Improving the performance of standard solvers for quadratic 0-1 programs by a tight convex reformulation: The QCR method

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Abstract

Let (QP) be a 0-1 quadratic program which consists in minimizing a quadratic function subject to linear equality constraints. In this paper, we present QCR, a general method to reformulate (QP) into an equivalent 0-1 program with a convex quadratic objective function. The reformulated problem can then be efficiently solved by a classical branch-and-bound algorithm, based on continuous relaxation. This idea is already present in the literature and used in standard solvers such as CPLEX. Our objective in this work was to find a convex reformulation whose continuous relaxation bound is, moreover, as tight as possible. From this point of view, we show that QCR is optimal in a certain sense. State-of-the-art reformulation methods mainly operate a perturbation of the diagonal terms and are valid for any {0, 1} vector. The innovation of QCR comes from the fact that the reformulation also uses the equality constraints and is valid on the feasible solution domain only. Hence, the superiority of QCR holds by construction. However, reformulation by QCR requires the solution of a semidefinite program which can be costly from the running time point of view. We carry out a computational experience on three different combinatorial optimization problems showing that the costly computational time of reformulation by QCR can however result in a drastically more efficient branch-and-bound phase. Moreover, our new approach is competitive with very specific methods applied to particular optimization problems.
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1. Introduction

Consider the following linearly-constrained zero-one quadratic program:

$$(QP): \text{ Min } \left\{ g(x) = x^t Q x + c^t x : Ax = b, \ x \in \{0, 1\}^n \right\}$$

where c is an n real vector, b is an m real vector, Q is a symmetric $n \times n$ real matrix and A is an $m \times n$ real matrix. Without loss of generality, we assume that all diagonal terms of Q are equal to 0.

Quadratic zero-one programming with linear constraints is a general model that allows to formulate numerous important problems in combinatorial optimization including, for example: quadratic assignment [19], graph partitioning [33], task allocation [5] and densest k-subgraph [31].

Various heuristics and exact methods have been proposed to solve (*QP*). Due to the nonconvexity of the objective function, (*QP*) is often reformulated before searching for its optimal solution. So, several methods have been developed to solve it exactly through 0-1 linear reformulations (see, for example, [1,2,20,22,39]) or 0-1 convex quadratic reformulations (see, for example, [7,12,24,34,37]). This paper is concerned with the latter type of reformulation. Although 0-1 linear reformulations of (*QP*) are the most common approaches, other methods have been proposed. Let us cite, for example, algebraic and dynamic programming methods [16,25], reformulation to a continuous concave minimization problem [29] and enumerative methods based on different types of relaxations such as lagrangian relaxation, semidefinite relaxation or convex quadratic relaxation [3,9,11,13,18,21,23,27,35].

In this paper we reformulate (*QP*) by an equivalent zero-one quadratic program with a convex objective function. Consequently, we can solve the transformed problem using general-purpose optimization software which implement branch-and-bound algorithms with a bounding procedure based on the optimal value of the continuous relaxation. We will show how to find the best convex reformulation of (*QP*), in a certain sense, by semidefinite programming.

The paper is organized as follows. In Section 2 we present QCR, a reformulation of (*QP*) by a zero-one quadratic program with a convex objective function. Section 3 reports computational experiments on the solution of the densest k-subgraph problem, the graph bisection problem and a task allocation problem. More precisely, we apply QCR on the one hand and the default preprocessing of CPLEX on the other hand in order to compare the efficiency of the two convexifications. Moreover, for the graph bisection problem, we compare QCR with a specific branch-and-bound algorithm, developed by Karisch, Rendl and Clausen [30]. Section 4 gives a conclusion.

2. QCR: A quadratic convex reformulation method

Let $X = \{x : Ax = b, \ x \in \{0, 1\}^n\}$ be the set of feasible solutions of problem (*QP*) and $\overline{X} = \{x : Ax = b, \ x \in [0, 1]^n\}$ be the set of feasible solutions of the continuous relaxation of (*QP*). The general term of matrix A is denoted by a_{ij} and the general term of Q by q_{ij}.

The objective function of (*QP*) is not convex since all diagonal terms of Q are equal to 0. Consider the following zero-one quadratic problem equivalent to (*QP*) and depending on two parameters $\alpha \in \mathbb{R}^{m \times n}$ and $u \in \mathbb{R}^n$:

$$(QP_{\alpha,u}) : \ \text{Min} \ \left\{ g_{\alpha,u}(x) : Ax = b, \ x \in \{0, 1\}^n \right\}$$

where

$$g_{\alpha,u}(x) = g(x) + \sum_{k=1}^{m} \left(\sum_{i=1}^{n} \alpha_{ki} x_i \right) \left(\sum_{j=1}^{n} a_{kj} x_j - b_k \right) + \sum_{i=1}^{n} u_i \left(x_i^2 - x_i \right)$$

$$= x^t Q_\alpha x + c_\alpha^t x + \sum_{i=1}^{n} u_i \left(x_i^2 - x_i \right)$$

$$= x^t Q_{\alpha,u} x + c_{\alpha,u}^t x$$

and

$$Q_\alpha = Q + \frac{1}{2} \left(\alpha^t A + A^t \alpha \right), \quad Q_{\alpha,u} = Q_\alpha + \text{Diag}(u),$$

$$c_\alpha = c - \alpha^t b, \quad c_{\alpha,u} = c_\alpha - u.$$

Diag(u) is a diagonal $n \times n$ matrix with the elements of u on the diagonal.

