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Improving an Upper Bound on the Stability Number of a Graph

CARLOS J. LUZ
Escola Superior de Tecnologia de Setúbal/Instituto Politécnico de Setúbal
Campus do IPS, Estefanilha, 2914-508 Setúbal, Portugal (e-mail: cluz@est.ips.pt)

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Abstract. In previous works an upper bound on the stability number of a graph based on quadratic programming was introduced and several of its properties were given. The graphs for which this bound is attained has been known as graphs with convex-QP stability number. This paper proposes a new upper bound on the stability number whose determination is also done by quadratic programming. It is proved that the new bound improves the above mentioned bound and several computational tests asserting its interest for large graphs are presented. In addition a necessary and sufficient condition for a graph to attain the new bound is proved. As a consequence a graph with convex-QP stability number also attains the new bound. On the other hand it is shown the existence of graphs attaining the new bound that do not belong to the class of graphs with convex-QP stability number. This allows to assert that the class of graphs with convex-QP stability number is strictly included in the class of graphs that attain the introduced bound. Some conclusions and lines for future work finalize the paper.

Key words: combinatorial optimization, graph theory, maximum stable set, quadratic programming

1. Introduction

Let $G = (V, E)$ be a simple undirected graph where $V = \{1, \ldots, n\}$ denotes the vertex set and E is the edge set. Throughout the paper it will be supposed that E is not empty. We will write $ij \in E$ to denote the edge linking nodes i and j of V. The adjacency matrix $A = [a_{ij}]$ of G is defined by

$$a_{ij} = \begin{cases} 1, & \text{if } ij \in E, \\ 0, & \text{if } ij \notin E. \end{cases}$$

A stable (or independent) set of G is a subset of nodes of V whose elements are pairwise nonadjacent. The stability number (or independence number) of G is defined as the cardinality of the largest stable set and is usually denoted by $\alpha(G)$. A maximum stable set of G is a stable set with $\alpha(G)$ nodes. The problem of finding $\alpha(G)$ is NP-*hard* and thus it is suspected that it cannot be solved in polynomial-time. However, several ways of approaching that number have been proposed in the literature, which were certainly motivated by the theoretical and practical interest of stable sets (see, for example, [2, 4, 7, 8, 13, 19]).

The aim of this paper is to improve the upper bound on the stability number of a graph introduced in previous works [16, 17]. For any graph G it was proved in [17] that $\alpha(G) \leqslant \upsilon(G)$, where $\upsilon(G)$ is the optimal value of the following convex quadratic programming problem:

$$\upsilon(G) = \max\{2e^{\mathrm{T}}x - x^{\mathrm{T}}(H + I)x : x \geqslant 0\}. \tag{1}$$

Here and hereinafter e is the $n \times 1$ all ones vector, T stands for the transposition operation, I is the identity matrix of order n and $H = A/(-\lambda_{\min}(A))$, where A is the adjacency matrix of G and $\lambda_{\min}(A)$ is its smallest eigenvalue. Assuming that G has at least an edge, we have $\lambda_{\min}(A) \leqslant -1$ (see [6]). Thus the definition of H implies that $\lambda_{\min}(H) = -1$.

This paper proposes a new upper bound on the stability number whose determination is also done by quadratic programming. The new bound, which will be denoted by $\upsilon'(G)$, is deduced in Section 2. In Section 3 it is proved that $\upsilon'(G)$ improves $\upsilon(G)$. This section discusses also the conditions under which this improvement is strict and presents examples illustrating this fact. The interest of the new bound is also shown by the inclusion of an empirical comparison with to the famous Lovász ϑ number introduced in [13] and discussed in many publications (see, for example [4, 9, 11, 14]). Although the proposed bound seems to be dominated by theta in the tests performed, it is computed in much smaller time. Moreover, it is computable in reasonable time for much larger graphs than the ϑ number. On the other hand, very large graphs are presented for which the stability number is obtained by computing the improved bound.

The class of graphs G verifying $\alpha(G) = \upsilon(G)$ was introduced in [16] and successively studied in [5, 15, 17, 18]. In [5] the graphs belonging to this class were coined as graphs with convex-QP stability number. We recall a necessary and sufficient condition that characterizes this class of graphs: a graph G verifies $\alpha(G) = \upsilon(G)$ if and only if for any maximum stable set S of G,

$$-\lambda_{\min}(A) \leqslant \min\{|N(i) \cap S| : i \notin S\}, \tag{2}$$

where $N(i)$ is the set of vertices of G which are adjacent to i (throughout the paper the number of elements of a finite set C is denoted by $|C|$). In Section 4 the class of graphs for which $\alpha(G) = \upsilon'(G)$ is introduced and an analogous necessary and sufficient condition for a graph to attain the new bound is proved. This condition (or alternatively the inequality $\upsilon'(G) \leqslant \upsilon(G)$) allows to conclude that the graphs G for which $\alpha(G) = \upsilon(G)$ (i.e., the graphs with convex-QP stability number) also verify $\alpha(G) = \upsilon'(G)$. On the other hand an example of a graph G is provided for which $\alpha(G) = \upsilon'(G) < \upsilon(G)$. This implies that the class of graphs with convex-QP stability number is strictly included in the class of graphs that attain the introduced bound. Finally, Section 5 presents some conclusions and lines for future work.

2. The Improved Bound

In [16], the upper bound $\upsilon(G)$ given in (1) was deduced by applying the theory of Lagrangian duality to the following quadratic programming problem:

$$\begin{aligned} \max \quad & e^{\mathrm{T}}x - \frac{1}{2}x^{\mathrm{T}}Hx \\ \text{s.t.} \quad & x^{\mathrm{T}}x \leqslant \alpha(G), \\ & x \geqslant 0, \end{aligned} \tag{3}$$

whose optimal value gives an upper bound on $\alpha(G)$. In fact the characteristic vector x of any maximum independent set S of G (defined by $x_i = 1$ if $i \in S$ and $x_i = 0$ otherwise) is a feasible solution of (3) and verifies $e^{\mathrm{T}}x - \frac{1}{2}x^{\mathrm{T}}Hx = \alpha(G)$, because $x^{\mathrm{T}}Hx = 0$.

To obtain the improved bound, the constraint $e^{\mathrm{T}}x = \alpha(G)$ is added to problem (3) and a procedure similar to that of [16] is followed. The resulting problem can be stated as

$$\begin{aligned} \max \quad & e^{\mathrm{T}}x - \frac{1}{2}x^{\mathrm{T}}Hx \\ \text{s.t.} \quad & e^{\mathrm{T}}x = \alpha(G), \\ & x^{\mathrm{T}}x \leqslant \alpha(G), \\ & x \geqslant 0. \end{aligned} \tag{4}$$

Clearly its optimal value constitutes also an upper bound on $\alpha(G)$ (to simplify the notation we will use several times α instead of $\alpha(G)$ as well as υ and υ' instead of $\upsilon(G)$ and $\upsilon'(G)$, respectively).

Consider now the restricted Lagrangian dual problem of (4), i.e.,

$$\begin{aligned} \min \quad & d(w) \\ \text{s.t.} \quad & w \geqslant 0, \end{aligned}$$

where

$$\begin{aligned} d(w) = \max \quad & (e + w)^{\mathrm{T}}x - \frac{1}{2}x^{\mathrm{T}}Hx \\ \text{s.t.} \quad & e^{\mathrm{T}}x = \alpha, \\ & x^{\mathrm{T}}x \leqslant \alpha. \end{aligned} \tag{5}$$

In order to eliminate the linear constraint $e^{\mathrm{T}}x = \alpha$ in this problem we need to introduce some additional notation.

Let $\bar{x}$ and $\bar{e}$ be the vectors formed by the last $n-1$ components of $x = (x_1, x_2, \ldots, x_n)^{\mathrm{T}}$ and e, respectively. Denote by F the matrix defined as

$$F = \begin{bmatrix} -\bar{e}^{\mathrm{T}} \\ \bar{I} \end{bmatrix}, \tag{6}$$

where $\bar{I}$ denotes the identity matrix of order $n-1$. Note that $F^{\mathrm{T}}F$ is a positive definite matrix since $F^{\mathrm{T}}F = \bar{I} + \bar{e}\bar{e}^{\mathrm{T}}$. Thus, a non-singular J can be found such that $F^{\mathrm{T}}F = J^{\mathrm{T}}J$ (for example, the Cholesky factorization could be performed with this purpose). However, in this particular case, we can choose J as the following symmetric matrix, which will be used in the sequel:

$$J = \bar{I} + \frac{\sqrt{n}-1}{n-1}\bar{e}\bar{e}^{\mathrm{T}}.$$

We can now give an alternative form to $d(w)$.

LEMMA 1. *Consider the problem given in* (5). *Then*

$$d(w) = \alpha + \frac{\alpha}{n}e^{\mathrm{T}}w - \frac{1}{2}\frac{\alpha^2}{n^2}e^{\mathrm{T}}He + g(w), \tag{7}$$

where

$$\begin{aligned} g(w) = \max \quad & \left(w - \frac{\alpha}{n}He\right)^{\mathrm{T}} FJ^{-1}\bar{y} - \frac{1}{2}\bar{y}^{\mathrm{T}}Q\bar{y} \\ \text{s.t.} \quad & \bar{y}^{\mathrm{T}}\bar{y} \leqslant \alpha\left(1 - \frac{\alpha}{n}\right), \end{aligned} \tag{8}$$

with

$$Q = J^{-1}F^{\mathrm{T}}HFJ^{-1}. \tag{9}$$

To facilitate the reading, the proof of this lemma is presented in the appendix. The same happens with the four technical lemmas stated in the sequel, which are needed to give the improved bound.

