
Solving Combinatorial Optimization Problems via Reformulation and Adaptive Memory Metaheuristics

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ABSTRACT— *Metaheuristics* — general search procedures whose principles allow them to escape the trap of local optimality using heuristic designs — have been successfully employed to address a variety of important optimization problems over the past few years. Particular gains have been achieved in obtaining high quality solutions to problems that classical *exact methods* (which guarantee convergence) have found too complex to handle effectively. Typically a metaheuristic method is crafted to suit the particular characteristics of the problem at hand, exploiting to the extent possible the structure available to enable a fruitful and efficient search process. An alternative to this problem specific solution approach is a more general methodology that recasts a given problem into a common modeling format, permitting solutions to be derived by a common, rather than tailor-made, heuristic method.

The optimization folklore strongly emphasizes the unproductive consequences of converting problems from a specific class to a more general representation, since the “domain-specific structure” of the original setting then becomes invisible and can not be exploited by a method for the more general problem representation. Nevertheless, there is a strong motivation to attempt such a conversion in many applications to avoid the necessity to develop a new method for each new class. We demonstrate the existence of a general problem representation that frequently overcomes the limitation commonly ascribed to such models. Contrary to expectation, when a specially structured problem is translated into this general form, it often does not become much harder to solve, and sometimes becomes even easier to solve provided the right type of solution approach is applied.

The model with this appealing property is the unconstrained binary quadratic binary programming problem, accompanied by the device of introducing quadratic infeasibility penalty functions to handle constraints. Not only is this model capable of representing a wide range of “special case” problem classes, but it can be advantageously exploited by adaptive memory (tabu search) metaheuristics and associated evolutionary (scatter search) methods. Computational outcomes disclose the effectiveness of this combined modeling and solution approach for problems from a diverse collection of challenging settings.

1. Introduction:

The unconstrained quadratic program can be written in the form:

$$\text{QUIP: } \min f(x) = xQx$$

where Q is an n by n matrix of constants and x is an n -vector of binary variables. QUIP is notable for its ability to represent a significant variety of important problems. The applicability of this representation has been reported in diverse settings such as social psychology (Harary [19]), financial analysis (Laughunn, [23], McBride and Yormak, [25]), computer aided design (Krarup and Pruzan [22]), traffic management (Gallo et al. [7], Witsgall, [32]), machine scheduling (Alidaee, Kochenberger, and Ahmadian, [1]), cellular radio channel allocation (Chardaire and Sutter [6]), and molecular conformation (Phillips and Rosen [30]). Moreover, many combinatorial optimization problems pertaining to graphs such as determining maximum cliques, maximum cuts, maximum vertex packing, minimum coverings, maximum independent sets, and maximum independent weighted sets are known to be capable of being formulated by the QUIP problem as documented in papers of Pardalos and Rodgers [28], and Pardalos and Xue [29].

The application potential of QUIP is yet substantially greater than this, however, due to reformulation methods that enable certain constrained models to be re-cast in the form of QUIP. Hammer and Rudeanu [16] and Hansen [17] show that any quadratic (or linear) objective in bounded integer variables and constrained by linear equations can be reformulated as a QUIP model. Our purpose is to report results that disclose this wide array of potential reformulations into the QUIP format is not merely a representational novelty, but is a source of practical consequences. The following material draws upon recent findings in by Kochenberger, Glover, Alidaee, and Amini [21] and in Glover, Kochenberger, Alidaee and Amini [12].

