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Maximum stable set formulations and heuristics based on continuous optimization*

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Abstract. The stability number $\alpha(G)$ for a given graph G is the size of a maximum stable set in G . The Lovász theta number provides an upper bound on $\alpha(G)$ and can be computed in polynomial time as the optimal value of the Lovász semidefinite program. In this paper, we show that restricting the matrix variable in the Lovász semidefinite program to be rank-one and rank-two, respectively, yields a pair of continuous, nonlinear optimization problems each having the global optimal value $\alpha(G)$. We propose heuristics for obtaining large stable sets in G based on these new formulations and present computational results indicating the effectiveness of the heuristics.

Key words. maximum stable set – maximum clique – minimum vertex cover – semidefinite program – semidefinite relaxation – continuous optimization heuristics – nonlinear programming

1. Introduction

Let $G = (V, E)$ be a simple, undirected graph. A stable (independent) set S in G is a set of vertices that are mutually nonadjacent, and the size of S is given by its cardinality $|S|$. The stability number of G , denoted by $\alpha(G)$, is the size of a maximum stable set in G . The maximum stable set problem, or MSS problem for short, on G is to find a maximum stable set in G . It is well known that the MSS problem on G is equivalent to the minimum vertex cover problem on G and to the maximum clique problem on the complement graph of G .

The MSS problem is a classical NP-Hard optimization problem which has been studied extensively. Numerous approaches for solving or approximating the MSS problem have been proposed. A survey paper [2] by Bomze et al. gives a broad overview of progress made on the maximum clique problem, or equivalently the MSS problem, in

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the last four decades. The authors describe several different formulations of the MSS problem, a number of exact algorithms (such as explicit and implicit enumeration), and a number of heuristic algorithms (such as sequential greedy approaches, local and random searches) for the MSS problem. Though many of these algorithms perform well on certain classes of instances, it seems clear that no single algorithm has demonstrated superiority on all classes of graphs. Hence, new formulations and algorithms are needed to strengthen our ability to solve or approximate the MSS problem in general.

An upper bound on the stability number $\alpha(G)$ was defined and studied by Lovász in [18] (see also [12] for further details). This upper bound is called the Lovász theta number $\vartheta(G)$ and can be computed as the optimal value of the following semidefinite program (SDP), called the Lovász theta SDP:

$$\max\{e^T X e : \text{trace}(X) = 1, X_{ij} = 0 \forall (i, j) \in E, X \succeq 0\}, \quad (1)$$

where X is a symmetric matrix of size $|V| \times |V|$, the constraint $X \succeq 0$ requires that X be positive semidefinite, and e is the $|V|$ -length column vector of all ones.

In addition to its theoretical value, the upper bound $\vartheta(G)$ could be practically useful in an implicit enumeration scheme such as branch-and-bound for solving the MSS problem as long as it can be computed efficiently. There are, however, practical difficulties in applying semidefinite programming to the MSS problem. For a graph having $|V|$ vertices and $|E|$ edges, the number of variables and constraints involved in the corresponding SDP (1) is on the order of $|V|^2 + |E|$. Solving such an SDP becomes increasingly expensive as the size of $|V|$ and $|E|$ increase. For example, for $|V| \geq 500$ and $|E| \geq 1,000$, solving (1) via traditional interior-point methods becomes excessively time-consuming and memory-intensive on today's computers. (For further details on semidefinite programming and the classical interior-point algorithms to solve them, we refer the reader to [24].) Even though there have been some recent advances in solving (1) for graphs having more than 1,000 vertices and 100,000 edges using non-traditional approaches (see, for example, [7, 6, 15]), solving (1) for large-scale instances is still a formidable challenge.

Besides providing a high-quality upper bound on $\alpha(G)$, can the Lovász theta SDP (1) be utilized in some way to provide a high-quality lower bound on $\alpha(G)$? More specifically, can (1) be exploited to find large stable sets in G ? Computational advances in this direction have been shown, for example, by Benson and Ye [1] and Gruber [13]. Benson and Ye have solved an alternative SDP formulation of the Lovász theta number $\vartheta(G)$ to generate stable sets in G via a Goemans-Williamson-type rounding method (see [11]), and Gruber has obtained stable sets via a specialized rounding procedure applied to the optimal solution of (1). Since both of these methods require the solution of an SDP, it is reasonable to ask whether the quality of stable sets delivered by such methods can be obtained without the expense of explicitly solving an SDP.

In a recent paper [5], the authors of the present paper have considered another combinatorial optimization problem — the Max-Cut problem on G — in a similar context as we now consider the MSS problem. The SDP relaxation of Max-Cut is well known to provide both a good upper bound on the maximum cut size as well as the ability to obtain guaranteed high-quality cuts in G via the Goemans-Williamson randomization scheme. The focus of [5] was to develop fast methods for finding high-quality cuts in G , and so

instead of solving the expensive SDP relaxation for Max-Cut, the authors restricted the rank of the matrix variable of the relaxation to be at most two and applied a modified Goemans-Williamson scheme to the “rank-two” problem. They provided strong computational evidence showing that this rank-two problem produces higher quality cuts than the SDP relaxation, while taking much less computer time and storage. A disadvantage of the rank-two approach, however, is that it is a nonconvex relaxation of Max-Cut (unlike the SDP relaxation) and hence there are many local maximizers that cannot be guaranteed to provide an upper bound on the size of a maximum cut. Nonetheless, [5] has shown that the rank-two Max-Cut relaxation is a powerful tool when one wishes to find high-quality approximate solutions to the Max-Cut problem of large size.

Since the strategy of replacing an expensive convex relaxation by an inexpensive nonconvex relaxation has worked surprisingly well for approximating the Max-Cut problem, it is natural to ask whether or not a similar strategy would also work well for the MSS problem. Hence, in this paper we apply the low-rank restriction strategy to the Lovász theta SDP and study the resulting issues. In particular, we will show that: (i) restricting the matrix variable X in (1) to be of low rank (more precisely, to be either rank one or two) has a meaningful correspondence with the MSS problem; (ii) any feasible solution of the low-rank problems can be used to obtain a stable set with size at least as large as the solution’s continuous objective value; and (iii) local optimizers of the low-rank problems can be obtained quickly, taking advantage of graph structure such as sparsity.

An additional focus of this paper is the application of the ideas of the previous paragraph to the development and implementation of a class of continuous optimization heuristics for solving the MSS problem, and it is worth noting that the heuristics introduced here follow in a successful line of continuous optimization heuristics for the MSS problem. See, for example, [20, 23] for the continuous Motzkin-Straus formulation of the MSS problem and [3, 9, 10, 16, 19] for several continuous heuristics. In particular, the recent paper [19] includes computational results on the same set of test graphs that we study in Section 4. For the general topic of solving discrete optimization problems using continuous approaches, see [22].

This paper is organized as follows. In Section 2, we develop and analyze the nonlinear program formed by restricting the matrix variable X of (1) to be rank one. In particular, we demonstrate how every feasible solution of this rank-one problem naturally leads to a stable set and also show that the optimal value of the rank-one problem is exactly the stability number $\alpha(G)$. In Section 3, we show the same results for the problem resulting from restricting X to be at most rank two. In Section 4, we discuss an implementation of the aforementioned heuristics based on the rank-one and rank-two formulations of MSS. By comparing their performance on a large set of benchmark instances, we conclude that the rank-two heuristic gives better stable sets than the rank-one formulation even though it generally requires more computation time. In Section 5, we conclude with a few final remarks.

2. The rank-one problem

The “rank-one” restriction of (1) is to require that X be a matrix of rank at most one; that is, to require that $X = xx^T$ for some $x \in \mathfrak{R}^n$. Making the substitution $X = xx^T$ in (1) yields the following nonlinear program:

$$\alpha_1 \equiv \max \left\{ (e^T x)^2 : x \in \mathcal{F}^1 \right\}, \quad (2)$$

where

$$\mathcal{F}^1 \equiv \left\{ x \in \mathfrak{N}^n : \|x\|^2 = 1, x_i x_j = 0 \forall (i, j) \in E \right\}$$

and where $\|\cdot\|$ denotes the Euclidean norm in \mathfrak{N}^n . The goal of this subsection is to establish that $\alpha_1 = \alpha(G)$ and to characterize all local and global maximizers of problem (2).

We start by stating two simple technical results. For any $x \in \mathfrak{N}^n$, define

$$S_x \equiv \{i \in V : x_i \neq 0\}.$$

Lemma 1. *Suppose that $x \in \mathfrak{N}^n$ and $S \subseteq V$ satisfy $\|x\|^2 = 1$ and $S_x \subseteq S$. Then $(e^T x)^2 \leq |S|$, and equality holds if and only if $S = S_x$ and $x = \pm x^S$, where*

$$x_i^S = \begin{cases} |S|^{-1/2}, & i \in S \\ 0, & \text{otherwise} \end{cases}$$

Proof. For any $m \geq 1$ and $(\gamma_1, \dots, \gamma_m) \in \mathfrak{N}^m$, we have $(\gamma_1 + \dots + \gamma_m)^2 \leq m(\gamma_1^2 + \dots + \gamma_m^2)$, with equality holding if and only if $\gamma_1 = \dots = \gamma_m$. The result follows immediately from this observation. \square

Lemma 2. *Let $x \in \mathfrak{N}^n$ be given such that $\|x\|^2 = 1$. Then $x \in \mathcal{F}^1$ if and only if S_x is a stable set of G , in which case*

$$(e^T x)^2 \leq |S_x| \leq \alpha(G). \quad (3)$$

Proof. S_x is a stable set if and only if $\{i, j\} \not\subseteq S_x$ for all $(i, j) \in E$, or equivalently, if and only if $x_i x_j = 0$ for all $(i, j) \in E$. Since we have by assumption that $\|x\|^2 = 1$, the latter condition is equivalent to the condition $x \in \mathcal{F}^1$. The two inequalities in (3) follow from Lemma 1 and the definition of $\alpha(G)$ as the size of a maximum stable set of G . \square

In the sequel, we will refer to S_x as the stable set *induced* by $x \in \mathcal{F}^1$. We are now ready to characterize the global maximizers of the rank-one problem (2).

Theorem 1. *The optimal value of (2) equals the stability number of G , i.e., $\alpha_1 = \alpha(G)$. Moreover, for $x^* \in \mathfrak{N}^n$ such that $\|x^*\|^2 = 1$, the following conditions are equivalent:*

- a) x^* is a global maximizer of (2);
- b) S_{x^*} is a maximum stable set of G and $(e^T x^*)^2 = |S_{x^*}|$;
- c) $x^* = \pm x^S$ for some maximum stable set $S \subseteq V$.

Proof. We first prove that $\alpha_1 = \alpha(G)$. By Lemma 2, we have $(e^T x)^2 \leq |S_x| \leq \alpha(G)$ for all $x \in \mathcal{F}^1$, from which we conclude that $\alpha_1 \leq \alpha(G)$. To show the reverse inequality, let S be a maximum stable set of G and let $x^* = \pm x^S$. Clearly $S_{x^*} = S$, and so by Lemma 2, $x^* \in \mathcal{F}^1$. Also, by Lemma 1, $(e^T x^*)^2 = |S| = \alpha(G)$. These two observations imply that $\alpha_1 \geq \alpha(G)$, and thus, the relation $\alpha(G) = \alpha_1$ follows. We have also proved that x^* is a global maximizer of (2), and hence that the implication (c) \Rightarrow (a) holds. The implication (a) \Rightarrow (b) follows from relation (3) with $x = x^*$ and the fact that, when (a) holds, $(e^T x^*)^2 = \alpha_1 = \alpha(G)$. The implication (b) \Rightarrow (c) follows from Lemma 1. \square

We remark that the relation $\alpha_1 = \alpha(G)$ was noted independently by Gruber and Rendl [14].

With Theorem 1 giving a characterization of the global maximizers of the rank-one problem (2), we now turn to the classification of their local maximizers. The main tool of this analysis is the following auxiliary problem, which is specified by a subset $\emptyset \neq S \subseteq V$:

$$(P_S^1) : \quad \max \left\{ (e^T x)^2 : x \in \mathcal{F}_S \right\},$$

where $\mathcal{F}_S \equiv \{x \in \mathfrak{R}^n : \|x\|^2 = 1, x_i = 0 \forall i \notin S\}$. Observe that the points $\pm x^S \in \mathfrak{R}^n$ are feasible for (P_S^1) . The following result gives several properties of the problem (P_S^1) .

Lemma 3. *Let $\emptyset \neq S \subseteq V$ be given. The following statements hold:*

- a) $\mathcal{F}_S \subseteq \mathcal{F}^1$ if and only if S is a stable set of G ;
- b) the optimal value of (P_S^1) is $|S|$, and its set of global maximizers equals $\{\pm x^S\}$;
- c) (P_S^1) has no local maximizers other than its global maximizers.

Proof. (a): Using Lemma 2 with $x = x^S$, we conclude that S is a stable set if and only if $x^S \in \mathcal{F}^1$, which in turn is easily seen to be equivalent to the condition that $\mathcal{F}_S \subseteq \mathcal{F}^1$.

(b): It is an immediate consequence of Lemma 1.