The next two lemmas characterize the matrix Q given in (9). Let

$$\lambda_{\min}(Q) = \lambda_1(Q) \leqslant \lambda_2(Q) \leqslant \cdots \leqslant \lambda_{n-1}(Q) = \lambda_{\max}(Q)$$

be the eigenvalues of Q. As Q is a symmetric matrix, there exists a set of $n-1$ orthonormal eigenvectors associated with the eigenvalues of Q. They will be represented by $u_1, \ldots, u_k, u_{k+1}, \ldots, u_{n-1}$, where the first k vectors $(k \leqslant n-1)$ correspond to $\lambda_{\min}(Q)$.

LEMMA 2. *Let G be a graph with at least an edge. Then the corresponding matrix Q verifies the following inequalities*:

$$-1 \leqslant \lambda_{\min}(Q) < 0.$$

In addition the lower bound -1 *is reached if and only if* $e^{\mathrm{T}}x = 0$, *for some eigenvector* x *of* H *associated to the smallest eigenvalue* $\lambda_{\min}(H) = -1$.

A graph is complete if every pair of vertices is joined by an edge. The complete graph with n vertices will be denoted by K_n. We have:

LEMMA 3. *Let G be a graph of order n with at least an edge. Then the smallest eigenvalue of the corresponding matrix Q has multiplicity* $n-1$ *if and only if* $G = K_n$.

The following lemma bounds the function $g(w)$ given in (8) from above.

LEMMA 4. *Consider a non-complete graph G with at least an edge. Associated with G, let*

$$W = \left\{ w{:}w \geqslant 0 \wedge \left(w - \frac{\alpha}{n} He\right)^{\mathrm{T}} FJ^{-1} u_i = 0, \quad \forall i = 1, \ldots, k \right\}.$$

Then, for any $w \in W$, the following inequality holds:

$$g(w) \leqslant \frac{1}{2} \left\{ \sum_{i=k+1}^{n-1} \frac{[(w - \frac{\alpha}{n} He)^{\mathrm{T}} FJ^{-1} u_i]^2}{\lambda_i(Q) - \lambda_{\min}(Q)} - \lambda_{\min}(Q)\, \alpha \left(1 - \frac{\alpha}{n}\right) \right\}.$$

Let G be a non-complete graph with at least an edge. Consider, associated with G, the following problem:

$$\eta = \min \left\{ \frac{\alpha}{n} e^{\mathrm{T}} w + \frac{1}{2} \sum_{i=k+1}^{n-1} \frac{\left[\left(w - \frac{\alpha}{n} He\right)^{\mathrm{T}} FJ^{-1} u_i \right]^2}{\lambda_i(Q) - \lambda_{\min}(Q)} : w \in W \right\}, \tag{10}$$

where W is defined in Lemma 4. The last lemma concerns with (10).

LEMMA 5. *Consider the quadratic function*

$$\phi(\bar{x}) = -[\bar{h}_{\cdot 1} + \lambda_{\min}(Q)\bar{e}]^{\mathrm{T}} \bar{x} - \frac{1}{2} \bar{x}^{\mathrm{T}} \hat{H} \bar{x},$$

where

$$\widehat{H} = F^{\mathrm{T}} HF - \lambda_{\min}(Q) F^{\mathrm{T}} F \tag{11}$$

and $\bar{h}_{\cdot 1}$ is the vector formed by the last $n-1$ components of the first column of H. Then the optimal value of problem (10) *can be given by*

$$\eta = \frac{1}{2} \frac{\alpha^2}{n^2} e^{\mathrm{T}} He + \frac{1}{2} \alpha^2 \frac{n-1}{n} \lambda_{\min}(Q) + \alpha^2 \phi^*, \tag{12}$$

with

$$\phi^* = \max\{\phi(\bar{x}){:}\bar{e}^{\mathrm{T}} \bar{x} \leqslant 1 \quad \text{and} \quad \bar{x} \geqslant 0\}. \tag{13}$$

The improved upper bound for $\alpha(G)$ is now presented.

THEOREM 1. *Let G be a graph with at least an edge and let Q and $\widehat{H}$ be the matrices defined in* (9) *and* (11) *respectively. Then*

$$\alpha(G) \leqslant \upsilon'(G) = \frac{\lambda_{\min}(Q)}{\lambda_{\min}(Q) + 2\phi^*},$$

where ϕ^* is given in (13).

Proof. If G is a complete graph then $\lambda_{\min}(Q) = -1$ (see the proof of Lemma 3 in the appendix). So, in this case, we have $\phi^* = 0$ since

$\bar{h}_{.1} + \lambda_{\min}(Q)\bar{e} = 0$ and $\widehat{H}$ is the null matrix in (13). Consequently, if G is a complete graph we obtain $\upsilon'(G) = 1$ and the theorem is true.

For the rest of the proof assume that G is a non-complete graph with at least an edge. Taking into account (7) in Lemma 1, i.e.,

$$d(w) = \alpha + \frac{\alpha}{n} e^{\mathrm{T}} w - \frac{1}{2}\frac{\alpha^2}{n^2} e^{\mathrm{T}} He + g(w),$$

we obtain, by Lemma 4,

$$d(w) \leqslant \alpha - \frac{1}{2}\frac{\alpha^2}{n^2} e^{\mathrm{T}} He - \frac{1}{2}\lambda_{\min}(Q)\,\alpha\left(1 - \frac{\alpha}{n}\right) + \left\{\frac{\alpha}{n} e^{\mathrm{T}} w + \frac{1}{2}\sum_{i=k+1}^{n-1} \frac{\left[\left(w - \frac{\alpha}{n} He\right)^{\mathrm{T}} FJ^{-1} u_i\right]^2}{\lambda_i(Q) - \lambda_{\min}(Q)}\right\}$$

for all $w \in W$. Therefore, using the Lagrangian duality and recalling (10) and (12) given in Lemma 5, it follows that

$$\begin{aligned}
\alpha \leqslant \min_{w \geqslant 0} d(w) &\leqslant \alpha - \frac{1}{2}\frac{\alpha^2}{n^2} e^{\mathrm{T}} He - \frac{1}{2}\lambda_{\min}(Q)\,\alpha\left(1 - \frac{\alpha}{n}\right) + \eta \\
&= \alpha - \frac{1}{2}\frac{\alpha^2}{n^2} e^{\mathrm{T}} He - \frac{1}{2}\lambda_{\min}(Q)\,\alpha\left(1 - \frac{\alpha}{n}\right) \\
&\quad + \frac{1}{2}\frac{\alpha^2}{n^2} e^{\mathrm{T}} He + \frac{1}{2}\alpha^2 \frac{n-1}{n}\lambda_{\min}(Q) + \alpha^2 \phi^* \\
&= \alpha - \frac{1}{2}\lambda_{\min}(Q)\,\alpha\left(1 - \frac{\alpha}{n}\right) + \frac{1}{2}\alpha^2\,\frac{n-1}{n}\lambda_{\min}(Q) + \alpha^2\,\phi^*.
\end{aligned}$$

Consequently, by subtracting α and then dividing by $\alpha > 0$, we arrive at

$$\begin{aligned}
& 0 \leqslant -\frac{1}{2}\lambda_{\min}(Q)\left(1 - \frac{\alpha}{n}\right) + \frac{1}{2}\alpha\,\frac{n-1}{n}\lambda_{\min}(Q) + \alpha\,\phi^* \\
\Leftrightarrow \quad & \lambda_{\min}(Q) \leqslant \alpha\left(\frac{1}{n} + \frac{n-1}{n}\right)\lambda_{\min}(Q) + 2\alpha\,\phi^* \\
\Leftrightarrow \quad & \lambda_{\min}(Q) \leqslant \alpha\,[\lambda_{\min}(Q) + 2\phi^*].
\end{aligned}$$

So, to conclude the proof it remains to see that $\lambda_{\min}(Q) + 2\phi^* < 0$. This can be done as follows.