It is easy to verify that for all $x \in X$, function $g_{\alpha,u}(x)$ is equal to $g(x)$. We are interested by the reformulations of $g(x)$ into $g_{\alpha,u}(x)$ if $g_{\alpha,u}(x)$ is convex over $\mathbb{R}^n$. This is always possible. Take α equal to the null matrix and $u = -\lambda e$ where λ is the smallest eigenvalue of matrix Q and e the n-vector of all ones. This amounts to the eigenvalue method introduced in [24].

The transformation of $g(x)$ into a convex function over $\mathbb{R}^n$ allows to solve ($QP_{\alpha,u}$) by a branch-and-bound algorithm based on continuous relaxation. It is well known that the behavior of such an algorithm is very dependent

upon the bound at the root of the search tree. This bound is equal to the optimum value of the continuous relaxation of $(QP_{\alpha,u})$ that can be solved in polynomial time with a given accuracy. So we are going to determine $\alpha \in \mathbb{R}^{m \times n}$ and $u \in \mathbb{R}^n$ such that $g_{\alpha,u}(x)$ is convex and the value of the continuous relaxation of $(QP_{\alpha,u})$ is as tight as possible. More precisely we have to solve the following problem:

$$(C(QP)) : \max_{\substack{\alpha \in \mathbb{R}^{m \times n}, u \in \mathbb{R}^n \\ Q_{\alpha,u} \succeq 0}} \min_{x \in \overline{X}} g_{\alpha,u}(x).$$

In the following theorem, we show that problem $(C(QP))$ is equivalent to the SDP-dual of a semidefinite relaxation $(SDQP)$ of problem (QP). Therefore, an optimal solution (α^*, u^*) of $(C(QP))$ can be obtained by solving $(SDQP)$, which can be done in polynomial time. For instance, Renegar [38] develops an interior point method for semidefinite programming, and shows that it can solve semidefinite programs to a prescribed accuracy in a polynomial number of arithmetic operations.

Theorem 1. *The optimum value of $(C(QP))$ is equal to the optimum value of the following semidefinite program $(SDQP)$, which is a semidefinite relaxation of (QP):*

$$(SDQP) \begin{cases} \text{Min} & c^t x + \sum_{i=1}^n \sum_{j=1}^n q_{ij} X_{ij} \\ s.t. & X_{ii} = x_i & i = 1, \ldots, n & (1) \\ & -b_k x_i + \sum_{j=1}^n a_{kj} X_{ij} = 0 & k = 1, \ldots, m; \; i = 1, \ldots, n & (2) \\ & Ax = b \\ & \begin{pmatrix} 1 & x^t \\ x & X \end{pmatrix} \succeq 0 \\ & x \in \mathbb{R}^n, \quad X \in \mathbf{S}_n \end{cases}$$

where $\mathbf{S}_n$ represents the set of $n \times n$ real symmetric matrices. For problem $(C(QP))$, optimal values u_i^* $(i = 1 \ldots, n)$ are given by the optimal values of the dual variables associated with constraints (1) *and optimal values α_{ki}^* ($k = 1, \ldots, m; i = 1, \ldots, n$) are given by the optimal values of the dual variables associated with constraints* (2).

Proof. Consider the quadratic function $z_{\alpha,u,\beta}(x) = g_{\alpha,u}(x) + \beta^t(Ax - b)$ depending on the three multidimensional parameters $\alpha \in \mathbb{R}^{m \times n}$, $u \in \mathbb{R}^n$ and $\beta \in \mathbb{R}^m$. Let $z_{\alpha,u,\beta}(x) = x^t Q_{\alpha,u} x + c_{\alpha,u,\beta}^t x - \beta^t b$ with $c_{\alpha,u,\beta}^t = c_{\alpha,u}^t + \beta^t A$. By observing that $x_i^2 \leq x_i$ is equivalent to $0 \leq x_i \leq 1$, our convexification problem $(C(QP))$ can be written as $(D1)$:

$$(D1) : \max_{\substack{\alpha \in \mathbb{R}^{m \times n}, u \in \mathbb{R}^n \\ Q_{\alpha,u} \succeq 0}} \min_{x \in \mathbb{R}^n} \left\{ g_{\alpha,u}(x) : Ax = b, x_i^2 \leq x_i \; (i = 1, \ldots, n) \right\}$$

$g_{\alpha,u}(x)$ is a convex function; the constraints $Ax = b$ and $x_i^2 \leq x_i$ define a convex set. Assuming the Slater's interiority condition is satisfied then, by Lagrangian duality, $(D1)$ is equivalent to $(D2)$:

$$(D2) : \max_{\substack{\alpha \in \mathbb{R}^{m \times n}, u \in \mathbb{R}^n, \beta \in \mathbb{R}^m, \lambda \in \mathbb{R}_+^n \\ Q_{\alpha,u} \succeq 0}} \min_{x \in \mathbb{R}^n} \left\{ g_{\alpha,u}(x) + \sum_{i=1}^n \lambda_i (x_i^2 - x_i) + \beta^t(Ax - b) \right\}$$

$(D2)$ is also equivalent to $(D3)$:

$$(D3) : \max_{\substack{\alpha \in \mathbb{R}^{m \times n}, u \in \mathbb{R}^n, \beta \in \mathbb{R}^m \\ Q_{\alpha,u} \succeq 0}} \min_{x \in \mathbb{R}^n} \left\{ g_{\alpha,u}(x) + \beta^t(Ax - b) \right\}$$
$$= \max_{\substack{\alpha \in \mathbb{R}^{m \times n}, u \in \mathbb{R}^n, \beta \in \mathbb{R}^m \\ Q_{\alpha,u} \succeq 0}} \min_{x \in \mathbb{R}^n} z_{\alpha,u,\beta}(x).$$

Indeed, if $(\alpha^*, u^*, \beta^*, \lambda^*)$ is an optimal solution of $(D2)$, $(\alpha^*, u^* = u^* + \lambda^*, \beta^*)$ is a feasible solution of $(D3)$ with the same value. Moreover, the optimal value of $(D2)$ is obviously greater than or equal to the optimal value of $(D3)$.