(c): Suppose that \bar{x} is a local maximizer of (P_S^1) . We claim that $e^T \bar{x} \neq 0$. Indeed, assume for contradiction that $e^T \bar{x} = 0$. Since \bar{x} is a local maximizer of (P_S^1) , we have $e^T x = 0$ for all $x \in \mathcal{F}_S$ sufficiently close to \bar{x} , which implies that \bar{x} is a stationary point of the related problem $\max\{e^T x : x \in \mathcal{F}_S\}$. Hence, by the constraint qualification of linear independence, there exists $\lambda \in \mathfrak{R}$ and $\sigma_i \in \mathfrak{R}$ for each $i \in V \setminus S$ such that

$$e - 2\lambda \bar{x} - \sum_{i \in V \setminus S} \sigma_i e_i = 0, \quad (4)$$

where e_i denotes the i -th column of the identity matrix. For $j \in S$, the j -th component of (4) implies that $\lambda \neq 0$. Moreover, using the fact that $\bar{x} \in \mathcal{F}_S$, (4) shows that $e^T \bar{x} = 2\lambda$, which contradicts our assumption that $e^T \bar{x} = 0$. Hence, the claim follows. Now considering the first-order necessary conditions for (P_S^1) and noting that the constraint qualification of linear independence holds at $\bar{x} \neq 0$, we conclude that there exists $\eta \in \mathfrak{R}$ such that $e^T \bar{x} = \eta \bar{x}_i$ for all $i \in S$. Since $e^T \bar{x} \neq 0$, this implies that $\eta \neq 0$, and so $\bar{x}_i = e^T \bar{x} / \eta$ for all $i \in S$. In other words, \bar{x}_i is constant over all $i \in S$. The constraint $\|\bar{x}\|^2 = 1$ thus implies that $\bar{x} = \pm x^S$. \square

A maximal stable set $S \subseteq V$ in G is a stable set that is not properly contained in any other stable set. We are now ready to state the main result concerning the local maximizers of the rank-one problem (2).

Theorem 2. *For $\bar{x} \in \mathfrak{R}^n$ such that $\|\bar{x}\|^2 = 1$, the following conditions are equivalent:*

- a) \bar{x} is a local maximizer of (2);
- b) $S_{\bar{x}}$ is a maximal stable set of G and $(e^T \bar{x})^2 = |S_{\bar{x}}|$;
- c) $\bar{x} = \pm x^S$ for some maximal stable set $S \subset V$.

Proof. (a) \Rightarrow (c): Assume that $\bar{x} \in \mathcal{F}^1$ is a local maximizer of (2), and let $S \equiv S_{\bar{x}}$. By Lemmas 2 and 3(a), S is a stable set, and the feasible region \mathcal{F}_S is contained in \mathcal{F}^1 .

Since \bar{x} is clearly in \mathcal{F}_S , it follows that \bar{x} is also a local maximizer of (P_S^1) . By (b) and (c) of Lemma 3, it follows that $\bar{x} = \pm x^S$. To show that S is a maximal stable set, assume for contradiction that there exists a stable set $\tilde{S} \subseteq V$ that properly contains S . Clearly $\bar{x} \in \mathcal{F}_S \subset \mathcal{F}_{\tilde{S}} \subseteq \mathcal{F}^1$, from which it follows that \bar{x} is also a local maximizer of $(P_{\tilde{S}}^1)$. By Lemma 3(b), this implies that $\bar{x} = \pm x^{\tilde{S}}$, which contradicts the earlier conclusion that $x = \pm x^S$.

(c) \Rightarrow (b): This implication is obvious.

(b) \Rightarrow (a): By Lemma 2, $\bar{x} \in \mathcal{F}^1$ since $S_{\bar{x}}$ is a stable set. Since $\bar{x}_i \neq 0$ for all $i \in S_{\bar{x}}$, there exists a neighborhood $\mathcal{N}_{\bar{x}}$ of \bar{x} in \mathfrak{R}^n such that $x_i \neq 0$ for all $x \in \mathcal{N}_{\bar{x}}$ and $i \in S_{\bar{x}}$, or equivalently, $S_x \supseteq S_{\bar{x}}$ for all $x \in \mathcal{N}_{\bar{x}}$. Now, if x is an arbitrary point in $\mathcal{N}_{\bar{x}} \cap \mathcal{F}^1$, then $S_x = S_{\bar{x}}$, due to the fact that $S_{\bar{x}}$ is a maximal stable set contained in S_x , which in turn is a stable set by Lemma 2. Using Lemma 1, we conclude that $(e^T x)^2 \leq |S_{\bar{x}}|$ for all $x \in \mathcal{N}_{\bar{x}} \cap \mathcal{F}^1$. Since $(e^T \bar{x})^2 = |S_{\bar{x}}|$ by assumption, it follows \bar{x} is a local maximizer of (2). \square

3. The rank-two problem

In this section we consider a ‘‘rank-two’’ formulation of MSS obtained by restricting the rank of the matrix variable X of the Lovász theta SDP (1) to be at most two, i.e., we require that X be equal to $xx^T + yy^T$ for some $x, y \in \mathfrak{R}^n$. Note that the rank-one formulation of the previous section can be obtained from the rank-two formulation by setting y to be a multiple of x . A surprising result that we will show in this section is that the optimal values of the two formulations are equal even though the feasible region of the rank-two problem is strictly larger than that of the rank-one problem. Moreover, we will show how global maximizers for the rank-two problem yield maximum stable sets of G , and we will give a partial classification of the local maximizers of the rank-two problem.

Making the substitution $X = xx^T + yy^T$ in the SDP problem (1) and defining

$$\mathcal{F}^2 \equiv \left\{ (x, y) \in \mathfrak{R}^{2n} : \|x\|^2 + \|y\|^2 = 1, x_i x_j + y_i y_j = 0 \forall (i, j) \in E \right\},$$

we obtain the following rank-two problem:

$$\alpha_2 \equiv \max \left\{ (e^T x)^2 + (e^T y)^2 : (x, y) \in \mathcal{F}^2 \right\}. \quad (5)$$

An alternative form of the above problem that will also prove useful is

$$\alpha_2 \equiv \max \left\{ f(z) : \sum_{i=1}^n \|z^i\|^2 = 1, (z^i)^T z^j = 0 \forall (i, j) \in E \right\}, \quad (6)$$

where $z \equiv (z^1, \dots, z^n)$, $z^i \equiv (x_i, y_i)^T \in \mathfrak{R}^2$ for all $i = 1, \dots, n$, and

$$f(z) = f(z^1, \dots, z^n) \equiv \left\| \sum_{i=1}^n z^i \right\|^2.$$

Formulation (6) highlights the fact that the rank-two problem has n vector variables in \mathfrak{R}^2 — one for each node in the graph. (Recall that the rank-one problem has a scalar

variable for each node.) In the sequel, we will use (x, y) and (z^1, \dots, z^n) interchangeably to denote the variable of the rank-two problem.

It is interesting to note that the level sets of problem (6) are rotationally invariant in the sense that, if (z^1, \dots, z^n) is feasible, then so is (Qz^1, \dots, Qz^n) for any orthogonal matrix $Q \in \mathfrak{R}^{2 \times 2}$, and moreover the objective value is unchanged. Hence, the problem does not have any strict local maximizers (or minimizers). Later in this section, we will establish results which show that any non-global local maximizer can be rotated to some saddle point having the same objective value from which we may further increase the objective function.

3.1. Global and local maximizers of the rank-two formulation

The main goal of this subsection is to establish that $\alpha_2 = \alpha_1 = \alpha(G)$ and to characterize the global maximizers of problem (5). We will also study some properties of the local maximizers of problem (5) and contrast them with the ones for the local maximizers of problem (2).

We start by introducing a few definitions. A graph $\tilde{G} = (\tilde{V}, \tilde{E})$ is *bipartite* if there exists a pair of disjoint stable sets \tilde{V}_1 and \tilde{V}_2 of \tilde{G} such that $\tilde{V} = \tilde{V}_1 \cup \tilde{V}_2$. In such a case we refer to $(\tilde{V}_1, \tilde{V}_2)$ as a *bipartition* of \tilde{G} . Also, given a graph $G = (V, E)$, the subgraph of G induced by a nonempty subset B of V is the graph $G_B = (B, E_B)$ where E_B consists of those edges in E having both endpoints in B . We say that $B \subseteq V$ is *bipartite for G* if $B \neq \emptyset$ and G_B is bipartite. In such a case, the connected components of G_B , say G_k for $k = 1, \dots, p$, are also bipartite, and if (S_k, T_k) is a bipartition of G_k such that $|S_k| \geq |T_k|$ for all $k = 1, \dots, p$, the family $\{(S_k, T_k); k = 1, \dots, p\}$ is referred to as a *component bipartition* of G_B . (Here we use the convention that $T_k = \emptyset$ whenever G_k consists of only one vertex.)

Observation 1. Assume that $B \subseteq V$ is bipartite for G and let $\{(S_k, T_k) : k = 1, \dots, p\}$ denote a component bipartition of G_B . Then the following statements hold:

- a) every stable set in G_B is also a stable set in G ;
- b) the set $S = \cup_{k=1}^p S_k$ is a maximal stable set in G_B of size $|S| = |S_1| + \dots + |S_p|$;
- c) other maximal stable sets in G_B of the same size can be obtained by interchanging S_k and T_k whenever $|S_k| = |T_k|$.

In what follows we will refer to a stable set S of G obtained according to Observation 1 as a stable set induced by B .

We now introduce an auxiliary problem that will play a major role throughout the analysis of the rank-two problem. Assume that $B \subseteq V$ is bipartite for G and let $\{(S_k, T_k) : k = 1, \dots, p\}$ denote a component bipartition of G_B . The auxiliary problem is

$$\begin{aligned}
 (P_B^2) \quad & \max_z \left\| \sum_{i=1}^n z^i \right\|^2 \\
 \text{s.t.} \quad & \sum_{i=1}^n \|z^i\|^2 = 1, \\
 & z^i = 0, \quad \forall i \notin B, \\
 & z^i \perp z^j, \quad \forall (i, j) \in S_k \times T_k, \quad \forall k = 1, \dots, p.
 \end{aligned}$$

Note that the auxiliary problem depends only on B and not on the actual component bipartition chosen (see Observation 1(c)). The following result summarizes the important properties of the auxiliary problem (P_B^2) .

Theorem 3. *Suppose that $B \subseteq V$ is bipartite for G and that $\{(S_k, T_k) : k = 1, \dots, p\}$ is a component bipartition of G_B . The following statements regarding problem (P_B^2) hold:*

- a) *the feasible region of (P_B^2) is contained in \mathcal{F}^2 ;*
- b) *the optimal value of (P_B^2) is equal to $|S|$, where S is a stable set induced by B ;*
- c) *a feasible solution $z = (z^1, \dots, z^n) \in \mathfrak{R}^{2n}$ of (P_B^2) is optimal if and only if there exist pairs of vectors $(u^k, v^k) \in \mathfrak{R}^2 \times \mathfrak{R}^2$, $k = 1, \dots, p$, and a unit-length vector $w \in \mathfrak{R}^2$ such that the following conditions hold for all $k = 1, \dots, p$:*

$$\begin{aligned} u^k + v^k &= w/\sqrt{|S|}, \\ |S_k| > |T_k| &\implies v^k = 0, \\ z^i &= \begin{cases} u^k, & i \in S_k, \\ v^k, & i \in T_k; \end{cases} \end{aligned}$$

- d) *(P_B^2) has no local maximizers other than its global maximizers.*

Proof. Here, we prove only (a) and (b). The proofs of (c) and (d) will be given in Appendix A.

(a): Assume that $z = (z^1, \dots, z^n)$ is a feasible solution of (P_B^2) and let $(i, j) \in E$ be given. If at least one of the endpoints of (i, j) is not in B , then $(z^i)^T z^j = 0$ since at least one of z^i and z^j is zero. If both endpoints of (i, j) are in B , then either (i, j) or (j, i) must be in $S_k \times T_k$ for some $k \in \{1, \dots, p\}$, and hence $(z^i)^T z^j = 0$. We have thus proved that $(z^i)^T z^j = 0$ for all $(i, j) \in E$. Clearly, this implies that $z \in \mathcal{F}^2$.