By (11) and (22) (see the proof of Lemma 2 in the appendix), we have

$$\widehat{H} = F^{\mathrm{T}} HF - \lambda_{\min}(Q) F^{\mathrm{T}} F = \bar{H} - \bar{h}_{.1}\bar{e}^{\mathrm{T}} - \bar{e}\bar{h}_{.1}^{\mathrm{T}} - \lambda_{\min}(Q)\left(\bar{I} + \bar{e}\bar{e}^{\mathrm{T}}\right). \qquad (14)$$

Thus

$$\begin{aligned}\phi(\bar{x}) &= -\bar{h}_{.1}^{\mathrm{T}}\bar{x} - \lambda_{\min}(Q)\bar{e}^{\mathrm{T}}\bar{x} - \frac{1}{2}\bar{x}^{\mathrm{T}}\widehat{H}\bar{x} \\ &= -\bar{h}_{.1}^{\mathrm{T}}\bar{x} - \lambda_{\min}(Q)\bar{e}^{\mathrm{T}}\bar{x} - \frac{1}{2}\bar{x}^{\mathrm{T}}\bar{H}x + \bar{x}^{\mathrm{T}}\bar{h}_{.1}\bar{e}^{\mathrm{T}}\bar{x} \\ &\quad + \frac{1}{2}\lambda_{\min}(Q)\left[(\bar{e}^{\mathrm{T}}\bar{x})^2 + \bar{x}^{\mathrm{T}}\bar{x}\right] \\ &= \bar{h}_{.1}^{\mathrm{T}}\bar{x}(\bar{e}^{\mathrm{T}}\bar{x} - 1) + \lambda_{\min}(Q)\left[\frac{1}{2}(\bar{e}^{\mathrm{T}}\bar{x})^2 - \bar{e}^{\mathrm{T}}\bar{x}\right] \\ &\quad - \frac{1}{2}\bar{x}^{\mathrm{T}}\bar{H}x + \frac{1}{2}\lambda_{\min}(Q)\bar{x}^{\mathrm{T}}\bar{x}.\end{aligned} \tag{15}$$

Denoting the solution of (13) by $\bar{x}^*$, (15) implies

$$\begin{aligned}2\phi^* + \lambda_{\min}(Q) &= 2\bar{h}_{.1}^{\mathrm{T}}\bar{x}^*(\bar{e}^{\mathrm{T}}\bar{x}^* - 1) + \lambda_{\min}(Q)[(\bar{e}^{\mathrm{T}}\bar{x}^*)^2 - 2\bar{e}^{\mathrm{T}}\bar{x}^* + 1] \\ &\quad - \bar{x}^{*\mathrm{T}}\bar{H}\bar{x}^* + \lambda_{\min}(Q)\bar{x}^{*\mathrm{T}}\bar{x}^* \\ &= 2\bar{h}_{.1}^{\mathrm{T}}\bar{x}^*(\bar{e}^{\mathrm{T}}\bar{x}^* - 1) + \lambda_{\min}(Q)[(\bar{e}^{\mathrm{T}}\bar{x}^* - 1)^2 + \bar{x}^{*\mathrm{T}}\bar{x}^*] - \bar{x}^{*\mathrm{T}}\bar{H}\bar{x}^*\end{aligned}$$

and, as $(\bar{e}^{\mathrm{T}}\bar{x}^* - 1)^2 + \bar{x}^{*T}\bar{x}^* > 0$, $\lambda_{\min}(Q) < 0$ (recall Lemma 2), $\bar{e}^{\mathrm{T}}\bar{x}^* - 1 \leqslant 0$ as well as $\bar{x}^* \geqslant 0$, it follows that $2\phi^* + \lambda_{\min}(Q) < 0$, as desired. The theorem is then proved. □

COROLLARY 1. *For an arbitrary graph with at least an edge, $\upsilon'(G)$ can be computed in polynomial-time.*

Proof. The corollary is obviously true when G is complete. In the opposite case, we have $\widehat{H} = JVD^{-1}VJ = J[Q - \lambda_{\min}(Q)]J$ (see (29) in the proof of Lemma 5 in the appendix) and thus $\widehat{H}$ is positive semidefinite. Therefore the quadratic problem (13) can be solved in polynomial-time and $\upsilon'(G)$ is polynomial-time computable. □

3. Showing that $\upsilon'(G)$ Improves $\upsilon(G)$

In this section it is shown that problem (13) can be written as a standard quadratic optimization problem (StQP), which is thoroughly studied in [3]. Additionally the Theorem 5 of this paper is used to offer an alternative formula to $\upsilon'(G)$ which allows to show that this bound is not worse than $\upsilon(G)$, for an arbitrary graph G.

Consider the problem (13). Introducing the slack variable $x_1 \in \mathbb{R}$ and setting

$$x = \begin{bmatrix} x_1 \\ \bar{x} \end{bmatrix}, \quad c = \begin{bmatrix} 0 \\ -\bar{h}_{.1} - \lambda_{\min}(Q)\bar{e} \end{bmatrix} \quad \text{and} \quad B = \left[\begin{array}{c|c} 0 & \bar{0}^T \\ \hline \bar{0} & -\hat{H} \end{array}\right],$$

with $x, c \in \mathbb{R}^n$ and $B \in \mathbb{R}^{n\times n}$, we can write (13) in the following form

$$\begin{aligned}\phi^* = \max \quad & c^{\mathrm{T}}x + \frac{1}{2}x^{\mathrm{T}}Bx \\ \text{s.t.} \quad & e^{\mathrm{T}}x = 1, \\ & x \geqslant 0\end{aligned}$$

or, equivalently,

$$\phi^* = \max\left\{c^{\mathrm{T}}x + \frac{1}{2}x^{\mathrm{T}}Bx : x \in \Delta\right\}$$

where Δ is the standard simplex in $\mathbb{R}^n$,

$$\Delta = \left\{x \in \mathbb{R}^n : e^{\mathrm{T}}x = 1 \quad \text{and} \quad x \geqslant 0\right\}.$$

This shows that (13) is a StQP problem. Additionally, considering the matrix

$$C = \frac{1}{2}\left(B + ce^{\mathrm{T}} + ec^{\mathrm{T}}\right),$$

we can write

$$\phi^* = \max\left\{x^{\mathrm{T}}Cx : x \in \Delta\right\} \tag{16}$$

and thus (13) can be viewed as a homogenized StQP problem. Using the Theorem 5 given in [3], the next result gives an alternative formula for computing $\upsilon'(G)$.

THEOREM 2. *Let $\upsilon'(G)$ be the bound given in Theorem* 1. *Then*

$$\upsilon'(G) = \max\left\{2e^{\mathrm{T}}x - x^{\mathrm{T}}\left(\frac{1}{\lambda_{\min}(Q)\lambda_{\min}(A)}A + I\right)x : x \geqslant 0\right\}, \tag{17}$$

where A is the adjacency matrix of G and Q is defined in (9).

Proof. First, using (16) we have

$$-\lambda_{\min}(Q) - 2\phi^* = \min\left\{x^{\mathrm{T}}\widetilde{C}x : x \in \Delta\right\},$$

where $\widetilde{C} = -2C - \lambda_{\min}(Q)ee^{\mathrm{T}}$. Using some algebra and taking into account the definitions of C, B and c as well as the Lemma 2, we can easily deduce that $\widetilde{C} = H - \lambda_{\min}(Q)I$. Therefore, $\widetilde{C}$ is a strictly $\mathbb{R}^n_+$-copositive matrix and by Theorem 5 of [3] we have

$$\begin{aligned}\upsilon'(G) &= \frac{\lambda_{\min}(Q)}{\lambda_{\min}(Q) + 2\phi^*} = -\lambda_{\min}(Q)\frac{1}{-\lambda_{\min}(Q) - 2\phi^*} \\ &= -\lambda_{\min}(Q)\frac{1}{\min\left\{x^{\mathrm{T}}\widetilde{C}x : x \in \Delta\right\}} \\ &= -\lambda_{\min}(Q)\max\left\{2e^{\mathrm{T}}p - p^{\mathrm{T}}\widetilde{C}p : p \geqslant 0\right\}.\end{aligned}$$

Consequently, since $p^{\mathrm{T}}\widetilde{C}p = p^{\mathrm{T}}Hp - \lambda_{\min}(Q)p^{\mathrm{T}}p$,

$$\begin{aligned} \upsilon'(G) &= -\lambda_{\min}(Q)\max\{2e^{\mathrm{T}}p - p^{\mathrm{T}}[H - \lambda_{\min}(Q)I]p : p \geqslant 0\} \\ &= \max\left\{2e^{\mathrm{T}}[-\lambda_{\min}(Q)p] - [-\lambda_{\min}(Q)p]^{\mathrm{T}}\left[\frac{H}{-\lambda_{\min}(Q)} + I\right][-\lambda_{\min}(Q)p] : p \geqslant 0\right\} \end{aligned}$$

Substituting x for $-\lambda_{\min}(Q)p$ in the last problem we obtain the desired result. □

Note that, when $\lambda_{\min}(Q) > -1$, the quadratic problem in (17) is not convex. Thus, the formula given in Theorem 1 must be used to compute $\upsilon'(G)$ in general. However, the utility of Theorem 2 becomes clear in the next result.