It is well known that a necessary condition for the quadratic function $z_{\alpha,u,\beta}(x)$ to have a minimum not equal to $-\infty$ is that matrix $Q_{\alpha,u}$ is positive semidefinite. Hence, ($D3$) is equivalent to ($D4$):

$$(D4) : \max_{\alpha \in \mathbb{R}^{m \times n}, u \in \mathbb{R}^n, \beta \in \mathbb{R}^m} \min_{x \in \mathbb{R}^n} z_{\alpha,u,\beta}(x).$$

This last problem is the Lagrangian dual obtained from (QP') by relaxing all the constraints:

$$(QP') : \min \left\{ g(x) : Ax = b, x_i^2 = x_i (i = 1, \ldots, n), x_i \left(\sum_{j=1}^{n} a_{kj} x_j - b_k \right) = 0 \ (i = 1, \ldots, n; k = 1, \ldots, m) \right\}.$$

Observe that (QP') is equivalent to the initial problem (QP). Following Lemaréchal and Oustry ([32], Corollary 4.2), the dual of (QP') is equivalent to the SDP problem ($D5$):

$$(D5) \begin{cases} \text{Max} \quad r \\ \text{s.t.} \quad \begin{pmatrix} -\beta^t b - r & \frac{1}{2} c_{\alpha,u,\beta}^t \\ \frac{1}{2} c_{\alpha,u,\beta} & Q_{\alpha,u} \end{pmatrix} \succeq 0 \\ \quad r \in \mathbb{R}, \alpha \in \mathbb{R}^{m \times n}, u \in \mathbb{R}^n, \beta \in \mathbb{R}^m. \end{cases}$$

Following again Lemaréchal and Oustry ([32], Theorem 4.4), if we apply SDP duality to problem ($D5$), we get ($SDQP$). Note that there is no duality gap since (i) the feasible domain of ($SDQP$) is nonempty (as (QP) admits a feasible solution) and then ($D5$) is bounded, (ii) ($D5$) satisfies Slater's condition. For example, by setting $\alpha = \beta = 0$ and taking the u_i components positive and large, and r negative with $|r|$ large, it is possible to build a feasible matrix of ($D5$) that is positive definite. □

Remark

We can observe that, since $\sum_{k=1}^{m} (\sum_{i=1}^{n} \alpha_{ki}^* x_i)(\sum_{j=1}^{n} a_{kj} x_j - b_k)$ is null for all $x \in \overline{X}$, then:

$$\underline{\text{Min}}_{x \in \overline{X}} \ g_{\alpha^*,u^*}(x) = \underline{\text{Min}}_{x \in \overline{X}} \ g_{O,u^*}(x)$$

where O is the $m \times n$-null matrix.

However, $g_{O,u^*}(x)$ is not necessarily convex over $\mathbb{R}^n$ and recall that our main objective is to convexify $g(x)$ over $\mathbb{R}^n$ in order to make the continuous relaxation easy to solve.

Example

Consider the following linearly constrained 0–1 quadratic programming problem whose optimal value is -80, obtained for $x_2 = x_3 = x_5 = 1$ and $x_1 = x_4 = 0$:

$$(E) : \quad \text{Min} \quad \phi(x) = -9x_1 - 7x_2 + 2x_3 + 23x_4 + 12x_5 - 48x_1 x_2 + 4x_1 x_3 + 36x_1 x_4$$
$$-24x_1 x_5 - 7x_2 x_3 + 36x_2 x_4 - 84x_2 x_5 + 40x_3 x_4 + 4x_3 x_5 - 88x_4 x_5$$
$$\text{s.t.}$$
$$x_1 + x_2 + x_4 + x_5 = 2$$
$$x_1, x_2, x_3, x_4, x_5 \in \{0, 1\}$$

The SDP relaxation of our example (E) is:

$$(SDE) : \quad \text{Min} \quad -9x_1 - 7x_2 + 2x_3 + 23x_4 + 12x_5 - 48X_{12} + 4X_{13} + 36X_{14}$$
$$-24X_{15} - 7X_{23} + 36X_{24} - 84X_{25} + 40X_{34} + 4X_{35} - 88X_{45}$$
$$\text{s.t.}$$
$$x_1 + x_2 + x_4 + x_5 = 2$$
$$X_{1i} + X_{2i} + X_{4i} + X_{5i} = 2x_i \quad i = 1, \ldots, 5 \quad \leftarrow \alpha_i^*$$
$$X_{ii} = x_i \quad i = 1, \ldots, 5 \quad \leftarrow u_i^*$$
$$\begin{pmatrix} cc1 & x^t \\ x & X \end{pmatrix} \succeq 0$$
$$x \in \mathbb{R}^5, \ X \in S_5$$

Parameters u^* and α^* that allow us to build the new problem are obtained from the solution of (*SDE*). The optimal solution value of (*SDE*) equals -88.02. It is therefore the optimal solution value of the continuous relaxation of the QCR-reformulated problem (E_{α^*,u^*}):

$$
\begin{aligned}
(E_{\alpha^*,u^*}): \quad \text{Min} \quad & \phi(x) \\
& + (14x_1 + 18.6x_2 - 1.4x_3 + 0.12x_4 + 29.26x_5)(x_1 + x_2 + x_4 + x_5 - 2) \\
& + 24.6(x_1^2 - x_1) + 3.38(x_2^2 - x_2) + 17.38(x_3^2 - x_3) + 111.46(x_4^2 - x_4) \\
& - 7.4(x_5^2 - x_5) \\
\text{s.t.} \quad & x_1 + x_2 + x_4 + x_5 = 2 \\
& x \in \{0, 1\}^5
\end{aligned}
$$

Note that the bound obtained by the preprocessing of CPLEX is -113.68.

