

SpeeDP: A new algorithm to compute the SDP relaxations of Max-Cut for very large graphs

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Abstract

We consider low-rank semidefinite programming (LRSDP) relaxations of unconstrained $\{-1, 1\}$ quadratic problems (or, equivalently, of Max-Cut problems) that can be formulated as the nonconvex nonlinear programming problem of minimizing a quadratic function subject to separable quadratic equality constraints. We prove the equivalence of the LRSDP problem with the unconstrained minimization of a new merit function and we define an efficient and globally convergent algorithm, called **SpeeDP**, for finding critical points of the LRSDP problem. We provide evidence of the effectiveness of **SpeeDP** by comparing it with other existing codes on an extended set of instances of the Max-Cut problem.

When the rank of solution matrix is bounded by a given value (independent on the problem size n), **SpeeDP** is still able to provide a valid upper bound for Max-Cut. This feature makes it possible to design an algorithm, called **SpeeDP-MC** and based on the Goemans-Williamson heuristic, that has two interesting features: (a) it provides heuristic solutions to Max-Cut along with a guaranteed optimality error; (b) it runs with a $\mathcal{O}(n + m)$ memory requirement (where m is the number of edges of the graph), thus overcoming a serious drawback of interior point based methods that demand $\mathcal{O}(n^2)$ memory. Exploiting the latter feature, we could run it on very large graphs with sizes of up to a million nodes, obtaining very small optimality error bounds in reasonable computation times.

keywords Semidefinite programming, low rank factorization, unconstrained binary quadratic programming, Max-Cut, nonlinear programming.

1 Introduction

We consider a semidefinite programming (SDP) problem in the form

$$\min_X \{Q \bullet X : \text{diag}(X) = e, X \succeq 0\}, \quad (1)$$

where $Q \in \mathcal{S}^n$ is given, $X \in \mathcal{S}^n$ (\mathcal{S}^n being the space of the $n \times n$ symmetric matrices), $e \in \mathbb{R}^n$ is the vector of all ones, $\text{diag}(X)$ denotes the n -vector corresponding to the main diagonal of X , and, finally, $X \succeq 0$ tells that X is required to be positive semidefinite.

Semidefinite Programming problems of this form arise as relaxations of unconstrained $\{-1, 1\}$ quadratic problems (see, e.g., [6], [10], [19]):

$$\min_x \{x^T Q x : x \in \{-1, 1\}^n\}, \quad (2)$$

which are equivalent to the Max-Cut problem. Given the weighted adjacency matrix A of a weighted graph $G = (V, E)$, the Max-Cut problem calls for a bipartition $(S, V \setminus S)$ of its vertices V so that the weight of the cut, i.e., of the edges joining the two sets of the bipartition, is maximized. Denote by L the Laplacian matrix associated with A and defined by $L := \text{diag}(Ae) - A$. Represent each bipartition $(S, V \setminus S)$ by an n -vector defined by $x_i = 1$ for $i \in S$ and $x_i = -1$ for $i \notin S$ (or, equivalently, by its opposite vector). Then the Max-Cut problem can be formulated as

$$\max_x \left\{ \frac{1}{4} x^T L x : x \in \{-1, 1\}^n \right\}. \quad (3)$$

Since $x^T L x = L \bullet x x^T$ and $x x^T \succeq 0$ with $\text{diag}(x x^T) = e$, it is clear that problem (1) with $Q = -\frac{1}{4}L$ provides a relaxation of Max-Cut. Efficient solution of problem (1) is then of great interest because it can be exploited for solving the corresponding integer problem (2) exactly or as a tool for defining good heuristics (see, e.g., [23], [25]).

The aim of this paper is twofold: on one side is to define an efficient algorithm for solving large scale instances of problem (1); on the other, exploiting this useful tool, is to find good solutions of problem (3), by defining a new heuristic algorithm and providing a measure of the distance of the solution weight from the optimal value.

It is well known that problem (1) can be solved by any interior point method, where the key idea consists in applying the Newton method to the optimality conditions of the primal-dual pair of problems.

The dual of problem (1) is

$$\min_y \{e^T y : \text{Diag}(y) + Q \succeq 0\}. \quad (4)$$

Unfortunately, the interior point methods require $\mathcal{O}(n^2)$ memory which makes it prohibitive to attack instances with, say, $n > 50\,000$. Moreover these methods typically require to perform a Cholesky factorization of a $n \times n$ matrix which require $\mathcal{O}(n^3)$ operations, a much too expensive task when the graph is very large. These limitations motivate searching for methods that are less demanding in terms of memory allocation and avoid the need of the Cholesky factorization. For this reason, the special structure of the constraints of problem (1) has been exploited in the literature to define ad-hoc algorithms. One possibility is to

eliminate the semidefiniteness constraint $\text{Diag}(y) + Q \succeq 0$ in the dual problem. At the end, the dual problem is reformulated as eigenvalue optimization problem which can be solved by spectral bundle methods [17]. The other option is to use nonlinear programming reformulations that eliminate the semidefiniteness constraint from the primal problem (1). The latter is the line of research this paper falls into. Indeed, using the Gramian representation, any given matrix $X \succeq 0$ with rank r can be written as $X = VV^T$, where V is a $n \times r$ real matrix. Therefore the positive semidefiniteness constraint can be eliminated, and problem (1) reduces to the Low Rank SDP formulation (LRSDP)

$$\min_V \{Q \bullet VV^T : \text{diag}(VV^T) = e\}. \quad (5)$$

For a fixed value of the rank r , problem (5) can be written as a Non Linear Programming problem (NLP_r)

$$\min_v \left\{ q_r(v) = \sum_{i=1}^n \sum_{j=1}^n q_{ij} v_i^T v_j : \|v_i\|^2 = 1, i = 1, \dots, n \right\}, \quad (6)$$

where $v_i, i = 1, \dots, n$, are the columns of the matrix V^T and $v = \text{vec}(V^T) \in \mathbb{R}^{nr}$. Indeed this formulation was first derived by Goemans-Williamson in [12], by replacing each variable x_i of problem (2) with a vector $v_i \in \mathbb{R}^n$ (or $v_i \in \mathbb{R}^r$ with $r \leq n$), obtaining problem (6). Although reformulation (5) results in the non convex problem (6), it is still possible to state conditions that ensure correspondence among global solutions of problem (6) and solutions of problem (1) and also optimality conditions which can be used to check global optimality [14], [21], [15], [5].

In most of the papers based on NLP approaches, the solution of problem (6) is achieved by means of an unconstrained reformulation (see [5], [15], [18] and Section 5).

Indeed, the first idea of an unconstrained formulation of problem (1) goes back to Homer and Peinado [18], but the dimension of the resulting problem made the method prohibitive for large scale problems. Burer and Monteiro in [5] combine the Homer and Peinado formulation with the ‘‘low rank idea’’. By introducing the change of variables $X_{ij} = v_i^T v_j / \|v_i\| \|v_j\|$, where $v_i \in \mathbb{R}^r$, $i = 1, \dots, n$, with $r \ll n$, they get the unconstrained formulation

$$\min_v \left\{ f_r(v) = \sum_{i=1}^n \sum_{j=1}^n q_{ij} \frac{v_i^T v_j}{\|v_i\| \|v_j\|}, \quad v_i \in \mathbb{R}^r \right\}. \quad (7)$$

The resulting algorithm **SDPLR-MC** was computationally efficient, but the underlying convergence theory was not deeply investigated.

In this paper, we start from the unconstrained formulation (7), to get an enhanced different unconstrained formulation, for which we prove complete equivalence with problem (1). The specific feature of this formulation is that we add to the function $f_r(v)$, where $v \in \mathbb{R}^{nr}$ as in [5], a shifted barrier penalty term that

ensures compactness of the level sets of the new merit function. This allows us to use standard unconstrained optimization algorithms. In particular, we define a globally convergent algorithm based on the nonmonotone Barzilai-Borwein gradient method proposed in [16]. The resulting algorithmic scheme **SpeedP** outperforms the best existing methods for solving problem (1). By fixing r to a value independent of n , Algorithm **SpeedP** requires $\mathcal{O}(n+m)$ memory; moreover, despite the limitation in the rank of the solution matrix, it is still possible to derive a valid lower bound for problem (1). Therefore, it is possible to produce a lower bound (close to the SDP bound) for very large instances of problem (2). In addition, **SpeedP** provides in output the Gramian matrix of a solution X to problem (1). This implies that, once **SpeedP** has produced a solution, the famous Goemans-Williamson algorithm proposed in [12] can be applied, essentially without any additional computational effort, to find a feasible cut that, in case of nonnegative weights, has weight at most 12.1% away from the weight of the optimum. Therefore, we designed a heuristic algorithm exploiting this feature in order to produce good cuts for very large graphs. In this algorithm the Goemans-Williamson cut is improved by applying a 1-opt local search and then by solving problem (1) again a few more times for a perturbed matrix Q' . As the computation time is concerned, contrary to what happens for the interior point methods, **SpeedP** has the ability of exploiting sparsity of matrix Q , thus making it possible to find cuts in sparse graphs with millions of nodes and edges, with optimality error lower than 5% (when the edge weights are all positive) in quite practical computation times.

