EXPEDIS: An Exact Penalty Method over Discrete Sets

Nicolò Gusmeroli∗† Angelika Wiegele∗

January 5, 2021

Abstract

We address the problem of minimizing a quadratic function subject to linear constraints over binary variables. We introduce the exact solution method called EXPEDIS where the constrained problem is transformed into a max-cut instance, and then the whole machinery available for max-cut can be used to solve the transformed problem. We derive the theory in order to find a transformation in the spirit of an exact penalty method; however, we are only interested in exactness over the set of binary variables. In order to compute the maximum cut we use the solver BiqMac. Numerical results show that this algorithm can be successfully applied on various classes of problems.

1 Introduction

We address the problem of solving linearly constrained binary quadratic problems of the following form:

\[
\hat{f}^* = \min \left\{ \hat{f}(y) = y^T \hat{F} y + \hat{c}^T y \mid \hat{A} y = \hat{b}, \ y \in \{0,1\}^n \right\}, \tag{BQP_01}
\]

where \( \hat{F} \in \mathbb{R}^{n \times n} \) is a symmetric matrix, \( \hat{c} \in \mathbb{R}^n \), and the linear equations are given via \( \hat{A} \in \mathbb{Z}^{m \times n} \) and \( \hat{b} \in \mathbb{Z}^m \).

Problem (BQP_01) encompasses 0/1 linear programming problems and unconstrained quadratic 0/1 problems, which are both known to be classes of NP-hard problems. Several well-known NP-hard problems from combinatorial optimization, like max-cut, stable set, graph partitioning, graph coloring, routing problems, knapsack problems etc. are explicit instances of these two classes, see, e.g., [10, 23, 28] for definitions and proofs.

All these problems have a wide range of applications and there is big interest in solution methods for (BQP_01) also outside the mathematical optimization area. Data science (clustering analysis), logistics (quadratic assignment problem, vehicle routing problem), telecommunications (several versions of frequency assignment problem), finance (portfolio optimization problem), etc. are some of the areas where solving the underlying linear or quadratic 0/1 problems is essential, see, e.g., the survey papers [11, 16].

∗Alpen-Adria-Universität Klagenfurt, Universitätsstraße 65-67, 9020 Klagenfurt, Austria.
Emails: {nicolo.gusmeroli,angelika.wiegele}@aau.at
†Part of this work has been done while the first author was employed at TU Dortmund.
Solving Problem (BQP) to optimality is always highly appreciated. Even when good solutions based on appropriate (meta)heuristics are acceptable for practical needs, the developers of such algorithms still need to evaluate them and this can be done only if optimal solutions on problems of (at least) medium size are available.

Global optimization solvers that can handle problems of this type are typically branch-and-bound algorithms. One can group them according to the different types of relaxations used in order to obtain lower bounds. Among them are relaxations based on reformulation-linearization techniques (RLT) but also relaxations based on semidefinite programming (SDP) have been successfully implemented.

In this paper we follow the idea introduced by J. B. Lasserre in . We will reformulate Problem (BQP) as a max-cut problem, which we then solve using the solver BiqMac developed by Rendl, Rinaldi and Wiegele . The crucial part is to find a penalty parameter used in the transformation large enough to get equality of the two problems but at the same time to be kept small in order to not run into numerical difficulties.

The max-cut problem is a well-studied combinatorial optimization problem. Hence, the whole machinery developed for max-cut can be used in order to solve the underlying problem. Transformation to max-cut is also beneficial since quantum annealers like D-Wave systems ask for max-cut problems as input type.

We introduce algorithm EXPEDIS that computes a penalty parameter and solves the transformed problem using the solver BiqMac. We derive the theory on what is necessary to get such a transformation to a max-cut instance. In particular, we state conditions on a minimal penalty parameter. Several variants of how the parameter can be computed as well as refinements with respect to infeasibility or known feasible solutions are presented. Numerical results demonstrate that this procedure works well on randomly generated instances as well as on several classes of instances from the literature, like the max k-cluster problem.

The remainder of this paper is structured as follows: in Section 2 we briefly describe a well-known procedure to derive relaxations based on semidefinite programming (SDP) and we give a formulation of the max-cut problem together with a short explanation of the exact solution method BiqMac; in Section 3 we begin the heart of this paper – we describe Algorithm EXPEDIS, an exact penalty method over discrete sets; in Section 4 we show that EXPEDIS is a generalization of the method introduced by Lasserre ; Section 5 states the necessary conditions on how to choose the parameters used in EXPEDIS while in Section 6 we give recipes on computing them; in Section 7 refinements of the algorithm are discussed before we present our numerical results in Section 8; Section 9 concludes this paper giving a summary and an outlook on future research.

**Notation** We denote by $e$ the vector of all ones, by $J$ the matrix of all ones, and by $e_j$ the unit vector with value 1 in the $j$-th component and 0 everywhere else. The 0-vector and the 0-matrix is denoted by $0$. Given a matrix $A$, $A_i,.$ is row $i$ of $A$ and $A_.,j$ is column $j$ of $A$. Matrix $A \in \mathbb{R}^{n \times n}$ is positive semidefinite, denoted $A \succeq 0$, if $x^\top Ax \geq 0$ for every $x \in \mathbb{R}^n$ and for $A, B \in \mathbb{R}^{n \times n}$, we define the inner product $\langle A, B \rangle = \text{tr} (B^\top A) = \sum_i \sum_j A_{ij}B_{ij}$. The vector holding the diagonal elements of a matrix $X \in \mathbb{R}^{n \times n}$ is denoted by $\text{diag}(X)_i$, i.e., $\text{diag}(X)_i = X_{ii}$, and given a vector $x \in \mathbb{R}^n$, by $\text{Diag}(x)$ we denote the $n \times n$ diagonal matrix

\[\text{Diag}(x) = \begin{bmatrix} x_1 & & \\ & \ddots & \\ & & x_n \end{bmatrix}\]
2 Preliminaries

2.1 Solving Max-Cut Problems

The max-cut problem is among the most studied combinatorial optimization problems. It has connections to various fields of discrete mathematics and has a wide range of applications. Max-cut is an NP-hard problem, but several approximation algorithms as well as exact methods using some kind of branch-and-bound type methods exist, see, e.g., [25] for more details and references. As several other combinatorial optimization problems, max-cut problems are easy to state. Let be given an undirected graph \( G = (V, E) \), having vertex set \( V \) and edge set \( E \) with weights \( w_e \in \mathbb{R} \) on the edges \( e \in E \). The max-cut problem asks to partition the vertex set into two parts \( (S, V \setminus S) \) in a way such that the sum of the weights on the edges having exactly one endpoint in \( S \) is maximized, i.e., we look for a subset of the edges

\[
\delta(S) = \{ e = uv \in E \mid u \in S, v \notin S \}
\]

where \( S \subseteq V \), such that \( \sum_{e \in \delta(S)} w_e \) is maximized. Let \( A = (a_{ij}) \) be the adjacency matrix of the graph, i.e., \( a_{ij} = w_e \) for \( e = \{i, j\} \). The Laplace matrix of the graph associated with \( A \) is given as

\[
L = \text{Diag}(Ae) - A
\]

and defines \( C = \frac{1}{4}L \). Then we can find the maximum cut by solving the binary quadratic problem

\[
\max \{ x^T C x \mid x \in \{-1, 1\}^{\left| V \right|} \}.
\]

(1)

Among the most efficient solvers for computing the maximum cut in a (medium-sized) graph is BiqMac [25]. BiqMac uses semidefinite relaxations in order to generate high quality upper bounds on the maximum cut. In particular, the approximate solution of the semidefinite relaxation

\[
\max \{ \langle C, X \rangle \mid X \succ 0, \ \text{diag}(X) = e, \ X \in \text{MET} \}
\]

(2)

serves as an upper bound in a branch-and-bound scheme (see Section 2.2).

In order to derive a lower bound (finding a cut in the graph with a large value), the Goemans-Williamson hyperplane rounding technique [13] is applied to the matrix obtained by solving the SDP (2). All details about the BiqMac algorithm can be found in [25].