A QCR variant

We consider the following transformation of $g(x)$:

$$
g_{\beta,u}(x) = g(x) + \beta \sum_{k=1}^{m} \left(\sum_{j=1}^{n} a_{kj} x_j - b_k \right)^2 + \sum_{i=1}^{n} u_i \left(x_i^2 - x_i \right)
$$

and so the new problem:

$$
(QP_{\beta,u}): \text{ Min} \left\{ g_{\beta,u}(x) : Ax = b, \ x \in \{0, 1\}^n \right\}.
$$

As for the above QCR method, the optimal parameters β^* and u^* are the ones that allow to convexify $g(x)$ and to obtain an optimal continuous value as tight as possible. They are given by solving the following semidefinite relaxation:

$$
(SDQP') \begin{cases}
\text{min} \quad c^t x + \sum_{i=1}^{n} \sum_{j=1}^{n} q_{ij} X_{ij} & \\
\text{s.t.} \quad X_{ii} = x_i \quad i = 1, \ldots, n & (1) \\
\sum_{k=1}^{m} \left(\sum_{i=1}^{n} \sum_{j=1}^{n} a_{ki} a_{kj} X_{ij} - 2 \sum_{j=1}^{n} b_k a_{kj} x_j + b_k^2 \right) = 0 & (4) \\
\begin{pmatrix} 1 & x^t \\ x & X \end{pmatrix} \succeq 0 & \\
x \in \mathbb{R}^n, \ X \in \mathbf{S}_n &
\end{cases}
$$

The u_i^* values are given by the optimal values of the dual variables associated with constraints (1) and the β^* value is given by the optimal value of the dual variable associated with constraint (4).

QCR and this new transformation provide the same lower bound since the associated semidefinite programs have the same optimal value [18]. So, this new semidefinite relaxation should be more efficient than (*SDQP*) because of its smaller size. However a preliminary experiment does not show that the resolution with this variant accelerates the global solution time.

3. Computational results

In this section, we present different applications of QCR: the densest k-subgraph problem (Section 3.1), the graph bisection problem (Section 3.2) and finally a task allocation problem (Section 3.3).

All the experiments have been carried out on a Pentium IV 2.2 GHz computer with 1 Go of RAM. For each instance, execution time limit is set to 1 hour.

We choose to solve semidefinite programs using SB ([26,28]), a software applying the spectral bundle method on eigenvalue optimization problems, developed by Helmberg and Rendl [28]. (QP_{α^*,u^*}) is modeled with AMPL and then solved by CPLEX9 [15]. Note that we use the default accuracy (10^{-5}) to solve the semidefinite problem and the continuous relaxation.

For convenience, we use 'QCR+CPLEX' to refer to CPLEX with QCR preprocessing and 'CPLEX' to refer to the direct execution of CPLEX. Indeed, CPLEX can solve problem (QP) by operating a convexification algorithm. A brief computational test led us to think that this algorithm is based on the smallest eigenvalue method of [24].

For all the results reported in the following tables, gap represents the average value of the gap at the root node, defined as $|\frac{bound-opt}{opt}| * 100$ where opt is the value of the optimal or the best known solution and bound is the optimal value of the continuous relaxation at the root node of the branch-and-bound algorithm.

3.1. Computational results for the densest k-subgraph problem

Given an undirected graph $G = (V, U)$ with n nodes $\{v_1, \ldots, v_n\}$ and a positive integer k in $\{3, \ldots, n - 2\}$, the densest k-subgraph problem consists in selecting a node subset $S \subseteq V$ of cardinality k and such that the subgraph of G induced by S contains as many edges as possible.

The densest k-subgraph problem can be formulated as the following linearly constrained 0–1 quadratic optimization problem (DS):

$$(DS) : \text{Max} \left\{ \sum_{i<j} \delta_{ij} x_i x_j : \sum_{j=1}^{n} x_j = k, \ x \in \{0, 1\}^n \right\}$$

where the binary coefficient $\delta_{ij} = 1$ if and only if $[v_i, v_j]$ is an edge of G. The binary variable x_i is equal to 1 if and only if vertex v_i is in the k-subgraph. (DS) is also known under the name of *k-cluster problem* [14]. It can be also considered as a special case of the *k-dispersion-sum problem* [36].

The densest k-subgraph problem can be rewritten as follows:

$$(DS') : \text{Min} \left\{ f(x) = x^t M x : \sum_{j=1}^{n} x_j = k, \ x \in \{0, 1\}^n \right\}$$

where the general term of M is $m_{ij} = -\frac{1}{2}\delta_{ij}, \ \forall i, j$. Problems (DS) and (DS') are equivalent and their optimal values are opposite.

Now, we can apply the QCR approach to problem (DS').

According to the general method presented in Section 2, the reformulation of (DS') is:

$$(DS'_{\alpha,u}) : \text{Min} \left\{ f_{\alpha,u}(x) : \sum_{j=1}^{n} x_j = k, \ x \in \{0, 1\}^n \right\}$$

where $f_{\alpha,u}(x) = x^t M x + \sum_{i=1}^{n} u_i(x_i^2 - x_i) + \sum_{i=1}^{n} \alpha_i x_i (\sum_{j=1}^{n} x_j - k)$.

Since problem (DS') has just one constraint, α is a vector with n components. The best parameters α^* and u^* are then computed by the SDP relaxation associated to (DS'), that we call $(SDDS')$ in the following.