(b): Let S be a stable set induced by B , and consider the vector $\bar{z} = (\bar{z}^1, \dots, \bar{z}^n)$ defined as

$$\bar{z}^i = \begin{cases} w/\sqrt{|S|}, & i \in S, \\ 0, & i \notin S, \end{cases}$$

where $w \in \mathfrak{R}^2$ is an arbitrary unit-length vector. It is easy to verify that \bar{z} is a feasible solution of (P_B^2) such that $f(\bar{z}) = |S|$, which implies that the optimal value of (P_B^2) is at least $|S|$. To complete the proof of (b), it is then sufficient to show that $f(z) \leq |S|$ for every feasible solution $z = (z^1, \dots, z^n)$ of (P_B^2) . Indeed, let z be as such, and define the following quantities for all $k = 1, \dots, p$:

$$p^k \equiv \sum_{i \in S_k} z^i, \quad q^k \equiv \sum_{i \in T_k} z^i, \quad (7)$$

$$\theta_{ak} \equiv \sum_{i \in S_k} \|z^i\|^2, \quad \theta_{bk} \equiv \sum_{i \in T_k} \|z^i\|^2, \quad \theta_k \equiv \theta_{ak} + \theta_{bk}. \quad (8)$$

Using the feasibility of (z^1, \dots, z^n) and the above identities, it is easy to see that $p^k \perp q^k$ for every $k = 1, \dots, p$, and $\sum_{k=1}^p \theta_k = 1$. Furthermore,

$$\|p^k\|^2 = \left\| \sum_{i \in S_k} z^i \right\|^2 \leq \left(\sum_{i \in S_k} \|z^i\| \right)^2 \leq |S_k| \left(\sum_{i \in S_k} \|z^i\|^2 \right) = \theta_{ak} |S_k|. \quad (9)$$

Similarly, we can show that

$$\|q^k\|^2 \leq \theta_{bk} |T_k|. \quad (10)$$

Using the fact that $z^i = 0$ for all $i \notin B$, relation (7), the triangle inequality for norms and the Pythagorean identity, we obtain

$$\left\| \sum_{i=1}^n z^i \right\|^2 = \left\| \sum_{k=1}^p (p^k + q^k) \right\|^2 \leq \left(\sum_{k=1}^p \|p^k + q^k\| \right)^2 = \left(\sum_{k=1}^p \sqrt{\|p^k\|^2 + \|q^k\|^2} \right)^2. \quad (11)$$

Using the two inequalities (9) and (10) and the fact that $|S_k| \geq |T_k|$ for all $k = 1, \dots, p$, we obtain

$$\left(\sum_{k=1}^p \sqrt{\|p^k\|^2 + \|q^k\|^2} \right)^2 \leq \left(\sum_{k=1}^p \sqrt{\theta_{ak} |S_k| + \theta_{bk} |T_k|} \right)^2 \leq \left(\sum_{k=1}^p \sqrt{\theta_k |S_k|} \right)^2. \quad (12)$$

Finally, using the Cauchy-Schwarz inequality and the fact that $\sum_{k=1}^p \theta_k = 1$, we have

$$\left(\sum_{k=1}^p \sqrt{\theta_k |S_k|} \right)^2 \leq \left(\sum_{k=1}^p |S_k| \right) \left(\sum_{k=1}^p \theta_k \right) = |S|. \quad (13)$$

Combining inequalities (11), (12) and (13), we conclude that the objective value of any feasible solution of (7) is bounded above by $|S|$, which completes the proof of (b). \square

It is worth mentioning that by considering the necessary and sufficient conditions for the inequalities (9) through (13) to be satisfied as equalities, we can prove Theorem 3(c). We postpone its proof, however, until Corollary A.3 in Appendix A since it can also be obtained as a by-product of our proof of Theorem 3(d).

Given $z = (z^1, \dots, z^n) \in \mathfrak{R}^{2n}$, define $B_z \equiv \{i \in V : z^i \neq 0\}$. Our next result gives a characterization for the point z to be in \mathcal{F}^2 , which is related to the bipartiteness of B_z for G .

Lemma 4. *A point $z = (z^1, \dots, z^n) \in \mathfrak{R}^{2n}$ is in \mathcal{F}^2 if and only if B_z is bipartite for G and z is feasible for problem (P_B^2) , in which case*

$$f(z) \leq |S| \leq \alpha(G), \quad (14)$$

where S is a stable set induced by $B(z)$.

Proof. The ‘if’ part of the lemma follows immediately from Theorem 3(a). To show the ‘only if’ part, assume that $z \in \mathcal{F}^2$. Let

$$B_z^+ \equiv \{i \in B_z : x_i = 0 \text{ or } x_i y_i > 0\} \quad \text{and} \quad B_z^- \equiv \{i \in B_z : y_i = 0 \text{ or } x_i y_i < 0\},$$

where $z^i = (x_i, y_i)$. We claim that G_{B_z} is a bipartite graph with bipartition (B_z^+, B_z^-) . Indeed, since $z^i = (x_i, y_i) \neq 0$ for all $i \in B$, we easily see that (B_z^+, B_z^-) is a partition of B . It remains to verify that B_z^+ and B_z^- are both stable sets of G . We concentrate only on B_z^+ since the proof for B_z^- is similar. Let $i, j \in B_z^+$ be given. Consider first the case in which $x_i = 0$ or $x_j = 0$, which easily implies that both y_i and y_j are nonzero. Hence, we have $x_i x_j + y_i y_j = y_i y_j \neq 0$. For the other case in which both x_i and x_j are nonzero, and hence $x_i y_i > 0$ and $x_j y_j > 0$, we also have $x_i x_j + y_i y_j \neq 0$ as one can easily verify. Now, using the assumption that $z \in \mathcal{F}^2$, we conclude that $(i, j) \notin E$. We have thus proved that B_z^+ is a stable set.

Relation (14) is an immediate consequence of Theorem 3(b) and the definition of $\alpha(G)$ as the size of a maximum stable set in G . \square

For a point $z = (z^1, \dots, z^n) \in \mathcal{F}^2$, we refer to a stable set S of G induced by B_z , which is bipartite for G , as a stable set *induced by* z . We are now ready to characterize the global and local maximizers of the rank-two problem (5).

Theorem 4. *The optimal value of (5) equals the stability number of G , i.e., $\alpha_2 = \alpha(G)$. Moreover, $z^* \in \mathfrak{R}^{2n}$ is a global maximizer of (5) if and only if $B \equiv B_{z^*}$ is bipartite for G , z^* is an optimal solution of (P_B^2) , and any stable set S induced by z^* is a maximum stable set, in which case $f(z^*) = |S|$.*

Proof. It follows immediately from Lemma 4 that $\alpha_2 \leq \alpha(G)$. By Theorem 1 and the fact that problem (5) is a relaxation of problem (2), we have $\alpha_2 \geq \alpha_1 = \alpha(G)$. Hence, $\alpha_2 = \alpha(G)$.

To show the ‘only if’ part of the second statement of the theorem, assume that z^* is a global maximizer of (5), or equivalently that $z^* \in \mathcal{F}^2$ and $\alpha(G) = \alpha_2 = f(z^*)$. Then, it follows from Lemma 4 that $B \equiv B_{z^*}$ is bipartite for G and that z^* is a feasible point for problem (P_B^2) . Since (P_B^2) is a restriction of (5) by Theorem 3, it follows that z^* is also a global maximizer of (P_B^2) and hence that $f(z^*) = |S|$ due to Theorem 3(b). We have thus shown that $\alpha(G) = |S|$, and hence that S is a maximum stable set of G .

To show the ‘if’ part, assume that $B \equiv B_{z^*}$ is bipartite for G , z^* is an optimal solution of (P_B^2) , and any stable set S induced by z^* is maximum. It follows from (a) and (b) of Theorem 3 that $z^* \in \mathcal{F}^2$ and that $f(z^*) = |S|$. Since S is a maximum stable set, which implies $|S| = \alpha(G) = \alpha_2$, we conclude that $f(z^*) = \alpha_2$. This shows that z^* is an optimal solution of (5). \square

Theorem 5. *Suppose that $\bar{z} = (\bar{z}^1, \dots, \bar{z}^n) \in \mathfrak{R}^{2n}$ is a local maximizer of problem (5). Then, $B \equiv B_{\bar{z}}$ is bipartite for G and \bar{z} is an optimal solution of (P_B^2) . Hence, $f(\bar{z}) = |S|$ for any stable set S induced by \bar{z} .*

Proof. Assume that \bar{z} is a local maximizer of (5). Then it follows from Lemma 4 that $B \equiv B_{\bar{z}}$ is bipartite for G and that \bar{z} is a feasible point for problem (P_B^2) . Since (P_B^2) is a restriction of (5) by Theorem 3(a), it follows that \bar{z} is also a local maximizer of (P_B^2) . By Theorem 3(d), we conclude that \bar{z} is a global maximizer of (P_B^2) . \square

Unlike the results obtained in Theorem 2 for the rank-one problem, Theorem 5 does not provide a full characterization for a local maximizer of the rank-two problem. At this point, it is natural to wonder if a stable set induced by a nonglobal local maximizer of problem (5) is maximal. It turns out that the answer is negative. An example illustrating this fact is given in Appendix B. It is also natural to question whether the reverse of the implication derived in Theorem 5 holds. It turns out that the answer in this case is also negative even if we assume that the stable set induced by \bar{z} is maximal. This is a consequence of a very general result (derived below), which establishes that, for every non-maximum maximal stable set S in G , there is an easily computable, “canonical” feasible point $z = (z^1, \dots, z^n)$ for the rank-two problem such that $B_z = S$ and $f(z) = |S|$, and yet z is not a local maximizer of the rank-two problem. Note that the condition $f(z) = |S|$ implies that z is an optimal solution of (P_B^2) . This is in direct contrast with the rank-one problem where the canonical solutions $\pm x^S$ associated with S , i.e., the ones that induce S and are optimal solutions of (P_S^1) , are necessarily local maximizers.

Before stating the result, we first state a lemma that gives conditions under which a point $z \in \mathcal{F}^2$ is not a local maximizer.

Lemma 5. *Let $\tilde{z}, \hat{z} \in \mathcal{F}^2$, and suppose that*

$$\tilde{z}^i = \tilde{\gamma}_i \tilde{w}, \quad \forall i = 1, \dots, n, \quad (15)$$

$$\hat{z}^i = \hat{\gamma}_i \hat{w}, \quad \forall i = 1, \dots, n, \quad (16)$$

for some $\tilde{\gamma}_i, \hat{\gamma}_i \in \mathfrak{R}$, $i = 1, \dots, n$, and some perpendicular, unit vectors $\tilde{w}, \hat{w} \in \mathfrak{R}^2$. In addition, let $\tilde{f} \equiv f(\tilde{z})$ and $\hat{f} \equiv f(\hat{z})$. Then, there exists a feasible path in \mathcal{F}^2 from \tilde{z} to \hat{z} along which the objective function $f(z)$ is strictly monotonic if $\tilde{f} \neq \hat{f}$ or is constant if $\tilde{f} = \hat{f}$.

Proof. For each $t \in [0, 1]$, define $\psi(t) \equiv [(1-t)^2 + t^2]^{-1/2}$ and

$$z(t) \equiv \psi(t) \left[(1-t)\tilde{z} + t\hat{z} \right]. \quad (17)$$

We will show that $z(t) \in \mathcal{F}^2$ and $f(z(t)) = f^t \equiv \psi(t)^2 \left[(1-t)^2 \tilde{f} + t^2 \hat{f} \right]$, for all $t \in [0, 1]$, from which the result of the lemma clearly follows. To show that $z(t) \in \mathcal{F}^2$, we first verify that $\|z(t)\|^2 = 1$. This follows directly from (17) and the equalities

$$\begin{aligned} \|z(t)\|^2 &= \psi(t)^2 \|(1-t)\tilde{z} + t\hat{z}\|^2 = \psi(t)^2 \left[(1-t)^2 \|\tilde{z}\|^2 + t^2 \|\hat{z}\|^2 \right] \\ &= \psi(t)^2 \left[(1-t)^2 + t^2 \right] = 1, \end{aligned}$$

where the second equality follows from (15), (16), and the orthogonality of \tilde{w} and \hat{w} and the third equality follows from the feasibility of \tilde{z} and \hat{z} . Next, we show that $z(t)$ satisfies $z^i(t) \perp z^j(t) = 0$ for all $(i, j) \in E$ and $t \in [0, 1]$. From (17) and the definition of $z(t)$, we easily see that

$$\begin{aligned} \left(z^i(t) \right)^T \left(z^j(t) \right) &= \psi(t)^2 \left((1-t)\tilde{z}^i + t\hat{z}^i \right)^T \left((1-t)\tilde{z}^j + t\hat{z}^j \right) \\ &= \psi(t)^2 \left[(1-t)^2 \left(\tilde{z}^i \right)^T \tilde{z}^j + (1-t)t \left[\left(\tilde{z}^i \right)^T \hat{z}^j + \left(\hat{z}^i \right)^T \tilde{z}^j \right] + t^2 \left(\hat{z}^i \right)^T \hat{z}^j \right], \end{aligned}$$

Noting that $(\tilde{z}^i)^T \tilde{z}^j = (\hat{z}^i)^T \hat{z}^j = 0$ due to the feasibility of \tilde{z} and \hat{z} and that $(\tilde{z}^i)^T \hat{z}^j = (\hat{z}^i)^T \tilde{z}^j = 0$ due to (15), (16), and the orthogonality of \tilde{w} and \hat{w} , we obtain $(z^i(t))^T z^j(t) = 0$, as desired. Hence, $z(t) \in \mathcal{F}^2$. We now evaluate $f(z(t))$. Since $f(z(t)) = \|\sum_{i=1}^n z^i(t)\|^2$, it follows from (17), the orthogonality of $\sum_{i=1}^n \tilde{z}^i$ and $\sum_{i=1}^n \hat{z}^i$ (due to the orthogonality of \tilde{w} and \hat{w}) and the definition of the objective values \tilde{f} and \hat{f} that

$$\begin{aligned} f(z(t)) &= \psi(t)^2 \left\| (1-t) \sum_{i=1}^n \tilde{z}^i + t \sum_{i=1}^n \hat{z}^i \right\|^2 \\ &= \psi(t)^2 \left[(1-t)^2 \left\| \sum_{i=1}^n \tilde{z}^i \right\|^2 + t^2 \left\| \sum_{i=1}^n \hat{z}^i \right\|^2 \right] \\ &= \psi(t)^2 \left[(1-t)^2 \tilde{f} + t^2 \hat{f} \right]. \end{aligned}$$

Hence, the result follows. \square

We are now ready to state the result mentioned earlier.