2.2 Semidefinite Relaxations of Binary Problems

There is a well-known procedure on how to derive semidefinite relaxations for the \( \pm 1 \) version of problem (BQPO1). (See Problem (BQP) in Section 3 for an explicit formulation in the \( \pm 1 \) setting.) The following equivalence is easy to prove.

\[
\{ xx^T : x \in \{-1, 1\}^n \} = \{ X \in S_n \mid X \succ 0, \ \text{diag}(X) = e, \ \text{rk}(X) = 1 \}
\]

(3)
Thus, problem (BQP) has an equivalent formulation as
\[
f^* = \min \left\{ \langle F, X \rangle + c^T x + \alpha \mid Ax = b, \begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \succeq 0, \ \text{diag}(X) = e, \ \text{rk}(X) = 1 \right\}.
\]
In this formulation, all non-convexity (from the objective function as well as from the binary conditions) is hidden in the rank-1 constraint. Hence, it is straightforward to derive a semidefinite relaxation by dropping the rank-condition,
\[
\min \left\{ \langle F, X \rangle + c^T x + \alpha \mid Ax = b, \begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \succeq 0, \ \text{diag}(X) = e \right\}.
\] (4)
In the absence of linear constraints, this is the Shor relaxation [27]. It can be solved in polynomial time using, e.g., interior point methods. For a more detailed study about semidefinite programming, we refer the reader to the handbooks [1, 29] and the references therein.

**Adding cutting planes.** Relaxation (4) can be tightened by adding polyhedral cuts. In particular, clique inequalities [20] turn out to strengthen relaxation (4) significantly.

Consider the vector \(b\) with entries from the set \([-1, 0, 1]^n\) and an odd number of nonzero entries. Then
\[
\min \left\{ (b^T x)^2 \mid x \in \{-1, 1\}^n \right\} = 1,
\]
hence the inequality \(b^T X b \geq 1\) is valid for Problem (BQP) and can be used to tighten relaxation (4).

When the vector \(b\) consists of three nonzero entries, the arising clique inequalities are the so called triangle inequalities, i.e., the set of constraints
\[
\begin{align*}
    x_{ij} + x_{ik} + x_{jk} &\geq -1 \\
    x_{ij} - x_{ik} - x_{jk} &\geq -1 \\
    -x_{ij} + x_{ik} - x_{jk} &\geq -1 \\
    -x_{ij} - x_{ik} + x_{jk} &\geq -1
\end{align*}
\]
for all \(1 \leq i < j < k \leq n\). The polytope containing all \(X\) that satisfy these triangle inequalities is called the metric polytope and is denoted by MET. Adding these constraints tightens the SDP relaxation significantly. However, solving this strengthened SDP comes with a serious computational effort. In [9, 25] a method to deal with such an SDP with a huge number of linear constraints has been developed. A (dynamic version) of a bundle method is used in order to obtain an approximate solution, giving a safe upper bound on the maximum cut of the graph.

In case all triangle inequalities are satisfied, we can achieve a further strengthening by considering vectors \(b\) with five nonzero entries, leading to 5-clique inequalities. Differently from the triangle inequalities, the 5-clique inequalities are too many to be enumerated hence we use a heuristic to separate them.

In this separation algorithm we create a set of random permutations of five elements. Then we run a minimization problem over this permutation for a finite number of swaps. The swaps are accepted if the solution improves, and they are accepted with a certain probability if the solution does not improve. This procedure creates a set of 5-clique inequalities with a potentially high violation. From this set, we add the most violated 5-clique inequalities to the relaxation.
3 Exact Penalty Method over Discrete Sets

Given a symmetric matrix \( \hat{F} \in \mathbb{R}^{n \times n} \) and a vector \( \hat{c} \in \mathbb{R}^n \), we define the objective function \( \hat{f}(y) = y^\top \hat{F} y + \hat{c}^\top y \). Moreover, we consider the linear equations \( \hat{A} y = \hat{b} \), where \( \hat{A} \in \mathbb{Z}^{m \times n} \) and \( \hat{b} \in \mathbb{Z}^m \). We want to find

\[
f^* = \min \{ \hat{f}(y) \mid \hat{A} y = \hat{b}, \ y \in \{0, 1\}^n \},
\]

i.e., we want to solve a linearly constrained binary quadratic problem.

We can reformulate problem (BQP_{01}) to an equivalent formulation with variables in \( \{-1, 1\} \). Consider the change of variables \( x = 2y - e \), and let \( A = \frac{1}{2} \hat{A}, \ b = \hat{b} - \frac{1}{2} \hat{A} e, \ c = \frac{1}{2} (\hat{c} + \hat{F} e) \) and \( F = \frac{1}{4} \hat{F} \) be the new parameters. Then

\[
f^* = \min \{ f(x) \mid Ax = b, \ x \in \{-1, 1\}^n \}
\]

where \( f(x) = x^\top F x + c^\top x + \alpha \) and \( \alpha = \frac{1}{2} \hat{c}^\top e + \frac{1}{4} e^\top \hat{F} e \). In case problem (BQP) is infeasible, we have \( f^* = +\infty \).

**Remark 1.** Note that since \( \hat{A} \) and \( \hat{b} \) are integer valued, for \( y \in \{0, 1\}^n \) the value of \( \hat{A} y - \hat{b} \) is an integer as well. The transformation ensures \( \hat{A} y - \hat{b} = Ax - b \). Therefore, for \( x \in \{-1, 1\}^n \), the value of \( Ax - b \) must also be integral, even though the values in \( A \) and \( b \) might be fractional.

In order to simplify notation, we denote by \( \Delta \) the set of feasible points of Problem (BQP), and by \( \Delta^c \) we denote the set of infeasible \( \{-1, 1\}^n \) vectors, i.e.,

\[
\Delta = \{ x \in \{-1, 1\}^n \mid Ax = b \}
\]

\[
\Delta^c = \{ x \in \{-1, 1\}^n \mid Ax \neq b \}.
\]

We now introduce a penalty parameter \( \sigma > 0 \) and add a quadratic penalty function to \( f(x) \), thus we have the function

\[
h(x) = f(x) + \sigma \| Ax - b \|^2
\]

and we consider the unconstrained binary quadratic problem

\[
h^* = \min \{ h(x) \mid x \in \{-1, 1\}^n \}.
\]

(UBQP)

Expanding terms, we can rewrite the objective function of Problem (UBQP)

\[
h(x) = f(x) + \sigma \| Ax - b \|^2 = \\
x^\top F x + c^\top x + \alpha + \sigma (Ax - b)^\top (Ax - b) = \\
x^\top (F + \sigma A^\top A) x + (c - 2\sigma A^\top b)^\top x + (\alpha + \sigma b^\top b) = \\
= \bar{x}^\top Q \bar{x}
\]

where \( \bar{x} = \begin{bmatrix} 1 \\ x \end{bmatrix} \) and

\[
Q = \begin{bmatrix} \alpha + \sigma b^\top b & (c - 2\sigma A^\top b)^\top / 2 \\ (c - 2\sigma A^\top b)/2 & F + \sigma A^\top A \end{bmatrix}.
\]
In this way we can restate Problem (UBQP) as

\[ h^* = \min \{ \bar{x}^\top Q \bar{x} \mid \bar{x} \in \{-1, 1\}^{n+1}, \bar{x}_0 = 1 \} \quad \text{(MC)} \]

which is a max-cut problem on a graph with \( n + 1 \) vertices. To see this, we define \( C = \text{Diag}(Qe) - Q \), which gives

\[
\begin{align*}
    h^* &= \min \{ \bar{x}^\top Q \bar{x} \mid \bar{x} \in \{-1, 1\}^{n+1} \} \\
    &= -\max \{ \bar{x}^\top (Q) \bar{x} \mid \bar{x} \in \{-1, 1\}^{n+1} \} \\
    &= e^\top Q e - \max \{ \bar{x}^\top C \bar{x} \mid \bar{x} \in \{-1, 1\}^{n+1} \}
\end{align*}
\]

where \( C = \frac{1}{4} L \) and \( L \) is the Laplace matrix of a graph with vertex set \( \{0, 1, \ldots, n\} \) and adjacency matrix \( A \) with

\[
A_{ij} = \begin{cases} 
0 & \text{if } i = j \\
2c_j - 4\sigma (A_{i,j})^\top b & \text{if } i = 0 \text{ and } i \neq j \\
2c_i - 4\sigma (A_{i,i})^\top b & \text{if } j = 0 \text{ and } j \neq i \\
4F_{i,j} + 4\sigma (A_{i,j})^\top A_{i,i} & \text{if } 1 \leq i, j \leq n \text{ and } i \neq j
\end{cases}
\]

We now state a theorem that allows us to obtain the solution to the constrained problem via an unconstrained one. This theorem is the key of the algorithm developed afterwards.

**Theorem 2.** Consider Problem (BQP) and Problem (UBQP) with optimal values \( f^* \) and \( h^* \), respectively. Furthermore, assume we have a threshold parameter \( \rho \) and a penalty parameter \( \sigma \), satisfying the following conditions:

(i) Problem (BQP) has no feasible solution with value bigger than the threshold \( \rho \);

(ii) given any vector \( x \in \Delta^c \), the value of the penalized function \( h(x) = f(x) + \sigma \|Ax - b\|^2 \) exceeds the threshold parameter \( \rho \).