We consider randomly generated instances of the densest k-subgraph problem. We take different graph sizes ($n = 40, 80, 100$), different densities ($d = 25\%, 50\%, 75\%$) and different k values ($k = \frac{n}{4}, \frac{n}{2}, \frac{3n}{4}$). For each couple (k, d), there are 5 instances (used in [4] for $n = 40$ and in [37] for $n = 80$). They are generated as follows: for a given density d and any pair of indexes (i, j) such that $i < j$, we generate a random number ρ from $[0, 1]$. If $\rho > d$ then δ_{ij} is set to 0, otherwise, δ_{ij} is set to 1.

All the results are reported in Table 1.

Legend of Table 1:

- d, density of the graph
- CPU, the average value of the CPU time, for five instances, required by CPLEX to solve (DS') or required by SB and CPLEX to solve $(SDDS')$ and (DS'_{α^*,u^*}) respectively. Note that a number $i < 5$ in brackets corresponds to the number of instances out of 5 solved within 1h. In this case, the corresponding CPU time is the average over these i instances.

The running times corresponding to the computation of (α^*, u^*) by the semidefinite programming solver SB are very small, always less than one second.

Table 1
Average results for 135 randomly generated instances of *k*-cluster

n	k	d (%)	QCR+CPLEX		CPLEX	
			CPU	gap (%)	CPU	gap (%)
40	$\lfloor \frac{n}{4} \rfloor$	25	0.16"	9.63	1'5"	91.4
		50	0.36"	9.32	–	154.53
		75	3.96"	12.28	–	257.40
	$\lfloor \frac{n}{2} \rfloor$	25	0.08"	3.06	5'41"	33.1
		50	0.22"	2.5	–	43.45
		75	0.10"	1.5	–	71.27
	$\lfloor \frac{3n}{4} \rfloor$	25	0.12"	1.08	13.88"	10.6
		50	0.04"	0.78	8'32" (4)	17.7
		75	0.03"	0.48	–	23.6
80	$\lfloor \frac{n}{4} \rfloor$	25	2'6"	9.16	–	114.4
		50	5'26"	8	–	170.7
		75	22'3"	6.44	–	225.3
	$\lfloor \frac{n}{2} \rfloor$	25	19.6"	2.96	–	42.9
		50	18.54"	1.8	–	62.1
		75	2'57"	1.32	–	78.2
	$\lfloor \frac{3n}{4} \rfloor$	25	0.92"	0.86	–	14.9
		50	2.09"	0.56	–	20.9
		75	3.6"	0.42	–	26.2
100	$\lfloor \frac{n}{4} \rfloor$	25	24'32"	9.1	–	124.1
		50	32'58"	7.88	–	180
		75	–	5.6	–	229.9
	$\lfloor \frac{n}{2} \rfloor$	25	7'54"	2.56	–	47.3
		50	6'32" (1)	2.18	–	67
		75	9'8"	1	–	79.3
	$\lfloor \frac{3n}{4} \rfloor$	25	9"	0.8	–	16.1
		50	50.81"	0.64	–	22.8
		75	14.32"	0.34	–	26.7

None of the five corresponding instances could be solved within 1 h (*i*): *i* instances out of 5 were solved within 1 h.

As a general remark, the gap of 'QCR+CPLEX' is about 20 times smaller than the one of 'CPLEX'. The CPU time is hence drastically improved. Indeed, 'CPLEX' solves only 19 out of the 135 instances within one hour of CPU time whereas 'QCR+CPLEX' allows to solve 126 instances.

Instances with 40 and 80 nodes have already been used in [37]: eigenvalue methods have been applied to solve (*DS*). Note that for all instances, QCR improves results presented in [37] (i.e the bound value and therefore the CPU time): the gap obtained with QCR is about 2 times smaller. In addition, the 'QCR+CPLEX' approach allows to solve all instances with $n = 80$ and $k = \lfloor \frac{n}{4} \rfloor$ whereas, with the reformulation studied in [37], only 3 instances out of 15 are solved in less than one hour.

Moreover, we can solve larger problems than in recent publications that use the same instances but different approaches. In [36], the reported results concern weighted instances with no more than 60 nodes. The integer linear programming approach presented in [4] and based on six different formulations does not allow to solve instances with 80 nodes, except for a density of 75%.

3.2. Computational results for the graph bisection problem

Let $G = (V, E)$ be an undirected graph with n nodes $\{v_1, \ldots, v_n\}$ and a set of weighted edges E. The graph bisection problem consists in dividing the nodes of G into two sets V_1 and V_2 such that $| V_1 |= p$ and $| V_2 |= n - p$ and such that the total weight of edges that have end-points in different sets is minimal. This problem can be formulated

as the following linearly constrained zero-one quadratic problem:

$$(BP): \text{ Min } \left\{ g(x) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} c_{ij} \left(x_i(1-x_j) + (1-x_i)x_j \right) : \sum_{i=1}^{n} x_i = p, \ x \in \{0,1\}^n \right\}$$

where c_{ij} is the weight of edge $[v_i, v_j]$. The binary variable x_i is equal to 1 if and only if the node v_i is in V_1.

(*BP*) is equivalent to the following problem where, in the objective function, linear terms are separated from quadratic terms:

$$(BP): \text{ Min } \left\{ g(x) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} -2c_{ij}x_i x_j + \sum_{i=1}^{n} C_i x_i : \sum_{i=1}^{n} x_i = p, \ x \in \{0,1\}^n \right\}$$

where $C_i = \sum_{j=1}^{i-1} c_{ji} + \sum_{j=i+1}^{n} c_{ij}$. According to the general method presented in Section 2, the reformulation of (*BP*) is:

$$(BP_{\alpha,u}): \text{ Min } \left\{ g_{\alpha,u}(x) : \sum_{i=1}^{n} x_i = p, \ x \in \{0,1\}^n \right\}$$

with:

$$g_{\alpha,u}(x) = g(x) + \sum_{i=1}^{n} u_i \left(x_i^2 - x_i \right) + \sum_{i=1}^{n} \alpha_i x_i \left(\sum_{j=1}^{n} x_j - p \right).$$

The best parameters α^* and u^* are computed by the SDP relaxation associated to *BP* that we call (*SDBP*) in the following.