Proposition 1. *Let S be a stable set in G , and for any $w \in \mathfrak{R}^2$ with unit-length, define*

$$\begin{aligned} z^i &= \frac{1}{\sqrt{|S|}} w \quad \forall i \in S, \\ z^i &= 0 \quad \forall i \notin S. \end{aligned}$$

Then, $z = (z^1, \dots, z^n) \in \mathcal{F}^2$, $f(z) = |S|$, $B(z) = S$ and S is induced by z . If, in addition, S is not a maximum stable set, then z is not a local maximizer.

Proof. Let the suggested solution z be called the *canonical solution* associated with (S, w) . It is easy to show that the first three conclusions of the proposition hold. The final statement can be shown as follows. Assume S is not maximum, and let S^* be a maximum stable set of G . Then Lemma 5 shows that there is a strictly increasing, feasible path between the canonical solution associated with (S, w) and the canonical solution associated with (S^*, w^\perp) , where w^\perp is orthogonal to w . Hence, z is not a local maximizer of (5). \square

On the surface, the above properties seem to be disadvantages of the rank-two formulation, since one would expect that finding a local maximizer of (5) should correspond to finding a maximal stable set. However, Proposition 1 actually shows a significant advantage of the rank-two problem over the rank-one problem. In the rank-one problem, if one obtains a local maximizer, then the induced stable set S is maximal, but one is “stuck” at the local maximizer. In the rank-two problem, on the other hand, if one obtains a local maximizer, the induced stable set S may or may not be maximal, but in either case one can easily move to a canonical feasible solution associated with S with the same objective value $|S|$. From this canonical solution which is not a local maximizer, it is possible to “escape” to a higher local maximizer corresponding to a larger stable set. Indeed, when this feature of the rank-two problem is exploited algorithmically, it allows us to find considerably larger stable sets than does the rank-one problem, as will be demonstrated in the computational results of the next section.

3.2. Extension to higher ranks?

Before closing our discussion of the rank-two problem, we address a question that arises naturally after we see the results for rank-one and rank-two problems. Is the optimal value of the rank-three problem — for variables $x, y, v \in \mathfrak{R}^n$,

$$\begin{aligned} & \text{maximize} && (e^T x)^2 + (e^T y)^2 + (e^T v)^2 \\ & \text{subject to} && \|x\|^2 + \|y\|^2 + \|v\|^2 = 1 \\ & && x_i x_j + y_i y_j + v_i v_j = 0, \quad \forall (i, j) \in E \end{aligned} \tag{18}$$

also equal to $\alpha(G)$? Although the answer may be “yes” for special classes of graphs (e.g., perfect graphs), the general answer is “no,” as the following example demonstrates. Consider the pentagon graph

$$G = (V, E) = (\{1, 2, 3, 4, 5\}, \{(1, 2), (2, 3), (3, 4), (4, 5), (5, 1)\}).$$

It is then straightforward to verify that the point

$$\begin{aligned} x &= (1/3, 0, 1/3, 1/3, 0) \\ y &= (0, 1/3, 0, 1/3, 1/3) \\ v &= (0, 0, 1/3, -1/3, 1/3) \end{aligned}$$

is feasible for the rank-three problem with objective value $2\frac{1}{9}$ which is greater than 2 — the stability number $\alpha(G)$ of the pentagon graph.

4. Computational results

Since the low-rank NLPs (2) and (5) are formulations of the MSS problem, it is natural to ask whether they can be employed in solving or approximating the MSS problem. Important are the following two principles that have been established in the previous sections: every feasible point of each NLP yields (or induces) a stable set in G ; and, in general, the higher the objective of the feasible point, the larger the size of the induced stable set. Hence, a reasonable approach is to optimize (2) and (5) using standard NLP techniques, which in turn optimizes the MSS problem, and in this section, we describe our computational experiences with these ideas. We also seek to characterize the practical advantages and disadvantages of the rank-one and rank-two formulations in the context of solving or approximating the MSS problem since we have shown that they have substantially different theoretical properties.

It is important to remember that both (2) and (5) are NP-Hard to optimize due to their equivalence with the MSS problem. Hence, using NLP techniques, one can only expect to “solve” (2) and (5) in the sense of obtaining stationary points or local maximizers.

Since the rank-one problem (2) can be seen as a restriction of the rank-two problem (5) in which the variable y is set to zero, our discussion of algorithmic techniques focuses on (5), from which direct applications to (2) are immediately available. In particular, we discuss an augmented Lagrangian method for obtaining a stationary point of (5) as well as a technique for extracting stable sets of G from points that are “nearly feasible” for

(5). Such a technique is necessary since an augmented Lagrangian algorithm will only produce a feasible point in the limit and since the theoretical discussion of Section 3 has only described how to obtain a stable set of G from a feasible solution. We conclude the section with a comparison of three heuristics (one for the rank-one problem and two for the rank-two problem) on a large set of benchmark instances, and we then discuss the relative advantages and disadvantages of each method.

4.1. The augmented Lagrangian algorithm

From a nonlinear programming perspective, the edge constraints of the rank-two problem (5) are difficult to enforce algorithmically, and so we employ the standard technique of placing these constraints into the objective function via the augmented Lagrangian function. (The unit-norm constraint, on the other hand, is easier to handle; see the details below.) The augmented Lagrangian method we will consider is based on the following maximization for fixed Lagrangian multipliers $\lambda = (\lambda_{ij})_{(i,j) \in E}$ and fixed penalty parameter $\sigma > 0$, where $c(x, y) = (x_i x_j + y_i y_j)_{(i,j) \in E}$ represents the edge-constraint violations:

$$\begin{aligned} \text{maximize } \mathcal{L}(x, y) &\equiv (e^T x)^2 + (e^T y)^2 + \left(\lambda - \frac{\sigma}{2} c(x, y) \right)^T c(x, y) \\ \text{subject to } \|x\|^2 + \|y\|^2 &= 1. \end{aligned} \quad (19)$$

Our algorithm to obtain a stationary point of (5) proceeds as detailed in Algorithm AL (or ‘‘Augmented Lagrangian’’) below. (See, for example, [21] for a full description of the standard augmented Lagrangian algorithm). First, however, we give two alternative sets of equations that are used by Algorithm AL:

$$\lambda^{k+1} = \lambda^k - \sigma_k c(x^k, y^k), \quad (20a)$$

$$\sigma_{k+1} = \sigma_k, \quad (20b)$$

$$v_{k+1} = v; \quad (20c)$$

and

$$\lambda^{k+1} = \lambda^k, \quad (21a)$$

$$\sigma_{k+1} = 10 \sigma_k, \quad (21b)$$

$$v_{k+1} = v_k. \quad (21c)$$

We now state the algorithm.

Algorithm AL:

Default Initialization: $G = (V, E)$, $\sigma_1 = 1$, $v_0 = \infty$

Input: $(x^0, y^0) \in \mathfrak{R}^{2n}$, $\lambda^1 \in \mathfrak{R}^{|E|}$

For $\ell = 1, 2, \dots$

- a. Solve (19) with $\lambda = \lambda^\ell$ and $\sigma = \sigma_\ell$ from the initial point $(x^{\ell-1}, y^{\ell-1})$, obtaining (x^ℓ, y^ℓ) . Set $v = \|c(x^\ell, y^\ell)\|$.
- b. If $v < 0.25 v_{\ell-1}$, then apply equations (20). Otherwise, apply (21).

End

A couple of comments are in order. First, Algorithm AL does not have a stopping criterion as stated. Instead of employing a standard stopping criterion, we will use a special criterion (see Algorithm AL' in the next subsection) that is tailored to (5) and the MSS problem. Second, theory dictates that, under some mild conditions, the augmented Lagrangian algorithm will converge to a stationary point of (5), though in practice one could expect convergence to a local maximizer. Indeed, we always observe that the algorithm converges to a point (\bar{x}, \bar{y}) which, in accordance with Theorem 5, has integer objective value.

A very important aspect of the algorithm proposed above is the procedure to solve (19), where “to solve” means to obtain a stationary point or local maximizer. We note that any $(\hat{x}, \hat{y}) \in \mathfrak{N}^{2n}$ can be easily scaled to $(x, y) \equiv (\hat{x}, \hat{y})/(\|\hat{x}\|^2 + \|\hat{y}\|^2)^{1/2}$, which is feasible for (19). Moreover, if $\|\hat{x}\|^2 + \|\hat{y}\|^2$ is already close to the feasible value of 1, then $\mathcal{L}(x, y)$ is close to $\mathcal{L}(\hat{x}, \hat{y})$. These two ideas can be used in the following procedure that can be iterated to solve (19): given (x, y) feasible for (19) and a direction (d_x, d_y) of ascent for \mathcal{L} at (x, y) , compute the projection (\bar{d}_x, \bar{d}_y) of (d_x, d_y) onto the tangent space of the unit ball at (x, y) and then select $\alpha > 0$ such that $\mathcal{L}(x_\alpha, y_\alpha)$ is greater than $\mathcal{L}(x, y)$, where

$$(x_\alpha, y_\alpha) \equiv \frac{(x + \alpha \bar{d}_x, y + \alpha \bar{d}_y)}{(\|x + \alpha \bar{d}_x\|^2 + \|y + \alpha \bar{d}_y\|^2)^{1/2}}$$

is feasible for (19). The procedure can be thought of as a line search on the surface of the unit sphere in \mathfrak{N}^{2n} , and it is not difficult to show that a suitable α exists and can be found with any standard line search strategy. (For example, these same ideas have been described in [4].) We have implemented the above ideas with a strong Wolfe-Powell line search and a first-order (or gradient-based) limited-memory BFGS technique for generating the search directions. The technique is based on the standard limited-memory BFGS approach for unconstrained optimization but has been adapted in a straightforward manner to incorporate the ideas of projection and spherical line searches mentioned above. These adaptations have been developed primarily for testing the feasibility of the nonlinear formulations presented in this paper, and though they have proven successful, we feel there may be opportunities for further performance improvements by more carefully considering the best way to incorporate limited-memory BFGS techniques into problems such as (19).

Finally, we mention that our choice of using a first-order approach for solving (19) is motivated by the fact that we do not need highly accurate local solutions of (5) (see the next subsection), that the function and gradient evaluations of the augmented Lagrangian are very fast especially when $|E|$ is small, and that the computation of second derivatives is very expensive relative to the computation of first derivatives.

4.2. Extracting stable sets from approximately feasible solutions

In order to implement the ideas presented at the beginning of this section, it is important to be able to generate stable sets from the optimization of (5), which, according to Section 3, requires (x, y) to be feasible. By the very nature of Algorithm AL, however, a feasible point of (5) will never be readily available. So we need a technique for extracting stable sets from the approximately feasible solutions that the algorithm does produce.

Each point obtained by the algorithm will have some or all of its edge constraints violated, but recall that the augmented Lagrangian algorithm will always maintain the unit-norm constraint of (5). Of course, as the algorithm progresses, the amount of infeasibility will decrease, but this infeasibility nonetheless complicates the computation of a stable set induced by $z = (x, y)$. Note that by Lemma 4, the set B_z is bipartite if and only if $z \in \mathcal{F}^2$. So, it is necessary to introduce an analogue of the set B_z that is always a stable set for G regardless of whether $z \in \mathcal{F}^2$ or not. First, given $z \in \mathfrak{R}^{2n}$, we define

$$\varepsilon_z \equiv \max_{(i,j) \in E} |x_i x_j + y_i y_j|$$

so that ε_z is a measure of the largest constraint violation. Next, letting the superscript I denote the idea of ‘‘infeasibility,’’ we define

$$B_z^I \equiv \left\{ i : x_i y_i = 0, \max(|x_i|, |y_i|) > \varepsilon_z^{1/2} \right\} \cup \left\{ i : \min(|x_i|, |y_i|) > \varepsilon_z^{1/2} \right\}.$$

Note that when $\varepsilon_z = 0$, i.e., when $z/\|z\| \in \mathcal{F}^{(2)}$, the definition of B_z^I matches the usual definition of B_z . We have the following proposition.