COROLLARY 2. *Let G be any arbitrary graph with at least an edge and the bounds $\upsilon'(G)$ and $\upsilon(G)$ given respectively in* (17) *and in* (1). *Then $\upsilon'(G) \leqslant \upsilon(G)$.*

Proof. The result follows immediately from Lemma 2 because

$$\begin{aligned} -\lambda_{\min}(Q) \leqslant 1 \quad &\Rightarrow \quad \lambda_{\min}(Q)\lambda_{\min}(A) \leqslant -\lambda_{\min}(A) \\ &\Rightarrow \quad \frac{1}{\lambda_{\min}(Q)\lambda_{\min}(A)} \geqslant \frac{1}{-\lambda_{\min}(A)} \\ &\Rightarrow \quad -\frac{1}{\lambda_{\min}(Q)\lambda_{\min}(A)} \leqslant -\frac{1}{-\lambda_{\min}(A)} \\ &\Rightarrow \quad -\frac{1}{\lambda_{\min}(Q)\lambda_{\min}(A)}A \leqslant -H. \end{aligned}$$

Since $-x^{\mathrm{T}}\left(\frac{1}{\lambda_{\min}(Q)\lambda_{\min}(A)}A + I\right)x \leqslant -x^{\mathrm{T}}(H+I)x$ the result follows. □

This corollary shows that $\upsilon'(G)$ is never worse that $\upsilon(G)$. However, from (17), we can conclude that $\upsilon'(G) = \upsilon(G)$ for the graphs such that $\lambda_{\min}(Q) = -1$. By Lemma 1, these are the graphs for which $e^{\mathrm{T}}\upsilon = 0$, for some eigenvector υ of H associated to $\lambda_{\min}(H) = -1$. As a consequence, any regular graph is a graph that satisfies $\lambda_{\min}(Q) = -1$, because the vector of ones e is an eigenvector associated to the largest eigenvalue of its adjacency matrix (see, for example [6]). Therefore, for a regular graph G with adjacency matrix A, we have

$$\upsilon'(G) = \upsilon(G) = \frac{-n\lambda_{\min}(A)}{\lambda_{\max}(A) - \lambda_{\min}(A)},$$

where $\lambda_{\min}(A)$ and $\lambda_{\max}(A)$ are, respectively, the smallest and the greatest eigenvalues of A. This is precisely the upper bound introduced by Hoffman (unpublished, see [6]) and Lovász [13] which, as proved in [16], equals

$\upsilon(G)$. Thus υ as well as υ' can be thought of as generalizations of the Hoffman–Lovász bound to arbitrary graphs (see [10] for other generalization deduced from the eigenvalues interlacing properties).

When $\lambda_{\min}(Q) > -1$ and $\alpha(G) < \upsilon'(G)$, it can be shown that $\upsilon'(G)$ strictly improves $\upsilon(G)$. In fact, let x^* an optimal solution of (17). Under those conditions and taking into account that $x^{*T}Ax^* > 0$, we have

$$\begin{aligned}\upsilon'(G) &= 2e^{\mathrm{T}}x^* - x^{*T}\left(\frac{1}{\lambda_{\min}(Q)\lambda_{\min}(A)}A + I\right)x^*\\ &< 2e^{\mathrm{T}}x^* - x^{*T}\left(\frac{1}{-\lambda_{\min}(A)}A + I\right)x^* = 2e^{\mathrm{T}}x^* - x^{*T}(H+I)x^*\\ &\leqslant \max\left\{2e^{\mathrm{T}}x - x^{\mathrm{T}}(H+I)x{:}x\geqslant 0\right\} = \upsilon(G),\end{aligned}$$

i.e., $\upsilon'(G) < \upsilon(G)$.

To illustrate that the improvement carried out by the new bound can be significant, the results of some tests are presented in Table 1. Each of the tested graphs of this table was generated as follows: for a specified number of vertices and a given edge density, a graph was randomly generated; then the vertex with the maximum degree was identified and edges were added (if necessary) from this vertex to all other vertices of the graph. For each tested graph of order n and density d the values of υ, υ' and $\lambda_{\min}(Q)$ were recorded.

The results of Table 1 suggest that the difference between υ and υ' is meaningful for low densities. This difference tends to have no practical value for high or even moderate densities independently of the graph's order. In fact, for the tested graphs, when the density is increased, $\lambda_{\min}(Q)$ tends to be near -1 and thus the two bounds become almost identical. In other tests on graphs of the same type not presented here, the same tendency was observed.

The improvement obtained by υ' is only one reason for asserting its interest. In fact, it can be used to design simple heuristics to approximate the independence number of a graph (similar to the ones designed for υ in previous papers). On the other hand, it serves as an alternative to the

Table 1. Comparing υ and υ'

n	d	υ	υ'	$\lambda_{\min}(Q)$	n	d	$\upsilon(G)$	$\upsilon'(G)$	$\lambda_{\min}(Q)$
10	0.05	8.489	8.281	−0.6124	100	0.05	63.393	52.428	−0.5618
10	0.1	9	9	−0.6000	100	0.1	42.955	41.841	−0.9369
10	0.5	4.447	4.442	−0.9885	100	0.5	18.570	18.567	−0.9997
20	0.05	15.696	13.949	−0.4711	150	0.05	90.561	72.971	−0.5439
20	0.1	15.089	13.271	−0.4978	150	0.1	54.864	54.503	−0.9870
20	0.5	7.168	7.149	−0.9942	150	0.5	22.626	22.625	−0.9999
50	0.05	37.814	33.007	−0.4999	200	0.05	106.342	86.138	−0.6004
50	0.1	27.158	25.665	−0.8336	200	0.1	64.717	64.677	−0.9988
50	0.5	12.808	12.804	−0.9995	200	0.5	25.924	25.922	−0.9999

Lovász ϑ bound for large graphs. To illustrate this point the numbers υ' and ϑ were computed for a set of randomly generated graphs. The tests were made on a Windows 98 PC, using the interactive matrix language MATLAB (version 5.3). The routine `quadprog.m` provided in the optimization toolbox was used to compute the optimal solution of (13). The ϑ number was computed using the MATLAB toolbox `sdppack` (version 0.9 beta) by Alizadeh et al. [1]. The scripts `lsdp.m`, `lsetopt.m` and `linit.n` were applied. The results are shown in Table 2 where, for each tested graph of order n and density d, the values of υ' and ϑ were recorded as well as the respective computation times (in seconds).

Although υ' seems to be dominated by the ϑ number in the performed tests, it compares favorably with this number in the following aspects:

- It can be computed in reasonable time for much larger instances than the Lovász ϑ number (this is understandable since to obtain ϑ, a semidefinite programming problem has to be solved and, as it is well known, solving problems of this type is a formidable computational task).
- For the same instance it spends much smaller time than the computation of the Lovász ϑ number.

Thus the proposed bound can be viewed as a real alternative to the ϑ bound for large graphs. Obviously, to appraise definitively the capabilities of υ' a theoretical study relating this bound with ϑ has to be done. This remains as an interesting question for future research.

Table 2. Comparing υ' and the Lovász ϑ number

n	d	υ'	Time (s)	ϑ	Time (s)
30	0.5	9.3	0.2	7	2.6
30	0.75	5.7	0.2	4	33.2
50	0.5	12.7	0.2	8	119.3
50	0.75	7.8	0.4	5	208.4
100	0.25	27.9	0.9	18.9	337.4
100	0.5	17.7	0.8	10.2	1190.2
100	0.75	11.1	1.6	6	17903.9
150	0.25	34.5	5.1	23.7	2480.3
150	0.5	21.9	4.5	–	*
200	0.5	26.7	11.4	–	*
300	0.5	32.9	62.1	–	*
500	0.5	43.1	352.2	–	*
600	0.5	46.7	583.9	–	*
800	0.5	54.9	1822.1	–	*
1000	0.25	102	4313.8	–	*
1000	0.5	61.1	5483.0	–	*
1000	0.75	36.9	4471.8	–	*

*Insufficient memory reported.

Table 3. Graphs for which υ' attains the stability number

n	m	υ'	Time (s)	n	m	υ'	Time (s)
61	367	9	0.5	571	9183	34	99.9
72	457	10	0.3	597	8931	38	101.3
86	628	11	0.4	666	11405	37	132.3
105	778	13	0.4	711	12979	37	222.9
189	1771	19	2.3	866	15366	47	342.2
190	1866	18	3.5	954	19829	44	491.4
198	2265	16	3.8	976	21229	43	659.7
206	2187	18	4.6	1112	24233	49	820.0
269	3255	21	10.2	1156	25630	50	960.4
304	3662	24	13.6	1229	27426	53	1130.3
343	4419	25	18.7	1304	29290	56	1352.1
376	5144	26	22.3	1483	36612	58	2489.3
403	5181	30	34.4	1562	38744	61	2746.7
472	7518	28	58.7	1984	55150	69	10917.9

The next section gives a characterization of the graphs for which $\alpha = \upsilon'$. Also, an infinite class of such graphs will be identified. The Table 3 presents the results of several tests performed with these graphs. The computations were made on the same machine as before. For each graph, the order n, the number of edges m, the bound υ' and the times spent (in seconds) were recorded. As Table 3 shows, υ' can be used to compute (in reasonable time) the stability number of very large graphs for which the computation of ϑ is prohibitive. This certainly contributes to consider the bound υ' as a reliable tool for approximating the stability number on large graphs.

4. The Class of Graphs for which $\alpha(G) = \upsilon'(G)$

A characterization for the graphs such that $\alpha = \upsilon'$ is now introduced. This is similar to the characterization for υ given in [16] and recalled in (2).

THEOREM 3. *Let G be a graph with at least an edge. Then $\alpha(G) = \upsilon'(G)$ if and only if there is a maximum stable set S of G, for which the following inequality holds,*

$$\lambda_{\min}(A)\lambda_{\min}(Q) \leqslant \min\{|N(i) \cap S| : i \notin S\}, \tag{18}$$

where Q is the matrix (9).