Note that one constraint is added to (*BP*) when $p = \frac{n}{2}$ in order to accelerate the branch-and-bound algorithm, which consists in fixing to 1 the variable corresponding to a largest degree node.

3.2.1. Randomly generated unweighted graphs

We first apply QCR to randomly generated unweighted graphs. They are generated as follows: for a given density $d \in [0, 1]$ and a pair of indices (i, j) such that $i < j$, we generate a random number ρ from $[0, 1]$. If $\rho > d$ then c_{ij} is set to 0, otherwise, c_{ij} is set to 1.

Table 2 shows the results for four graph sizes ($n = 40, 80, 90, 100$), three densities ($d = 25\%, 50\%, 75\%$) and three p values ($p = \lfloor \frac{n}{8} \rfloor, \lfloor \frac{n}{4} \rfloor, \lfloor \frac{n}{2} \rfloor$). For each triplet ($n, p, d$), we solve 5 instances.

Legend of Table 2:

- d, density of the graph.
- CPU, average value of the total CPU time required by CPLEX to solve (*BP*) or required by SB and CPLEX to solve (*SDBP*) and (BP_{α^*,u^*}) respectively. Note that a number $i < 5$ in brackets corresponds to the number of instances out of 5 solved within 1h. In this case, the corresponding CPU time is the average over these i instances.

For Table 2, the running times corresponding to the computation of (α^*, u^*) by semidefinite programming are very small: they are always much smaller than the running time of the branch-and-bound phase.

We can observe that the gap obtained with the QCR approach are rather small and whatever the graph sizes are, the best gap values are obtained for largest densities. The average gap is equal to 9% for $d = 25\%$, 4% for $d = 50\%$ and 3% for $d = 75\%$.

With 'CPLEX', the gap is always equal to 100%, except when $p = \lfloor \frac{n}{2} \rfloor$, where a constraint is added to (*BP*). Note that if this constraint is not added, then the gap will be 100%. Because of these results, 'CPLEX' allows to solve few instances within 1 hour whereas with 'QCR+CPLEX', the first CPU times higher than 1 hour are obtained when $n \geq 90$ and $p \neq \lfloor \frac{n}{8} \rfloor$.

Observe that the longest running times are obtained for the graph equicut problem (i.e. $p = \lfloor \frac{n}{2} \rfloor$): intuitively, we can think that the partition size p increases the difficulty of the problem when it tends towards the value $\frac{n}{2}$ since the number of feasible solutions is equal to the number of combinations of p objects taken among n.

Table 2
Average results for 180 randomly generated unweighted instances of the graph bipartition problem

n	p	d (%)	QCR+CPLEX		CPLEX	
			CPU	gap (%)	CPU	gap (%)
40	$\lfloor \frac{n}{8} \rfloor$	25	0.04"	12.45	1.17"	100
		50	0.07"	7.22	8.2"	100
		75	0.08"	4.32	53.4"	100
	$\lfloor \frac{n}{4} \rfloor$	25	0.15"	10.2	2'6"	100
		50	0.25"	6.33	–	100
		75	0.36"	3.36	–	100
	$\lfloor \frac{n}{2} \rfloor$	25	0.54"	8.05	13'9" (3)	89.37
		50	0.64"	3.08	–	93
		75	0.53"	2.02	–	93.7
80	$\lfloor \frac{n}{8} \rfloor$	25	5.7"	8.48	–	100
		50	3.8"	4.98	–	100
		75	14.8"	3.26	–	100
	$\lfloor \frac{n}{4} \rfloor$	25	2'18"	8.4	–	100
		50	4'04"	4.54	–	100
		75	5'09"	2.6	–	100
	$\lfloor \frac{n}{2} \rfloor$	25	24'21"	6.52	–	95.3
		50	10'51"	3.26	–	96.5
		75	6'49"	1.62	–	96.9
90	$\lfloor \frac{n}{8} \rfloor$	25	41.2"	10.04	–	100
		50	25.3"	5.14	–	100
		75	29.6"	3.08	–	100
	$\lfloor \frac{n}{4} \rfloor$	25	19'31" (4)	8.76	–	100
		50	13'40" (4)	3.48	–	100
		75	9'46" (3)	2.56	–	100
	$\lfloor \frac{n}{2} \rfloor$	25	36'1" (3)	5.92	–	96.2
		50	9'48" (1)	3.14	–	97
		75	23'18" (3)	1.6	–	97.4
100	$\lfloor \frac{n}{8} \rfloor$	25	1'22"	9.54	–	100
		50	2'9"	5.36	–	100
		75	3'4"	3	–	100
	$\lfloor \frac{n}{4} \rfloor$	25	27'13" (1)	7.9	–	100
		50	26'34" (1)	4.4	–	100
		75	22'40" (2)	2	–	100
	$\lfloor \frac{n}{2} \rfloor$	25	–	5.92	–	96.7
		50	–	3	–	97.5
		75	–	1.7	–	97.7

None of the five corresponding instances could be solved within 1 h (i): i instances out of 5 were solved within 1 h.