Then, for \( f^* < +\infty \), \( f^* \) is the optimal value of Problem (UBQP), i.e., \( h^* = f^* \). Moreover Problem (BQP) has no feasible solution if and only if \( h^* > \rho \).

**Proof.** From Remark 1 it follows that \( Ax - b = 0 \) for \( x \in \Delta \) and \( \|Ax - b\|^2 \in \mathbb{Z}^+ \) for \( x \in \Delta^c \). Combining this with the assumptions on the parameters \( \rho \) and \( \sigma \) we have

\[
h(x) = \begin{cases} 
f(x) + 0 \leq \rho & \text{for } x \in \Delta \\
f(x) + \sigma \|Ax - b\|^2 > \rho & \text{for } x \in \Delta^c
\end{cases}
\]

We know that \( h^* \) is the minimum of Problem (UBQP), hence we have \( h^* > \rho \) if and only if \( \Delta = \emptyset \), meaning that Problem (BQP) is infeasible. On the other hand, if \( \Delta \neq \emptyset \), then the minimizer of Problem (UBQP) must lie in the set \( \Delta \) and it follows that \( h^* = \min \{h(x) \mid x \in \Delta\} = \min \{f(x) + 0 \mid x \in \Delta\} = f^* \).

Figure 1 illustrates the role of the parameters \( \rho \) and \( \sigma \); if \( x \in \Delta \) we have \( h(x) = f(x) \leq \rho \). On the other hand, if \( x \in \Delta^c \), adding the penalty term to \( f(x) \) yields \( h(x) = f(x) + \sigma \|Ax - b\|^2 > \rho \).
\[ h(x) = f(x) + \sigma \| Ax - b \|^2 > \rho \]

\[ h(\hat{x}) = f(\hat{x}) \leq \rho \]

\[ h(x) \text{ for } x \in \Delta \]

\[ h(x) \text{ for } x \in \Delta^c \]

Figure 1: The values of \( h(x) \) for \( x \in \Delta \) and \( x \in \Delta^c \) are separated by \( \rho \).

---

**Algorithm 1**: Scheme of an exact penalty method over discrete sets

1. **Algorithm**: EXPEDIS

   **Data**: \( \hat{F} \in \mathbb{R}^{n \times n}, \hat{c} \in \mathbb{R}^n, \hat{A} \in \mathbb{Z}^{m \times n}, \hat{b} \in \mathbb{Z}^m \) defining problem
   \[ \min \{ y^\top \hat{F} y + \hat{c}^\top y \mid \hat{A} y = \hat{b}, \, y \in \{0, 1\}^n \} \]

   **Result**: optimal solution or certificate of infeasibility

2. transform to problem \( \min \{ x^\top F x + c^\top x + \alpha \mid Ax = b, \, x \in \{-1, 1\}^n \} \);

3. compute a **threshold parameter** \( \rho \);

4. compute a **penalty parameter** \( \sigma \);

5. set up the **max-cut** problem as given in (MC);

6. solve the max-cut problem giving optimal value \( h^* \);

7. **if** \( h^* > \rho \) **then**

8. problem infeasible;

9. **else**

10. transform the optimal cut to the optimal solution of the 0/1 problem;

11. **end**
Having such a pair of parameters at hand, Theorem 2 allows us to formulate an exact penalty method over discrete sets which we call EXPEDIS and outline in Algorithm 1.

Algorithm EXPEDIS reformulates a constrained binary quadratic problem into a max-cut instance. The solution of the max-cut problem either gives a certificate for infeasibility of the original problem or provides the optimal solution. Taking a closer look at the computations in EXPEDIS, all steps beside Steps 3, 4, and 6 are straightforward and computationally cheap.

To perform Step 6, which is solving the max-cut problem, we will use the solver BiqMac (see Section 2.1).

The description on how to perform Steps 3 and 4 is given in Section 6, after we develop in Section 5 the necessary conditions on choosing $\rho$ and $\sigma$.

4 Relation to the Work of Lasserre

Lasserre [19] showed that solving problem \( \text{BQP}_01 \) is equivalent to minimizing a quadratic form in \( n + 1 \) variables on the hypercube \( \{-1, 1\}^{n+1} \). In this section we show that this work of Lasserre falls into our concept of an exact penalty method over discrete sets. In fact, we will show that the choice of the parameters $\rho_{\text{Las}}$ and $\sigma_{\text{Las}}$ in [19] satisfies the assumptions of Theorem 2.

The parameters $\rho_{\text{Las}}$ and $\sigma_{\text{Las}}$ in [19] are defined using the minimum and the maximum of the standard SDP relaxation (ignoring the linear constraints $Ax = b$), i.e.,

\[
\hat{\ell} = \min \left\{ \langle F, X \rangle + c^\top x + \alpha \mid \begin{bmatrix} 1 & x^\top \\ x & X \end{bmatrix} \succ 0, \ \text{diag}(X) = e \right\}, \quad (9a)
\]

\[
\hat{u} = \max \left\{ \langle F, X \rangle + c^\top x + \alpha \mid \begin{bmatrix} 1 & x^\top \\ x & X \end{bmatrix} \succ 0, \ \text{diag}(X) = e \right\}. \quad (9b)
\]

The threshold and the penalty parameter are defined as $\rho_{\text{Las}} = \max \{|\hat{\ell}|, |\hat{u}|\}$ and $\sigma_{\text{Las}} = 2 \cdot \max \{|\hat{\ell}|, |\hat{u}|\} + 1$, respectively.

**Lemma 3.** The parameters $\rho_{\text{Las}}$ and $\sigma_{\text{Las}}$ satisfy the assumptions of Theorem 2.

**Proof.** Since Problem \( (9b) \) is a relaxation of $\max \{f(x) \mid x \in \Delta\}$, it is easy to see that

$\rho_{\text{Las}} = \max \{|\hat{\ell}|, |\hat{u}|\} \geq |\hat{u}| \geq \hat{u} \geq \max \{f(x) \mid x \in \Delta\}$.

Hence, every feasible solution of Problem \( \text{BQP} \) is bounded by $\rho_{\text{Las}}$, which is assumption (i) of Theorem 2.

Assume now $x \in \Delta^c$, then the penalty added is at least $\sigma_{\text{Las}}$ because, by Remark 1 $\|Ax - b\|^2 \in \mathbb{Z}^+$. Therefore, and by the definition of $\hat{\ell}$, it follows that

$\hat{h}(x) \geq \hat{\ell} + \sigma_{\text{Las}} = \hat{\ell} + 2 \cdot \max \{|\hat{\ell}|, |\hat{u}|\} + 1 \geq \max \{|\hat{\ell}|, |\hat{u}|\} + 1 > \rho_{\text{Las}}$

and thus the parameters $\rho_{\text{Las}}$ and $\sigma_{\text{Las}}$ satisfy also assumption (ii) of Theorem 2.

Figure 2 depicts the proof of Lemma 3: if $x \in \Delta$, then $\|Ax - b\|^2 = 0$, thus $\hat{h}(x) = f(x) \leq \rho_{\text{Las}}$; for $x \in \Delta^c$ the penalty added is at least $\sigma_{\text{Las}}$, thus $\hat{h}(x) \geq \hat{\ell} + \sigma_{\text{Las}} > \rho_{\text{Las}}$.

Combining the above lemma and Theorem 2 we can now restate [19, Theorem 2.2] as...
Corollary 4. Consider Problem (BQP) and Problem (UBQP) with optimal values $f^*$ and $h^*$, respectively, the threshold parameter $\rho_{\text{Las}} = \max\{|\ell|, |\hat{\ell}|\}$ and the penalty parameter $\sigma_{\text{Las}} = 2 \cdot \max\{|\ell|, |\hat{\ell}|\} + 1$.

If $f^* < +\infty$, then it follows $h^* = f^*$. Moreover (BQP) has no feasible solutions if and only if $h^* > \rho_{\text{Las}}$.

Summarizing, by solving two semidefinite programs with variables $X \in S_n$ and $x \in \mathbb{R}^n$, we can define a threshold and a penalty parameter satisfying the assumptions in Theorem 2 and thus apply Algorithm EXPEDIS.