Proposition 2. *The set B_z^I is bipartite for G for every $z \in \mathfrak{R}^{2n}$.*

Proof. To simplify notation, let $B \equiv B_z^I$. In a similar fashion as Lemma 4, we define

$$B^+ \equiv \{i \in B : x_i = 0 \text{ or } x_i y_i > 0\} \quad \text{and} \quad B^- \equiv \{i \in B : y_i = 0 \text{ or } x_i y_i < 0\}.$$

It is easy to see that B^+ and B^- form a bipartition of B , and we also claim that (B^+, B^-) is a bipartition of G_B , i.e., B^+ and B^- are stable sets in G_B (or equivalently of G). To show this in the case of B^+ , let $i, j \in B^+$ be given; we will show that $(i, j) \notin E$. Using the definition of B^+ , it is straightforward to see that $|x_i x_j + y_i y_j| = |x_i||x_j| + |y_i||y_j|$. Suppose first that $x_i = 0$ or $x_j = 0$. Then it is easy to see that $\min\{|y_i|, |y_j|\} > \varepsilon_z^{1/2}$, which implies that

$$|x_i x_j + y_i y_j| = |y_i||y_j| > \varepsilon_z^{1/2} \varepsilon_z^{1/2} = \varepsilon_z.$$

Since ε_z is the largest edge constraint violation, we conclude that $(i, j) \notin E$. Now consider the case in which $x_i y_i > 0$ and $x_j y_j > 0$. It is then easy to see that $\min\{|x_i|, |x_j|, |y_i|, |y_j|\} > \varepsilon_z^{1/2}$. Hence,

$$|x_i x_j + y_i y_j| = |x_i||x_j| + |y_i||y_j| \geq \varepsilon_z + \varepsilon_z = 2\varepsilon_z > \varepsilon.$$

As before, we conclude that $(i, j) \notin E$. This completes the proof that B^+ is a stable set, and the proof that B^- is a stable set is similar. Overall, we conclude that B is a bipartition of G_B . \square

Since B_z^I is bipartite for G , we can define the notion of a stable set induced by infeasible point $z = (x, y)$ by employing the same kind of construction illustrated in Observation 1. In fact, this process of extracting a large stable set using B_z^I allows us to define a variant of Algorithm AL that includes a stopping criterion:

Algorithm AL':**Default Initialization:** $G = (V, E)$, $\sigma_1 = 1$, $v_0 = \infty$, $\text{flag} = 0$ **Input:** $(x^0, y^0) \in \mathfrak{N}^{2n}$, $\lambda^1 \in \mathfrak{N}^{|E|}$ **Output:** S , λ^ℓ **For** $\ell = 1, 2, \dots$ and while $\text{flag} = 0$ a. Solve (19) with $\lambda = \lambda^\ell$ and $\sigma = \sigma_\ell$ from initial point $(x^{\ell-1}, y^{\ell-1})$, obtaining (x^ℓ, y^ℓ) . Set $v = \|c(x^\ell, y^\ell)\|$.b. If $v < 0.25 v_{\ell-1}$, then apply equations (20). Otherwise, apply (21).c. Let S be an induced stable set of (x^ℓ, y^ℓ) and set $\text{flag} = 1$ if $|f(x^\ell, y^\ell) - |S|| < 0.01$.**End**

In words, Algorithm AL' executes Algorithm AL with an important enhancement. In particular, after (19) is solved for the point (x^ℓ, y^ℓ) , an induced stable set S of (x^ℓ, y^ℓ) is calculated, and if the objective function $f(x^\ell, y^\ell)$ and the size of S are comparable up to two decimal places (in particular, $f(x^\ell, y^\ell)$ is approximately integer), then the algorithm is stopped via the use of a simple flag. Although there is no theoretical guarantee that Algorithm AL' will terminate when the sequence of points $\{(x^\ell, y^\ell)\}_{\ell \geq 1}$ is converging to a stationary point of (5), the algorithm will terminate if convergence is to a local maximizer, and in practice, we always observe that Algorithm AL' terminates.

4.3. Comparison of three heuristics

In this subsection, we present rank-one and rank-two heuristics for finding large stable sets in G based on the ideas of the previous two subsections as well as — in the rank-two case — the ideas of escaping from canonical solutions mentioned at the end of Subsection 3.1. We then present computational results comparing the heuristics and discuss the relative advantages and disadvantages of each.

The rank-two heuristic we present is motivated by Theorem 5 and Proposition 1 for the rank-two problem (5). Once Algorithm AL' has terminated with a large stable set S , it may be possible to improve upon S by using ideas from Proposition 1. In particular, Proposition 1 shows that there is a collection of easily computable canonical solutions associated with S that have objective value $|S|$ but are not local maximizers of (5). Restarting Algorithm AL' at or near one of these points may allow the method to “escape” from the stable set S to another stable set of larger size.

We propose the following rank-two heuristic based on the above ideas:

MSS Heuristic (rank-two):**Default Initialization:** $G = (V, E)$, $S = \emptyset$ **Input:** $K \geq 1$, $(x, y) \in \mathfrak{N}^{2n}$, $\lambda \in \mathfrak{N}^{|E|}$ **Output:** S **For** $k = 1, \dots, K$ a. Run Algorithm AL' with input $(x^0, y^0) = (x, y)$ and $\lambda^1 = \lambda$ and receive output \tilde{S} and $\lambda = \lambda^\ell$.b. If $|\tilde{S}| > |S|$, set $S = \tilde{S}$.

- c. Set (x, y) to be a slight perturbation of a canonical solution of S associated with a random unit vector $w \in \mathfrak{R}^2$.

End

We stress that there is no theory guaranteeing that an “escape” would always be achievable for the rank-two problem. In fact, although “escapes” were often observed in our experiments, sometimes the algorithm did fail to escape from a non-maximum stable set.

Since the idea of escaping is not theoretically applicable to the rank-one problem, we present a rank-one heuristic that employs Algorithm AL' by setting the variable y to zero and achieves a single stable set since improvement is unlikely due to Theorem 2. We note, however, that in the implementation discussed below, the variable $y = 0$ is not explicitly carried in the computations.

MSS Heuristic (rank-one):

Default Initialization: $G = (V, E)$, $S = \emptyset$

Input: $x \in \mathfrak{R}^n$, $\lambda \in \mathfrak{R}^{|E|}$

Output: S

Run Algorithm AL' with input $(x^0, y^0) = (x, 0)$ and $\lambda^1 = \lambda$ and receive output S .

We implemented the above heuristics in an ANSI C code which we call “Max-AO” and have tested it on an SGI Origin2000 with sixteen 300MHz R12000 processors at Rice University, although we note that Max-AO utilizes only one processor. In order to test the difference between the rank-one and rank-two formulations and to establish the effectiveness of the “escaping” procedure, we tested the rank-one heuristic as well as two realizations of the rank-two heuristic. In particular, we investigated the rank-two heuristics arising from the choice of parameter $K = 1$ and $K = 5$. We refer to the three resulting heuristics as h1, h21 and h25, respectively.

We ran all three heuristics on a set of 64 graphs obtained from the Center for Discrete Mathematics and Theoretical Computer Science (DIMACS) [8]. These graphs were used as test instances for the maximum clique problem in the Second DIMACS Implementation Challenge. Since the maximum clique problem on a graph is the MSS problem on the complement graph, we actually run Max-AO on the complements of the 64 graphs.

Since each run of Max-AO is randomized, we have run h1, h21 and h25 ten times each on all 64 graphs. In Tables 1 and 2, we report the results of these experiments. Each table has thirteen columns which are divided into four groups. The first group contains information about the test graphs including the name of the graph, the number of vertices and edges, and the size of the largest stable set known for the graph, which has been verified by other researchers to equal $\alpha(G)$ for 55 of the 64 graphs. Note that, if the exact value of $\alpha(G)$ is unknown, then the previously best known stable set size is prefixed with an asterisk (*). The next group of columns gives the size of the largest stable set found by each of the three heuristics over all ten runs. The third group of columns gives the average size (rounded to the nearest integer) of the stable sets found by each heuristic during the ten runs, and the final set of columns gives the average time (in seconds) for each of the heuristics during the ten runs.

A few comments regarding the data in the tables are in order. First and foremost, the data shows that each heuristic is capable of finding large stable sets in a short amount

Table 1. Results of ten runs of each heuristic on the first set of 32 graphs

| name | GRAPH | | | MAX OVERALL | | | AVERAGE SIZE | | | AVERAGE TIME | | |
|------------------|-------|--------|----------|-------------|-----|-----|--------------|-----|-----|--------------|-----|-----|
| | V | E | α | h1 | h21 | h25 | h1 | h21 | h25 | h1 | h21 | h25 |
| MANN-a9.co | 45 | 72 | 16 | 16 | 16 | 16 | 16 | 16 | 16 | 0 | 0 | 0 |
| MANN-a27.co | 378 | 702 | 126 | 118 | 125 | 126 | 100 | 124 | 126 | 0 | 3 | 24 |
| MANN-a45.co | 1035 | 1980 | 345 | 45 | 45 | 344 | 45 | 45 | 343 | 2 | 2 | 390 |
| brock200-1.co | 200 | 5066 | 21 | 20 | 21 | 21 | 20 | 21 | 21 | 0 | 2 | 13 |
| brock200-2.co | 200 | 10024 | 12 | 10 | 11 | 11 | 10 | 11 | 11 | 0 | 3 | 16 |
| brock200-3.co | 200 | 7852 | 15 | 13 | 14 | 14 | 13 | 13 | 14 | 0 | 2 | 13 |
| brock200-4.co | 200 | 6811 | 17 | 15 | 16 | 16 | 15 | 16 | 16 | 0 | 3 | 12 |
| brock400-1.co | 400 | 20077 | 27 | 22 | 24 | 25 | 22 | 24 | 24 | 2 | 12 | 75 |
| brock400-2.co | 400 | 20014 | 29 | 24 | 25 | 25 | 23 | 24 | 24 | 2 | 11 | 81 |
| brock400-3.co | 400 | 20119 | 31 | 24 | 25 | 25 | 22 | 24 | 24 | 2 | 17 | 65 |
| brock400-4.co | 400 | 20035 | 33 | 23 | 24 | 25 | 23 | 24 | 24 | 2 | 13 | 70 |
| brock800-1.co | 800 | 112095 | 23 | 20 | 21 | 21 | 19 | 20 | 20 | 12 | 104 | 490 |
| brock800-2.co | 800 | 111434 | 24 | 20 | 20 | 20 | 19 | 19 | 20 | 13 | 815 | 476 |
| brock800-3.co | 800 | 112267 | 25 | 19 | 21 | 21 | 19 | 20 | 20 | 14 | 92 | 476 |
| brock800-4.co | 800 | 111957 | 26 | 18 | 21 | 21 | 18 | 20 | 20 | 15 | 78 | 500 |
| c-fat200-1.co | 200 | 18366 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 0 | 1 | 5 |
| c-fat200-2.co | 200 | 16665 | 24 | 24 | 24 | 24 | 24 | 24 | 24 | 0 | 3 | 10 |
| c-fat200-5.co | 200 | 11427 | 58 | 58 | 58 | 58 | 58 | 58 | 58 | 0 | 1 | 9 |
| c-fat500-1.co | 500 | 120291 | 14 | 14 | 14 | 14 | 14 | 14 | 14 | 5 | 13 | 83 |
| c-fat500-2.co | 500 | 115611 | 26 | 26 | 26 | 26 | 26 | 26 | 26 | 3 | 13 | 81 |
| c-fat500-5.co | 500 | 101559 | 64 | 64 | 64 | 64 | 64 | 64 | 64 | 3 | 22 | 75 |
| c-fat500-10.co | 500 | 78123 | 126 | 126 | 126 | 126 | 126 | 126 | 126 | 3 | 18 | 68 |
| hamming6-2.co | 64 | 192 | 32 | 32 | 32 | 32 | 31 | 32 | 32 | 0 | 0 | 0 |
| hamming6-4.co | 64 | 1312 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 0 | 0 | 0 |
| hamming8-2.co | 256 | 1024 | 128 | 128 | 128 | 128 | 124 | 128 | 128 | 0 | 0 | 0 |
| hamming8-4.co | 256 | 11776 | 16 | 16 | 16 | 16 | 15 | 16 | 16 | 0 | 1 | 4 |
| hamming10-2.co | 1024 | 5120 | 512 | 512 | 512 | 512 | 512 | 512 | 512 | 2 | 3 | 4 |
| hamming10-4.co | 1024 | 89600 | *40 | 40 | 40 | 40 | 34 | 35 | 36 | 47 | 185 | 643 |
| johnson8-2-4.co | 28 | 168 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 0 | 0 | 0 |
| johnson8-4-4.co | 70 | 560 | 14 | 14 | 14 | 14 | 14 | 14 | 14 | 0 | 0 | 0 |
| johnson16-2-4.co | 120 | 1680 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 0 | 0 | 0 |
| johnson32-2-4.co | 496 | 14880 | 16 | 16 | 16 | 16 | 14 | 16 | 16 | 11 | 2 | 12 |

of time. Second, the “average size” column shows that, on average, h21 finds better stable sets than h1, which indicates that the rank-two formulation is more useful than the rank-one formulation, and that h25 finds better stable sets than h21, which indicates that the escaping procedure works well. Third, even though the ranking of the heuristics in terms of quality of solutions is h1 (good), h21 (better) and h25 (best), the average times show that h25 is the most expensive and h1 is the least expensive. Hence, the data demonstrates the standard trade-off between quality of solution and computation time.

Regarding the “max overall” column, we see that h1 found the maximum stable set 23 times out of the 55 instances for which the exact value of α is known. Thus, h1 found a maximum stable set about 42% of the time. The percentages for h21 and h25 are about 65% and 75%, respectively. Moreover, the three heuristics replicated (or surpassed, as for the graph p-hat1000-3.co) the best known stable set in 38%, 69%, and 78% of the 64 graphs, respectively. From a general perspective, then, we see that the heuristics are highly effective in finding large stable sets, although there is much room for improvement on some graphs — for example, the “brock” instances.