3.2.2. Comparison with Karisch, Rendl and Clausen (KRC) method

In this section, we compare our method with the one of Karisch, Rendl and Clausen (KRC) who designed an exact solution method for the graph bisection problem [30]. Their approach is a specific branch-and-bound algorithm based on semidefinite programming and polyhedral relaxations.

Comparison with the KRC method based on Brunetta, Conforti and Rinaldi instances

Karisch, Rendl and Clausen tested their approach on a library created by Brunetta, Conforti and Rinaldi (BCR) [10]. We choose to solve instances from it (ftp://ftp.math.unipd.it/pub/Misc/equicut) and compare our results with the ones of KRC. The instances correspond to $p = \lfloor \frac{n}{2} \rfloor$ and are divided into 4 classes: *Random Instances*, *Toroidal Grid Instances*, *Mixed grid Instances*, *Instances with Negative Weights*. We only present results for *Toroidal Grid Instances*. For more information, all results and more complete details are available in [8].

Table 3
Equicut of toroidal grid instances from the BCR-library

Problem	n	d (%)	opt	KRC $\mathrm{CPU_{KRC}}$	QCR+CPLEX $\overline{\mathrm{CPU_{QCR}}}$	$\mathrm{gap_{QCR}}$ (%)
$4 \times 5t$	20	21	28	0.06"	0.01"	12.6
$6 \times 5t$	30	14	31	0.2"	0.02"	26.9
$8 \times 5t$	40	10	33	0.4"	0.09"	38.5
$12 \times 2t$	42	10	9	0.34"	0.05"	66.5
$23 \times 2t$	46	9	9	8.3"	0.2"	78
$4 \times 12t$	48	9	24	1.13"	0.14"	54.2
$5 \times 10t$	50	8	33	0.4"	0.25"	50
$10 \times 6t$	60	7	42	23.33"	2.22"	53.5
$7 \times 10t$	70	6	45	38.13"	3.69"	54.2
$10 \times 8t$	80	5	43	1'3"	2.29"	47.7
	Average value			13.53"	0.9"	48.21

Table 4
Randomly generated unweighted instances

Graph	n	p	opt	KRC $\mathrm{CPU_{KRC}}$	QCR+CPLEX $\overline{\mathrm{CPU_{QCR}}}$	$\mathrm{gap_{QCR}}$ (%)
ex36a	36	$\lfloor \frac{n}{2} \rfloor$	117	3"	0.22"	4.5
ex60a	60		367	20"	11.39"	3.4
ex84a	84		742	2h02'55"	40'06"	3.5
ex36a	36	$\lfloor \frac{3n}{4} \rfloor$	85	31"	0.13"	7.8
ex60a	60		268	9'56"	8.95"	5.96
ex84a	84		548	8'20"	12'24"	4.9
ex36a	36	$\lfloor \frac{7n}{12} \rfloor$	112	0.67"	0.21"	5
ex60a	60		351	22.53"	3.56"	2.9
ex84a	84		721	37'7"	2h17'24"	4.08
ex36a	36	$\lfloor \frac{13n}{24} + \frac{1}{2} \rfloor$	114	0.2"	0.13"	4.5
ex60a	60		360	21.2"	8.72"	3.1
ex84a	84		735	20'15"	1h52'48"	3.8
	Average value			16'41"	25'16"	

Note that our computer is about 15 times faster than the one of Karisch, Rendl and Clausen whose experiments were performed on a HP 9000/735. So, in the following tables, we report CPU times required by the KRC method divided by 15.

Legend of Tables 3 and 4:

- opt, value of the optimal solution
- $\mathrm{CPU_{QCR}}$, total CPU time required by the 'QCR+CPLEX' method
- $\mathrm{gap_{QCR}} = |\frac{\mathrm{bound}-\mathrm{opt}}{\mathrm{opt}}|$ where bound is the optimal value of the continuous relaxation of the QCR reformulated problem
- $\mathrm{CPU_{KRC}}$, total CPU time required by the KRC method on a HP 9000/735 (divided by 15).

We solve all instances to optimality. For all instances, the CPU time required to find the optimal solution is drastically improved compared with the results found by KRC: $\mathrm{CPU_{QCR}}$ can be up to 40 times smaller than $\mathrm{CPU_{KRC}}$ taking into account the difference of computers.

Our method is 15 times faster in average and in spite of a rather large gap, the CPU time is very small.

Comparison with the KRC results obtained on their randomly generated instances

Finally, we apply our method on random instances, generated by Karisch et al. [30]. The graphs are unweighted random graphs with uniform edge probability $\frac{1}{2}$. Instances have a number of nodes varying from 36 to 84, and the p values are $\lfloor \frac{n}{2} \rfloor$, $\lfloor \frac{3n}{4} \rfloor$, $\lfloor \frac{7n}{12} \rfloor$ and $\lfloor \frac{13n}{24} + \frac{1}{2} \rfloor$. Table 4 presents the results.

As Karisch et al. noted, randomly generated instances of this type constitute the most difficult classes. All instances are solved to optimality. By 'QCR+PLEX', the solution time for the different p values are very small for $n = 36$ (less than 1") and $n = 60$ (less than 11.39"). For $n = 84$, several minutes and even hours are required (between 12' and 2h17'). Note that, for all instances, the gap is rather small.

Now, if we compare our results with the ones of KRC, our method is not always better. For instance, when $n = 84$ and $p = \lfloor \frac{7n}{12} \rfloor$, the optimal value is found 3.7 times faster with their approach than with the QCR one. But we can say that Karisch et al. apply a specific method to the graph bisection problem whereas QCR is a very general approach which can be applied to many combinatorial optimization problems.

3.3. Computational results for the task allocation problem

Let $P = \{P_1, \ldots, P_n\}$ be a set of nonidentical processors of a distributed system and $T = \{T_1, \ldots, T_m\}$ be a set of tasks that must be run over this distributed system. Some of these tasks have to communicate.