5 Conditions on the Threshold and the Penalty Parameter

In Section 4 we proved that the parameters chosen in [19] are a particular choice for $\rho$ and $\sigma$ in our algorithm EXPEDIS. In this section we investigate necessary conditions on the parameters to satisfy the assumptions of Theorem 2 in order to give a wider choice on computing $\rho$ and $\sigma$. Large penalty parameters can lead to huge numbers in the Laplacian of the graph which in turn can have negative effects on the computational time for finding the maximum cut. Hence, we aim in finding small parameters $\rho$ and $\sigma$, still large enough to satisfy the assumptions of Theorem 2. To this end, we define

\begin{align}
\ell^* &= \min \{f(x) \mid x \in \Delta^c\}, \\
u^* &= \max \{f(x) \mid x \in \Delta\}.
\end{align}

Observation 5. If $u^* < \ell^*$, then $f(\hat{x}) < f(\bar{x})$ for any $\hat{x} \in \Delta$ and any $\bar{x} \in \Delta^c$. Hence, any minimizer over $\{-1, 1\}^n$ will satisfy $Ax = b$, i.e., $f^* = \min \{f(x) \mid x \in \{-1, 1\}^n\}$ and we can simply ignore all the equality constraints because minimization forces $Ax = b$ to hold.

Due to this observation, from now on we assume $\ell^* < u^*$ throughout this paper.

Lemma 6. The parameters $\rho^* = u^*$ and $\sigma^* = u^* - \ell^* + \epsilon$ satisfy the assumptions of Theorem 2.

Proof. To satisfy assumption (i) in Theorem 2, the threshold parameter $\rho$ must be an upper bound on the feasible values of Problem (BQP). Hence it follows $\rho \geq u^*$. Since there are no
other constraints on ρ, the smallest value of a threshold parameter satisfying the assumption of Theorem \ref{thm:penalized} is \( u^* \). Thus we set \( \sigma^* = u^* \).

To satisfy assumption \( \text{(ii)} \) in Theorem \ref{thm:penalized} we have to show that \( h(x) > \rho^* \) for all \( x \in \Delta^c \). Let \( x \in \Delta^c \), thus \( \|Ax - b\|^2 \) is a nonnegative integer (see Remark \ref{remark:integer}) and the penalization added is at least \( \sigma \), hence \( h(x) \geq \ell^* + \sigma \). By setting \( \sigma^* = u^* - \ell^* + \epsilon \) it follows

\[
h(x) \geq \ell^* + u^* - \ell^* + \epsilon = \rho^* + \epsilon > \rho^*.
\]

Thus assumption \( \text{(ii)} \) is satisfied.

The value \( \sigma^* \) cannot be further decreased, i.e., it is the smallest possible formulation of the penalty parameter in order to have the assumptions of Theorem \ref{thm:penalized} satisfied.

**Proposition 7.** Let \( \ell^* \) and \( u^* \) be the bounds defined in \( \text{(10)} \) and assume the penalty parameter to be \( \hat{\sigma} = u^* - \ell^* \). Then there exist binary quadratic problems for which (UBQP) is minimized by some vector \( x \in \Delta^c \), while \( \Delta \) is nonempty.

**Proof.** Let the parameters be \( \hat{A} = 1, \hat{b} = 1, \hat{c} = 2 \) and \( \hat{F} = 0 \), i.e., the problem is one-dimensional. The transformed parameters are \( A = 0.5, b = 0.5, c = 1 \) and \( F = 0 \), while the additive constant is \( \alpha = 1 \). Let \( x = 1 \) be the (unique) optimal solution and \( y = -1 \) be a (the unique) point in \( \Delta^c \). It follows \( f(x) = 2 \) and \( f(y) = 0 \). It is easy to see that \( \ell^* = \min \{ f(x) \mid x \in \Delta^c \} = 0 \) and \( u^* = \max \{ f(x) \mid x \in \Delta \} = 2 \). Assuming \( \hat{\sigma} = u^* - \ell^* = 2 \), it follows that \( h(x) = f(x) + 0 = 2 \) and \( h(y) = f(y) + \hat{\sigma} \|Ax - b\|^2 = 2 \). Thus Problem (BQP) is feasible but the penalized problem is minimized by a vector in the set \( \Delta^c \).

Clearly, finding \( u^* \) is as hard as solving Problem (BQP) and computing \( \ell^* \) is also out of reach. But any bounds \( \ell \leq \ell^* \) and \( u \geq u^* \) also give rise to a pair of parameters \( \rho \) and \( \sigma \) that ensures our desired assumptions to hold.

**Proposition 8.** Let \( \ell \) and \( u \) be a lower and an upper bound, respectively, such that \( \ell \leq \ell^* \) and \( u \geq u^* \). Moreover, the parameters and the penalized function are defined similar as above, i.e., \( \rho = u, \sigma = u - \ell + \epsilon \). Then the parameters satisfy the assumptions of Theorem \ref{thm:penalized}.

**Proof.** Since \( u \geq u^* \), we have that \( \rho = u \) clearly ensures assumption \( \text{(i)} \) to hold. And since \( \ell \leq \ell^* \), the second assumption also holds, by using the same arguments as in the proof of Lemma \ref{lemma:penalized} for \( \sigma = u - \ell + \epsilon \).

### 5.1 Comparison to the Parameters of Lasserre

We now compare the choices of the parameters \( \rho \) and \( \sigma \) given in Lemma \ref{lemma:lasserre} and Lemma \ref{lemma:penalized}. Note that the values of the parameters \( \rho \) and \( \sigma \) are obtained through some bounds \( \ell \) and \( u \). In \cite{lasserre2011}, \( \ell \) and \( u \) as defined in \( \text{(9)} \) are used. However, Proposition \ref{prop:comparison} shows that any \( \ell \leq \ell^* \) and any \( u \geq u^* \) give rise to valid parameters \( \rho \) and \( \sigma \). In order to compare the two different formulations of \( \rho \) and \( \sigma \), we fix a pair \( (\ell, u) \). The following proposition shows that our choice of parameters is always less (or equal) to the ones proposed by Lasserre \cite{lasserre2011}.
Proposition 9. Let \( \ell \) and \( u \) be any pair of lower and upper bounds such that \( \ell \leq \ell^* \) and \( u \geq u^* \). We denote the Lasserre and our new formulations of the parameters as follows.

\[
\begin{align*}
\rho_{\text{Las}} &= \max\{|\ell|, |u|\} & \sigma_{\text{Las}} &= 2 \cdot \max\{|\ell|, |u|\} + 1 \\
\rho_{\text{GW}} &= u & \sigma_{\text{GW}} &= u - \ell + \epsilon
\end{align*}
\]

Then \( \rho_{\text{GW}} \leq \rho_{\text{Las}} \) and \( \sigma_{\text{GW}} < \sigma_{\text{Las}} \).

Proof. The first inequality holds since \( \rho_{\text{GW}} = u \leq |u| \leq \max\{|\ell|, |u|\} = \rho_{\text{Las}} \).

And the following arguments prove the second inequality: \( \sigma_{\text{GW}} = u - \ell + \epsilon < |u - \ell| + 1 \leq |u| + |\ell| + 1 \leq 2 \cdot \max\{|u|, |\ell|\} + 1 = \sigma_{\text{Las}} \).

6 Choosing \( \ell \) and \( u \) efficiently

In Section 5 we give a recipe for computing a pair of parameters \( \rho \) and \( \sigma \) that satisfies the assumptions of Theorem 2 by using bounds on \( \ell^* = \min\\{f(x) \mid x \in \Delta^c\} \) and \( u^* = \max\\{f(x) \mid x \in \Delta\} \). The bounds \( \hat{\ell} \) and \( \hat{u} \), as introduced in Section 4, are candidates since clearly \( \hat{\ell} \leq \ell^* \) and \( \hat{u} \geq u^* \).

The time for solving the max-cut instance is influenced by the penalty parameter \( \sigma \). We aim in finding small values for \( \sigma \) (but sufficiently large to satisfy the assumptions in Theorem 2) in order to solve the max-cut problem in reasonable time. In this section we will present alternatives to compute tight bounds on \( \ell^* \) and \( u^* \).

6.1 Adding Cutting Planes

The bounds \( \hat{\ell} \) and \( \hat{u} \) defined in (9) are the solution of the standard SDP relaxation. These bounds can be strengthened by adding cutting planes. We denote the upper and lower bound computed by solving the standard SDP relaxation with the addition of triangle inequalities and, possibly, of a set of 5-clique inequalities (see Section 2.2) by \( \tilde{\ell} \) and \( \tilde{u} \), i.e.,

\[
\begin{align*}
\tilde{\ell} &= \min \left\{ \langle F, X \rangle + c^\top x + \alpha \mid \begin{bmatrix} \begin{array}{c} 1 \\ x \end{array} & X \end{bmatrix} \succeq 0, \ \diag(X) = e, \ X \in \text{MET} \cap X_I \right\}, \quad (11a) \\
\tilde{u} &= \max \left\{ \langle F, X \rangle + c^\top x + \alpha \mid \begin{bmatrix} \begin{array}{c} 1 \\ x \end{array} & X \end{bmatrix} \succeq 0, \ \diag(X) = e, \ X \in \text{MET} \cap X_I \right\}. \quad (11b)
\end{align*}
\]

where \( X_I \) is the set of 5-clique inequalities generated by the heuristic procedure described in Section 2.2.