Proof. To prove the "only if" part consider the characterization (17) and suppose that $\alpha(G) = \upsilon'(G)$. Let S be a maximum stable set of G and consider the characteristic vector $x = (x_1, \ldots, x_n)^{\mathrm{T}}$ associated to S. Substituting this vector in the objective function of (17), the value of $\alpha(G)$ is obtained, as $x^{\mathrm{T}}Ax = 0$. Thus the vector x solves (17), since, from the hypothesis,

$\alpha(G) = \upsilon'(G)$. The Karush–Kuhn–Tucker conditions guarantee that there exists a vector $y \geqslant 0$ such that the equality

$$\left(\frac{1}{\lambda_{\min}(Q)\lambda_{\min}(A)}A + I\right)x = e + y$$

holds true. Therefore, denoting by $\left(\frac{1}{\lambda_{\min}(Q)\lambda_{\min}(A)}A + I\right)_i$ the row of matrix $\frac{1}{\lambda_{\min}(Q)\lambda_{\min}(A)}A + I$ corresponding to node i, it follows from the last equality that, for each $i \notin S$,

$$\left(\frac{1}{\lambda_{\min}(Q)\lambda_{\min}(A)}A + I\right)_i x = \frac{|N(i) \cap S|}{\lambda_{\min}(Q)\lambda_{\min}(A)} = 1 + y_i.$$

This implies (18) because $y \geqslant 0$.

To prove the "if part" suppose that the inequality (18) holds for a maximum stable set S of G. Let S be a maximum stable set of G and denote by x, as before, the characteristic vector of S. The following two cases need to be considered:

Case 1: The vertex 1 does not belong to S.

Let $\bar{x} = (x_2, \ldots, x_n)^{\mathrm{T}}$ be the vector formed by the last $n-1$ components of x, consider $\bar{w} = \frac{1}{\alpha}\bar{x}$ and the vector $\bar{y} = (y_2, \ldots, y_n)^{\mathrm{T}}$ as well as the scalar μ given by

$$y_i = \begin{cases} \frac{1}{\alpha}\left[\frac{|N(i)\cap S|}{-\lambda_{\min}(A)} + \lambda_{\min}(Q)\right], & \text{if } i \notin S, \\ 0, & \text{if } i \in S \end{cases}$$

and

$$\mu = \frac{1}{\alpha}\left[\frac{|N(1) \cap S|}{-\lambda_{\min}(A)} + \lambda_{\min}(Q)\right].$$

The definitions on $\bar{w}$, $\bar{y}$ and μ as well as (18) imply

$$\bar{H}\bar{w} - \bar{e}\bar{h}_{.1}^{\mathrm{T}}\bar{w} - \lambda_{\min}(Q)\bar{w} = -\mu\bar{e} + y,$$

$$\bar{w}^{\mathrm{T}}\bar{y} = 0, \quad \bar{w} \geqslant 0, \quad \bar{y} \geqslant 0, \quad \mu \geqslant 0 \text{ and } \mu\left(1 - \bar{e}^{\mathrm{T}}\bar{w}\right) = 0.$$

In fact, these are the Karush–Kuhn–Tucker conditions associated to problem (13). To see this, it suffices to prove that first equality coincides with

$$\widehat{H}\bar{w} + \bar{h}_{.1} = -\lambda_{\min}(Q)\bar{e} - \mu\bar{e} + \bar{y},$$

as the other conditions are evident. Using (14) this last equality can be written in the form

$$\bar{H}\bar{w} - \bar{h}_{.1}\bar{e}^{\mathrm{T}}\bar{w} - \bar{e}\bar{h}_{.1}^{\mathrm{T}}\bar{w} - \lambda_{\min}(Q)\bar{e}\bar{e}^{\mathrm{T}}\bar{w} - \lambda_{\min}(Q)\bar{w} + \bar{h}_{.1} = -\lambda_{\min}(Q)\bar{e} - \mu\bar{e} + \bar{y}.$$

But this equality entails

$$\bar{H}\bar{w} - \bar{e}\bar{h}_{.1}^{\mathrm{T}}\bar{w} - \lambda_{\min}(Q)\bar{w} = -\mu\bar{e} + \bar{y},$$

because $\bar{e}^{\mathrm{T}}\bar{w} = 1$ (recall that $1 \notin S$).

Therefore $\bar{w}$ solves the quadratic problem (13) as the Hessian $-\widehat{H}$ is negative semidefinite. So, using (15) and the equality $\bar{e}^{\mathrm{T}}\bar{w} = 1$, the optimal value of (13) is

$$\begin{aligned}\phi^* = \phi(\bar{w}) &= \bar{h}_{.1}^{\mathrm{T}}\bar{w}(\bar{e}^{\mathrm{T}}\bar{w}-1)+\lambda_{\min}(Q)\left[\frac{1}{2}(\bar{e}^{\mathrm{T}}\bar{w})^2-\bar{e}^{\mathrm{T}}\bar{w}\right]-\frac{1}{2}\bar{w}^{\mathrm{T}}\bar{H}\bar{w}+\frac{1}{2}\lambda_{\min}(Q)\bar{w}^{\mathrm{T}}\bar{w}\\ &= 0+\lambda_{\min}(Q)\left(\frac{1}{2}-1\right)-0+\frac{1}{2}\lambda_{\min}(Q)\frac{1}{\alpha}\\ &= \lambda_{\min}(Q)\frac{1-\alpha}{2\alpha}.\end{aligned}$$

Consequently, $\alpha = \frac{\lambda_{\min}(Q)}{\lambda_{\min}(Q)+2\phi^*} = \upsilon'(G)$ as required.

Case 2: The vertex 1 belongs to S.

Let $\bar{x} = (x_2, \ldots, x_n)^{\mathrm{T}}$ be the vector formed by the last $n-1$ components of x, consider $\bar{w} = \frac{1}{\alpha}\bar{x}$ and the vector $\bar{y} = (y_2, \ldots, y_n)^{\mathrm{T}}$ given as in the previous case. The definitions on $\bar{w}$ and $\bar{y}$ as well as (18) and the scalar $\mu = 0$ imply

$$\begin{aligned}&\bar{H}\bar{w}+\bar{h}_{.1}\frac{1}{\alpha}-\lambda_{\min}(Q)\bar{w} = -\lambda_{\min}(Q)\bar{e}\frac{1}{\alpha}+\bar{y},\\ &\bar{w}^{\mathrm{T}}\bar{y}=0, \quad \bar{w}\geqslant 0, \quad \bar{y}\geqslant 0 \quad \text{and} \quad \mu\big(1-\bar{e}^{\mathrm{T}}\bar{w}\big)=0.\end{aligned}$$

In fact, these are the Karush–Kuhn–Tucker conditions associated to problem (13). Similarly to the previous case, it can be easily verified, using (14), that the first equality is equivalent to

$$\widehat{H}\bar{w}+\bar{h}_{.1} = -\lambda_{\min}(Q)\bar{e}+\bar{y},$$

taking into account that $\bar{e}^{\mathrm{T}}\bar{w} = \frac{\alpha-1}{\alpha}$ and $\bar{h}_{.1}^{\mathrm{T}}\bar{x} = 0$ (recall that $1 \in S$).

Therefore $\bar{w}$ solves the quadratic problem (13) as the Hessian $-\widehat{H}$ is negative semidefinite. So, using (15) and the equality $\bar{e}^{\mathrm{T}}\bar{w} = \frac{\alpha-1}{\alpha}$, the optimal value of (13) is

$$\begin{aligned}\phi^* = \phi(\bar{w}) &= \bar{h}_{.1}^{\mathrm{T}}\bar{w}(\bar{e}^{\mathrm{T}}\bar{w}-1)+\lambda_{\min}(Q)[\frac{1}{2}(\bar{e}^{\mathrm{T}}\bar{w})^2-\bar{e}^{\mathrm{T}}\bar{w}]\\ &\quad -\frac{1}{2}\bar{w}^{\mathrm{T}}\bar{H}\bar{w}+\frac{1}{2}\lambda_{\min}(Q)\bar{w}^{\mathrm{T}}\bar{w}\\ &= 0+\lambda_{\min}(Q)\left[\frac{1}{2}\left(\frac{\alpha-1}{\alpha}\right)^2-\frac{\alpha-1}{\alpha}\right]-0+\frac{1}{2}\lambda_{\min}(Q)\frac{\alpha-1}{\alpha^2}\\ &= \lambda_{\min}(Q)\frac{1-\alpha}{2\alpha}.\end{aligned}$$

Consequently, we also arrive at $\alpha = \frac{\lambda_{\min}(Q)}{\lambda_{\min}(Q)+2\phi^*} = \upsilon'(G)$. □

As a corollary of this theorem, it can be concluded that the graphs for which $\alpha = \upsilon$ also satisfy $\alpha = \upsilon'$.

COROLLARY 3. *Let G a graph with at least an edge such that $\alpha(G) = \upsilon(G)$. Then $\alpha(G) = \upsilon'(G)$.*

Proof. As recalled in (2), the equality $\alpha(G) = \upsilon(G)$ is true if and only if, for any maximum stable set S of G,

$$-\lambda_{\min}(A) \leqslant \min\{|N_G(i) \cap S|: i \notin S\}.$$

By Lemma 2, $-\lambda_{\min}(Q) \in]0, 1]$ and thus

$$\lambda_{\min}(A)\lambda_{\min}(Q) \leqslant -\lambda_{\min}(A) \leqslant \min\{|N_G(i) \cap S|: i \notin S\}.$$

The condition (18) is satisfied and consequently $\alpha(G) = \upsilon'(G)$. □

Note that this result can also be immediately concluded from the Theorem 1 and Corollary 2. In fact assuming that $\alpha = \upsilon$, as $\alpha \leqslant \upsilon' \leqslant \upsilon$, we have $\alpha = \upsilon'$.