The task allocation problem can be formulated as the following linearly constrained 0–1 quadratic optimization problem (TA):

$$(TA) : \text{Min} \left\{ l(x) = \sum_{i=1}^{m} \sum_{k=1}^{n} e_{ik} x_{ik} + \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} \sum_{k=1}^{n} \sum_{\ell=1}^{n} c_{ikjl} x_{ik} x_{jl} : \right.$$
$$\left. \sum_{k=1}^{n} x_{ik} = 1 \ (i = 1, \ldots, m), x \in \{0, 1\}^{m \times n} \right\}$$

where the real coefficient e_{ik} represents the execution cost of task T_i when it is assigned to processor P_k and the real coefficient c_{ikjl} represents the communication cost between two tasks T_i and T_j (respectively assigned to processors P_k and P_ℓ). The binary variable x_{ik} is equal to 1 if and only if task T_i is assigned to processor P_k.

According to the general method presented in Section 2, the reformulation of (TA) is:

$$(TA_{\alpha,u}) : \ \text{Min} \left\{ l_{\alpha,u}(x) : \sum_{k=1}^{n} x_{ik} = 1, \ (i = 1, \ldots, m), x \in \{0, 1\}^{m \times n} \right\}$$

with:

$$l_{\alpha,u}(x) = l(x) + \sum_{i=1}^{m} \sum_{k=1}^{n} u_{ik} \left(x_{ik}^2 - x_{ik} \right) + \sum_{i=1}^{m} \left(\sum_{j=1}^{m} \sum_{l=1}^{n} \alpha_{ijl} x_{jl} \right) \left(\sum_{k=1}^{n} x_{ik} - 1 \right).$$

Optimal parameters α^* and u^* are computed by the SDP relaxation associated to (TA) that we call $(SDTA)$ in the following. For comparison of 'CPLEX' and 'QCR+CPLEX', we consider randomly generated instances: we choose the parameters m and n who define the problem dimension and then the coefficients e_{ik} and c_{ikjl} are randomly selected from an interval $[-50, 50]$. These instances have been already used in [6] and can be obtained from http://cedric.cnam.fr/oc/TAP/TAP.html.

Table 5 presents results for all instances that we have considered: 3 values of n (3, 4, 5) and 4 values of m (10, 15, 18, 20). For each pair (m, n), average values (over 10 instances) of computation time and gap are reported.

Legend of Table 5:

- CPU, average value of the total CPU time required by CPLEX to solve (TA) or required by SB and CPLEX to solve $(SDTA)$ and (TA_{α^*, u^*}) respectively. Note that a number i in brackets corresponds to the number of instances out of 10 solved within 1h. In this case, the corresponding CPU time is the average of these i instances.

For all instances, QCR drastically improves the default preprocessing of CPLEX. More complete comparisons are presented in [17]. In this reference, our 'QCR+CPLEX' method is compared with a sophisticated linear programming based method. For the $m = 20$ and $n = 5$ instances, it is observed that the average gap (resp. CPU time) of the linear programming based method is 84% (resp. 36'46") versus 34% (resp. 9'59").

Table 5
Average results for 70 randomly generated instances of the task allocation problem

m	n	QCR+CPLEX		CPLEX	
		CPU	gap (%)	CPU	gap (%)
15	5	21"	30	4'16"	63
18	4	27"	22	4'34"	60
20	4	35"	24	21'4"	62
20	5	9'59"	34	–	67
25	4	9'14"	24	–	59
25	5	48'27"(1)	35	–	67
25	6	–	46	–	76

None of the ten corresponding instances could be solved within 1 h (i): i instances out of 10 were solved within 1 h.

4. Conclusion

In this paper, we have considered the problem (QP) of minimizing a quadratic 0-1 function $g(x)$ subject to linear equality constraints $\sum_{j=1}^{n} a_{kj} x_j = b_k \ \forall k = 1, \ldots, m$. We have proposed a reformulation of this problem into an equivalent 0–1 program with a convex quadratic objective function $g_{\alpha,u}(x)$ depending on two parameters α and u and obtained by adding to $g(x)$ the two following functions, null on the feasible solution set, $g_1(x) = \sum_{i=1}^{n} u_i (x_i^2 - x_i)$ and $g_2(x) = \sum_{k=1}^{m} (\sum_{i=1}^{n} \alpha_{ki} x_i)(\sum_{j=1}^{n} a_{kj} x_j - b_k)$. The n-vector u and the $m \times n$-matrix α are determined by semidefinite programming in order to make $g_{\alpha,u}(x)$ convex and to maximize its minimum value over the relaxed domain $\overline{X}$. This reformulation, that we call QCR (Quadratic Convex Reformulation), can be viewed as a preprocessing of (QP) in order to solve it by a general-purpose (MIQP) solver. We applied QCR to three difficult combinatorial optimization problems: the densest k-subgraph, the graph bisection and a task allocation problem. For all the considered instances of these problems, QCR largely outperforms the method consisting to directly submit the quadratic 0-1 problem to CPLEX.

Moreover, for the densest k-subgraph problem, QCR also outperforms the methods proposed in the literature (specific algorithms or linearizations). For the graph bisection problem, QCR is competitive with the best method – to our knowledge – proposed in the literature: the one of Karisch, Rendl and Clausen (KRC) that is a specific branch-and-bound algorithm based on semidefinite programming and polyhedral relaxations.

Finally, QCR is a general approach which can be applied to a lot of combinatorial optimization problems. We are currently trying to extend QCR to quadratic 0-1 programs involving linear inequality constraints.

Acknowledgment

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