Since there are many varied techniques for the maximum stable set problem (or equivalently, the maximum clique problem) a direct comparison of the running times of

Table 2. Results of ten runs of each heuristic on the second set of 32 graphs

| name | GRAPH | | | MAX OVERALL | | | AVERAGE SIZE | | | AVERAGE TIME | | |
|-----------------|-------|--------|----------|-------------|-----|-----|--------------|-----|-----|--------------|------|------|
| | $ V $ | $ E $ | α | h1 | h21 | h25 | h1 | h21 | h25 | h1 | h21 | h25 |
| keller4.co | 171 | 5100 | 11 | 7 | 11 | 11 | 7 | 10 | 11 | 0 | 3 | 10 |
| keller5.co | 776 | 74710 | 27 | 16 | 24 | 27 | 16 | 21 | 25 | 560 | 391 | 1306 |
| p-hat300-1.co | 300 | 33917 | 8 | 7 | 8 | 8 | 7 | 8 | 8 | 2 | 19 | 64 |
| p-hat300-2.co | 300 | 22922 | 25 | 25 | 25 | 25 | 25 | 25 | 25 | 1 | 22 | 66 |
| p-hat300-3.co | 300 | 11460 | 36 | 35 | 36 | 36 | 35 | 36 | 36 | 1 | 11 | 46 |
| p-hat500-1.co | 500 | 93181 | 9 | 9 | 9 | 9 | 8 | 9 | 9 | 11 | 55 | 192 |
| p-hat500-2.co | 500 | 61804 | 36 | 36 | 36 | 36 | 36 | 36 | 36 | 6 | 83 | 338 |
| p-hat500-3.co | 500 | 30950 | *50 | 48 | 50 | 50 | 48 | 49 | 50 | 4 | 33 | 188 |
| p-hat700-1.co | 700 | 183651 | 11 | 9 | 11 | 11 | 8 | 9 | 10 | 28 | 139 | 1175 |
| p-hat700-2.co | 700 | 122922 | 44 | 44 | 44 | 44 | 44 | 44 | 44 | 18 | 193 | 850 |
| p-hat700-3.co | 700 | 61640 | *62 | 60 | 62 | 62 | 60 | 62 | 62 | 10 | 117 | 524 |
| p-hat1000-1.co | 1000 | 377247 | 10 | 9 | 10 | 10 | 9 | 9 | 10 | 45 | 371 | 1410 |
| p-hat1000-2.co | 1000 | 254701 | *46 | 45 | 46 | 46 | 45 | 46 | 46 | 45 | 599 | 2580 |
| p-hat1000-3.co | 1000 | 127754 | *66 | 63 | 68 | 68 | 63 | 68 | 68 | 21 | 348 | 1445 |
| p-hat1500-1.co | 1500 | 839327 | 12 | 10 | 11 | 11 | 10 | 10 | 10 | 204 | 2214 | 6237 |
| p-hat1500-2.co | 1500 | 555290 | *65 | 64 | 65 | 65 | 64 | 65 | 65 | 148 | 1687 | 7098 |
| p-hat1500-3.co | 1500 | 277006 | *94 | 93 | 94 | 94 | 93 | 93 | 94 | 81 | 1155 | 4917 |
| san200-0.7-1.co | 200 | 5970 | 30 | 15 | 30 | 30 | 15 | 24 | 30 | 0 | 1 | 2 |
| san200-0.7-2.co | 200 | 5970 | 18 | 12 | 18 | 18 | 12 | 15 | 18 | 0 | 2 | 12 |
| san200-0.9-1.co | 200 | 1990 | 70 | 70 | 70 | 70 | 67 | 70 | 70 | 0 | 0 | 0 |
| san200-0.9-2.co | 200 | 1990 | 60 | 36 | 60 | 60 | 35 | 60 | 60 | 0 | 0 | 0 |
| san200-0.9-3.co | 200 | 1990 | 44 | 44 | 44 | 44 | 39 | 40 | 44 | 0 | 1 | 5 |
| san400-0.5-1.co | 400 | 39900 | 13 | 7 | 9 | 13 | 6 | 8 | 11 | 10 | 22 | 68 |
| san400-0.7-1.co | 400 | 23940 | 40 | 20 | 40 | 40 | 19 | 22 | 40 | 226 | 72 | 17 |
| san400-0.7-2.co | 400 | 23940 | 30 | 15 | 19 | 30 | 15 | 16 | 30 | 3 | 11 | 51 |
| san400-0.7-3.co | 400 | 23940 | 22 | 12 | 18 | 22 | 12 | 15 | 18 | 3 | 185 | 98 |
| san400-0.9-1.co | 400 | 7980 | 100 | 52 | 100 | 100 | 52 | 100 | 100 | 1 | 2 | 2 |
| san1000.co | 1000 | 249000 | 15 | 8 | 9 | 10 | 7 | 7 | 9 | 391 | 3401 | 3090 |
| sanr200-0.7.co | 200 | 6032 | 18 | 17 | 18 | 18 | 17 | 17 | 18 | 0 | 4 | 18 |
| sanr200-0.9.co | 200 | 2037 | *42 | 41 | 42 | 42 | 41 | 41 | 42 | 0 | 1 | 8 |
| sanr400-0.5.co | 400 | 39816 | 13 | 12 | 13 | 13 | 12 | 12 | 13 | 2 | 22 | 102 |
| sanr400-0.7.co | 400 | 23931 | *21 | 20 | 21 | 21 | 20 | 21 | 21 | 2 | 17 | 86 |

Table 3. DIMACS processor speed benchmarks (in seconds)

| instance | r100.5 | r200.5 | r300.5 | r400.5 | r500.5 |
|----------|--------|--------|--------|--------|--------|
| time | 0.00 | 0.16 | 1.36 | 8.30 | 31.57 |

our heuristics with those of other heuristics is not readily available. Instead, we adopt a strategy employed by the Second DIMACS Implementation Challenge which is to provide machine timings of a particular DIMACS computer algorithm on five different instances of increasing size. By doing so, running times can be somewhat calibrated, thus allowing solution quality to be compared. Table 3 lists the results for the DIMACS program on the SGI Origin2000 upon which our code has been run. (Please see [8] for more information and [17] for other heuristics which use the same technique for comparison.)

We do, however, believe that it is worth mentioning that the quality of stable sets produced by our heuristics compares well with other heuristics in the literature; in particular, those in [17]. For example, our heuristic h25 achieves the same size stable set on essentially all test instances as the code developed by Balas and Niehaus, which finds large stable sets using the idea of maximum matchings in bipartite subgraphs of G . In

addition, our heuristic compares favorably with the heuristic developed in Benson and Ye [1], which is based on solving an SDP relaxation of the MSS problem that is different from (1). In their paper, they report the size of the best stable set found by their heuristic on twelve of the graphs that are listed in Tables 2 and 3. We remark that the size of the stable set found by our heuristic was at least as large as theirs on all twelve instances. In particular, our heuristic h25 found stable sets which matched theirs on nine of the twelve instances and exceeded theirs on the remaining three (sanr200-0.7, 18 versus 11; sanr200-0.9, 42 versus 34; brock200-1, 21 versus 14).

5. Final remarks

In this paper, we have extended the path laid in [5] by providing yet another example in which low-rank, nonconvex formulations serve as efficient tools for obtaining high-quality approximate (and often exact) solutions to NP-hard combinatorial optimization problems. As is the case in [5] with the Max-Cut problem, our experimental results with the maximum stable set problem indicate that the semidefinite program (1), or its equivalents, is unlikely to be a cost-effective vehicle for finding stable sets in the graph G because of the high computational costs associated with solving such a semidefinite program. Instead, the rank-one and rank-two formulations are more attractive alternatives for that task. We stress, however, that the upper bound $\vartheta(G)$ that (1) provides on $\alpha(G)$ can be highly valuable in its own right as mentioned in the introduction.

We believe that the ideas developed in this paper can be applied to the maximum weight stable set problem. In particular, if each node i in the graph G has an associated weight $w_i > 0$, then the problem of finding a stable set with maximum total weight on its nodes can still be formulated as (2) and (5) by simply replacing the vector e in the objective functions by the vector $(\sqrt{w_1}, \dots, \sqrt{w_n})$ while keeping the constraints unchanged. For example, in the weighted case the canonical solutions of Lemma 1 become $x = \pm x^{S,w}$ where $x_i^{S,w} = \sqrt{w_i/W(S)}$ for $i \in S$ (where $W(S)$ is defined as $\sum_{i \in S} w_i$) and $x_i^{S,w} = 0$ for $i \notin S$.

The continuous formulations and heuristics detailed in this paper add novel techniques to those already available for solving or approximating the MSS problem. We believe that these new techniques are of particular interest because in our tests they consistently produce high-quality stable sets. Nonetheless, there are still many interesting avenues for further improvement. For example, can we devise a more efficient local optimization method than the augmented Lagrangian method (e.g., a trust-region method)? Can we obtain better heuristics by combining the continuous heuristics with some discrete heuristics? Is it possible to escape more reliably from the saddle points corresponding to sub-optimal stable sets? We believe that these questions deserve further investigations.

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A. Complete proof of Theorem 3

Before we give the complete proof of Theorem 3, we wish to point out a simplification that we have employed in the derivation of the results of this section. In particular, the

definition of problem (P_B^2) allows that $T_k = \emptyset$ for one or more $k \in \{1, \dots, p\}$, but in the proofs of this section, we will often implicitly assume that $T_k \neq \emptyset$ so as to reduce the complexity of the proofs. Each result, however, is stated to include the cases that $T_k = \emptyset$, and the proofs are valid even when the equations $T_k = \emptyset$ are considered. As a rule of thumb, each result can be interpreted by noting that $T_k = \emptyset$ implies, for example, that $|T_k| = 0$ or that the variables and constraints corresponding to T_k are nonexistent.

Our first result establishes some characteristics of every local maximizer of (P_B^2) .

Lemma 6. *Let $\bar{z} \equiv (\bar{z}^1, \dots, \bar{z}^n)$ be a local maximizer of (P_B^2) . Then, for each $k = 1, \dots, p$, there exist \bar{u}^k and \bar{v}^k such that*

$$\bar{z}^i = \begin{cases} \bar{u}^k, & i \in S_k, \\ \bar{v}^k, & i \in T_k. \end{cases} \quad (22)$$

Proof. To show the lemma, let $k \in \{1, \dots, p\}$ be given. Note that (22) is obviously true when $|T_k| = 0$ since then $|S_k| = 1$. So assume that $|T_k| > 0$. Since \bar{z} is a local maximizer, the point $(\bar{z}^i)_{i \in U_k}$ is a local maximizer of the problem

$$\max \left\{ \left\| \sum_{i \in U_k} z^i + a^k \right\|^2 : z^i \perp z^j \ \forall (i, j) \in S_k \times T_k, \sum_{i \in U_k} \|z^i\|^2 = \delta_k \right\}, \quad (23)$$

where $U_k \equiv S_k \cup T_k$, $a^k \equiv \sum_{i \notin U_k} \bar{z}^i$ and $\delta_k \equiv 1 - \sum_{i \notin U_k} \|\bar{z}^i\|^2$. Note that if $\delta_k = 0$ then (22) obviously hold with $\bar{u}^k = \bar{v}^k = 0$. Hence, we assume that $\delta_k \neq 0$. We now examine (23) in the three cases in which the span of $\{\bar{z}^i : i \in S_k\}$ is either zero-, one- or two-dimensional.

If the span is zero-dimensional, then $\bar{z}^i = 0$ for all $i \in S_k$, in which case $(\bar{z}^j)_{j \in T_k}$ is a local maximizer of the problem

$$\max \left\{ \left\| \sum_{i \in T_k} z^i + a^k \right\|^2 : \sum_{i \in T_k} \|z^i\|^2 = \delta_k \right\}. \quad (24)$$

Analyzing the first-order necessary conditions of (24) at $(\bar{z}^j)_{j \in T_k}$, we see that there exists $\lambda \in \Re$ such that $\sum_{i \in T_k} \bar{z}^i + a^k = \lambda \bar{z}^j$ for all $j \in T_k$. If $\lambda \neq 0$ then it follows from these conditions that (22) holds with $\bar{u}^k = 0$ and $\bar{v}^k = (\sum_{i \in T_k} \bar{z}^i + a^k)/\lambda$. Suppose now that $\lambda = 0$. Then, we have $\sum_{i \in T_k} \bar{z}^i + a^k = 0$. Since $(\bar{z}^j)_{j \in T_k}$ is a local maximizer of (24), this implies that the objective function of every feasible solution sufficiently close to $(\bar{z}^j)_{j \in T_k}$ is zero. Thus, $(\bar{z}^j)_{j \in T_k}$ is also a local maximizer of $\max\{\sum_{i \in T_k} e^T(z^i + a^k) : \sum_{i \in T_k} \|z^i\|^2 = \delta_k\}$. First-order optimality conditions for this problem then imply the existence of $\eta \in \Re$ such that $e = \eta \bar{z}^j$ for all $j \in T_k$. This implies that when $\lambda = 0$, (22) also holds with $\bar{u}^k = 0$ and $\bar{v}^k = e/\eta$.

If the span is two-dimensional, then $\bar{z}^i = 0$ for all $i \in T_k$. Hence, a similar argument as in the zero-dimensional case shows that \bar{z}^i is constant over all $i \in S_k$.