From this corollary we can conclude that there is an infinite number of graphs satisfying $\alpha = \upsilon'$. In fact, as proved in [5], there is an infinity of graphs satisfying $\alpha = \upsilon$, which constitute the so called class of graphs with convex-QP stability number (one member of this class can be constructed by considering $L(L(G))$, where $L(G)$ is the line graph of a connected graph G with an even number of edges). As these graphs also verify $\alpha = \upsilon'$, the class of graphs satisfying this equality has an infinite number of members. On the other hand, there are graphs for which $\alpha = \upsilon' < \upsilon$ as is the case of the graph depicted in Figure 1. In fact, for this graph, $S = \{2, 5, 7, 10, 12\}$ is a maximum stable set, $\upsilon = 5.2771$, $\lambda_{\min}(A) = -2.2972$ and

$$\lambda_{\min}(Q)\lambda_{\min}(A) = 2 = \min\{|N(i) \cap S| : i \notin S\}.$$

Consequently, $\alpha = \upsilon' = 5 < \upsilon$, and this allows to assert that the class of graphs verifying $\alpha = \upsilon'$ strictly includes the class of graphs with convex-QP stability number.

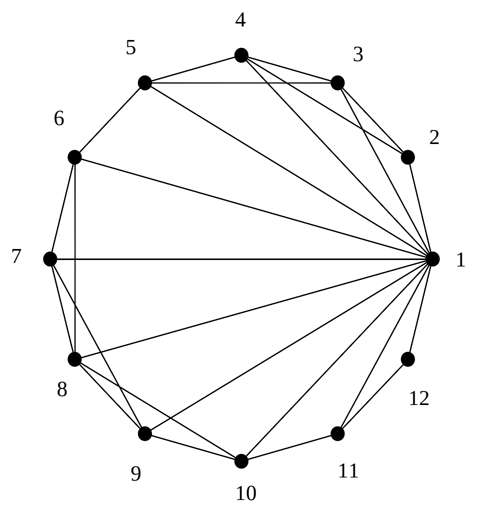

Figure 1. A graph G such that $\alpha(G) = \upsilon'(G) < \upsilon(G)$.

5. Conclusions

In this paper a new upper bound on the stability number of a graph was introduced developing ideas included in previous papers. The new bound improves the bound given in [16] which was studied in several subsequent papers. The improvement carried out by the introduced bound can be strict as it is presented in Table 1. The interest of the new bound is stressed by tables 2 and 3, which show that it is computable for much larger graphs than the ϑ number and that it can be used to compute the stability number on certain very large graphs.

Additionally, the existence of graphs for which $\alpha = \upsilon' < \upsilon$, jointly with Corollary 3, allows to enlarge the so called class of graphs with convex-QP stability number considered in [5]. The problem of recognizing the graphs of this last class in polynomial-time is yet an important open question. The results of this paper lead to the companion problem of polynomially recognizing the graphs that verify $\alpha = \upsilon'$.

Another topic worthwhile to be considered is how the new bound compares with other well known bounds on the stability number. A positive answer in this direction was given before. In fact, it was observed in section 3 that, when applied to regular graphs, the proposed bound υ' coincides with υ and thus with the well known Hoffman and Lovász upper bound. As referred also in Section 3, it appears as an interesting research question to study how υ' compares theoretically with the famous Lovász ϑ number.

6. Appendix

Proof of Lemma 1. As

$$e^{\mathrm{T}}x = \alpha \quad \Leftrightarrow \quad x_1 = \alpha - \bar{e}^{\mathrm{T}}\bar{x}$$

and

$$x^{\mathrm{T}}x \leqslant \alpha \quad \Leftrightarrow \quad \bar{x}^{\mathrm{T}}\bar{x} + \left(\alpha - \bar{e}^{\mathrm{T}}\bar{x}\right)^2 \leqslant \alpha \quad \Leftrightarrow \quad \bar{x}^{\mathrm{T}}\bar{x} + \alpha^2 - 2\alpha\bar{e}^{\mathrm{T}}\bar{x} + \bar{x}^{\mathrm{T}}\bar{e}\bar{e}^{\mathrm{T}}\bar{x} \leqslant \alpha$$
$$\Leftrightarrow \quad \bar{x}^{\mathrm{T}}\left(\bar{I} + \bar{e}\bar{e}^{\mathrm{T}}\right)\bar{x} - 2\alpha\bar{e}^{\mathrm{T}}\bar{x} + \alpha^2 \leqslant \alpha,$$

we can substitute in (5) $\alpha - \bar{e}^{\mathrm{T}}\bar{x}$ for x_1, as follows:

$$\begin{aligned} d(w) = \max \quad & (e+w)^{\mathrm{T}}\begin{bmatrix} \alpha - \bar{e}^{\mathrm{T}}\bar{x} \\ \bar{x} \end{bmatrix} - \frac{1}{2}\begin{bmatrix} \alpha - \bar{e}^{\mathrm{T}}\bar{x} \\ \bar{x} \end{bmatrix}^{\mathrm{T}} H \begin{bmatrix} \alpha - \bar{e}^{\mathrm{T}}\bar{x} \\ \bar{x} \end{bmatrix} \\ \text{s.t.} \quad & \bar{x}^{\mathrm{T}}\left(\bar{I} + \bar{e}\bar{e}^{\mathrm{T}}\right)\bar{x} - 2\alpha\bar{e}^{\mathrm{T}}\bar{x} + \alpha^2 \leqslant \alpha. \end{aligned} \tag{19}$$

Therefore, setting $a = \begin{bmatrix} \alpha \\ \bar{0} \end{bmatrix}$, where $\bar{0}$ represents the subvector of the null vector with exactly $n-1$ components, it follows that

$$\begin{bmatrix} \alpha - \bar{e}^{\mathrm{T}}\bar{x} \\ \bar{x} \end{bmatrix} = a + F\bar{x}.$$

Thus (19) is equivalent to the problem

$$\begin{aligned} d(w) = \max \quad & (e+w)^{\mathrm{T}}(a+F\bar{x}) - \frac{1}{2}(a+F\bar{x})^{\mathrm{T}}H(a+F\bar{x}) \\ \text{s.t.} \quad & \bar{x}^{\mathrm{T}}F^{\mathrm{T}}F\bar{x} - 2\alpha\bar{e}^{\mathrm{T}}\bar{x} + \alpha^2 \leqslant \alpha. \end{aligned}$$

Substituting $\bar{r} + (\alpha/n)\bar{e}$ for $\bar{x}$ in this problem, we obtain

$$d(w) = (e+w)^{\mathrm{T}}\Big(a + \frac{\alpha}{n}F\bar{e}\Big) - \frac{1}{2}\Big(a + \frac{\alpha}{n}F\bar{e}\Big)^{\mathrm{T}}H\Big(a + \frac{\alpha}{n}F\bar{e}\Big) + g(w),$$

where

$$\begin{aligned} g(w) = \max \quad & (e+w)^{\mathrm{T}}F\bar{r} - \Big(a + \frac{\alpha}{n}F\bar{e}\Big)^{\mathrm{T}}HF\bar{r} - \frac{1}{2}\bar{r}^{\mathrm{T}}F^{\mathrm{T}}HF\bar{r} \\ \text{s.t.} \quad & \bar{r}^{\mathrm{T}}F^{\mathrm{T}}F\bar{r} \leqslant \alpha(1 - \frac{\alpha}{n}). \end{aligned}$$

Taking into account that

$$a + \frac{\alpha}{n}F\bar{e} = \frac{\alpha}{n}e \quad \text{and} \quad e^{\mathrm{T}}F = 0, \tag{20}$$

we can write

$$d(w) = \alpha + \frac{\alpha}{n}e^{\mathrm{T}}w - \frac{1}{2}\frac{\alpha^2}{n^2}e^{\mathrm{T}}He + g(w)$$

and

$$\begin{aligned} g(w) = \max \quad & (w - \frac{\alpha}{n}He)^{\mathrm{T}}F\bar{r} - \frac{1}{2}\bar{r}^{\mathrm{T}}F^{\mathrm{T}}HF\bar{r} \\ \text{s.t.} \quad & \bar{r}^{\mathrm{T}}F^{\mathrm{T}}F\bar{r} \leqslant \alpha\Big(1 - \frac{\alpha}{n}\Big). \end{aligned} \tag{21}$$

Finally, as $\bar{r}^{\mathrm{T}}F^{\mathrm{T}}F\bar{r} = (J\bar{r})^{\mathrm{T}}J\bar{r}$, the substitution of $J\bar{r}$ by $\bar{y}$ allows to write (21) as the trust region problem (8) and the lemma follows. □

Proof of Lemma 2. To prove that $\lambda_{\min}(Q) < 0$, note first that $\lambda_{\min}(F^{\mathrm{T}}HF) < 0$. In fact by (6),

$$F^{\mathrm{T}}HF = \bar{H} - \bar{h}_{.1}\bar{e}^{\mathrm{T}} - \bar{e}\bar{h}_{.1}^{\mathrm{T}}, \tag{22}$$

where $\overline{H}$ is the matrix obtained by deleting the first row and the first column of H and $\bar{h}_{.1}$ is the vector formed by the last $n-1$ components of the first column of H. As the trace of $\overline{H}$ is zero (recall that $H = A/(-\lambda_{\min}(A))$), the trace of $F^{\mathrm{T}}HF$ is negative or zero. In the first case $\lambda_{\min}(F^{\mathrm{T}}HF) < 0$. If the trace is zero, $\bar{h}_{.1}$ is the null vector and thus $\lambda_{\min}(F^{\mathrm{T}}HF) = \lambda_{\min}(\overline{H}) < 0$, since G has at least an edge which is not incident on vertex 1.