Papers describing heuristics for Max-Cut abound in the literature. However, only in a few cases the algorithms they describe provide a bound on the optimality error for the generated solutions. Excluding the heuristics with a certified a priori bound (like the one of Goemans and Williamson) the only cases when this bound is computed are those of the exact algorithms, that compute an upper bound on the value of optimal solution, by solving a relaxation of the problem. If these algorithms are interrupted prematurely, they provide, as a side product, a heuristic cut along with an upper bound on the optimal value. Unfortunately, the computational studies based on these types of algorithms consider graphs much smaller than those used for the test bed of this paper (see, e.g., [20] for the polyhedral relaxations and [25] for a combination of SDP and polyhedral relaxation), therefore no comparison of the computational results provided here with other approaches is possible at the time.

The paper is structured as follows: in Section 2 we report some useful results about the low rank reformulation of problem (1). In Section 3 we define the new unconstrained reformulation of problem (LRSDP), while in Section 4 we define formally the solution algorithm **SpeedP** employed for solving this formulation.

In Section 5 we define our heuristic for finding good solutions of large sparse instances of Max-Cut.

In Section 6 we report the numerical results. We compare the performance of **SpeedP** against other existing approaches for problem (1). Then we use the heuristic to find good solutions of large and huge instances of the Max-Cut problem for random graphs.

Throughout the paper, given an $m \times p$ matrix M we denote by $\text{vec}(M) \in \mathbb{R}^{mp}$ the vector corresponding to the elements of M ordered by column index and then by row index. Given a vector $v \in \mathbb{R}^m$, we denote by $\text{Diag}(v)$ the diagonal matrix having as diagonal the vector v and by $B_\rho(v)$ the closed ball centered in v with radius $\rho > 0$, namely $B_\rho(v) = \{y \in \mathbb{R}^m : \|y - v\| \leq \rho\}$. For a given scalar x we denote by $(x)_+$ the maximum between x and zero, namely $(x)_+ \equiv \max(x, 0)$.

2 Some useful results about the low rank SDP formulation

In this section we report the main results on the Low Rank SDP formulation (LRSDP) defined in (5).

A global minimum point of problem (5) is a solution of problem (1) provided that

$$r \geq r_{\min} = \min_{X \in \mathcal{X}_{\text{SDP}}^*} \text{rank}(X),$$

where $\mathcal{X}_{\text{SDP}}^*$ denotes the optimal solution set of problem (1). Although the value of r_{\min} is not known, an upper bound can easily be computed by exploiting the result proved in [24], [2], [22], that gives

$$r_{\min} \leq \hat{r} = \frac{\sqrt{8n+1} - 1}{2}. \quad (8)$$

Thus, in order to get a problem equivalent to problem (1), the dimension of the matrix V in problem (5) can be fixed to $n \times r$ with $r \geq \hat{r}$.

We say that a point $v^* \in \mathbb{R}^{nr}$ solves problem (1) if $X^* = V^*V^{*T}$ is an optimal solution of problem (1). This implies, by definition, that $r \geq r_{\min}$.

Although reformulation (5) results in the non convex problem (6), the primal-dual optimality conditions for (1) combined with necessary optimality conditions for (6) lead to some global optimality conditions that can be exploited from the computational point of view [14], [21], [15], [5].

The Karush-Kuhn-Tucker conditions for problem (6) are written as follows for some $\lambda \in \mathbb{R}^n$

$$\begin{aligned} \sum_{j=1}^n q_{ij} v_j + \lambda_i v_i &= 0, & i = 1, \dots, n \\ \|v_i\|^2 &= 1, & i = 1, \dots, n. \end{aligned} \quad (9)$$

We define stationary point of problem (6) a point $\hat{v} \in \mathbb{R}^{nr}$ satisfying (9) with a suitable multiplier $\hat{\lambda} \in \mathbb{R}^n$. Given a local minimizer $\hat{v} \in \mathbb{R}^{nr}$ of problem (6), the KKT conditions are necessary conditions for optimality and there exists a unique $\hat{\lambda} \in \mathbb{R}^n$ such that $(\hat{v}, \hat{\lambda})$ satisfies (9). This feature has been exploited first in [15] and later for slightly more general constraints in [21]. Indeed, given

a pair (v, λ) satisfying the conditions (9), the multiplier λ can be expressed uniquely as a function of v , namely

$$\lambda_i(V) = \lambda_i = -E_{ii}Q \bullet VV^T = -v_i^T \sum_{j=1}^n q_{ij}v_j, \quad i = 1, \dots, n. \quad (10)$$

By substituting the expression of λ in the first condition of (9), we get

$$\sum_{j=1}^n q_{ij} (I_r - v_i v_i^T) v_j = 0 \quad i = 1, \dots, n. \quad (11)$$

The next proposition that extends the sufficient conditions given in [5] and was proved in in [15] and for more general problems in [14], [21], states the global optimality conditions obtained by exploiting the primal-dual properties for problem (1).

Proposition 3 (Global optimality conditions). *A point $v^* \in \mathbb{R}^{nr}$ is a global minimizer of problem (6) that solves problem (1) if and only if it is a stationary point of problem (6) and satisfies*

$$Q + \text{Diag}(\lambda(V^*)) \succeq 0,$$

where $\lambda(V^*)$ is computed according to (10).

Thanks to the above proposition, given a stationary point of problem (6), we can prove its optimality just checking that a certain matrix is positive semidefinite.

Another global condition has been proved in [21] for a slightly more general convex SDP problem which includes as a special case problem (1). It is proved that the $n \times r$ local minimizer \widehat{V} of the LRSDP problem provides a global solution $\widehat{X} = \widehat{V}\widehat{V}^T$ of the original SDP problem if \widehat{V} is rank deficient, namely if $\text{rank}(\widehat{V}) < r$. Actually looking at the proof, it turns out that the assumption of \widehat{V} being a local minimizer can be relaxed to satisfying the second order necessary conditions for the LRSDP problem. Hence we restate their proposition (only in the special case of problem (1), although a generalization to linear constraints and convex objective function easily follows).

Proposition 4. *Let \widehat{V} be the $n \times r$ matrix satisfying the first and second order necessary conditions of problem (5), namely (9) and*

$$\left(Q + \text{Diag}(\widehat{\lambda})\right) \bullet ZZ^T \geq 0 \quad \text{for all } Z \in \mathbb{R}^{n \times r} : E_{ii} \bullet \widehat{V}Z^T = 0 \quad i = 1, \dots, n.$$

If the matrix \widehat{V} is rank deficient, then it provides a global solution $\widehat{X} = \widehat{V}\widehat{V}^T$ of problem (1). If $r = n$, any $n \times n$ matrix \widehat{V} satisfying the second order necessary conditions of problem (5) provides a global solution $\widehat{X} = \widehat{V}\widehat{V}^T$ of problem (1).

For sake of completeness we report the proof in Appendix 14 although it is only a special case of the proof presented in [21]. We note for $r = n$ it was already proved in [18] that there exists no local minimizer \widehat{V} of problem (5) which is not global.

5 A new unconstrained formulation of the SDP problem

In most papers considering problem (6), its solution is achieved by means of an unconstrained reformulation of it. In particular, the augmented Lagrangian function proposed in [5] for a semidefinite programming problem with general linear constraints can be specified to problem (1) and takes the form

$$\mathcal{L}(V, \lambda; \varepsilon) = Q \bullet VV^T + \sum_{i=1}^n \lambda_i (\|v_i\|^2 - 1) + \frac{1}{2\varepsilon} \sum_{i=1}^n (\|v_i\|^2 - 1)^2,$$

where $\varepsilon > 0$ is a penalty parameter and $\lambda_i \in \mathbb{R}$, $i = 1, \dots, n$. This function is minimized for a sequence of suitable values of $(\lambda^k, \varepsilon^k)$, where ε^k is increasing and λ^k is obtained with some updating rule. In [15], the structure of the constraints in problem (6) has been exploited to get the closed expression (10) of the multipliers $\lambda_i(V)$ as a function of the variables v . Replacing the multipliers λ_i with the closed expression $\lambda_i(V)$ in the augmented Lagrangian function $\mathcal{L}(V, \lambda; \varepsilon)$ and fixing the penalty parameter to a value $\bar{\varepsilon} > 0$, they get an exact penalty function

$$P(V) = Q \bullet VV^T + \sum_{i=1}^n \lambda_i(V) (\|v_i\|^2 - 1) + \frac{1}{2\bar{\varepsilon}} \sum_{i=1}^n (\|v_i\|^2 - 1)^2.$$

In this case a single unconstrained minimization of the twice continuously differentiable function $P(V)$ is enough to find a stationary point of problem (6). Computational experiments with the resulting algorithmic scheme, called EXPA in [15], showed that this unconstrained approach compares favorably with the best codes available in literature. More recently, Journée et al. in [21] use a trust region method for optimizing over a manifold [1], which relies on a particular quotient manifold. Their algorithm is defined for a slightly more general problem than (1) since they consider a generic convex objective function and general linear constraints. Their method relies on exploiting the special structure of the constraints to find a closed expression of the multipliers, which in the special case of problem (6) returns the same expression found in [15].