2. Transformations:

We take as our starting point the constrained problem

$$\min x_0 = xQx$$

subject to

$$Ax = b, x \text{ binary}$$

This model describes both the quadratic and linear case since the linear case results when Q is a diagonal matrix. Problems with inequality constraints can also be put into this form by representing their bounded slack variables by a binary expansion. These constrained quadratic optimization models are converted into equivalent QUIP models by adding a quadratic infeasibility penalty function to the objective function in place of explicitly imposing the constraints $Ax = b$.

$$\begin{aligned} x_0 &= xQx + P(Ax - b)'(Ax - b) \\ &= xQx + xDx + c \\ &= x\hat{Q}x + c \end{aligned}$$

where the matrix D and the additive constant c result directly from the matrix multiplication indicated. Dropping the additive constant, the equivalent unconstrained version of our constrained problem becomes

$$QUIP(PEN) : \min_x \hat{Q}x, x \text{ binary}$$

From a theoretical standpoint, a suitable choice of the penalty scalar P can always be chosen such that the optimal solution to $QUIP(PEN)$ is the optimal solution to the original constrained problem. (Hammer and Rudeanu [16]). Similar theoretical outcomes apply to many types of representations other than the QUIP model, of course, and the issue of interest is whether there is any practical merit in undertaking such a transformation in the QUIP case. The same question arises by reference to another transformation, which likewise falls within the context of the QUIP model.

We refer to the preceding general transformation as transformation # 1. A very important special class of constraints that arise in many applications can be handled by an alternative approach, given below, which we call transformation #2.

Many problems have considerations that isolate two specific alternatives and prohibit both from being chosen. That is, for a given pair of alternatives, one or the other but not both *may* be chosen. If x_j and x_k are binary variables denoting whether or not alternatives j and k are chosen, the standard constraint that allows one choice but precludes both is:

$$x_j + x_k \leq 1$$

Then, for a positive scalar P , adding the penalty function Px_jx_k to the objective function is a simple alternative to imposing the constraint in a traditional manner. This penalty function has sometimes been used by to convert certain optimization problems on graphs (e.g., the maximum clique problem) into an equivalent QUIP model. Its potential application, however, goes far beyond graph problems as we demonstrate in later sections of this paper.

3. Examples:

Before highlighting a variety of problem classes to which we have successfully applied the foregoing transformation approaches, we give two small examples from classical problem settings to provide concrete illustrations:

Example 1: Set Partitioning.

$$\min x_0 = 3x_1 + 2x_2 + x_3 + x_4 + 3x_5 + 2x_6$$

subject to

$$\begin{aligned} x_1 + x_3 + x_6 &= 1 \\ x_2 + x_3 + x_5 + x_6 &= 1 \\ x_3 + x_4 + x_5 &= 1 \\ x_1 + x_2 + x_4 + x_6 &= 1 \end{aligned}$$

and x binary. Applying transformation #1 with $P = 10$ gives the equivalent QUIP model:

$$QUIP(PEN) : \min x \hat{Q}x, x \text{ binary}$$

where the additive constant, c , is 40 and

$$\hat{Q} = \begin{bmatrix} -17 & 10 & 10 & 10 & 0 & 20 \\ 10 & -18 & 10 & 10 & 10 & 20 \\ 10 & 10 & -29 & 10 & 20 & 20 \\ 10 & 10 & 10 & -19 & 10 & 10 \\ 0 & 10 & 20 & 10 & -17 & 10 \\ 20 & 20 & 20 & 10 & 10 & -28 \end{bmatrix}$$

Solving QUIP(PEN) by the method of Glover et al. [11]¹ we obtain an optimal solution $x_1 = x_5 = 1$ for which $x_0 = 6$. In the straightforward application of transformation #1 to this example, it is to be noted that the replacement of the original problem formulation by the QUIP(PEN) model did not involve the introduction of new variables. In many applications, transformation #1 and transformation #2 can be used in concert to produce an equivalent QUIP model, as demonstrated next.

