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Introduction to special xQx issue

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The Unconstrained Binary Quadratic Programming (UBQP) problem is notable for encompassing a remarkable range of applications in combinatorial optimization. As observed in Kochenberger et al. (2013), classes of problems that can be formally expressed using UBQP formulations include: 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, Number Partitioning Problems, and Linear Ordering Problems.

Even more remarkable is the fact that, once given a UBQP formulation, these problems can be solved by a UBQP method which is not specialized to exploit the problem domain of any individual class of problems, to yield solutions whose quality in many cases rivals or even surpasses the quality of the solutions produced by the best specialized methods, while achieving this outcome with an efficiency that likewise rivals or surpasses the efficiency of leading specialized methods. Moreover, these outcomes typically dominate those produced by current state-of-the-art commercial solvers for mixed integer linear and quadratic optimization, sometimes consuming two orders of magnitude less solution time to yield solutions superior to those of competing approaches. In other cases, where specialized methods edge out general UBQP methods for certain classes of problems, the UBQP formulation often still

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provides a useful framework for representing and analyzing various features of these problems.

The papers of this current issue provide significant advances in the UBQP area, consisting of several types (some papers belonging to more than one category): (1) new and highly effective methods for special classes of UBQP problems; (2) new UBQP formulations for problems not previously identified as UBQP problems, together with characterization of special properties and associated algorithms; (3) new methods for general UBQP problems or that specialize naturally for UBQP problems; (4) landscape analysis for UBQP problems that can be used to explain the behavior of certain methods.

Category (1): New methods for special UBQP problem classes

There are five papers in this category starting with *Metaheuristics for Robust Graph Coloring* by F. Wang and Z. Hu. In this paper the authors present an unconstrained quadratic programming formulation of the graph coloring problem and report on extensive computational experience with several metaheuristic methods for efficiently solving the problem.

The second paper in this category is Test *Assignment: A Quadratic Coloring Problem* by J. Duives, A. Lodi, and E. Malaguti. In this paper the authors describe the problem of assigning slightly different exams to desks in a university classroom so that neighbors have different exam variants. The problem is modeled in the form of UBQP and is solved by a Tabu Search metaheuristic. Extensive computational experience is provided including comparisons with CPLEX.

The third paper in this set is *Solving Large Scale Max Cut Problems via Tabu Search*, by G. Kochenberger, J-K. Hao, Z. LU, Haibo Wang, and F. Glover. In this paper the authors adopt a UBQP modeling representation for the Max Cut problem and apply a new Tabu Search metaheuristic to test problems ranging in size from 800 variables to 10,000 variables. Extensive computational experience is presented and comparisons are made with several well-known methods from the literature.

The forth paper in category (1) is *Quadratic Bottleneck Knapsack Problems* by R. Zhang and A. Punnen. The authors present a "min–max" variation of the quadratic knapsack problem along with complexity analysis and extensive computational experience with both heuristic and exact methods. Special polynomially solvable cases along with variations of the basic model are also identified.

The last paper in this set is *Heuristics and Metaheuristics for the Maximum Diversity Problem* by R. Marti, M. Gallego, A. Duarte, and E. G. Pardo. Here the authors study the well-known problem of selecting the maximum diverse subset of a specified size from a given set of objects. The paper provides extensive computational results and analysis together with computational comparisons among 30 different methods reported in the literature. A survey of applications along with the introduction of new benchmark library, MDPLIB, is also provided in the paper.

Category (2): New UBQP formulations and characterization of special algorithm properties

Our second category contains two papers starting with "*D-optimal Matrices via Quadratic Integer Optimization*," by I. S. Kotsireas, P. M. Pardalos. In this paper the authors describe the problem of searching for D-Optimal matrices and show how the problem can be approached via quadratic integer programming. A special focus is given to the case where the where the submatrices used to construct the D-optimal matrices are of size 3. Explicit examples and test problems are provided.

The second paper in this category is "*On characterization of maximal independent sets via quadratic optimization*," F. M. Pajouh, B. Balasundaram, O. Prokopyev, which studies the box constrained quadratic formulation of the maximum independent set problem. Based on properties developed for local maxima for the box-constrained case, necessary and sufficient conditions are presented for a binary point to be a local maximizing solution. Additional analysis of these conditions in the context of Hamming-1 and Hamming-2 neighborhoods motivate the development of new metaheuristic methods for this class of problems.

Category (3): New general UBQP methods and experimentation

This third set of papers contains three contributions starting with "*Several versions of the Devour Digest Tidy-up Heuristic for Unconstrained Binary Quadratic Problems*," by S. Hanafi, A. R. Rebai, M. Vasquez. In this paper the authors present and test a variety of alternative implementations of the basic one-pass framework of Devour, Digest, and Tidy-up. Efficient implementations of one and two—flip moves in the context of the one-pass framework are also presented. Extensive computational testing and comparisons are presented on problems ranging up to 7,000 variables.

The second paper in this category is "*Backbone Guided Tabu Search for Solving the UBQP problem*," Y. Wang, A. Lu, F. Glover, and J-K. Hao. The authors present a two-phase metaheuristic for solving UBQP that alternates between a basic Tabu Search that generates a set of local solutions and a methodology for fixing or freeing strongly determined backbone variables as the search proceeds. Substantial computational experience indicates that this procedure is very successful on a wide variety of test problems in terms of solution efficiency and solution quality.

The last paper in this set is "*Variable Objective Search*" by S. Butenko, O. Yezerska, and B. Balasundaram. The authors exploit the notion that many combinatorial optimization problems have alternative objective function formulations while sharing a common feasible region to be searched. While a local optimizing point for one formulation may not be locally optimal for another formulation, all formulations share the same global optima. The paper presents a solution process that alternates between formulations to conduct a robust search of the solution space. The viability of the approach is illustrated via computational experience on a standard test bed of maximum independent set problems.

Category (4): Landscape analysis to explain UBQP algorithm behavior

Our last category contains the single paper "*Elementary Landscape Decomposition of the 0-1 Unconstrained Quadratic Optimization*," by F. Chicano and E. Alba. In this paper the authors analyze the landscape of the UBQP model and prove that in general it can be written as the sum of two elementary landscapes. Theoretical results useful in estimating the performance of local search methods along with practical insights for improved algorithm design are given. Along the way the authors give an overview of Landscape theory and show how the decomposition of UBQP allows the average value of the objective function in a bit-flip neighborhood of a solution to be computed using only a single evaluation of the elementary components.

Reference

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