective function is optimized in the original single-objective UBQP. As a consequence, the single-objective UBQP can only formulate the aforementioned single-objective problems. However, in many situations, more than one objectives might be optimized simultaneously, for example, the bi-objective coloring problem that needs to select a legal vertex coloring of a graph while minimizing both the number and the sum of colors [14]. The single-objective UBQP is obviously not suitable for these scenarios. To increase the expressive ability of UBQP, a multi-objective extension of UBQP (denoted as mUBQP) [14] is proposed recently. Given m matrices $Q^k = (q_{ij}^k)$ of size $n \times n$, $k \in \{1, \ldots, m\}$, the objective of mUBQP is to maximize m $(m \geq 2)$ functions defined as follows [14]:

$$f_k(\boldsymbol{x}) = \sum_{i=i}^{n} \sum_{j=1}^{n} q_{ij}^k x_i x_j,\ \ k \in \{1, \ldots, m\} \tag{2}$$

subject to $x_i \in \{0,\ 1\}$, $i \in \{1, \ldots, n\}$.

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Many multi-objective optimization problems can be converted to mUBQP, including multi-objective knapsack problem, multi-objective max-cut problem [15] and bi-objective coloring problem [14]. Due to the multi-objective nature of mUBQP, it is necessary to utilize multi-objective methodology to obtain a set of solutions that show the tradeoffs between the objectives.

Several multi-objective algorithms have been implemented for mUBQP. Liefooghe et al. [14] proposed a hybrid metaheuristic algorithm (HM) to solve mUBQP. It incorporates a single-objective tabu search procedure based on scalarizing function and an elitist multi-objective evolutionary algorithm. Thereafter, in [1], several local search methods were proposed for the bi-objective UBQP, including a Pareto-based approach, two scalarizing approaches and a hybrid approach. Zangari et al. [15] proposed a multi-objective optimization algorithm based on the decomposition approach and the probabilistic model binary ant colony optimization, then carried out experiments on some small-scale instances (up to $n = 1000$). Moreover, our preliminary work [16] proposed a directional-biased tabu search algorithm (DTS) and showed competitive results on mUBQP cases. However, DTS cannot generate solutions that are well-distributed over the Pareto front, i.e., most of the non-dominated solutions obtained by DTS distribute only in a small region of objective space.

The decomposition-based method is one of the most widely used multi-objective approaches to tackle the multi-objective optimization problem (MOP). Moreover, most of the aforementioned algorithms for mUBQP are decomposition-based algorithms, i.e., a transformation of mUBQP to a single-objective optimization problem is performed by aggregating all objectives. Since an optimal solution to an aggregated single-objective problem is Pareto-optimal to mUBQP, a set of Pareto optimal solutions can be obtained by solving a set of single-objective problems with a set of weight vectors [17]. The decomposition-based algorithms are quite appropriate for mUBQP, since the single-objective UBQP has been tackled by lots of metaheuristic methods. The key points that affect the performance of such kind of algorithms are : 1) weight vectors and 2) scalarizing methods. According to [18–24], the diversity of the Pareto optimal solutions is controlled by the weight vectors. Hence, it is crucial to obtain appropriate weight vectors in decomposition-based algorithms [22].

Another important implementation issue of decomposition-based algorithms is the choice of a scalarizing function, because this choice can greatly affect the performance of an algorithm [25]. There are a number of scalarizing approaches for decomposition [26]. Among them, two of the most widely and highly accepted approaches for combinatorial problems are the weighted sum approach and the Tchebycheff approach [15]. In the case of maximization such as mUBQP, the weighted sum approach is effective on concave Pareto fronts. However in the case of non-concave Pareto fronts, this approach cannot find all Pareto optimal vectors. In contrast, the Tchebycheff approach can handle non-concave Pareto fronts, however, it is inferior to the weighted sum approach in terms of convergence property [27]. Since both scalarizing approaches have certain drawbacks, it is not easy to select an appropriate method for different multi-objective problems [25,27–29].

To tackle the aforementioned issues and provide a more effective approach, this paper proposes a decomposition-based multi-objective tabu search algorithm (DMTS) for mUBQP. Details about the proposed DMTS are presented as follows.

1. To tackle the first issue, a novel weight vector generation method is designed in DMTS. It combines the simplex-lattice design with a random approach to obtain a set of initial weight vectors. Then, uniform weight vectors are selected from the initial weight vectors based on Euclidean distance. To enhance the diversity property, this procedure is invoked in the beginning of each iteration to generate different uniform weight vectors for decomposition. Experiment is carried out to show that the proposed strategy is more effective than the simplex-lattice design.
2. Consider the second issue, both the weighted sum approach and the Tchebycheff approach are utilized in an adaptive manner in DMTS. Therefore, the advantages of both methods can be taken. The effectiveness of this strategy will also be shown in this paper.
3. In order to access better performance, an outstanding approach for the single-objective UBQP problem, i.e., TS, is utilized to optimize all scalarizing functions simultaneously at each iteration. As a consequence, a better Pareto set approximation is expected to be generated.
4. The proposed DMTS is tested on 50 mUBQP cases [14]. Experimental results indicate that DMTS gets better performance than current state-of-the-art algorithms.

The contributions of this paper are summarized as follows.

1. A novel decomposition-based multi-objective algorithm is proposed for mUBQP, and superior results are obtained.
2. The proposed weight vector generation method and adaptive use of scalarizing approaches can make decomposition-based methods more effective in terms of convergence and diversity.
3. A comprehensive experimental comparison of the proposed DMTS with current state-of-the-art algorithms is provided.

This paper is an extension of the previous preliminary version [30]. The differences between the previous version and this paper are presented as follows. First, this paper provides a different way to generate weight vectors, and proposes a novel strategy to use two scalarizing approaches adaptively for decomposition and optimization. Second, this paper provides more information about the proposed algorithm, including more details, analysis of the complexity and discussions on the behavior of the proposed algorithm. Third, more experimental results on 50 mUBQP cases are presented in this paper.

The remaining sections of this paper are organized as follows. Background is presented in Section 2, including some concepts of multi-objective optimization, two scalarizing approaches utilized in this paper, and current state-of-the-art approaches for mUBQP. The proposed DMTS is presented in Section 3. In Section 4, experimental results are presented. Finally, in Section 5, conclusion is provided.

2. Background

In this section, some concepts of multi-objective optimization are first presented. Then, the scalarizing approaches utilized in the proposed algorithm are described. Finally, current state-of-the-art approaches for comparison in this paper are briefly reviewed.

2.1. Multi-objective optimization

The formulation of MOP is presented as follows:

$$\text{maximize } F(x) = \{f_1(x), \ldots, f_m(x)\} \tag{3}$$

subject to $x \in \Omega$, where Ω represents the decision variable space. F: $\Omega \rightarrow R^m$ consists of m objective functions, and these functions are often in conflict. Let $x, y \in R^m$, x is said to dominate y if and only if $f_i(x) \geq f_i(y)$ for every $i \in \{1, \ldots, m\}$, and $f_j(x) > f_j(y)$ for at least one $j \in \{1, \ldots, m\}$. If there is no solution $x \in \Omega$ such that x dominates x^*, then the solution x^* is Pareto optimal, and $F(x^*)$ is a Pareto optimal objective vector. *Pareto set* is the set of all Pareto optimal solutions, and *Pareto front* is the set of all Pareto optimal objective vectors. The multi-objective algorithms need to find a number