Example 2: P-Median Problem:

The P-Median problem can be modeled as:

$$\min x_0 = \sum_{i=1}^m \sum_{j=1}^n c_{ij} x_{ij}$$

subject to

$$\sum_{j=1}^n x_{ij} = 1, \quad i = 1, m$$

$$\sum_{j=1}^n y_j = p$$

$$x_{ij} \leq y_j \text{ for all } (i, j) \text{ pairs}$$

¹ Almost any method will work for this simple example.

where c_{ij} is the weighted distance from facility i to demand node j , $y_j = 1$ if a facility is located at location j , and $x_{ij} = 1$ if demand node i is assigned to the facility at location j . The first two sets of constraints can clearly be accommodated by transformation #1. The last set of constraints can be handled by transformation #2 by a “trick” of replacing the y variables by their compliments. (This same approach can be employed to model many fixed charge problems.)

To illustrate, consider the 12 variable example with $m = n = 3$, $p = 2$ and the C matrix

$$C = \begin{bmatrix} 0 & 2 & 3 \\ 2 & 0 & 1 \\ 3 & 1 & 0 \end{bmatrix}$$

For $P = 20$, the additive constant c is 80 and the \hat{Q} matrix for the equivalent QUIP model is

$$\hat{Q} = \begin{bmatrix} -20 & 20 & 20 & 0 & 0 & 0 & 0 & 0 & 0 & 10 & 0 & 0 \\ 20 & -18 & 20 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 10 & 0 \\ 20 & 20 & -17 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 10 \\ 0 & 0 & 0 & -18 & 20 & 20 & 0 & 0 & 0 & 10 & 0 & 0 \\ 0 & 0 & 0 & 20 & -20 & 20 & 0 & 0 & 0 & 0 & 10 & 0 \\ 0 & 0 & 0 & 20 & 20 & -19 & 0 & 0 & 0 & 0 & 0 & 10 \\ 0 & 0 & 0 & 0 & 0 & 0 & -17 & 20 & 20 & 10 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 20 & -19 & 20 & 0 & 10 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 20 & 20 & -20 & 0 & 0 & 10 \\ 10 & 0 & 0 & 10 & 0 & 0 & 10 & 0 & 0 & -20 & 20 & 20 \\ 0 & 10 & 0 & 0 & 10 & 0 & 0 & 10 & 0 & 20 & -20 & 20 \\ 0 & 0 & 10 & 0 & 0 & 10 & 0 & 0 & 10 & 20 & 20 & -20 \end{bmatrix}$$

Solving QUIP(PEN) gives $x_1 = x_6 = x_9 = y_1 = y_3 = 1$ for which $x_0 = 1$, which is optimal for the original problem.

4. Solution Approaches:

Due to its computational challenge and application potential, QUIP has been the focus of a considerable number of research studies in recent years, including both exact and heuristic solution approaches. Notable recent studies addressing QUIP are those by Williams [31], Pardalos and Rodgers [27], Boros, Hammer and Sun [5], Chardaire and

Sutter [6], Glover, Kochenberger and Alidaee [14], Glover, Kochenberger, Alidaee, and Amini [11], Alkhamis, Hasan and Ahmed [2], Beasley [4], Lodi, Allemand and Liebling [24], Amini, Alidaee and Kochenberger [3], and Glover, Amini, Kochenberger and Alidaee [3]. Other promising work is reported by Katayama, Tani and Narihisa [20] and Merz and Freisleben [26]. These various studies approach the problem by branch and bound, decomposition, tabu search, simulated annealing, and evolutionary methods such as genetic algorithms and scatter search. Each of these approaches exhibits some degree of success. However, the exact methods degrade rapidly with problem size, and have meaningful application to general QUIP problems with no more than 100 variables. For larger problems, heuristic methods are required. Two methods we have found to be particularly successful for a wide variety of problems are based on tabu search and on the related evolutionary strategy scatter search [3]. In the following we highlight our tabu search approach.

4.1 Tabu Search Overview:

Our TS method for QUIP is centered around the use of strategic oscillation, which constitutes one of the primary strategies of tabu search. The variant of strategic oscillation we employ may be sketched in overview as follows.

The method alternates between constructive phases that progressively set variables to 1 (whose steps we call “add moves”) and destructive phases that progressively set variables to 0 (whose steps we call “drops moves”). To control the underlying search process, we use a memory structure that is updated at *critical events*, identified by conditions that generate a subclass of locally optimal solutions. Solutions corresponding to critical events are called *critical solutions*.