However, the original idea of an unconstrained formulation of problem (1) goes back to Homer and Peinado [18], where the change of variables $X_{ij} = v_i^T v_j / \|v_i\| \|v_j\|$ for the elements of X with $v_i \in \mathbb{R}^n$, $i = 1, \dots, n$ has been used to formulate an unconstrained optimization problem equivalent to the original problem (6). Their approach led to a problem of dimension n^2 which was solved by a parallel gradient method, but turned out to be impractical for large values of n .

In [5] the unconstrained formulation proposed by Homer and Peinado has been resumed and combined it with the “low rank idea”, by introducing the change of variables $X_{ij} = v_i^T v_j / \|v_i\| \|v_j\|$ where $v_i \in \mathbb{R}^r$, $i = 1, \dots, n$, with $r < n$. The resulting unconstrained problem (7) was solved to obtain a solution of problem (5). The practical performance of the resulting algorithm, that

we called, SDPLR-MC was pretty good, but the underlying convergence theory was not deeply investigated. Indeed, it is easy to show that problem (7) is equivalent to problem (5) in the sense that a one-to-one correspondence among local/global/stationary point of the two problems can be stated (see [13]). However, problem (7) presents some peculiarities that make standard convergence results not immediately applicable. Indeed, standard unconstrained algorithms can be proved to be globally convergent if the objective function is continuously differentiable and has compact level sets. Function $f_r(v)$ is not even defined at points where $\|v_i\| = 0$ for at least one index i . In principle, it is possible to modify standard algorithms by looking not at the sequence $\{(v_1, \dots, v_n)^k\}$ but at the normalized sequence $\{(v_1/\|v_1\|, \dots, v_n/\|v_n\|)^k\}$. However, this may cause difficulties in proving convergence of standard optimization algorithms.

In this paper we propose to modify f_r in such a way to get an unconstrained problem that can be solved by standard methods. In particular, we add a shifted barrier penalty term

$$\sum_{i=1}^n \frac{(\|v_i\|^2 - 1)^2}{d(v_i)}, \quad (12)$$

where

$$d(v_i) \equiv \delta^2 - (1 - \|v_i\|^2)_+^2, \quad 0 < \delta < 1. \quad (13)$$

For a fixed $\varepsilon > 0$, we consider the unconstrained minimization problem

$$\min_v \left\{ f_\varepsilon(v) = f_r(v) + \frac{1}{\varepsilon} \sum_{i=1}^n \frac{(\|v_i\|^2 - 1)^2}{d(v_i)}, v \in S_\delta \right\}, \quad (14)$$

where $f_r(v)$ is given in (7) and the open set S_δ is defined as

$$S_\delta \equiv \{v \in \mathbb{R}^{nr} : \|v_i\|^2 > 1 - \delta, \quad i = 1, \dots, n\}.$$

The added term (12) ensures that the level sets of f_ε are contained in the set S_δ and are compact. Hence, problem (14) allows us to overcome all the theoretical drawbacks of problem (7). In particular, we will show that solving problem (14) for a single value of ε is equivalent to solving problem (6).

We start by investigating the theoretical properties of the function $f_\varepsilon(v)$. Function $f_\varepsilon(v)$ is continuously differentiable on the open set S_δ with gradient

$$\nabla_{v_i} f_\varepsilon(v) = \nabla_{v_i} f_r(v) + \frac{4}{\varepsilon} \frac{(\|v_i\|^2 - 1)}{d(v_i)} \left[1 - \frac{(\|v_i\|^2 - 1)(1 - \|v_i\|^2)_+}{d(v_i)} \right] v_i$$

where

$$\nabla_{v_i} f_r(v) = \frac{2}{\|v_i\|} \left[\sum_{j=1}^n q_{ij} \left(I_r - \frac{v_i v_i^T}{\|v_i\| \|v_i\|} \right) \frac{v_j}{\|v_j\|} \right].$$

The first important property is the compactness of the level sets of function $f_\varepsilon(v)$, that guarantees the existence of a solution of problem (14).

Proposition 6. For every given $\varepsilon > 0$ and for every given $v^0 \in S_\delta$, the level sets $\mathcal{L}_\varepsilon(v^0) = \{v \in S_\delta : f_\varepsilon(v) \leq f_\varepsilon(v^0)\}$ are compact and

$$\mathcal{L}_\varepsilon(v^0) \subseteq \{v \in \mathbb{R}^{nr} : \|v_i\|^2 \leq C(\varepsilon\delta), \quad i = 1, \dots, n\},$$

with $C(\varepsilon\delta) > 0$ positive constant depending from ε and δ .

The proof can be found in Appendix 14.

An interesting property of the objective function $f_r(v)$ of problem (7) is that, given a point v in S_δ , its gradient with respect to v_i is orthogonal to the vector v_i , namely, for every $v \in S_\delta$ and for every $i = 1, \dots, n$

$$v_i^T \nabla_{v_i} f_r(v) = 2 \left[\sum_{j=1}^n q_{ij} \left(\frac{v_i^T}{\|v_i\|} - \frac{v_i^T v_i}{\|v_i\|^2} \frac{v_i^T}{\|v_i\|} \right) \frac{v_j}{\|v_j\|} \right] = 0. \quad (15)$$

The following theorem states the equivalence between stationary points, local/global minimizers of (14) and the corresponding stationary points, local/global minimizers of (6).

Theorem 7 (Exactness properties of (14)). For any $\varepsilon > 0$ and for any fixed $r \geq 1$, the following correspondences hold:

- (i) a point $\hat{v} \in \mathbb{R}^{nr}$ is a stationary point of problem (14) if and only if it is a stationary point of problem (6).
- (ii) a point $\hat{v} \in \mathbb{R}^{nr}$ is a global minimizer of problem (14) if and only if it is a global minimizer of problem (6).
- (iii) a point $\hat{v} \in \mathbb{R}^{nr}$ is a local minimizer of problem (14) if and only if it is a local minimizer of problem (6).

Proof. First, we recall that, for every $v \in S_\delta$, $v_i \neq 0$ for all $i = 1, \dots, n$. Furthermore, by definition of $\nabla_{v_i} f_\varepsilon$ and by (15), we get for every v_i and for $i = 1, \dots, n$

$$v_i^T \nabla_{v_i} f_\varepsilon(v) = \frac{4(\|v_i\|^2 - 1)v_i^T v_i}{\varepsilon d(v_i)} \left(1 - \frac{(\|v_i\|^2 - 1)(1 - \|v_i\|^2)_+}{d(v_i)} \right).$$

Therefore we get, if $\|v_i\|^2 \geq 1$,

$$v_i^T \nabla_{v_i} f_\varepsilon(v) = \frac{4(\|v_i\|^2 - 1)\|v_i\|^2}{\varepsilon \delta^2}, \quad (16)$$

otherwise

$$v_i^T \nabla_{v_i} f_\varepsilon(v) = \frac{4(\|v_i\|^2 - 1)\|v_i\|^2}{\varepsilon d(v_i)} \left(1 + \frac{(\|v_i\|^2 - 1)^2}{d(v_i)} \right). \quad (17)$$

Furthermore, if $v \in \mathcal{F}$

$$\begin{aligned} f_\varepsilon(v) &= f_r(v) = q_r(v) & (18) \\ \nabla_{v_i} f_\varepsilon(v) &= 2 \sum_{j=1}^n q_{ij} (I_r - v_i v_i^T) v_j, \quad i = 1, \dots, n. & (19) \end{aligned}$$

Now we can prove the three statements.

(i) *Sufficiency.* Let \hat{v} be a stationary point for problem (6). Therefore \hat{v} satisfies (11) and $\hat{v} \in \mathcal{F}$. Then (19) implies

$$\nabla_{v_i} f_\varepsilon(\hat{v}) = 2 \sum_{j=1}^n q_{ij} (I_r - \hat{v}_i \hat{v}_i^T) \hat{v}_j = 0, \quad i = 1, \dots, n.$$

(i) *Necessity.* By (16) and (17), $\hat{v} \in S_\delta$ being a stationary point of f_ε implies $\hat{v} \in \mathcal{F}$. Hence, as a result of (19), \hat{v} is stationary point also for problem (6).

(ii) *Necessity.* By Proposition 6, the function f_ε admits a global minimizer \hat{v} , which is obviously a stationary point of f_ε and hence we have that $\hat{v} \in \mathcal{F}$, so that $f_\varepsilon(\hat{v}) = q_r(\hat{v})$. We proceed by contradiction. Assume that a global minimizer \hat{v} of f_ε is not a global minimizer of problem (6). Then there exists a point $v^* \in \mathcal{F}$, global minimizer of problem (6), such that

$$f_\varepsilon(\hat{v}) = q_r(\hat{v}) > q_r(v^*) = f_\varepsilon(v^*),$$

but this contradicts the assumption that \hat{v} is a global minimizer of f_ε .

(ii) *Sufficiency.* True by similar arguments.

(iii) *Necessity.* Since \hat{v} is a local minimizer of f_ε , it is a stationary point of f_ε , so that $\hat{v} \in \mathcal{F}$. Thus, $f_\varepsilon(\hat{v}) = q_r(\hat{v})$. Since \hat{v} is a local minimizer of f_ε , there exists a $\rho > 0$ such that for all $v \in S_\delta \cap B_\rho(\hat{v})$ such that

$$q_r(\hat{v}) = f_\varepsilon(\hat{v}) \leq f_\varepsilon(v).$$

Therefore, by using (18), for all $v \in v \in \mathcal{F} \cap B_\rho(\hat{v})$ we have that

$$q_r(\hat{v}) \leq f_\varepsilon(v) = q_r(v).$$

and hence \hat{v} is a local minimizer for problem (6).