6.2 Including the Constraints \( Ax = b \)

The optimizer leading to \( u^* \) is in the set \( \Delta \), therefore it satisfies the constraints \( Ax = b \). In order to take these constraints into account when computing a bound on \( u^* \), we follow an idea introduced by S. Burer in [6] and add the equality constraints to the standard SDP relaxation.
Proposition 10. Let $Y$ be the matrix $Y = \begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix}$ and suppose $Y \succ 0$. Moreover let $M$ be defined as $M = [b, -A]$. Then the following are equivalent:

(i) $Ax = b$ and $\text{diag}(AXA^\top) = b^2$

(ii) $MYM^\top = 0$

(iii) $MY = 0$

Proof. First we show $(i) \implies (ii)$. We have $[b_i, -A_i]Y[b_i, -A_i]^\top = b_i^2 - 2b_iA_iX + A_iXA_i^\top = b_i^2 - 2b_i^2 + b_i^2 = 0$. Considering all the rows of $Ax = b$ it follows that $\text{diag}(MYM^\top) = 0$. Since $Y \succ 0$, $MYM^\top \succ 0$. Thus $MYM^\top = 0$.

Next we prove $(ii) \implies (iii)$. Since $Y \succ 0$, let $Y = VV^\top$ be its Gram representation. Then, it follows $0 = \text{tr}(MYM^\top) = \text{tr}(MVV^\top M^\top) = \|MV\|^2$. Thus $MV = 0$. Hence $MY = (MV)V^\top = 0V^\top = 0$.

Now we show $(iii) \implies (i)$. Let us consider the first column of $MY$. It is the zero vector $0$, hence we have $0 = (MY)_{1,1} = [b, -A][1, x]^\top = b - Ax$, so $Ax = b$. Moreover $MY = 0$ implies $MYM^\top = 0$, hence $0 = (MYM^\top)_{ii} = [b_i, -A_i]Y[b_i, -A_i]^\top$. Expanding $Y$ we have $b_i^2 - 2b_iA_iX + A_iXA_i^\top$. Since we proved above $Ax = b$, we can rewrite $0 = b_i^2 - 2b_iA_iX + A_iXA_i^\top$ because $(AXA^\top)_{ii} = A_iXA_i^\topi$. Thus $\text{diag}(AXA^\top) = b_i^2$.

As a consequence of Proposition 10 we can compute the upper bound $u_\Delta$ by solving the SDP

$$u_\Delta = \max \left\{ \langle F, X \rangle + c^T x + \alpha \mid \begin{bmatrix} 1 & x^T \\ x & X \end{bmatrix} \succeq 0, \ \text{diag}(X) = e, \ MY = 0 \right\},$$

where $0$ is an $m \times (n + 1)$ matrix.

We now take a closer look on the inclusion of the equality constraints $MY = 0$. In fact, we can transform SDP (12) into a semidefinite program of smaller dimension and less constraints by projecting out the null space. We define the null space of $M$, denoted $\text{null}(M)$, as the set of vectors that are mapped to $0$, i.e., $\text{null}(M) = \{x \in \mathbb{R}^n \mid MX = 0\}$. We restate Lemma 1 as

Lemma 11. Let $M = [b, -A]$ and define the closed, convex cone $\mathcal{J} = \{Z \succ 0 \mid MZM^\top = 0\}$. Then $\mathcal{J} = \{NPN^\top \mid P \succ 0\}$ where $N$ is the matrix whose columns form an orthonormal basis of $\text{null}(M)$.

In order to simplify notation, we define the matrix $F' = \begin{bmatrix} \alpha & (c/2)^\top \\ c/2 & F \end{bmatrix}$ to obtain $\langle F, X \rangle + c^T x + \alpha = \langle F', Y \rangle$. Reformulating (12) using Lemma 11 we obtain

$$u_\Delta = \max \{\langle F', Y \rangle \mid Y \succeq 0, \ \text{diag}(Y) = e, \ MY = 0\}$$

$$= \max \{\langle F', NPN^\top \rangle \mid P \succ 0, \ \text{diag}(NPN^\top) = e\}$$

$$= \max \{\langle F', NPN^\top \rangle \mid P \succ 0, \ \langle e_je_j^\top, NPN^\top \rangle = 1, \ j \in \{1, \ldots, n + 1\}\}$$

$$= \max \{\langle N^\top F'N, P \rangle \mid P \succ 0, \ \langle N^\top e_j e_j^\top N, P \rangle = 1, \ j \in \{1, \ldots, n + 1\}\}$$

$$= \max \{\langle N^\top F'N, P \rangle \mid P \succ 0, \ \langle (N_{j,\cdot})^\top N_{j,\cdot}, P \rangle = 1, \ j \in \{1, \ldots, n + 1\}\}.$$
Thus, in order to compute \( u_\Delta \), we have to solve an SDP of size \( \dim(N) = n + 1 - \text{rk}(M) \) with \( n + 1 \) constraints.

**Observation 12.** In case the SDP for computing \( u_\Delta \) is infeasible, clearly Problem (BQP) is infeasible as well.

### 7 Refinements of the Algorithm

#### 7.1 Detecting (In)feasibility

The threshold parameter \( \rho \) has a key role in Algorithm 1, because it certifies (in)feasibility of Problem (BQP). An important difference between Problems (BQP) and (MC) is that the first one can be infeasible, while for the latter one any \( \{−1, 1\} \) vector is a feasible solution. We present a condition that allows early stopping of the branch-and-bound algorithm for solving Problem (MC) in case of infeasibility of Problem (BQP).

**Proposition 13.** Let \( Q \) be defined as in (6) and let \( z_{\text{ub}} \) denote the global upper bound of the max-cut problem throughout the branch-and-bound algorithm. If \( z_{\text{ub}} < e^\top Qe - \rho \), then Problem (BQP) is infeasible.

**Proof.** Let \( z_{\text{max-cut}} = \max\{x^\top Cx \mid x \in \{-1, 1\}^{n+1}\} \) where \( C = \frac{1}{4}L \) and \( L \) is the Laplace matrix of the graph with adjacency matrix as given in (7). We know that \( h^* = e^\top Qe - z_{\text{max-cut}} \). Moreover, by Theorem 2 Problem (BQP) is infeasible if and only if \( h^* > \rho \). Combining these two considerations, it follows that \( z_{\text{max-cut}} < e^\top Qe - \rho \) is equivalent to saying that Problem (BQP) has no feasible solution. By definition \( z_{\text{max-cut}} \leq z_{\text{ub}} \), hence \( z_{\text{ub}} < e^\top Qe - \rho \) implies infeasibility of the original problem. \( \square \)

On the other hand, the following lemma shows that any cut with value above a certain threshold gives rise to a feasible solution of Problem (BQP).

**Lemma 14.** Let \( z_{\text{lb}} \) be the value of some cut, i.e., a lower bound on \( z_{\text{max-cut}} \). If \( z_{\text{lb}} \geq e^\top Qe - \rho \), we can derive a feasible vector \( x_{\text{lb}} \in \Delta \) from the cut associated with \( z_{\text{lb}} \).

**Proof.** Let \( x_{\text{lb}} \) be the vector associated with \( z_{\text{lb}} \), i.e., \( z_{\text{lb}} = x_{\text{lb}}^\top Cx_{\text{lb}} \). Since \( x_{\text{lb}} \) is a cut, by the transformations presented in Section 3 it follows that \( h(x_{\text{lb}}) = x_{\text{lb}}^\top Qx_{\text{lb}} = e^\top Qe - x_{\text{lb}}^\top Cx_{\text{lb}} \). Thus, \( z_{\text{lb}} \geq e^\top Qe - \rho \) implies \( h(x_{\text{lb}}) \leq \rho \). By Theorem 2 it follows that \( x_{\text{lb}} \) is a feasible vector for Problem (BQP). \( \square \)

#### 7.2 Known Feasible Solutions

In case a feasible solution of (BQP) is known, e.g., if the assumption of Lemma 14 holds, we can use this information to update the penalty parameter. Obviously, detecting infeasibility is not needed anymore, hence we omit the threshold parameter \( \rho \). Given \( x' \in \Delta \) and \( \ell \leq \ell^* \), we define the penalty parameter \( \sigma' \) as follows.

\[
\sigma' = f(x') - \ell + \epsilon
\]
Note that \( f(x') \leq u^* \) and therefore \( \sigma' \) is smaller than the penalty parameter defined before in Section 5.