If the span is one-dimensional, then there exist perpendicular unit vectors $w^a, w^b \in \Re^2$ and scalars $\bar{\gamma}_i$ for all $i \in U_k$ such that $\bar{z}^i = \bar{\gamma}_i w^a$ for all $i \in S_k$ and $\bar{z}^i = \bar{\gamma}_i w^b$ for all

$i \in T_k$. It then follows that $(\bar{\gamma}_j)_{j \in U_k}$ is a local maximizer of the problem that originates from (23) by adding the extra constraints $z^i = \gamma_i w^a$ for all $i \in S_k$ and $z^i = \gamma_i w^b$ for all $i \in T_k$, or equivalently, the following maximization problem whose variables are $(\gamma_i)_{i \in U_k}$:

$$\max \left\{ \left\| \sum_{i \in S_k} \gamma_i w^a + \sum_{i \in T_k} \gamma_i w^b + a^k \right\|^2 : \sum_{i \in U_k} \gamma_i^2 = \delta_k \right\}. \quad (25)$$

Analyzing the first-order necessary conditions of the above maximization, we see that there exists $\lambda \in \Re$ such that

$$\begin{aligned} (w^a)^T \left(\sum_{i \in S_k} \bar{\gamma}_i w^a + \sum_{i \in T_k} \bar{\gamma}_i w^b + a^k \right) &= \lambda \bar{\gamma}_j \quad \forall j \in S_k, \\ (w^b)^T \left(\sum_{i \in S_k} \bar{\gamma}_i w^a + \sum_{i \in T_k} \bar{\gamma}_i w^b + a^k \right) &= \lambda \bar{\gamma}_j \quad \forall j \in T_k. \end{aligned}$$

If $\lambda \neq 0$ then the above conditions imply that $\bar{\gamma}_j$ is constant over $j \in S_k$ as well as over $j \in T_k$. Suppose now that $\lambda = 0$. Then the vector $\hat{w} \equiv \sum_{i \in S_k} \bar{\gamma}_i w^a + \sum_{i \in T_k} \bar{\gamma}_i w^b + a^k$ is perpendicular to both w^a and w^b . Since w^a and w^b are themselves perpendicular nonzero vectors in \Re^2 , it follows that $\hat{w} = 0$ in which case the objective value of (25) at $(\bar{\gamma}_i)_{i \in U_k}$ is 0. Using this fact together with an argument very similar to the one used in the zero-dimensional case above, one can also show for this case that $\bar{\gamma}_j$ is constant over $j \in S_k$ as well as over $j \in T_k$.

Hence, in each of the three cases pertaining to the assumption that $|T_k| > 0$, we have shown that \bar{z}^i is constant over $i \in S_k$ and \bar{z}^i is constant over $i \in T_k$, and the lemma follows. \square

In view of the above lemma, when we identify z^i with $i \in S_k$ (respectively, $i \in T_k$) with a single variable u^k (respectively, v^k), any local maximizer of problem (P_B^2) becomes a local maximizer of the problem

$$\begin{aligned} \text{maximize } g(Z) &\equiv \left\| \sum_{k=1}^p (|S_k| u^k + |T_k| v^k) \right\|^2 \\ \text{subject to } \sum_{k=1}^p (|S_k| \|u^k\|^2 + |T_k| \|v^k\|^2) &= 1, \\ u^k \perp v^k, \quad \forall k &= 1, \dots, p, \end{aligned} \quad (26)$$

whose variables are $Z \equiv (u^1, v^1, \dots, u^p, v^p)$.

Lemma 7. *Let $\bar{Z} = (\bar{u}^1, \bar{v}^1, \dots, \bar{u}^p, \bar{v}^p) \in \Re^{2p}$ be a local maximizer of (26). Then $g(\bar{Z}) > 0$ and, for every $k = 1, \dots, p$, at least one of the vectors \bar{u}^k or \bar{v}^k is nonzero.*

Proof. To show that $g(\bar{Z}) > 0$, assume for contradiction that $g(\bar{Z}) = 0$. Then, since $g(Z)$ is a nonnegative function, it follows that $g(Z)$ is zero within a neighborhood of \bar{Z} . Hence, \bar{Z} is also a local maximizer of

$$\max \left\{ \sum_{k=1}^p w^T (|S_k|u^k + |T_k|v^k) : \sum_{k=1}^p (|S_k| \|u^k\|^2 + |T_k| \|v^k\|^2) = 1, \right. \\ \left. u^k \perp v^k \forall k = 1, \dots, p \right\}$$

for an arbitrary nonzero $w \in \mathfrak{R}^2$. Examining the first-order optimality condition for this problem, we see that there exist $\lambda, \lambda_1, \dots, \lambda_p \in \mathfrak{R}$ such that, for each $k = 1, \dots, p$,

$$|S_k|w + 2\lambda|S_k|\bar{u}^k + \lambda_k \bar{v}^k = 0, \quad |T_k|w + 2\lambda|T_k|\bar{v}^k + \lambda_k \bar{u}^k = 0. \quad (27)$$

Taking the inner product of each of these equations with \bar{u}^k and \bar{v}^k , respectively, employing the orthogonality of \bar{u}^k and \bar{v}^k , and then summing over all k , we see that

$$\sum_{k=1}^p w^T (|S_k|\bar{u}^k + |T_k|\bar{v}^k) + 2\lambda \sum_{k=1}^p (|S_k| \|\bar{u}^k\|^2 + |T_k| \|\bar{v}^k\|^2) = 0. \quad (28)$$

Since $\sum_{k=1}^p (|S_k|\bar{u}^k + |T_k|\bar{v}^k) = 0$ by the assumption that $g(\bar{Z}) = 0$ and since

$$\sum_{k=1}^p (|S_k| \|\bar{u}^k\|^2 + |T_k| \|\bar{v}^k\|^2) = 1$$

by the feasibility of \bar{Z} for (26), we see from (28) that $\lambda = 0$. Now using (27) with the knowledge that $\lambda = 0$, we see that each \bar{u}^k and \bar{v}^k is a nonzero multiple of w . Since $0 \neq w \in \mathfrak{R}^2$ was chosen arbitrarily, however, this implies that \bar{u}^k and \bar{v}^k are nonzero multiples of every nonzero vector in \mathfrak{R}^2 , which is impossible. Hence, we have a contradiction of our assumption that $g(\bar{Z}) = 0$.

To show the second claim of the lemma, let $l \in \{1, \dots, p\}$ and assume that $\bar{v}^l = 0$; we will show $\bar{u}^l \neq 0$. We have that \bar{Z} is a local maximizer of the problem formed by setting $v^l = 0$, i.e.,

$$\begin{aligned} & \text{maximize} \quad \left\| |S_l|u^l + \sum_{k \neq l} (|S_k|u^k + |T_k|v^k) \right\|^2 \\ & \text{subject to} \quad |S_l| \|u^l\|^2 + \sum_{k \neq l} (|S_k| \|u^k\|^2 + |T_k| \|v^k\|^2) = 1, \quad (29) \\ & \quad \quad \quad u^k \perp v^k, \quad \forall k \neq l \end{aligned}$$

The first-order optimality conditions for this problem reveal that $\bar{r} = \eta \bar{u}^l$ for some $\eta \in \mathfrak{R}$, where

$$\bar{r} \equiv \sum_{k=1}^p (|S_k|\bar{u}^k + |T_k|\bar{v}^k) = |S_l|\bar{u}^l + \sum_{k \neq l} (|S_k|\bar{u}^k + |T_k|\bar{v}^k). \quad (30)$$

Since $0 < g(\bar{Z}) = \|\bar{r}\|^2 = \eta^2 \|\bar{u}^l\|^2$, we conclude that $\bar{u}^l \neq 0$. By employing an analogous argument, we may also conclude that $\bar{u}^l = 0$ implies $\bar{v}^l \neq 0$. Hence, it is not possible that $\bar{u}^l = \bar{v}^l = 0$, which proves the second claim of the lemma. \square

Lemma 8. *Let $Z = (u^1, v^1, \dots, u^p, v^p) \in \Re^{2p}$ be a point such that, for all $k = 1, \dots, p$,*

$$u^k + v^k = \gamma_k w, \quad u^k \perp v^k, \quad (31)$$

$$|S_k| > |T_k| > 0 \implies u^k = 0 \text{ or } v^k = 0, \quad (32)$$

where $w \in \Re^2$ is a vector of unit-length and $\gamma_1, \dots, \gamma_p$ are scalars. Let

$$\mathcal{K} \equiv \mathcal{K}(Z) \equiv \{k : |S_k| > |T_k| > 0, v^k \neq 0\}. \quad (33)$$

Then,

$$\sum_{k=1}^p (|S_k| u^k + |T_k| v^k) = \left(\sum_{k \notin \mathcal{K}} \gamma_k |S_k| + \sum_{k \in \mathcal{K}} \gamma_k |T_k| \right) w, \quad (34)$$

$$g(Z) = \left(\sum_{k \notin \mathcal{K}} \gamma_k |S_k| + \sum_{k \in \mathcal{K}} \gamma_k |T_k| \right)^2. \quad (35)$$

Moreover, Z is a feasible solution for problem (26) if and only if

$$\sum_{k \notin \mathcal{K}} |S_k| \gamma_k^2 + \sum_{k \in \mathcal{K}} |T_k| \gamma_k^2 = 1.$$

Proof. Using (31), (32) and the definition of \mathcal{K} , it is easy to see that for all $k = 1, \dots, p$,

$$\begin{aligned} |S_k| \|u^k\|^2 + |T_k| \|v^k\|^2 &= \begin{cases} |S_k| \|u^k + v^k\|^2, & k \notin \mathcal{K}, \\ |T_k| \|u^k + v^k\|^2, & k \in \mathcal{K}, \end{cases} \\ |S_k| u^k + |T_k| v^k &= \begin{cases} |S_k| (u^k + v^k), & k \notin \mathcal{K}, \\ |T_k| (u^k + v^k), & k \in \mathcal{K}. \end{cases} \end{aligned}$$

Hence, we have

$$\begin{aligned} \sum_{i=1}^p |S_k| \|u^k\|^2 + |T_k| \|v^k\|^2 &= \sum_{k \notin \mathcal{K}} |S_k| \|u^k + v^k\|^2 + \sum_{k \in \mathcal{K}} |T_k| \|u^k + v^k\|^2 \\ &= \sum_{k \notin \mathcal{K}} |S_k| \|\gamma_k w\|^2 + \sum_{k \in \mathcal{K}} |T_k| \|\gamma_k w\|^2 \\ &= \sum_{k \notin \mathcal{K}} |S_k| \gamma_k^2 + \sum_{k \in \mathcal{K}} |T_k| \gamma_k^2 \end{aligned}$$

and

$$\begin{aligned} \sum_{i=1}^p (|S_k| u^k + |T_k| v^k) &= \sum_{k \notin \mathcal{K}} |S_k| (u^k + v^k) + \sum_{k \in \mathcal{K}} |T_k| (u^k + v^k) \\ &= \left(\sum_{k \notin \mathcal{K}} |S_k| \gamma_k + \sum_{k \in \mathcal{K}} |T_k| \gamma_k \right) w. \end{aligned}$$

The expression for $g(Z)$ and the if-and-only-if statement of the lemma now follow immediately from the above two identities. \square

We will now give the complete proof of parts (c) and (d) of Theorem 3.