(iii) *Sufficiency.* Since $\hat{v} \in \mathcal{F}$ and is a local minimizer of (6), there exists a $\rho > 0$ such that for all $v \in \mathcal{F} \cap B_\rho(\hat{v})$

$$q_r(\hat{v}) = f_\varepsilon(\hat{v}) \leq q_r(v) = f_\varepsilon(v).$$

We want to show that there exists γ such that for all $v \in S_\delta \cap B_\gamma(\hat{v})$ we get

$$f_\varepsilon(\hat{v}) \leq f_\varepsilon(v).$$

It is sufficient to show that there is a $\gamma > 0$ such that for all $v \in S_\delta \cap B_\gamma(\hat{v})$, we have that $p(v) \in B_\gamma(\hat{v})$, where

$$p(v) \equiv \begin{pmatrix} \frac{v_1}{\|v_1\|} \\ \vdots \\ \frac{v_n}{\|v_n\|} \end{pmatrix}.$$

Actually in this case we have

$$q_r(\hat{v}) = f_\varepsilon(\hat{v}) \leq q_r(p(v)) = \overline{f_\varepsilon}(p(v)) \leq f_\varepsilon(v).$$

It is well known that, given any point $x \neq 0 \in \mathbb{R}^n$, its projection over the unit norm set is simply $\frac{x}{\|x\|}$. Hence, for any $\gamma \leq \frac{\rho}{2}$ we can write

$$\begin{aligned} \|p(v) - \hat{v}\|^2 &= \sum_{i=1}^n \left\| \hat{v}_i - \frac{v_i}{\|v_i\|} \right\|^2 = \sum_{i=1}^n \left\| \hat{v}_i - \frac{v_i}{\|v_i\|} + v_i - v_i \right\|^2 \\ &\leq \sum_{i=1}^n \left(\|\hat{v}_i - v_i\|^2 + \left\| v_i - \frac{v_i}{\|v_i\|} \right\|^2 + 2\|\hat{v}_i - v_i\| \left\| v_i - \frac{v_i}{\|v_i\|} \right\| \right) \\ &\leq \sum_{i=1}^n 4\|\hat{v}_i - v_i\|^2 = 4\|\hat{v} - v\|^2 \leq 4\gamma^2 \leq \rho^2 \end{aligned}$$

Therefore, for a proper γ , we have for all $v \in S_\delta \cap B_\gamma(\hat{v})$

$$f_\varepsilon(\hat{v}) \leq f_\varepsilon(v),$$

so that \hat{v} is a local minimum also for (14). \square

Theorem 7 states a tight relation between problem (14) and (6) and hence allows us to solve problem (6) by minimizing $f_\varepsilon(v)$. We stress that all the properties of problem (14) hold for any given $\varepsilon > 0$.

Proposition 7 implies that we can solve problem (6) by solving problem (14), and Proposition 6 implies that any standard global convergent unconstrained minimization method can be used for solving it (see, e.g., [4] for a complete review of unconstrained algorithms). Since $f_\varepsilon(v)$ is continuously differentiable over the set S_δ and, by Proposition 6, it has compact level sets, by applying a convergent unconstrained procedure, we can easily state the following convergence result.

Proposition 8. *Let r be given and $v^0 \in \mathcal{F}$. Assume we apply to problem (14) any unconstrained procedure that produces a sequence $\{v^k\}$ such that (i) v^k stays in the initial level set, (ii) it admits at least an accumulation point, (iii) every accumulation point is a stationary point of the objective function. Then*

- (i) $\{v^k\}$ is bounded and it admits at least an accumulation point;
- (ii) every accumulation point is a stationary point of problem (6);
- (iii) if \hat{v} is an accumulation point then $q_r(\hat{v}) \leq q_r(v^0)$.

Proof. Function $f_\varepsilon(v)$ is continuously differentiable over the set S_δ and Proposition 6 implies that it has compact level sets. Therefore the assumptions made on the unconstrained procedure imply that it produces a sequence that has at least an accumulation point and all the accumulation points are stationary points of problem (14). Finally, Theorem 7 implies that the stationary points of f_ε are stationary points of problem (6), and we have

$$q_r(\hat{v}) = f_\varepsilon(\hat{v}) \leq f_\varepsilon(v^0) = q_r(v^0).$$

□

9 SpeedP: an efficient algorithm for solving the SDP problem

In this section, we define an algorithm for solving problem (1) that exploits the results stated in the previous sections.

In Section 2 we have seen that for $r \geq r_{\min}$ a global solution of problem (6) provides a solution of problem (1). Moreover, Proposition 7 states a complete correspondence between problems (6) and (14). Finally, Proposition 8 ensures that we can find a stationary point of problem (14) by applying any global convergent unconstrained minimization procedure.

In our algorithm we select a nonmonotone gradient method defined by an iteration of the form

$$v_i^{k+1} = v_i^k - \alpha^k \nabla_{v_i} f_\varepsilon(v^k) \quad i = 1, \dots, n, \quad (20)$$

where $\alpha^k > 0$ is obtained by a suitable line-search procedure satisfying

$$f_\varepsilon(v^{k+1}) \leq f_\varepsilon(v^0), \quad (21)$$

with $v^0 \in \mathcal{F}$.

This choice is motivated by the fact that, using a gradient method and for ε sufficiently large, the produced sequence stays in the set $\{v \in \mathbb{R}^{nr} : \|v_i\|^2 \geq 1, i = 1, \dots, n\}$. This result implies that the barrier term (12), that may affect negatively the performance behavior of any optimization method when the produced sequence gets closer to the boundary of S_δ , reduces simply to a penalty term on the feasibility of problem (6).

In particular, the following proposition holds whose proof can be found in Appendix 14.

Proposition 10. *Let $v^0 \in \mathcal{F}$ and let $\{v^k\}$ be the sequence generated with the iterative scheme (20), where each α^k satisfies (21) and $\alpha^k \leq \alpha_M$. Then, there exists $\bar{\varepsilon} > 0$ such that, for any $\varepsilon \geq \bar{\varepsilon}$, we have for $k = 1, 2, \dots$*

$$\|v_i^k\| \geq 1, \quad i = 1, \dots, n.$$

The value of r_{\min} is not known. In principle, the only value of r that can be calculated and that guarantees the correspondence between solutions of (1) and global solutions of (6), is \hat{r} as defined in (8). However, this value is usually larger than the actual value needed to obtain a solution of problem (1). Hence, following the idea in [5] and [15], we choose $r \ll \hat{r}$, and use the global optimality condition of Proposition 3 to prove optimality. We use an incremental rank scheme as in algorithm EXPA defined in [15].

ALGORITHM SpeedP

Initialization. Set integers $2 \leq r^1 < r^2 < \dots < r^p$ with $r^p \in [\hat{r}, n]$ where \hat{r} is given by (8). Choose $\bar{\varepsilon} > 0$, $\bar{\delta} \in [0, 1]$ and $tol_\varepsilon > 0$.

For $j = 1, \dots, p$ **do:**

S.0 Set $r = r^j$ in problem (5).

S.1 Starting from $V^0 \in \mathbb{R}^{n \times r^j}$, find a stationary point $\hat{V} \in \mathbb{R}^{n \times r^j}$ of problem (14) with $\varepsilon = \bar{\varepsilon}$ and $\delta = \bar{\delta}$.

S.2 Compute $\lambda(\hat{V})$ with (10) and the minimum eigenvalue $\lambda_{\min}(\hat{V})$ of $Q + \text{Diag}(\lambda(\hat{V}))$.

S.3 If $\lambda_{\min}(\hat{V}) \geq -tol_\varepsilon$, then exit.

Return $\hat{V} \in \mathbb{R}^{n \times r^j}$ and $\lambda_{\min}(\hat{V})$

SpeedP returns \hat{V} , and $\lambda_{\min}(\hat{V})$. If $\lambda_{\min}(\hat{V}) \geq -tol_\varepsilon$, then the matrix $Q + \text{Diag}(\lambda(\hat{V}))$ is positive semidefinite within a tolerance tol_ε so that a solution of problem (1) is obtained as $X^* = \hat{V}\hat{V}^T$. If the optimality condition is not met, namely $\lambda_{\min}(\hat{V}) < -tol_\varepsilon$, a bound can be easily computed. Indeed, since $(\lambda(\hat{V}) + \lambda_{\min}(\hat{V}))e$ is feasible for the dual problem (4), the value $z_{LB} = Q \bullet \hat{V}\hat{V}^T + n\lambda_{\min}(\hat{V})$, provides a lower bound on the solution of problem (1) (see, e.g, [27], [15]).

In practice, however, in all the computational experiments performed the stopping condition $\lambda_{\min}(\hat{V}) \geq -tol_\varepsilon$ was always met with satisfactory accuracy, so that SpeedP always converged to a solution of (1), as we will illustrate in the Section 12.

11 SpeedP-MC: a heuristic for large scale Max-Cut

Our heuristic is essentially the one due to Goemans and Williamson and described in [12], integrated with SpeedP and a few simple details.