Theorem 15. Consider Problem (BQP) and Problem (UBQP) with optimal values \( f^* \) and \( h^* \), respectively. Furthermore, assume that we have a feasible solution \( x' \in \Delta \) and we define the penalty parameter \( \sigma' = f(x') - \ell + \epsilon \) where \( \ell \leq \ell^* \). Then \( h^* = f^* \).

Proof. Suppose \( h^* \neq f^* \). Let \( \tilde{x} \) be the vector minimizing \( h(x) \) over the set \( \{-1, 1\}^n \), i.e., \( h^* = h(\tilde{x}) \). For any \( x \in \Delta \) the equality \( f(x) = h(x) \) holds, hence we have \( \tilde{x} \in \Delta^c \). By definition of \( h(x) \), \( \sigma' \) and \( \ell \) it follows \( h(\tilde{x}) = f(\tilde{x}) + \sigma'\|Ax - b\|^2 \geq \ell + \sigma' = \ell + f(x') - \ell - \epsilon > f(x') \). Thus \( h(x') < h(\tilde{x}) = h^* \), hence a contradiction.

7.3 Least Violated Solution

In case of an infeasible instance, it is possible to detect the point with the least violation by relaxing the condition on the parameter \( u \). Let \( (\ell, u) \) be any pair of values such that \( \ell \leq \ell^* \) and \( u \geq \max\{f(x) \mid x \in \{-1, 1\}^n\} \). Given \( \sigma = u - \ell + \epsilon \), let \( \tilde{x} \) be the minimizer of \( h(x) \). Then \( \tilde{x} \in \arg\min\{\|Ax - b\| \mid x \in \{-1, 1\}^n\} \), i.e., the point with the least violation. This information can be helpful in case one is interested in some measure of infeasibility.

Lemma 16. Let \( x_1 \) and \( x_2 \) be any two vectors in \( \{-1, 1\}^n \). Furthermore, let \( h(x) \) be defined using \( \sigma = u - \ell + \epsilon \) where \( \ell \leq \ell^* \) and \( u \geq \max\{f(x) \mid x \in \{-1, 1\}^n\} \). Then, if \( h(x_1) \leq h(x_2) \), it follows \( \|Ax_1 - b\| \leq \|Ax_2 - b\| \).

Proof. The set \( \{-1, 1\}^n \) is partitioned into \( \Delta \) and \( \Delta^c \). Let \( x_1 \) and \( x_2 \) be any two vectors in \( \{-1, 1\}^n \) with \( h(x_1) \leq h(x_2) \). If \( x_1 \in \Delta \), then \( 0 = \|Ax_1 - b\| \leq \|Ax_2 - b\| \). If \( x_2 \in \Delta \), by Theorem 2 we have \( h(x_1) \leq h(x_2) \leq \rho \) and therefore \( x_1 \) is in \( \Delta \) as well. Thus \( \|Ax_1 - b\| = 0 = \|Ax_2 - b\| \). Hence, we study the remaining (and only interesting) case, namely \( x_1, x_2 \in \Delta^c \). By the definition of \( u \) and \( \ell \) we have

\[
\ell + \sigma\|Ax_1 - b\|^2 \leq f(x_1) + \sigma\|Ax_1 - b\|^2 \leq f(x_2) + \sigma\|Ax_2 - b\|^2 \leq u + \sigma\|Ax_2 - b\|^2.
\]

Hence it follows \( \sigma(\|Ax_1 - b\|^2 - \|Ax_2 - b\|^2) \leq u - \ell < \sigma \). Dividing the inequality by \( \sigma \) and rearranging the terms we have \( \|Ax_1 - b\|^2 < \|Ax_2 - b\|^2 + 1 \). By Remark 1 we know that \( \|Ax - b\|^2 \in \mathbb{Z}^+ \) for any vector \( x \in \{-1, 1\}^n \), thus \( \|Ax_1 - b\|^2 \leq \|Ax_2 - b\|^2 \).

8 Experimental Results

We implemented the bound computations and the computations of the transformed problem in Matlab. As max-cut solver we use BiqMac, as described in Section 2.1. All experiments were done on an Intel Xeon W-2195 CPU @ 2.30GHz and 512 GB RAM running under Linux.

Several problems can be stated as a BQP with equality constraints. In this section we present results for randomly generated instances, for the max \( k \)-cluster problem and for the quadratic boolean cardinality problem.
8.1 Description of the Instances

8.1.1 Randomly Generated Instances

In order to test the efficiency of our algorithm we created two families of randomly generated instances, denoted RGI, using Matlab. Since for binary vectors \( y \) the equality \( y = y^2 \) holds, it is possible to exchange \( \hat{c} \) and diag(\( \hat{F} \)), hence we assume \( \hat{c} = 0 \). Given a scalar value \( b_v \) we define \( \hat{b} = [b_v, \ldots, b_v]^\top \). For the choice of \( \hat{A}_{ij} \) we pick random integer numbers in the interval \([\hat{A}_l, \hat{A}_u]\). Similarly \( \hat{F}_{ij} \) is randomly chosen in \( \mathbb{Z} \cap [\hat{F}_l, \hat{F}_u] \). We assume \( \hat{F} \) to be symmetric.

In the first family we choose \([\hat{A}_l, \hat{A}_u]\) as \([-1, 1] \), \([-3, 3] \) and \([-7, 7] \). Similarly, we choose \([\hat{F}_l, \hat{F}_u]\) as \([-1, 1] \), \([-3, 3] \) and \([-7, 7] \). Moreover, we set \( b_v = 0 \), hence there is always a feasible vector, namely \( y = 0 \).

In the second family we choose the elements in \( \hat{A} \) to be from the intervals \([0, 1] \) and \([0, 3] \) and we choose the scalar \( b_v \in \{10, 15, 20\} \). For the choice of \( \hat{F} \) we use different intervals, namely \([0, 5] \), \([-5, 5] \), \([0, 10] \) and \([-10, 10] \).

For every combination of \( \hat{A}, \hat{F} \) and \( b_v \), we form two sets of instances with size \( n \in \{80, 100\} \). For each of these sets we create 15 instances having one to 15 constraints.

In total this gives 270 instances in the first family and 720 instances in the second family. All the randomly generated instances can be downloaded from [15].

8.1.2 \( k \)-Cluster Problem and Cardinality Boolean Quadratic Problem

The max \( k \)-cluster problem, sometimes called densest \( k \)-subgraph problem asks, given a graph \( G \), to find the induced subgraph on \( k \) vertices with the largest number of induced edges, i.e.,

\[
\max \left\{ \frac{1}{2} y^\top A y \mid y \in \{0, 1\}^n, \ y^\top e = k \right\}
\]

where \( A \in \mathbb{R}^{n \times n} \) is the adjacency matrix of the graph and \( k \) is an integer number in \([1, n]\).

We use the max \( k \)-cluster instances from [13] where \( n \in \{120, 140, 160\} \), \( k \in \{n/4, n/2, 3n/4\} \), and densities \( d \in \{0.25, 0.50, 0.75\} \).

A slightly more general problem is the cardinality boolean quadratic problem (CBQP). The CBQP is a minimization problem similar to the \( k \)-cluster problem, with the addition of a linear term in the objective function, i.e.,

\[
\min \left\{ y^\top Q y + q^\top y \mid y \in \{0, 1\}^n, \ y^\top e = k \right\}.
\]

A collection of CBQP instances can be found at [22]. These instances have different sizes \( n \in \{50, 75, 100, 200, 300\} \) and densities \( d \in \{0.10, 0.50, 0.75, 1.00\} \). Following the study of Grossmann and Lima [21] we set \( k = n/5 \) and \( k = 4n/5 \).