Now, assume that $\lambda_{\min}(Q) \geqslant 0$. Let $\bar{y}$ be any vector of $\mathbb{R}^{n-1}$ and consider $\bar{x} = J\bar{y}$. As J is non singular and $\bar{y}^{\mathrm{T}}F^{\mathrm{T}}HF\bar{y} = \bar{x}^{\mathrm{T}}J^{-1}F^{\mathrm{T}}HFJ^{-1}\bar{x} = \bar{x}^{\mathrm{T}}Q\bar{x} \geqslant 0$, we conclude that $F^{\mathrm{T}}HF$ is positive semidefinite, an absurd because $\lambda_{\min}(F^{\mathrm{T}}HF) < 0$. Consequently, $\lambda_{\min}(Q) < 0$.

To prove that $\lambda_{\min}(Q) \geqslant -1$ suppose the contrary. Let $\bar{x}$ be an eigenvector of Q associated to $\lambda_{\min}(Q)$ and consider $\bar{y} = J^{-1}\bar{x}$. As $JJ = F^{\mathrm{T}}F$,

$$\begin{aligned} Q\bar{x} = \lambda_{\min}(Q)\bar{x} \quad &\Leftrightarrow \quad J^{-1}F^{\mathrm{T}}HFJ^{-1}\bar{x} = \lambda_{\min}(Q)\bar{x} \\ \Leftrightarrow \quad F^{\mathrm{T}}HFJ^{-1}\bar{x} = \lambda_{\min}(Q)J\bar{x} \quad &\Leftrightarrow \quad F^{\mathrm{T}}HF\bar{y} = \lambda_{\min}(Q)F^{\mathrm{T}}F\bar{y} \\ \Leftrightarrow \quad F^{\mathrm{T}}[H - \lambda_{\min}(Q)I]F\bar{y} = 0 \quad &\Rightarrow \quad \bar{y}^{\mathrm{T}}F^{\mathrm{T}}[H - \lambda_{\min}(Q)I]F\bar{y} = 0. \end{aligned}$$

Since we are assuming that $\lambda_{\min}(Q) < -1$, the matrix $H - \lambda_{\min}(Q)I$ is positive definite because $\lambda_{\min}(H) = -1$. Thus the equality $\bar{y}^{\mathrm{T}}F^{\mathrm{T}}[H - \lambda_{\min}(Q)I]F\bar{y} = 0$ implies that $F\bar{y} = 0$. But this entails $\bar{y} = 0$, an absurd, because $\bar{x}$ is an eigenvector of Q and J is non-singular. Consequently, $\lambda_{\min}(Q) \geqslant -1$.

To prove the last part of the lemma, let x be a unit eigenvector of H associated to $\lambda_{\min}(H)$ such that $e^{\mathrm{T}}x = 0$. The definition of Q and the Rayleigh–Ritz ratio [12] imply

$$\lambda_{\min}(Q) = \min_{\bar{z} \neq 0} \frac{\bar{z}^{\mathrm{T}}Q\bar{z}}{\bar{z}^{\mathrm{T}}\bar{z}} = \min_{\bar{z} \neq 0} \frac{\bar{z}^{\mathrm{T}}J^{-1}F^{\mathrm{T}}HFJ^{-1}\bar{z}}{\bar{z}^{\mathrm{T}}\bar{z}}$$

or, setting $\bar{y} = J^{-1}\bar{z}$,

$$\lambda_{\min}(Q) = \min_{\bar{y} \neq 0} \frac{\bar{y}F^{\mathrm{T}}HF\bar{y}}{\bar{y}^{\mathrm{T}}F^{\mathrm{T}}F\bar{y}} \leqslant \frac{\bar{y}F^{\mathrm{T}}HF\bar{y}}{\bar{y}^{\mathrm{T}}F^{\mathrm{T}}F\bar{y}}, \quad \forall \bar{y} \neq 0. \tag{23}$$

Denoting by $\bar{x}$ the subvector of the last $n-1$ components of x, we have that $\bar{x} \neq 0$ (otherwise, $e^{\mathrm{T}}x = 0$ should imply $x = 0$, an absurd since x is an eigenvector) and

$$Fx = \begin{bmatrix} -\bar{e}^{\mathrm{T}} \\ \bar{I} \end{bmatrix} \bar{x} = \begin{bmatrix} -\bar{e}^{\mathrm{T}}\bar{x} \\ \bar{x} \end{bmatrix} = \begin{bmatrix} x_1 \\ \bar{x} \end{bmatrix} = x.$$

Consequently, by (23)

$$\lambda_{\min}(Q) \leqslant \frac{\bar{x}F^{\mathrm{T}}HF\bar{x}}{\bar{x}^{\mathrm{T}}F^{\mathrm{T}}F\bar{x}} = \frac{x^{\mathrm{T}}Hx}{x^{\mathrm{T}}x} = -1$$

and then $\lambda_{\min}(Q) = -1$, taking into account the first part of the lemma.

To prove the reverse implication of the last part of the lemma, assume that $\lambda_{\min}(Q) = -1$. Then there exists a unit vector $\bar{x}$ of Q such that $\bar{x}^{\mathrm{T}}Q\bar{x} = -1$ or

$$\bar{x}^{\mathrm{T}}J^{-1}F^{\mathrm{T}}HFJ^{-1}\bar{x} = -1 \Leftrightarrow \bar{y}^{\mathrm{T}}F^{\mathrm{T}}HF\bar{y} = -1,$$

where $\bar{y} = J^{-1}\bar{x}$. Therefore $F\bar{y}$ is an eigenvector of H associated to $\lambda_{\min}(H) = -1$, since

$$(F\bar{y})^{\mathrm{T}}F\bar{y} = \bar{y}^{\mathrm{T}}F^{\mathrm{T}}F\bar{y} = \bar{y}^{\mathrm{T}}JJ\bar{y} = \bar{x}^{\mathrm{T}}\bar{x} = 1.$$

As $e^{\mathrm{T}}F\bar{y} = 0$ by (20), the last part of the lemma is proved. □

Proof of Lemma 3. If $G = K_n$ then $H = ee^{\mathrm{T}} - I$. Recalling the right equality of (20) and the definition of J, it follows

$$Q = J^{-1}F^{\mathrm{T}}(ee^{\mathrm{T}} - I)FJ^{-1} = -J^{-1}F^{\mathrm{T}}FJ^{-1} = -\bar{I}.$$

Thus the smallest eigenvalue of Q has multiplicity $n-1$ and is equal to -1.

Conversely, suppose that the smallest eigenvalue of Q has multiplicity $n-1$. Then $Q = \lambda_{\min}(Q)\bar{I}$ and taking into account (22) we have

$$F^{\mathrm{T}}HF = \lambda_{\min}(Q)F^{\mathrm{T}}F \quad \Leftrightarrow \quad \overline{H} - \bar{h}_{.1}\bar{e}^{\mathrm{T}} - \bar{e}\bar{h}_{.1}^{\mathrm{T}} = \lambda_{\min}(Q)\bar{I} + \lambda_{\min}(Q)\bar{e}\bar{e}^{\mathrm{T}}.$$

Thus

$$\overline{H} - \lambda_{\min}(Q)\bar{I} - \lambda_{\min}(Q)\bar{e}\bar{e}^{\mathrm{T}} = \bar{h}_{.1}\bar{e}^{\mathrm{T}} + \bar{e}\bar{h}_{.1}^{\mathrm{T}}$$

and, since $\lambda_{\min}(Q) < 0$ by Lemma 2, we must have $\bar{h}_{.1} = -\lambda_{\min}(Q)\bar{e}$ (otherwise the principal diagonals of these matrices would not coincide). Therefore, $\overline{H} = -\lambda_{\min}(Q)(\bar{e}\bar{e}^{\mathrm{T}} - \bar{I})$ and then $H = -\lambda_{\min}(Q)(ee^{\mathrm{T}} - I)$. From this equality we conclude that the adjacency matrix of G is necessarily equal to $ee^{\mathrm{T}} - I$, i.e., $G = K_n$, as required. □

Proof of Lemma 4. Let w be an element of W and suppose that the optimal value of problem (8), $g(w)$, is attained for $\bar{y}^* = \sum_{i=1}^{k} \beta_i u_i + \sum_{i=k+1}^{n-1} \gamma_i u_i$. Then, as $\bar{y}^{*\mathrm{T}}\bar{y}^* \leqslant \alpha(1 - \alpha/n)$,

$$\sum_{i=1}^{k} \beta_i^2 \leqslant \alpha\left(1 - \frac{\alpha}{n}\right) - \sum_{i=k+1}^{n-1} \gamma_i^2.$$