The Goemans-Williamson algorithm is very well known and actually contributed to making SDP techniques popular; nevertheless, we briefly outline it here for the sake of completeness.

Let X be the optimal solution to (1), $-z_P$ be its optimal value (for the Max-Cut problem the objective function has to be maximized), and let $v_1, v_2, \dots, v_n \in \mathbb{R}^r$ be vectors whose Gramian matrix coincides with X . Let $h^T x = 0$ define a hyperplane of \mathbb{R}^r generated by drawing the value of the r components of h from a uniform random distribution. Then the algorithm outputs the node bipartition $(S, V \setminus S)$ where $S = \{i : h^T v_i \geq 0\}$.

We assume here that all components of the weighted adjacency matrix A of G are non-negative. The expected weight \overline{W} of the cut defined by the bipartition $(S, V \setminus S)$ is given by

$$\overline{W} = \sum_{i \in S, j \notin S} A_{ij} p_{ij},$$

where p_{ij} is the probability that edge ij belongs to the cut or, equivalently, the probability that v_i and v_j lay on opposite sides with respect to the hyperplane defined by $h^T x = 0$. Such a probability is proportional to the angle defined by the two vectors. Finally, using the inequality $\arccos(\alpha)/\pi \geq 0.87856(1 - \alpha)/2$, we can write

$$\overline{W} = \sum_{ij} A_{ij} \frac{\arccos(v_i^T v_j)}{\pi} \geq 0.87856 \sum_{ij} A_{ij} \frac{1 - v_i^T v_j}{2} = 0.87856 z_P.$$

In conclusion the gap (in percentage with respect to the SDP bound) obtained by using the relaxation (1) and the Goemans-Williamson algorithm is around 12.1%.

Once the SDP bound has been computed, the main computational effort of the Goemans-Williamson algorithm, is essentially devoted to finding the vectors v_i , with $i = 1, \dots, n$. This task can be accomplished by a truncated Cholesky decomposition of the matrix X which requires time proportional to n^3 and space proportional to n^2 . Therefore the algorithm cannot be applied to very large instances with size, say, of the order of one hundred thousand nodes.

To the contrary, **SpeedP** makes it possible to apply the Goemans-Williamson approximation algorithm to very large graphs since on the one hand it is able to solve problem (1) in reasonable time also for very large graphs, and on the other hand, it outputs the vectors v_i , avoiding the need of a Cholesky factorization. In our procedure the cut provided by the Goemans-Williamson algorithm is then improved by means of a 1-opt local search, where all possible moves of a single vertex to the opposite set of the partition are checked and moved are made until no further improvement is possible.

In [8], where a similar heuristic is described but problem (1) is solved by interior point algorithm, a particularly successful step is proposed to further improve on the solution. The whole procedure is repeated a few times where the solution matrix X of problem (1) is replaced by the convex combination $X' = \alpha X + (1 - \alpha) \hat{x} \hat{x}^T$, $0 < \alpha < 1$, where \hat{x} is the representative vector of the current best cut. The idea behind this step is to bias the Goemans-Williams

rounding with the current best cut, or put it differently, to force the rounding procedure to generate a cut in a neighborhood of the current best solution.

This step does not require to solve problem (1) again, but needs the Cholesky factorization of the matrix X' .

We use a similar technique in our procedure. However, to avoid the Cholesky factorization, which is not suitable for very large instances, we solve a new problem (1) after perturbing the objective function. Matrix Q is replaced by the perturbed matrix Q' given by $Q' = Q + \beta \hat{x} \hat{x}^T$ with $\beta > 0$.

Such a perturbation has again the effect of moving the solution of problem (1) and hence of the Goemans-Williamson rounding, towards a neighborhood of the current best integral solution. With the new objective function Q' we solve problem (1) with **SpeedDP** and repeat the rounding and the 1-opt improvement as well. The whole procedure is repeated a few times with different values of β .

Summarizing, the scheme of our heuristic algorithm is as follows:

ALGORITHM SpeedDP-MC

Data: Q , $\hat{x} = e$, $\alpha > 0$, k_{\max} , $\bar{Q} = \sum_{i,j} |Q_{ij}|/|E|$.

For $k = k_{\max}, \dots, 0$ **do** :

S.0 Set $\beta = k\alpha\bar{Q} \cdot J$ and $Q' = Q + \beta(\hat{x}\hat{x}^T)$

S.1 Apply **SpeedDP** to problem (1) with $Q = Q'$ and let v_i , $i = 1, \dots, n$ be the returned solution and the valid bound ϕ on problem (3) with objective function corresponding to Q' .

S.2 Apply the Goemans-Williamson hyperplane rounding technique to the vectors v_i , $i = 1, \dots, n$. This gives a bipartition representative vector \bar{x} .

S.3 Apply the 1-opt improvement to \bar{x} . This gives a new bipartition representative vector \tilde{x} . If $Q' \bullet \tilde{x}\tilde{x}^T < Q' \bullet \hat{x}\hat{x}^T$, set $\hat{x} = \tilde{x}$.

Return Best cut \hat{x} , lower bound $-Q' \bullet \hat{x}\hat{x}^T$, upper bound ϕ .

Note that the amount of perturbation decreases when the iteration counter increases, getting to zero in the last iteration. We stress that Step 1 is not expensive since we use a warm start technique: at each iteration we start **SpeedDP** from the solution found at the previous step, so that each minimization is computationally cheaper than the first one.

Besides the ability of treating graphs of very large sizes, another advantage of **SpeedDP-MC** is that it also provides a solution with a guaranteed optimality error bound, since it outputs an upper and lower bound on the value of the optimal cut.

Numerical results for this heuristic are reported in next section.

12 Numerical Results

In this section, we describe our computational experience both with algorithm **SpeeDP** for solving problem (1), and with the heuristic based on it for finding good cuts for large graphs.

SpeeDP is implemented in Fortran 90 and all the experiments have been run on a PC with processor Core2 DUO E6750 2.66Ghz, and RAM of 2.00 GB.

The parameter δ that appears in the definition of the open set S has been set to 0.25. This value has been chosen after some experiments for different values of δ . The parameter ε is set equal to $10^3/\delta$ for all the tests.

As unconstrained optimization procedure we use a Fortran 90 implementation of the non monotone Barzilai-Borwein gradient method proposed in [16] which falls in the iterative scheme (20), (21) and satisfies the assumption of Proposition 8. The termination criteria in the minimization procedure are standard ones with tolerance in the range 10^{-5} .

As for the choice of the starting value r^1 of the rank we use the same values as in [15], reported in Table 1. The values of the rank r^j are chosen with the simple rule $r^{j+1} = \min \{ \lfloor r^j \cdot 1.5 \rfloor, \hat{r} \}$ where \hat{r} is given in (8).

$n \leq 200$	$200 < n$ $n \leq 800$	$800 < n$ $n \leq 1000$	$1000 < n$ $n \leq 5000$	$5000 < n$ $n \leq 20000$	$n > 20000$
8	10	15	18	25	30

Table 1: Values of r^1 depending on the dimension of the problem.

In order to check positive semidefiniteness of $Q + \text{Diag}(\lambda(\hat{V}))$, we use the ARPACK subroutines `dsaupd` and `dseupd` to compute the minimum eigenvalue of this matrix. We set the tolerance $tol_\varepsilon = -10^{-3}$.

As a first step, we consider **SpeeDP** for solving problem (1). We compare the performance of **SpeeDP** with the best codes in literature in the main classes of methods for solving problem (1): interior point methods, Spectral Bundle methods and low rank NLP methods.

As an interior point method we select the dual-scaling algorithm defined in [3] and implemented in the software **DSDP**(version 5.8) downloaded from the web page <http://www-unix.mcs.anl.gov/DSDP/>. **DSDP** is considered particularly efficient for solving problems where the solution is known to have low rank (as it is the case for Max-Cut instances), since it exploits low-rank structure and sparsity in the data. Further, **DSDP** has relatively low memory requirements for an interior-point method, and is indeed able to solve instances up to 10 000 nodes. We also include the Spectral Bundle method **SB** can be found in [17] and downloadable <http://www-user.tu-chemnitz.de/~helmberg/>.

Among the NLP based methods, we choose as a term of comparison the code **SDPLR-MC**, proposed by Burer and Monteiro in [5] downloadable from the web page <http://dollar.biz.uiowa.edu/~burer/software/SDPLR-MC>, and **EXPA** proposed in [15].

Both **EXPA** and **SDPLR-MC** have a structure similar to **SpeeDP**. Indeed, the main scheme differs in the way of finding a stationary point for problem (6).

For any fixed value of r , EXPA uses the nonmonotone Barzilai-Borwein gradient proposed in [16] (the same one used in `SpeedP`) to minimize an exact penalty function for (6). SDPLR–MC uses an L-BFGS method to obtain a stationary point of (7). We remark again that SDPLR–MC does not certify global optimality of the produced solution in the sense that it does not check the global optimality condition $Q + \text{Diag}(\lambda(\widehat{V})) \succeq 0$, while both EXPA and `SpeedP` do it.