8.2 Comparing the Penalty Parameters

In this section we study different penalty parameters obtained from the bounds that we introduced in the previous sections. First we compare the values of different penalty parameters
and their computational times. We compare the following penalty parameters:

\[
\begin{align*}
\sigma_{\text{Las}} &= 2 \max\{|\hat{l}|, |\hat{u}|\} + 1 \\
\sigma_{\text{CLI}} &= \hat{u} - \hat{l} + \epsilon \\
\sigma_{\text{GW}} &= u_\Delta - \hat{l} + \epsilon
\end{align*}
\]

as described in Sections 4 and 6. In Table 1 we list in columns 2 and 3 the average of the ratios \(\frac{\sigma_{\text{CLI}}}{\sigma_{\text{Las}}}\) and \(\frac{\sigma_{\text{GW}}}{\sigma_{\text{Las}}}\) in percent. Columns 4 to 6 give the average time in seconds to compute the relevant \(\sigma\).

| Set of instances       | \(\text{avg } \frac{\sigma_{\text{CLI}}}{\sigma_{\text{Las}}}(\%)\) | \(\text{avg } \frac{\sigma_{\text{GW}}}{\sigma_{\text{Las}}}(\%)\) | \(\text{avg } t_{\text{Las}}(s)\) | \(\text{avg } t_{\text{CLI}}(s)\) | \(\text{avg } t_{\text{GW}}(s)\) |
|------------------------|-------------------------------------------------|-------------------------------------------------|-----------------|-----------------|-----------------|
| RGI with \(n = 80\)    | 41.94                                           | 15.89                                           | 0.15            | 126.53          | 31.18           |
| RGI with \(n = 100\)   | 25.03                                           | 13.20                                           | 0.20            | 142.36          | 45.08           |
| \(k\)-cluster          | 49.89                                           | 37.48                                           | 0.34            | 16.93           | 7.02            |
| CBQP with \(Q(\geq 0)\)| 50.17                                           | 17.92                                           | 0.51            | 28.71           | 63.48           |
| CBQP with \(Q(\in \mathbb{R})\)| 89.89 | 76.00                                           | 0.54            | 31.91           | 52.88           |

Table 1: Comparison of different penalty parameters and computational times

We already proved in Proposition 9 that \(\sigma_{\text{Las}} \geq \max\{\sigma_{\text{GW}}, \sigma_{\text{CLI}}\}\), but there is no relation between \(\sigma_{\text{CLI}}\) and \(\sigma_{\text{GW}}\). From Table 1 we observe that, for all our instances, on average the latter is always smaller than the former one.

As expected, the computational time for computing \(\sigma_{\text{CLI}}\) and \(\sigma_{\text{GW}}\) is clearly larger than the one for computing \(\sigma_{\text{Las}}\). However, compared to the time for solving the max-cut problem, the time for computing \(\sigma\) is negligible. Comparing the times for computing \(\sigma_{\text{CLI}}\) and \(\sigma_{\text{GW}}\), there is no clear winner.

We now show the impact of using a smaller penalty parameter on the overall performance of our algorithm. To do so, we study the running times of EXPEDIS with different choices for the penalty parameter. We only compare the two penalty parameters \(\sigma_{\text{Las}}\) and \(\sigma_{\text{GW}}\) since \(\sigma_{\text{Las}} \geq \sigma_{\text{CLI}} \geq \sigma_{\text{GW}}\).

Furthermore, we experiment with the effect of updating the penalty parameter \(\sigma_{\text{GW}}\) when a feasible solution is found at the root node, as described in Section 7.2.

In Figures 3 and 4 we show the results for the randomly generated instances of size \(n = 80\) and \(n = 100\), respectively; we set a time limit of 1.5 hours.

We see that decreasing the value of the penalty parameter improves the average computational time of the algorithm. Also, updating the penalty parameter at the root node improves the overall running time. We also observe that with an increasing number of variables, the effect of a smaller penalty parameter is even more significant.

### 8.3 Settings of EXPEDIS

The experiments in the previous section suggest to choose in our algorithm \(\sigma_{\text{GW}}\), with a possible update if some feasible solution is known, as penalty parameter. In order to possibly
avoid the preprocessing calculation of the parameters, we enhance the algorithm as follows. We first use a trivial penalty parameter to set up the max-cut problem as given in (MC). Then we run the Goemans-Williamson heuristic and we locally improve the resulting cut vector by checking all possible moves of a single vertex to the opposite partition block. Given as input a feasible problem, this heuristic often finds a cut whose vector associated with BQP is feasible.

Let $x'$ be the vector associated to the cut found by the rounding heuristic. If $x' \notin \Delta$, we set the threshold and the penalty parameter as described in Section 5, i.e.,

$$\rho_{GW} = u_\Delta \quad \text{and} \quad \sigma_{GW} = u_\Delta - \tilde{\ell} + \epsilon,$$

where $\tilde{\ell}$ and $u_\Delta$ are the bounds presented in Section 6. If $x' \in \Delta$, i.e., $x'$ is a feasible vector for Problem (BQP), we redefine the penalty parameter as described in Section 7.2, i.e.,

$$\sigma' = f(x') - \tilde{\ell} + \epsilon.$$

We outline our settings in Algorithm 2.

### 8.4 Comparison to other solvers

In this section we compare the performance of our algorithm with other generic solvers. We tested the instances using BiqCrunch [17], COUENNE [2], CPLEX [8], GUROBI [14], SCIP [12] and SMIQP [3]. In all these solvers we input Problem (BQP) and we keep the default settings. We use the data sets described in Section 8.1 above.

In Figure 5 we present the performance profile of the different solvers on all the randomly generated instances. Clearly, for these instances EXPEDIS outperforms all the other solvers. Within the time limit EXPEDIS and GUROBI solve almost 70% and 60% of the instances, respectively, BiqCrunch solves slightly less than 50% of them, while the other solvers less than 30% of them.
Algorithm 2: Scheme of our algorithm

1 Algorithm: Refined EXPEDIS

Data: \( \hat{F} \in \mathbb{R}^{n \times n}, \hat{c} \in \mathbb{R}^n, \hat{A} \in \mathbb{Z}^{m \times n}, \hat{b} \in \mathbb{Z}^m \) defining problem

\[
\min \{ y^\top \hat{F} y + \hat{c}^\top y \mid \hat{A} y = \hat{b}, \ y \in \{0,1\}^n \}
\]

Result: optimal solution or certificate of infeasibility

2 transform to problem \( \min \{ x^\top F x + c^\top x + \alpha \mid Ax = b, \ x \in \{-1,1\}^n \} \);

3 choose a trivial penalty parameter and set up the max-cut problem as given in (MC);

4 run the rounding heuristic and extract the cut \( x' \);

5 if \( x' \notin \Delta \) then

6 compute the threshold parameter \( \rho_{GW} = u_\Delta \);

7 compute the penalty parameter \( \sigma_{GW} = u_\Delta - \bar{\ell} + \epsilon \);

8 set up and solve the max-cut problem giving optimal value \( h^* \);

9 if \( z_{ub} < e^\top Q e - \rho_{GW} \) then

10 terminate the algorithm: problem infeasible;

11 end

12 if \( h^* > u_\Delta \) then

13 terminate the algorithm: problem infeasible;

14 end

15 else

16 update the penalty parameter: \( \sigma' = f(x') - \bar{\ell} + \epsilon \);

17 set up and solve the max-cut problem giving optimal value \( h^* \);

18 end

19 transform the optimal cut to the optimal solution of the 0/1 problem;
Next, we compare the performance of the different solvers for structured instances, namely the max $k$-cluster instances.

From the literature, two prominent solvers for the max $k$-cluster problem are BiqCrunch and SMIQP. The former has a tailored version for the max $k$-cluster problem, which reinforces the model with additional product constraints. The specialized version of BiqCrunch outperforms EXPEDIS on the max $k$-cluster instances, while the comparison with SMIQP and the general version of BiqCrunch is clearly dominated by EXPEDIS.

We report only the running times of EXPEDIS on the 135 instances of the max $k$-cluster problem as described in Section 8.1.2 in Table 2 below, since none of the other solvers was able to solve any of these instances within the time limit of 3 hours.

For every combination $(n, k)$ there are 15 instances. In the third column of Table 2, we present the average running time over the instances solved within the time limit of 3 hours. Note that all the instances with $k = 3n/4$ are solved within 3 hours and that the problem gets more complicated for small $k$.

In Figure 6 we compare the running times for solving the instances of the cardinality boolean quadratic problem, for which we set a time limit 1.5 hours. Since CBQP is essentially the same problem as the max $k$-cluster, i.e., a binary quadratic problem with a cardinality constraints, and from the considerations on the max $k$-cluster, we do not proceed further in solving the CBQP instances by using SMIQP and BiqCrunch. We do not present the results for $n = 50$ because all the solvers solve all the small size instances. Moreover, for the combination of parameters $(n, k) \in \{(200, n/5), (300, n/5), (300, 4n/5)\}$ none of the solvers manages to find the optimum of any instance within the time limit. Hence we omit these instances as well. We show the results in Figure 6. Within the time limit, EXPEDIS can solve almost all instances (95 %), whereas GUROBI manages to solve slightly less than 70% and all the other solvers at most half of them.
Figure 5: Performance profile of the different solvers on all the randomly generated instances

9 Conclusions and Future Work

In this paper we present EXPEDIS, a new algorithm for solving binary quadratic problems with linear equality constraints. EXPEDIS transforms the binary quadratic problem into a max-cut instance, computes the optimal cut, and then provides either the optimal solution of the binary quadratic problem or gives a certificate of infeasibility.

At the heart of the algorithm is a penalty parameter used for the transformation. We investigate conditions on the penalty parameter and present different ways to choose it. We also present numerical experiments showing the effect of the different choices.