A parameter *span* is used to indicate the amplitude of oscillation about a critical event. We begin with *span* equal to 1 and gradually increase it to some limiting value. For each value of *span*, a series of alternating constructive and destructive phases is executed before progressing to the next value. At the limiting point, *span* is gradually decreased, allowing again for a series of alternating constructive and destructive phases. When *span* reaches a value of 1, a *complete span cycle* has been completed and the next cycle is launched.

Information stored at critical events is used to influence the search process by penalizing potentially attractive add moves (during a constructive phase) and inducing drop moves (during a destructive phase) associated with assignments of values to variables in recent critical solutions. Cumulative critical event information is used to introduce a subtle long term bias into the search process by means of additional penalties and inducements similar to those discussed above. A complete description of the framework for the method is given in Glover, Kochenberger, Alidaee and Amini [11].

5. Computational Experience:

Our results of applying the tabu search and associated scatter search metaheuristics to combinatorial problems recast in QUIP form have uniformly attractive in terms of both solution quality and computation times. As intimated earlier, although our methods are designed for the completely general form of QUIP, without any specialization to take advantage of particular types of problems reformulated in this general representation, our outcomes have typically proved competitive with or even superior to those of specialized methods designed for the specific problem structure at hand. Our broad base

of experience with QUIP as a modeling and solution framework includes a substantial range of problem classes including:

- Quadratic Assignment Problems
- Capital Budgeting Problems
- Multiple Knapsack Problems
- Task Allocation Problems (distributed computer systems)
- Maximum Diversity Problems
- P-Median Problems
- Asymmetric Assignment Problems
- Symmetric Assignment Problems
- Side Constrained Assignment Problems
- Quadratic Knapsack Problems
- Constraint Satisfaction Problems (CSPs)
- Set Partitioning Problems
- Fixed Charge Warehouse Location Problems
- Maximum Clique Problems
- Maximum Independent Set Problems
- Maximum Cut Problems
- Graph Coloring Problems
- Graph Partitioning Problems

Details of our experience with these and other problems are documented in the paper by Kochenberger, Glover, Alidaee, and Rego [21]. We are currently solving problems via QUIP with more than 10,000 variables in the quadratic representation. The significance of this is underscored by that fact that the well-known transformation of the binary quadratic representation into a binary linear programming representation produces problems containing more than 50,000,000 zero-one variables. Currently we are working on enhancements that will permit larger instances to be solved.

6. Summary:

We have demonstrated how a variety of disparate combinatorial problems can be solved by first re-casting them into the common modeling framework of the unconstrained quadratic binary program. Once in this unified form, the problems can be solved effectively by adaptive memory tabu search metaheuristics and associated evolutionary (scatter search) procedures.

Our findings challenge the conventional wisdom that places high priority on preserving linearity and exploiting specific structure. Although the merits of such a priority are well-founded in many cases, the QUIP domain appears to offer a partial exception. In forming QUIP(PEN), we destroy any linearity that the original problem may have exhibited. Moreover, any exploitable structure that may have existed originally is “folded” into the \hat{Q} matrix, and the general solution procedure we apply takes no advantage of it. Nonetheless, our solution outcomes have been remarkably successful, yielding results that rival the effectiveness of the best specialized methods.

This combined modeling/solution approach provides a unifying theme that can be applied in principle to all linearly constrained quadratic and linear programs in bounded integer variables, and the computational findings for a broad spectrum of problem classes raises the possibility that similarly successful results may be obtained for even wider ranges of problems. As the research community continues to provide improved solution methodologies for the QUIP model, the unified framework that QUIP represents for modeling and solving combinatorial problems via reformulation will become an increasingly attractive alternative to traditional specialized representations. These developments, with their apparent promise, open up a new set of research challenges and opportunities for the optimization community.

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