We do not include in our comparison neither the code SDPLR defined in [5] nor the manifold optimization method `GenRTR` defined in [21]. Indeed the computational results in [5] show that SDPLR–MC outperforms SDPLR on the Max-Cut problem. Further, in [21] the authors report a comparison of a matlab implementation of `GenRTR` and SDPLR on some Max-Cut instances which are a subset of those used as benchmark set here and in [15]. Although the direct comparison in terms of computational time is not really fair, the authors stated that the two methods, `GenRTR` and SDPLR, may be considered to have comparable performances. Since SDPLR is always worse than SDPLR–MC, this implies that on the special structured problem (1) that comes out from Max-Cut, `GenRTR` should have worse performances than SDPLR–MC.

Our benchmark set consists in standard instances of the Max-Cut problem, with number of nodes ranging from 100 to 20 000, with different degrees of sparsity. The first set of problems belongs to the SDPLIB collection of semidefinite programming test problems (hosted by B. Borchers) that can be downloaded from the web page <http://infohost.nmt.edu/~sdplib>. The smallest problems (mcp set) have been contributed by Fujisawa [9], while the maxG problems were supplied by Benson [3]. The second set of problems belongs to the Gset of randomly generated problems by means of a machine-independent graph generator *rudy* [26]. These problems can also be downloaded from Burer’s web page <http://dollar.biz.uiowa.edu/~burer/software/SDPLR>.

`SpeedP`, EXPA, SDPLR–MC, and SB solve all the test problems, whereas DSDP runs out of memory on the two largest problems (G77 and G81 of the Gset collection). Hence we eliminate these two test problems in the comparison with DSDP.

We compare the different codes on the basis of the level of accuracy and of the computational time.

As for the accuracy, we report in Table 2 the primal and/or dual objective function value obtained by the five methods on all the instances. We note that SDPLR–MC only reports the primal objective value, while SB produces a value of the dual objective function that is a bound on the optimal value of problem (1). Similarly, for `SpeedP` we report the primal objective function value, and the dual, where the dual is obtained by adding $n\lambda_{\min}(Q + \text{Diag}(\lambda(\widehat{V})))$ to the primal value whenever $\lambda_{\min}(Q + \text{Diag}(\lambda(\widehat{V})))$ is negative.

As regards the computational time, in order to have a better flavor of the results, we follow the approach proposed in [7] and we draw the cpu time performance profile of the five methods. To be more precise, let p denote a particular problem and s a particular solver. The idea is to compare the performance of solver s on problem p with the best performance by any solver on this particular

	SpeedP		EXPA		SDPLR-MC		SB		DSDP	
	primal	dual obj	primal	dual	primal	dual	primal	dual	primal	dual
mcp100	226.157349	226.157303	226.15735	226.157394	226.15127	226.1592	226.15733	226.15735		
mcp124_1	141.990463	141.990494	141.99045	141.990402	141.99002	141.9937	141.99044	141.99048		
mcp124_2	269.880157	269.880890	269.88016	269.883087	269.88011	269.8822	269.88012	269.88017		
mcp124_3	467.750092	467.750092	467.75009	467.750092	467.75000	467.7537	467.75004	467.75012		
mcp124_4	864.411682	864.411682	864.41187	864.411926	864.41045	864.4156	864.41166	864.41187		
mcp250_1	317.264313	317.264313	317.26425	317.264313	317.26415	317.2708	317.26429	317.26435		
mcp250_2	531.930054	531.930115	531.92999	531.929993	531.92949	531.9349	531.92998	531.93009		
mcp250_3	981.172546	981.172607	981.17242	981.172424	981.17207	981.1780	981.17239	981.17257		
mcp250_4	1681.959595	1681.959595	1681.95960	1681.961426	1681.95581	1681.9750	1681.95995	1681.96011		
mcp500_1	598.148499	598.148499	598.14789	598.147888	598.14749	598.1588	598.14840	598.14852		
mcp500_2	1070.056152	1070.056152	1070.05615	1070.056152	1070.04501	1070.0759	1070.05660	1070.05677		
mcp500_3	1847.969971	1847.970093	1847.96936	1847.974731	1847.92925	1847.9836	1847.96947	1847.97003		
mcp500_4	3566.737549	3566.766357	3566.73779	3566.737793	3566.72863	3566.7479	3566.73765	3566.73806		
G01	12083.196289	12083.197266	12083.19727	12083.19727	12082.93730	12083.2650	12083.19640	12083.19770		
G60	15222.267578	15222.267578	15222.25488	15222.25488	15221.90950	15223.1930	15222.25710	15222.26810		
G11	629.146118	629.146118	629.14722	629.147217	629.15795	629.1701	629.16472	629.16478		
G14	3191.564209	3191.656982	3191.56567	3192.163574	3191.55893	3191.5847	3191.56609	3191.56681		
G22	14135.945312	14136.145508	14135.94336	14135.97754	14135.77440	14136.0440	14135.94470	14135.94570		
G32	1567.605591	1567.605591	1567.59265	1567.592651	1567.61532	1567.6519	1567.63942	1567.63965		
G35	8014.738770	8014.738770	8014.73584	8014.766602	8014.55729	8014.8070	8014.73758	8014.73972		
G36	8005.962891	8005.962891	8005.95850	8007.056152	8005.91627	8006.0213	8005.96316	8005.96379		
G43	7032.221680	7032.221680	7032.21973	7032.223145	7032.19023	7032.2749	7032.22079	7032.22185		
G48	5999.998047	6000.000000	5999.99561	5999.995605	5999.79596	6000.0000	5999.99852	6000.00000		
G51	4006.247559	4006.248291	4006.25391	4006.253906	4006.21749	4006.2745	4006.25460	4006.25553		
G52	4009.634766	4009.672363	4009.63696	4009.645264	4009.60292	4009.6574	4009.63834	4009.63877		
G55	11039.45898	11039.45898	11039.44922	11039.44922	11039.20140	11040.1590	11039.44910	11039.46050		
G57	3885.31787	3885.317871	3885.33887	3885.338867	3885.36524	3885.5197	3885.48675	3885.48917		
G58	20136.17383	20136.17383	20136.16992	20141.125	20135.59150	20136.2870	20136.18060	20136.18980		
G62	5430.506348	5430.506348	5430.79688	5430.796875	5430.72287	5430.9512	5430.90837	5430.91042		
G63	28244.353516	28244.458984	28244.30664	28260.37695	28243.63720	28244.5770	28244.40560	28244.41790		
G64	10465.827148	10469.678711	10465.87891	10472.86621	10465.82000	10465.9700	10465.89790	10465.90440		
G65	6205.268555	6205.268555	6205.32861	6205.328613	6205.28798	6205.5822	6205.53219	6205.53820		
G66	7076.871582	7076.871582	7076.92676	7076.926758	7076.93516	7077.2640	7077.20904	7077.21373		
G67	7744.033203	7744.033203	7744.14697	7744.146973	7744.06409	7744.4942	7744.42783	7744.43649		
G70	9861.485352	9861.485352	9861.48340	9861.483398	9861.24740	9861.7747	9861.51431	9861.52455		
G72	7808.015137	7808.015137	7808.04541	7808.04541	7808.16545	7808.5914	7808.53427	7808.53926		
G77	11044.382812	11044.983398	11045.36621	11045.36621	11045.08100	11045.7510	****	****		
G81	15655.122070	15655.122070	15655.44238	15655.44238	15655.12500	15656.2790	****	****		

Table 2: Objective function values obtained by the three NLP based methods, SB and DSDP

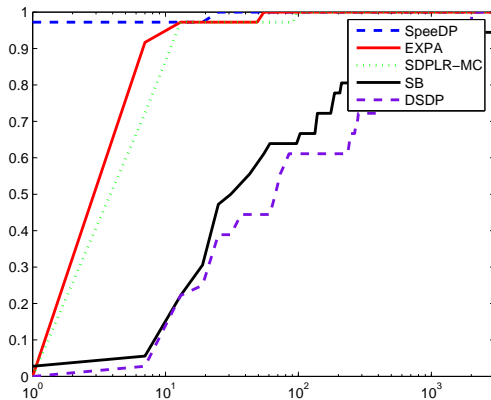


Figure 1: Comparison between NLP based methods, SB and DSDP

problem. To this aim, consider the performance ratio

$$r_{p,s} = \frac{t_{p,s}}{\min\{t_{p,s'} : s' \in S\}},$$

where $t_{p,s}$ is the CPU time in seconds needed by solver s to solve problem p . Given this performance ratio, a cumulative distribution function $\rho_s(\tau)$ is defined as:

$$\rho_s(\tau) = \frac{1}{n_p} \text{size}\{p \in P : r_{p,s} \leq \tau\}.$$

We draw $\rho_s(\tau)$ with respect to τ , that is reported on the x-axis in a logarithmic scale.

In the picture, the higher the method the better, and the efficiency is measured by how fast the method reaches the value of 1 (since all the methods solve all the problems, all the methods reach the performance value 1 allowing a sufficiently large τ).

In Figure 1 we compare all the five methods on the test problems solved by all of them (i.e. all the problems except G77 and G80).

In Figure 2, we report the comparison among the three low rank based methods and SB on all the test problems. It emerges from the profiles that SpeedP outperforms the other methods.