In order to demonstrate the strength EXPEDIS we perform numerical experiments on several types of instances. These experiments clearly show the dominance of EXPEDIS over CPLEX, COUENNE, GUROBI and SCIP.

Computing the max-cut is done using the solver BiqMac. Hence, advancing BiqMac will also result in a speedup of EXPEDIS. Therefore we are currently working on improving BiqMac by adding more polyhedral cuts in the bounding procedure. Another line of research is to make an extended parallel version of EXPEDIS and run it on a high-performance computer. This algorithm will then be available via BiqBin at the web page [http://biqbin.eu](http://biqbin.eu).

It would be interesting to generalize our algorithm to linear inequality constraints as well as to quadratic constraints. In particular, we would like to understand whether ellipsoidal relaxations [4] can be used to further improve the penalty parameter. These topics are currently under investigation.

Acknowledgments

This project was supported by the Austrian Science Fund (FWF): I3199-N31 and by the Slovenian Research Agency (ARRS): N1-0057. Furthermore, this project has received funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 764759. The authors are grateful to Franz
Table 2: Running times for solving the $k$-cluster instances. For each $(n, k)$ we consider 15 instances, in brackets we give the number of instances solved within the time limit of 3 hours.

| $(n, k)$  | instances | avg time (s) |
|-----------|-----------|--------------|
| (120, 30) | 15 (14)   | 2394         |
| (120, 60) | 15 (15)   | 1748         |
| (120, 90) | 15 (15)   | 198          |
| (140, 35) | 15 (5)    | 5108         |
| (140, 70) | 15 (12)   | 2922         |
| (140, 105) | 15 (15)  | 509          |
| (160, 40) | 15 (2)    | 7050         |
| (160, 80) | 15 (6)    | 5704         |
| (160, 120) | 15 (15) | 1145         |

Rendl for helpful discussions. Part of this work has been carried out during a research stay of the first author at the University of Iowa hosted by Sam Burer. The authors would like to thank Sam Burer for discussions and suggestions that improved the results significantly. The authors also thank two anonymous referees for their valuable comments.

References

[1] Miguel F. Anjos and Jean B. Lasserre (eds.), *Handbook on semidefinite, conic and polynomial optimization.*, vol. 166, New York, NY: Springer, 2012 (English).

[2] P. Belotti, J. Lee, L. Liberti, F. Margot, and A. Wächter, *Branching and bounds tightening techniques for non-convex MINLP*.

[3] Alain Billionnet, Sourour Elloumi, Amélie Lambert, and Angelika Wiegele, *Using a conic bundle method to accelerate both phases of a quadratic convex reformulation.*, INFORMS J. Comput. 29 (2017), no. 2, 318–331 (English).

[4] Christoph Buchheim, Marianna De Santis, Laura Palagi, and Mauro Piacentini, *An exact algorithm for nonconvex quadratic integer minimization using ellipsoidal relaxations*, SIAM J. Optim. 23 (2013), no. 3, 1867–1889.

[5] Christoph Buchheim and Angelika Wiegele, *Semidefinite relaxations for non-convex quadratic mixed-integer programming*, Math. Program. 141 (2013), no. 1-2, Ser. A, 435–452.

[6] Samuel Burer, *Optimizing a polyhedral-semidefinite relaxation of completely positive programs*, Mathematical Programming Computation 2 (2010), no. 1, 1–19.
Figure 6: Performance profile of the different solvers on 400 CBQP instances.

[7] Samuel Burer and Dieter Vandenbussche, *A finite branch-and-bound algorithm for non-convex quadratic programming via semidefinite relaxations*, Mathematical Programming 113 (2008), no. 2, 259–282.

[8] IBM Developer, *Cplex version 12.8*, www.cplex.com.

[9] Ilse Fischer, Gerald Gruber, Franz Rendl, and Renata Sotirov, *Computational experience with a bundle approach for semidefinite cutting plane relaxations of max-cut and equipartition*, Mathematical Programming 105 (2006), no. 2, 451–469.

[10] Michael R. Garey and David S. Johnson, *Computers and intractability*, W. H. Freeman and Co., San Francisco, Calif., 1979, A guide to the theory of NP-completeness, A Series of Books in the Mathematical Sciences. MR 519066 (80g:68056)

[11] Krasimira Genova and Vassil Guliashki, *Linear integer programming methods and approaches—a survey*, Cybern. Inf. Technol. 11 (2011), no. 1, 3–25.

[12] Ambros Gleixner, Michael Bastubbe, Leon Eifler, Tristan Gally, Gerald Gamrath, Robert Lion Gottwald, Gregor Hendel, Christopher Hojný, Thorsten Koch, Marco E. Lübbecke, Stephen J. Maher, Matthias Miltenberger, Benjamin Müller, Marc E. Pfetsch, Christian Puchert, Daniel Rehfeldt, Franziska Schlösser, Christoph Schubert, Felipe Serrano, Yuji Shinano, Jan Merlin Viernickel, Matthias Walter, Fabian Wegscheider, Jonas T. Witt, and Jakob Witzig, *The SCIP Optimization Suite 6.0*, Technical report, Optimization Online, July 2018.

[13] Michel X. Goemans and David P. Williamson, *Improved approximation algorithms for maximum cut and satisfiability problems using semidefinite programming*, J. ACM 42 (1995), no. 6, 1115–1145.

[14] LLC Gurobi Optimization, *Gurobi optimizer reference manual*, http://www.gurobi.com.
[15] Nicolò Gusmeroli, *Randomly Generated Instances*, https://www.aau.at/en/mathematics/publications/software/ 2019.

[16] Gary Kochenberger, Jin-Kao Hao, Fred Glover, Mark Lewis, Zhipeng Lü, Haibo Wang, and Yang Wang, *The unconstrained binary quadratic programming problem: a survey*, J. Comb. Optim. **28** (2014), no. 1, 58–81.

[17] Nathan Krislock, Jérôme Malick, and Frédéric Roupin, *BigCrunch: a semidefinite branch-and-bound method for solving binary quadratic problems*, ACM Trans. Math. Softw. **43** (2017), no. 4, 23 (English).

[18] Amélie Lambert, *Max k-cluster benchmark instances*, http://cedric.cnam.fr/~lamberta/Library/k-cluster.html 2018, Accessed: 2018-02-27.

[19] Jean B. Lasserre, *A MAX-CUT formulation of 0/1 programs*, Oper. Res. Lett. **44** (2016), no. 2, 158–164.

[20] Monique Laurent and Svatopluk Poljak, *Gap inequalities for the cut polytope*, Eur. J. Comb. **17** (1996), no. 2-3, 233–254 (English).

[21] Ricardo M. Lima and Ignacio E. Grossmann, *On the solution of nonconvex cardinality Boolean quadratic programming problems: a computational study*, Comput. Optim. Appl. **66** (2017), no. 1, 1–37 (English).

[22] _____, *CBQP benchmark instances*, https://sites.google.com/site/cbqppaper/ 2017, Accessed: 2019-12-12.

[23] George L. Nemhauser and Laurence A. Wolsey, *Integer and combinatorial optimization*, Wiley-Interscience Series in Discrete Mathematics and Optimization, John Wiley & Sons, Inc., New York, 1988, A Wiley-Interscience Publication.

[24] Svatopluk Poljak, Franz Rendl, and Henry Wolkowicz, *A recipe for semidefinite relaxation for (0,1)-quadratic programming*, Journal of Global Optimization **7** (1995), no. 1, 51–73.

[25] Franz Rendl, Giovanni Rinaldi, and Angelika Wiegele, *Solving Max-cut to optimality by intersecting semidefinite and polyhedral relaxations*, Math. Program. **121** (2010), no. 2 (A), 307–335 (English).

[26] Hanif D. Sherali and Warren P. Adams, *A hierarchy of relaxations between the continuous and convex hull representations for zero-one programming problems*, SIAM J. Discrete Math. **3** (1990), no. 3, 411–430.

[27] Naum Z. Shor, *Quadratic optimization problems*, Sov. J. Comput. Syst. Sci. **25** (1987), no. 6, 1–11 (English).

[28] Annegret K. Wagler, *Combinatorial optimization: the interplay of graph theory, linear and integer programming illustrated on network flow*, Large-scale networks in engineering and life sciences, Model. Simul. Sci. Eng. Technol., Springer, Heidelberg, 2014, pp. 225–262.
[29] Henry Wolkowicz, Romesh Saigal, and Lieven Vandenberghe (eds.), *Handbook of semidefinite programming. Theory, algorithms, and applications.*, vol. 27, Dordrecht: Kluwer Academic Publishers, 2000 (English).