Proof. We start by proving (d). Let $\bar{z} \equiv (\bar{z}^1, \dots, \bar{z}^n)$ be a local maximizer of (P_B^2) . We will show that $\bar{f} \equiv f(\bar{z}) = |S_1| + \dots + |S_p|$, from which part (d) of the theorem follows immediately due to Theorem 3(b). Define the point $\bar{Z} \equiv (\bar{u}^1, \bar{v}^1, \dots, \bar{u}^p, \bar{v}^p)$ whose two-dimensional vector components satisfy the conditions of Lemma 6. Using the fact that \bar{z} is a local maximizer of (P_B^2) , one can easily verify that \bar{Z} is a local maximizer of problem (26). Now let \bar{r} be the vector defined as in (30) and note that $\bar{f} = g(\bar{Z}) = \|\bar{r}\|^2$. The first-order optimality conditions that hold at \bar{Z} are:

$$|S_k|\bar{r} = \lambda|S_k|\bar{u}^k + \lambda_k\bar{v}^k, \quad (36)$$

$$|T_k|\bar{r} = \lambda|T_k|\bar{v}^k + \lambda_k\bar{u}^k, \quad (37)$$

for all $k = 1, \dots, p$, where $\lambda, \lambda_1, \dots, \lambda_p \in \Re$ are the Lagrange multipliers. (The constraint qualification that the gradients of the constraints of (26) at the point \bar{Z} are linearly independent can be easily verified.) By taking the dot product of (36) and (37) with \bar{u}^k and \bar{v}^k , respectively, then adding the two resultant equations, and finally summing all such equations over the index k , we easily obtain that $\lambda = \bar{f}$. Hence, in what follows, we replace λ by \bar{f} . Now multiplying (36) by $|T_k|$ and (37) by $|S_k|$, and subtracting the two resulting equations, we obtain

$$\bar{f}|S_k||T_k|(\bar{u}^k - \bar{v}^k) = \lambda_k(|S_k|\bar{u}^k - |T_k|\bar{v}^k).$$

Taking the dot product of the last equation with \bar{u}^k and \bar{v}^k , and using the fact that $\bar{u}^k \perp \bar{v}^k$, we obtain respectively that

$$|S_k|(|T_k|\bar{f} - \lambda_k)\|\bar{u}^k\|^2 = 0, \quad (38)$$

$$|T_k|(|S_k|\bar{f} - \lambda_k)\|\bar{v}^k\|^2 = 0. \quad (39)$$

By Lemma 7, we know that for all $k = 1, \dots, p$, at least one of the vectors \bar{u}^k and \bar{v}^k is nonzero. If $\bar{u}^k \neq 0$ then by (38) we have $\lambda_k = |T_k|\bar{f}$, which together with (37) implies that $\bar{u}^k + \bar{v}^k = \bar{r}/\bar{f}$. In a similar manner, using (39) and (36) we conclude that if $\bar{v}^k \neq 0$ and $|T_k| > 0$ then we have $\lambda_k = |S_k|\bar{f}$ and $\bar{u}^k + \bar{v}^k = \bar{r}/\bar{f}$. These two observations clearly imply that for all $k = 1, \dots, p$, we have

$$\bar{u}^k + \bar{v}^k = \frac{1}{\bar{f}^{1/2}} \frac{\bar{r}}{\|\bar{r}\|},$$

$$|S_k| > |T_k| > 0 \implies \text{either } \bar{u}^k = 0 \text{ or } \bar{v}^k = 0.$$

Therefore, letting $\bar{\mathcal{K}} \equiv \mathcal{K}(\bar{Z}) \equiv \{k : |S_k| > |T_k| > 0, \bar{v}^k \neq 0\}$, it follows from Lemma 8 with $\gamma_k = \bar{f}^{-1/2}$ for all $k = 1, \dots, p$ that

$$\bar{f} = \sum_{k \notin \bar{\mathcal{K}}} |S_k| + \sum_{k \in \bar{\mathcal{K}}} |T_k|. \quad (40)$$

To conclude the proof of assertion (d), it remains to show that $\bar{\mathcal{K}} = \emptyset$, in which case (40) reduces to $\bar{f} = \sum_{k=1}^p |S_k| = |S|$, which in turn implies the proposition by Theorem 3(b). Indeed, assume for contradiction that $\bar{\mathcal{K}} \neq \emptyset$ and note that in this case $\bar{f} < |S|$. Consider the point $\hat{Z} = (\hat{u}^1, \hat{v}^1, \dots, \hat{u}^p, \hat{v}^p)$ defined as

$$\hat{u}^k = \begin{cases} (\bar{f}/|S|)^{1/2} Q \bar{u}^k, & k \notin \bar{\mathcal{K}} \\ (|S|\bar{f})^{-1/2} Q \bar{r}, & k \in \bar{\mathcal{K}} \end{cases}, \quad \hat{v}^k = \begin{cases} (\bar{f}/|S|)^{1/2} Q \bar{v}^k, & k \notin \bar{\mathcal{K}} \\ 0, & k \in \bar{\mathcal{K}} \end{cases},$$

where $Q \in \mathfrak{N}^{2 \times 2}$ is defined as

$$Q \equiv \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

It is a simple verification to see that, for all $k = 1, \dots, p$, we have $\hat{u}^k \perp \hat{v}^k$ and $\hat{u}^k + \hat{v}^k = w/\sqrt{|S|}$, where w is the unit-length vector $w \equiv Q \bar{r}/\|Q \bar{r}\| = Q \bar{r}/\bar{f}^{1/2}$. Moreover, we have that $\hat{\mathcal{K}} \equiv \mathcal{K}(\hat{Z}) = \emptyset$, and so it follows that \hat{Z} is a feasible solution of (26). Using all these facts along with Lemma 8, we conclude that $g(\hat{Z}) = |S|$. Consider now the path $Z : [0, 1] \rightarrow \mathfrak{N}^{2p}$ defined as

$$Z(t) \equiv \psi(t) \left[(1-t)\bar{Z} + t\hat{Z} \right]$$

for all $t \in [0, 1]$, where $\psi(t) \equiv [(1-t)^2 + t^2]^{-1/2}$. We claim that $Z(t)$ is feasible for problem (26) for all $t \in [0, 1]$. Indeed, writing $Z(t) = (u^1(t), v^1(t), \dots, u^p(t), v^p(t))$ and noting that $\hat{u}^k \perp \hat{v}^k$ for all $k = 1, \dots, p$, we have for every $k \notin \bar{\mathcal{K}}$ that

$$\begin{aligned} (u^k(t))^T v^k(t) &= \psi(t)^2 \left((1-t)\bar{u}^k + t\hat{u}^k \right)^T \left((1-t)\bar{v}^k + t\hat{v}^k \right) \\ &= \psi(t)^2 t(1-t) \left((\bar{u}^k)^T \bar{v}^k + (\hat{z}^k)^T \bar{v}^k \right) \\ &= \psi(t)^2 t(1-t) (\bar{f}/|S|)^{1/2} (\bar{u}^k)^T (Q + Q^T) \bar{v}^k = 0, \end{aligned}$$

since $Q + Q^T = 0$. Noting that $\bar{v}^k = \bar{r}/\bar{f}$ for $k \in \bar{\mathcal{K}}$ and using the relation $\bar{r}^T Q \bar{r} = 0$, we easily see that the above inner product is also zero when $k \in \bar{\mathcal{K}}$. Hence, it follows that $u^k(t) \perp v^k(t)$ for all $t \in [0, 1]$. We also have, using $\hat{u}^k \perp \bar{u}^k$ and $\hat{v}^k \perp \bar{v}^k$, that

$$\begin{aligned} &\sum_{k=1}^p \left(|S_k| \|u^k(t)\|^2 + |T_k| \|v^k(t)\|^2 \right) \\ &= \psi(t)^2 \sum_{k=1}^p \left(|S_k| \|(1-t)\bar{u}^k + t\hat{u}^k\|^2 + |T_k| \|(1-t)\bar{v}^k + t\hat{z}^k\|^2 \right) \\ &= \psi(t)^2 \sum_{k=1}^p \left(|S_k| \left[(1-t)^2 \|\bar{u}^k\|^2 + t^2 \|\hat{z}^k\|^2 \right] + |T_k| \left[(1-t)^2 \|\bar{v}^k\|^2 + t^2 \|\hat{z}^k\|^2 \right] \right) \\ &= \psi(t)^2 \left[(1-t)^2 \sum_{k=1}^p \left(|S_k| \|\bar{u}^k\|^2 + |T_k| \|\bar{v}^k\|^2 \right) + t^2 \sum_{k=1}^p \left(|S_k| \|\hat{z}^k\|^2 + |T_k| \|\hat{v}^k\|^2 \right) \right] \\ &= \psi(t)^2 \left[(1-t)^2 + t^2 \right] = 1. \end{aligned}$$

We have thus established the feasibility of $Z(t)$ with respect to (26) for all $t \in [0, 1]$. We now claim that $g(Z(t))$ is a strictly increasing function of $t \in [0, 1]$. Note that this claim implies that $\bar{Z} = Z(0)$ is not a local maximizer of (26), thereby giving the desired contradiction. To prove the claim, note that

$$\begin{aligned}
g(Z(t)) &= \left\| \sum_{k=1}^p \left(|S_k| u^k(t) + |T_k| v^k(t) \right) \right\|^2 \\
&= \psi(t)^2 \left\| \sum_{k=1}^p \left(|S_k| \left((1-t)\bar{u}^k + t\hat{u}^k \right) + |T_k| \left((1-t)\bar{v}^k + t\hat{v}^k \right) \right) \right\|^2 \\
&= \psi(t)^2 \left\| (1-t) \sum_{k=1}^p \left(|S_k| \bar{u}^k + |T_k| \bar{v}^k \right) + t \sum_{k=1}^p \left(|S_k| \hat{u}^k + |T_k| \hat{v}^k \right) \right\|^2 \\
&= \psi(t)^2 \left[(1-t)^2 \left\| \sum_{k=1}^p \left(|S_k| \bar{u}^k + |T_k| \bar{v}^k \right) \right\|^2 + t^2 \left\| \sum_{k=1}^p \left(|S_k| \hat{u}^k + |T_k| \hat{v}^k \right) \right\|^2 \right] \\
&= \frac{(1-t)^2 \bar{f} + t^2 |S|}{(1-t)^2 + t^2}.
\end{aligned}$$

The fourth equality follows from the orthogonality between the vectors $\sum_{k=1}^p (|S_k| \bar{u}^k + |T_k| \bar{v}^k)$ and $\sum_{k=1}^p (|S_k| \hat{u}^k + |T_k| \hat{v}^k)$, which is guaranteed by Lemma 8 and the fact that \bar{r} is orthogonal to $Q\bar{r}$. This completes the proof of part (d) of the theorem.

Part (c) of the theorem can now be easily extracted from the analysis used to prove part (d). \square

B. An example

We provide an example in which (x, y) is a local maximizer in (5) but the induced stable set A is not maximal in G . Consider the example having $V = \{1, 2, 3, 4, 5, 6, 7, 8\}$ and

$$E = \{(1, 2), (1, 5), (1, 8), (2, 6), (2, 7), (3, 4), (3, 5), (3, 7), (4, 6), (4, 8)\},$$

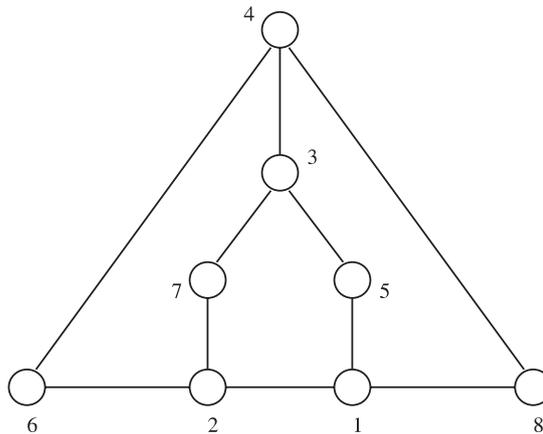
i.e., G is the following graph: Let $w \in \mathfrak{R}^2$ be any vector of unit-length, and consider any feasible (x, y) satisfying

$$(x_1, y_1) + (x_2, y_2) = (x_3, y_3) + (x_4, y_4) = \frac{1}{\sqrt{2}} w,$$

$$(x_5, y_5) = (x_6, y_6) = (x_7, y_7) = (x_8, y_8) = 0,$$

and the following: (i) none of $x_i, y_i, i = 1, 2, 3, 4$, is zero; and (ii) (x_i, y_i) and (x_j, y_j) are linearly independent for all non-edges (i, j) in the collection $(1, 3), (2, 4), (2, 3), (1, 4)$. For example, one could take $w = (1/\sqrt{2}, 1/\sqrt{2})$ and

$$\begin{aligned}
(x_1, y_1) &= \left(\frac{1}{4}, \frac{1}{4} - \frac{1}{2\sqrt{2}} \right), & (x_2, y_2) &= \left(\frac{1}{4}, \frac{1}{4} + \frac{1}{2\sqrt{2}} \right), \\
(x_3, y_3) &= \left(\frac{1}{4} + \frac{1}{2\sqrt{2}}, \frac{1}{4} \right), & (x_4, y_4) &= \left(\frac{1}{4} - \frac{1}{2\sqrt{2}}, \frac{1}{4} \right).
\end{aligned}$$



In such a case, it can be easily seen that $f(x, y) = 2$. In addition, $V_0 = \{5, 6, 7, 8\}$, which implies $p = 2$, $A_1 = \{1\}$, $B_1 = \{2\}$, $A_2 = \{3\}$ and $B_2 = \{4\}$.

By continuity, any nearby feasible point (\hat{x}, \hat{y}) satisfies the following: (a) none of \hat{x}_i, \hat{y}_i , $i = 1, 2, 3, 4$, is zero; and (b) (\hat{x}_i, \hat{y}_i) and (\hat{x}_j, \hat{y}_j) are linearly independent for all non-edges (i, j) in the collection $(1, 3)$, $(2, 4)$, $(2, 3)$, and $(1, 4)$. In fact, because of items (a) and (b) as well as the orthogonality constraints on the edges in the set $E \setminus \{(1, 2), (3, 4)\}$, it is straightforward to see that (\hat{x}_5, \hat{y}_5) , (\hat{x}_6, \hat{y}_6) , (\hat{x}_7, \hat{y}_7) and (\hat{x}_8, \hat{y}_8) must all equal 0. Thus, (\hat{x}, \hat{y}) gives rise to the same set V_0 as (x, y) , and so $f(\hat{x}, \hat{y}) \leq |A_1| + |A_2| = 2$. This implies that $f(\hat{x}, \hat{y}) \leq f(x, y)$ for all nearby feasible points (\hat{x}, \hat{y}) . We conclude that (x, y) is a local maximizer. Even though (x, y) is a local maximizer, however, its induced stable set $A = A_1 \cup A_2$ is not maximal in G . In fact, none of its alternate induced stable sets — $A_1 \cup A_2$, $A_1 \cup B_2$, $B_1 \cup A_2$ or $B_1 \cup B_2$ — are maximal.

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