Finally, we report the numerical results obtained by the heuristic described in Section 11 on some large random graphs. We used the graph generator *rudyl* [26] to define instances with growing dimension and density and different weights. We first considered graphs with number of nodes n equal to $500 + i \cdot 250$, for $i = 0, \dots, 8$ and with edge *density* equal to $10\% + i \cdot 10\%$ for $i = 0, \dots, 9$. For each pair $(n, \text{density})$ we generated three different graphs with positive weights ranging between 1 and 100. In Table 3 we report in each row the average values on the three problems in each class of CPU time, cut value, gap %, and the value

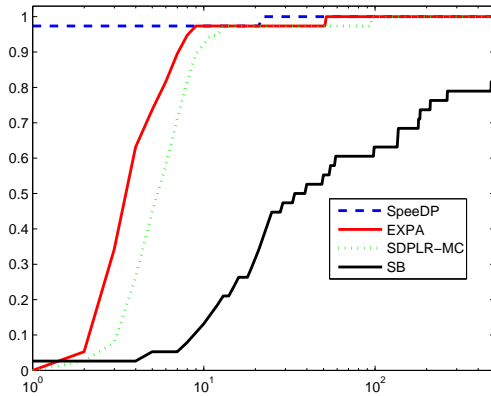


Figure 2: Comparison among the NLP based methods, and **SB**

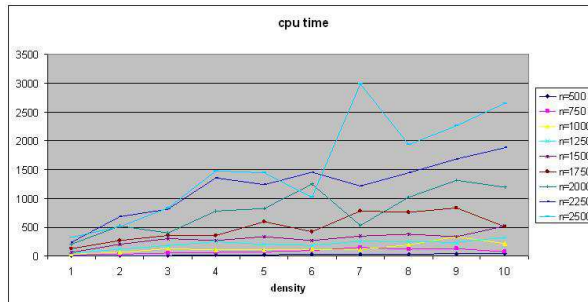


Figure 3: Average CPU time of the heuristic on the random graphs

$0.87856 \times (\text{upper bound})$, which represents the expected value of the Goemans-Williamson algorithm. We also draw in Figure 3 the average CPU time as a function of the density of the graph. As it emerges from the figure and the table, the heuristic is able to produce a good cut in a small amount of time, and as expected the performance of the heuristic is better on sparse graphs in term of time, but the gap decreases when the density of the graph increases.

Furthermore, we consider huge graphs, in order to verify how far we can go with the number of nodes. For this set of instances we run **SpeedP** on a machine with 6G of RAM.

We generate three random graphs with 100 001 nodes, 7 050 827 edges and different weights. The results are in Table 4 where we report the ranges of the weights, the total time, the value of the bound, the best cut obtained and the % gap.

We also generated 6-regular graphs (3D toroidal grid graphs) with 1 030 301 nodes and 3 090 903 edges and different weights. The results are reported in

	cut	time	gap %	0.87856*ub
n=500				
	388004.6667	6.21666667	4.59566667	356550.8369
	730297.3333	8.36666667	3.42113333	663560.8102
	1063049	13.4	2.76106667	959739.3467
	1391196.333	18.6266667	2.39476667	1251519.1163
	1714089	19.3766663	1.99266667	1535937.3951
	2032992.333	36.21333233	1.75293333	1817416.2683
	2347809	27.9200033	1.5559	2094784.6522
	2661106	30.53333433	1.29536667	2368226.2755
	2971604.333	44.373333	1.0805	2638941.8736
	3279198.333	47.4766667	0.88096667	2906354.3058
n=750				
	846281.6667	19.56000067	3.95533333	772917.3149
	1602525.667	34.23999967	3.0752	1451210.8624
	2344842.667	52.066667	2.40793333	2109690.0815
	3075792	62.92333367	2.038	2757341.3049
	3800724.667	71.54666633	1.73516667	3397102.7666
	4515431.333	100.419998	2.21953333	4055145.0852
	5223831.667	154.16333	1.95116667	4679018.8875
	5932074	117.4766693	2.15896667	5324216.9517
	6632193.667	126.8666653	1.42106667	5909605.1404
	7324080.333	81.35666933	1.5842	6536586.5558
n=1000				
	1470304.333	27.2766667	3.84216667	1341381.6741
	2804656.667	60.929999	2.8092	2533278.8535
	4116964	129.2566707	2.23743333	3697925.6641
	5407801.667	109.0300037	1.90816667	4841737.4244
	6694033	109.6433357	1.63916667	5977511.9713
	7971429.333	115.23333	1.9694	7141286.9576
	9234082.333	115.013331	1.6857	8249405.7535
	10487245	194.3833363	1.93753333	9392157.2383
	11727142.33	341.6733297	1.63603333	10471585.0468
	12962878.33	220.37	1.03856667	11506962.7354
n=1250				
	2261240.667	55.766665	3.55536667	2057267.4313
	4338898	117.859998	2.58416667	3910489.3026
	6376438.667	180.5166627	2.10673333	5720104.4340
	8396040.667	250.316666	1.7218	7503431.5860
	10395843	205.3633373	3.4118	9444982.7083
	12378616	179.5900063	1.23963333	11010166.9265
	14350605	256.8466697	2.52263333	12925918.8415
	16314387.67	247.2799987	1.7555	14584779.8125
	18264800	243.693334	1.49526667	16286651.5669
	20200056	321.730001	1.5469	18021482.4997
n=1500				
	3220711	60.03666533	3.39463333	2925643.823
	6195972	203.75	2.44333333	5576536.602
	9128485.333	305.3333283	1.93263333	8174914.701
	12020693.33	267.9600067	1.6445	10734573.2
	14899393	338.5299987	1.35426667	13267285.67
	17760397.33	272.16333	2.6834	16022282.32
	20603549.33	347.5099997	2.34436667	18525817.52
	23430844.67	384.0266673	2.01643333	21000489.11
	26236188	341.8233337	1.70753333	23443644.4
	29026448	521.1066593	1.41456667	25862214.06
n=1750				
	4344770.667	125.839999	3.21623333	3939910.081
	8382268	270.2400007	2.3461	7537097.712
	12355222.33	362.8666637	1.85843333	11056530.88
	16297722.33	356.3966677	2.1337	14624054.96
	20215156.67	602.439992	1.85056667	18088909.05
	24101639.33	422.2233273	2.4925	21702521.8
	27971634	777.3833313	1.7368	25001570.83
	31820130	760.8966573	1.88133333	28481837.5
	35640165.33	832.783315	1.59156667	31810367.49
	39437790.67	515.2300007	1.31226667	35103136.57
n=2000				
	5630775.667	208.1233367	3.07266667	5098977.742
	10892119.33	516.519989	2.17603333	9777614.603
	16076290	400.5799963	3.12513333	14565327.62
	21216458.67	778.7866413	2.03626667	19019499.13
	26329037.33	828.900004	2.1775	23635357.9
	31404458	1246.920024	1.91546667	28119172.62
	36443104	535.9733173	2.04013333	32670659.3
	41470418.67	1019.960002	1.77756667	37081879.77
	46475704	1320.056641	1.5193	41452038.69
	51442052	1198.696635	1.2375	45754212.3
n=2250				
	7092778.333	239.7566683	2.9204	6413414.787
	13724521.67	681.0033367	2.14573333	12316544.65
	20282490	817.880005	1.6331	18110391.01
	26779226	1363.850026	1.3677	23848933.49
	33236806	1234.75002	2.1361	29824281.87
	39660752	1457.619995	1.3802	35325275.19
	46049029.33	1214.609985	1.92916667	41237316.29
	52409853.33	1443.710001	1.64633333	46803264.48
	58740968	1682.113363	1.40903333	52334639.59
	65042482.67	1877.176676	1.17176667	57813304.6
n=2500				
	8707864.333	326.813334	2.86613333	7869652.293
	16883800	512.99999	2.05923333	15138884.38
	24971508.67	834.2133483	2.19943333	22421516.56
	32984345.33	1475.053324	1.82393333	29507260.52
	40946184	1444.76001	2.44776667	36854243.7
	48873544	1019.210001	1.72533333	43679150.81
	56771676	2992.886719	1.48626667	50618557.71
	64627920	1933.013305	1.55836667	57664353.54
	72453770.67	2257.273397	1.35233333	64515830.64
	80230896	2650.269979	0.90563333	71126099.68

Table 3: Random graphs with weights in $[1, 100]$ and density from 10% to 100%

Weights	Total CPU time	Upper Bound	Best Cut	gap%
1	15 043.98	4 113 227.8	3 959 852	3.87
[1, 100]	15 142.22	212 076 831.2	203 236 495	4.35
[-1000, 1000]	15 919.40	21 006 071 437.9	20 129 935 523	4.35

Table 4: Random sparse graphs with 100 001 nodes and 7 050 827 edges

Weights	Total CPU time	Upper Bound	Best Cut	gap%
1	4 723	3 090 133	3 060 300	0.97
[1, 10]	22 042	15 454 739	15 338 007	0.76
[1, 1000]	29 072	1 545 550 679	1 534 441 294	0.72
[-100, 100]	47 491	57 288 795	49 111 079	14.27

Table 5: 6-regular graphs with 1 030 301 nodes and 3 090 903 edges

Table 5. To the best of our knowledge, no other methods can achieve this accuracy for graphs of this size.

13 Concluding Remarks and future works

In this paper, we define a fast globally convergent algorithm for solving problem (1), called **SpeeDP**, which falls in the low rank nonlinear programming approach. **SpeeDP** outperforms existing methods for solving the special structured semidefinite programming problem (1) and provides both a primal and a dual solution. We also define an heuristic to compute a cut which is an enhanced version of the Goemans-Williamson algorithm, and is suitable for graphs up to millions of nodes and edges. The heuristic provides both a feasible cut and a valid bound, hence hence it is able to provide a cut and a guaranteed bound on how much its weight deviates from the optimum. As a next step, we intend to include **SpeeDP** within a branch-and-bound scheme similarly to what has been done in the BiqMac code of [25], in such a way aiming at increasing the size of Max-Cut instances that can be solved exactly exploiting semidefinite programming.

14 Appendix: Technical proofs and results

Proposition 4. The first condition in (9) can be written in matrix form as:

$$(Q + \text{Diag}(\hat{\lambda})) \hat{V} = 0 \tag{22}$$

where \hat{V} is the $n \times p$ matrix with rows v_i^T . Let \hat{V} be the $n \times r$ matrix satisfying (22) and the second order necessary condition

$$(Q + \text{Diag}(\hat{\lambda})) \bullet ZZ^T \geq 0 \quad \text{for all } Z \in \mathbb{R}^{n \times r} : E_{ii} \bullet \hat{V}Z^T = 0 \quad i = 1, \dots, n.$$

Assume the $\text{rank}(\widehat{V}) = p < r$, namely \widehat{V} is rank deficient, then there exists a $n \times p$ matrix \widehat{V}_1 such that

$$\widehat{V} = \widehat{V}_1 M^T \quad M \in \mathbb{R}^{r \times p}.$$

Let $M_\perp \in \mathbb{R}^{r \times (r-p)}$ be a matrix such that

$$M^T M_\perp = 0 \quad M_\perp^T M_\perp = I_{r-p}$$

For any matrix $Z_1 \in \mathbb{R}^{n \times (r-p)}$, the matrix $Z = Z_1 M_\perp^T$ satisfies

$$E_{ii} \bullet \widehat{V} Z^T = E_{ii} \bullet \widehat{V}_1 M^T M_\perp Z_1^T = 0$$

so that we must have

$$\left(Q + \text{Diag}(\widehat{\lambda}) \right) \bullet Z Z^T = \left(Q + \text{Diag}(\widehat{\lambda}) \right) \bullet Z_1 Z_1^T \geq 0$$

for any $n \times (r-p)$ matrix Z_1 , which is equivalent to $Q + \text{Diag}(\widehat{\lambda}) \geq 0$, so that global optimality of \widehat{V} follows from Theorem 3. If $r = n$ and $\text{rank}(\widehat{V}) < n$, the result follows from above. If instead $\text{rank}(\widehat{V}) = n$, the first order condition (22) implies $Q + \text{Diag}(\widehat{\lambda}) \equiv 0_{n \times n}$, so that global optimality of \widehat{v} follows from Theorem 3. \square

We prove Proposition 6. We split it into two propositions.

Proposition 15. *For every $v \in S_\delta$ and for every given $\varepsilon > 0$, the following condition holds*

$$f_\varepsilon(v) \geq -C + \frac{1}{\varepsilon} \frac{(\|v_i\|^2 - 1)^2}{\delta^2}, \quad \text{for all } i = 1, \dots, n, \quad (23)$$

where $C = \sum_{i=1}^n \sum_{j=1}^n |q_{ij}|$. Furthermore, for every given $\varepsilon > 0$ and for every given $v^0 \in S_\delta$, the level sets

$$\mathcal{L}_\varepsilon(v^0) = \{v \in S_\delta : f_\varepsilon(v) \leq f_\varepsilon(v^0)\}$$

of function $f_\varepsilon(v)$ are compact.

Proof. First, for every v , we have that

$$\begin{aligned} f_r(v) &= \sum_{i=1}^n \sum_{j=1}^n q_{ij} \frac{v_i^T v_j}{\|v_i\| \|v_j\|} \geq - \sum_{i=1}^n \sum_{j=1}^n |q_{ij}| \frac{|v_i^T v_j|}{\|v_i\| \|v_j\|} \\ &\geq - \sum_{i=1}^n \sum_{j=1}^n |q_{ij}| \frac{\|v_i\| \|v_j\|}{\|v_i\| \|v_j\|} = -C. \end{aligned}$$

Hence, (23) follows from simple majorizations. Now, we prove boundedness of $\mathcal{L}_\varepsilon(v^0)$. Let $\{v^k\} \in \mathcal{L}_\varepsilon(v^0)$ be a sequence of points such that $\|v^k\| \rightarrow \infty$. Assume without loss of generality that $\|v_1^k\| \rightarrow \infty$. By using (23), we can write:

$$f_\varepsilon(v^k) \geq -C + \frac{1}{\varepsilon} \frac{(\|v_1^k\|^2 - 1)^2}{\delta^2},$$

so that $f_\varepsilon(v)$ is coercive and the level set is bounded. On the other hand, any limit point of a sequence cannot belong to the boundary of S_δ . Indeed, if $\|\hat{v}_i\|^2 = 1 - \delta$ for some i , then (13) implies $d(\hat{v}_i) = 0$, and hence

$$\lim_{k \rightarrow \infty} f_\varepsilon(v^k) = \infty,$$

but this contradicts $v^k \in \mathcal{L}_\varepsilon(v^0)$ for k sufficiently large. Therefore the level set $\mathcal{L}_\varepsilon(v^0)$ is also closed, and the thesis follows. \square

Next proposition gives a bound on the value of $\|v_i\|$ for all $i = 1, \dots, n$ in the level set.

Proposition 16. *Let $\varepsilon > 0$ and $v^0 \in \mathcal{F}$. Then, we have*

$$\mathcal{L}_\varepsilon(v^0) \subseteq \left\{ v \in \mathbb{R}^{nr} : \|v_i\|^2 \leq (2C\varepsilon\delta^2)^{\frac{1}{2}} + 1, \quad i = 1, \dots, n \right\}.$$

Proof. For any given $v \in \mathcal{L}_\varepsilon(v^0)$, because $v^0 \in \mathcal{F}$, we can write

$$f_\varepsilon(v) \leq f_\varepsilon(v^0) = f_r(v^0) \leq C,$$

where C is defined in Proposition 6. Moreover, using (23), we have

$$f_\varepsilon(v) \geq -C + \frac{1}{\varepsilon} \frac{(\|v_j\|^2 - 1)^2}{\delta^2}, \quad j = 1, \dots, n,$$

so that

$$\|v_j\|^2 \leq (2C\varepsilon\delta^2)^{\frac{1}{2}} + 1, \quad j = 1, \dots, n.$$

\square

Proposition 10. By (21), for a fixed value $\varepsilon > 0$ the sequence $\{v^k\}$ stays in the compact level set $\mathcal{L}_\varepsilon(v^0)$. The proof is by induction. Assume that there exists $\bar{\varepsilon} > 0$ such that, for any $\varepsilon \geq \bar{\varepsilon}$, it is true that $\|v_i^k\|^2 \geq 1$. We show that is true also for $k + 1$. We can write

$$\begin{aligned} \|v_i^{k+1}\|^2 &= \|v_i^k\|^2 + (\alpha^k)^2 \|\nabla_{v_i} f_\varepsilon(v^k)\|^2 - 2\alpha^k (v_i^k)^T \nabla_{v_i} f_\varepsilon(v^k) \\ &= \|v_i^k\|^2 + (\alpha^k)^2 \|\nabla_{v_i} f_\varepsilon(v^k)\|^2 - \frac{8\alpha^k (\|v_i^k\|^2 - 1) \|v_i^k\|^2}{\varepsilon \delta^2} \\ &\geq \|v_i^k\|^2 - \frac{8\alpha_M}{\varepsilon \delta^2} (\|v_i^k\|^2 - 1) \|v_i^k\|^2, \end{aligned}$$

where the second equality derives from (16), keeping in mind that $\|v_i^k\| \geq 1$. If $\|v_i^k\| = 1$, then $\|v_i^{k+1}\|^2 \geq 1$. Otherwise, if $\|v_i^k\| > 1$, we need to verify that a value of $\bar{\varepsilon}$ exists such that for all $\varepsilon \geq \bar{\varepsilon}$

$$(\|v_i^k\|^2 - 1) - \frac{8\alpha_M}{\varepsilon\delta^2}(\|v_i^k\|^2 - 1)\|v_i^k\|^2 \geq 0,$$

namely

$$1 - \frac{8\alpha_M}{\varepsilon\delta^2}\|v_i^k\|^2 \geq 0. \quad (24)$$

By Proposition 16, we have that for all k

$$\|v_i^k\|^2 \leq (2C\varepsilon\delta^2)^{\frac{1}{2}} + 1 \quad i = 1, \dots, n. \quad (25)$$

Therefore (25) combined with (24) implies

$$\varepsilon - 8\frac{\alpha_M}{\delta^2} \left((2C\varepsilon\delta^2)^{\frac{1}{2}} + 1 \right) \geq 0$$

which is satisfied for all $\varepsilon \geq \bar{\varepsilon}$. \square

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