Substituting $\bar{y}^*$ in the objective function for (8), using the above inequality and the negativity of $\lambda_{\min}(Q)$ (by Lemma 2) yields

$$\begin{aligned}
g(w) &= \left(w - \frac{\alpha}{n}He\right)^{\mathrm{T}} FJ^{-1}\bar{y}^* - \frac{1}{2}\bar{y}^{*\mathrm{T}}Q\bar{y}^* \\
&= \left(w - \frac{\alpha}{n}He\right)^{\mathrm{T}} FJ^{-1}\sum_{i=1}^{n-1}(\bar{y}^{*\mathrm{T}}u_i)u_i - \frac{1}{2}\sum_{i=1}^{n-1}\lambda_i(Q)(\bar{y}^{*\mathrm{T}}u_i)^2 \\
&= \sum_{i=1}^{n-1}(\bar{y}^{*\mathrm{T}}u_i)\left(w - \frac{\alpha}{n}He\right)^{\mathrm{T}} FJ^{-1}u_i - \frac{1}{2}\lambda_{\min}(Q)\sum_{i=1}^{k}\beta_i^2 - \frac{1}{2}\sum_{i=k+1}^{n-1}\lambda_i(Q)\gamma_i^2 \\
&\leqslant \sum_{i=k+1}^{n-1}\gamma_i\left(w - \frac{\alpha}{n}He\right)^{\mathrm{T}} FJ^{-1}u_i - \frac{1}{2}\lambda_{\min}(Q)\,\alpha\left(1 - \frac{\alpha}{n}\right) + \frac{1}{2}\lambda_{\min}(Q)\sum_{i=k+1}^{n-1}\gamma_i^2 \\
&\quad - \frac{1}{2}\sum_{i=k+1}^{n-1}\lambda_i(Q)\gamma_i^2.
\end{aligned}$$

As G is not a complete graph, we have $k < n-1$ by Lemma 3. Thus we can write

$$g(w) \leqslant -\frac{1}{2}\lambda_{\min}(Q)\alpha\Big(1-\frac{\alpha}{n}\Big) + \sum_{i=k+1}^{n-1}\gamma_i\Big(w-\frac{\alpha}{n}He\Big)^{\mathrm{T}}FJ^{-1}u_i - \frac{1}{2}\sum_{i=k+1}^{n-1}[\lambda_i(Q)-\lambda_{\min}(Q)]\gamma_i^2$$

$$-\frac{1}{2}\sum_{i=k+1}^{n-1}\frac{\Big[\big(w-\frac{\alpha}{n}He\big)^{\mathrm{T}}FJ^{-1}u_i\Big]^2}{\lambda_i(Q)-\lambda_{\min}(Q)} + \frac{1}{2}\sum_{i=k+1}^{n-1}\frac{\Big[\big(w-\frac{\alpha}{n}He\big)^{\mathrm{T}}FJ^{-1}u_i\Big]^2}{\lambda_i(Q)-\lambda_{\min}(Q)}$$

$$= -\frac{1}{2}\lambda_{\min}(Q)\alpha(1-\frac{\alpha}{n}) + \frac{1}{2}\sum_{i=k+1}^{n-1}\frac{\Big[\big(w-\frac{\alpha}{n}He\big)^{\mathrm{T}}FJ^{-1}u_i\Big]^2}{\lambda_i(Q)-\lambda_{\min}(Q)}$$

$$-\frac{1}{2}\sum_{i=k+1}^{n-1}[\lambda_i(Q)-\lambda_{\min}(Q)]\left[\gamma_i - \frac{\big(w-\frac{\alpha}{n}He\big)^{\mathrm{T}}FJ^{-1}u_i}{\lambda_i(Q)-\lambda_{\min}(Q)}\right]^2.$$

Consequently,

$$g(w) \leqslant \frac{1}{2}\left\{\sum_{i=k+1}^{n-1}\frac{\Big[\big(w-\frac{\alpha}{n}He\big)^{\mathrm{T}}FJ^{-1}u_i\Big]^2}{\lambda_i(Q)-\lambda_{\min}(Q)} - \lambda_{\min}(Q)\,\alpha(1-\frac{\alpha}{n})\right\}$$

as required. □

Proof of Lemma 5. Recall the orthonormal eigenvectors $u_1 \ldots, u_k, u_{k+1}, \ldots, u_{n-1}$, associated to the eigenvalues of matrix Q, where the first k correspond to the smallest eigenvalue $\lambda_{\min}(Q)$. Denote by $V = [u_{k+1}\cdots u_{n-1}]$ the $(n-1)\times(n-1-k)$ matrix whose columns are the eigenvectors not corresponding to $\lambda_{\min}(Q)$.

Let $w \in W$. Thus $(w-\frac{\alpha}{n}He)^{\mathrm{T}}FJ^{-1}u_i = 0$, for $i = 1, \ldots, k$, where, by Lemma 3, $k < n-1$ since G is a non-complete graph. So, bearing in mind the definition of matrix V there exists $s \in \mathbb{R}^{n-1-k}$ such that

$$\begin{aligned} &J^{-1}F^{\mathrm{T}}\Big(w-\frac{\alpha}{n}He\Big) = Vs \quad \Leftrightarrow \quad F^{\mathrm{T}}\Big(w-\frac{\alpha}{n}He\Big) = JVs \\ &\Leftrightarrow -w_1\bar{e} + \bar{w} - \frac{\alpha}{n}F^{\mathrm{T}}He = JVs \quad \Leftrightarrow \quad \bar{w} = w_1\bar{e} + \frac{\alpha}{n}F^{\mathrm{T}}He + JVs, \end{aligned} \tag{24}$$

where w_1 is the first component of w and $\bar{w}$ is the vector of the remaining components. Therefore, as $w \geqslant 0$, we have

$$w \in W \quad \Longleftrightarrow \quad \begin{cases} w_1\bar{e} + \frac{\alpha}{n}F^{\mathrm{T}}He + JVs \geqslant 0 \\ w_1 \geqslant 0 \end{cases}.$$

and, taking into account (24), it follows that

$$e^{\mathrm{T}}w = w_1 + \bar{e}^{\mathrm{T}}\bar{w} = nw_1 + \frac{\alpha}{n}\bar{e}^{\mathrm{T}}F^{\mathrm{T}}He + \bar{e}^{\mathrm{T}}JVs.$$

Consequently, problem (10) can be written in the following equivalent form:

$$\begin{aligned}\eta = \frac{\alpha^2}{n^2}\bar{e}^{\mathrm{T}}F^{\mathrm{T}}He + \min \quad & \alpha w_1 + \frac{\alpha}{n}\bar{e}^{\mathrm{T}}JVs + \frac{1}{2}s^{\mathrm{T}}Ds \\ \text{s.t.} \quad & w_1\bar{e} + \frac{\alpha}{n}F^{\mathrm{T}}He + JVs \geqslant 0, \\ & w_1 \geqslant 0,\end{aligned}$$

where D is the diagonal matrix whose entries are $1/[\lambda_i(Q) - \lambda_{\min}(Q)]$ with $i = k+1, \ldots, n-1$ (note that D is well defined because $k < n-1$). Substituting αt for w_1 and αz for s, this problem can be written as

$$\begin{aligned}\eta = \frac{\alpha^2}{n^2}\bar{e}^{\mathrm{T}}F^{\mathrm{T}}He + \min \quad & \alpha^2 t + \frac{1}{n}\alpha^2\bar{e}^{\mathrm{T}}JVz + \frac{1}{2}\alpha^2 z^{\mathrm{T}}Dz \\ \text{s.t.} \quad & \alpha t\bar{e} + \frac{\alpha}{n}F^{\mathrm{T}}He + \alpha JVz \geqslant 0, \\ & \alpha t \geqslant 0\end{aligned}$$

or

$$\begin{aligned}\eta = \frac{\alpha^2}{n^2}\bar{e}^{\mathrm{T}}F^{\mathrm{T}}He + \alpha^2 \min \quad & t + \frac{1}{n}\bar{e}^{\mathrm{T}}JVz + \frac{1}{2}z^{\mathrm{T}}Dz \\ \text{s.t.} \quad & t\bar{e} + \frac{1}{n}F^{\mathrm{T}}He + JVz \geqslant 0, \\ & t \geqslant 0.\end{aligned} \tag{25}$$

We now proceed with the proof by showing that η can be expressed as in (12).

Consider the Lagrangian dual of the minimization problem given in (25),

$$\begin{aligned}\max \quad & \rho(\bar{x}, x_1) \\ \text{s.t.} \quad & \bar{x}, x_1 \geqslant 0,\end{aligned} \tag{26}$$

where $\bar{x} \in \mathbb{R}^{n-1}$, $x_1 \in \mathbb{R}$ and

$$\rho(\bar{x}, x_1) = \min_{z \in \mathbb{R}^{n-1-k}, t \in \mathbb{R}} t + \frac{1}{n}\bar{e}^{\mathrm{T}}JVz + \frac{1}{2}z^{\mathrm{T}}Dz - \bar{x}^{\mathrm{T}}\left(t\bar{e} + \frac{1}{n}F^{\mathrm{T}}He + JVz\right) - x_1 t.$$

The function ρ is separated and linear in t and convex quadratic in z. As $\rho(\bar{x}, x_1)$ is finite only if the gradient with respect to (z, t) vanishes, i.e.,

$$\begin{cases} \frac{1}{n}V^{\mathrm{T}}J\bar{e} + Dz - V^{\mathrm{T}}J\bar{x} = 0 \\ 1 - \bar{e}^{\mathrm{T}}\bar{x} - x_1 = 0 \end{cases} \quad \Leftrightarrow \quad \begin{cases} z = D^{-1}V^{\mathrm{T}}J\left(\bar{x} - \frac{1}{n}\bar{e}\right) \\ 1 - \bar{e}^{\mathrm{T}}\bar{x} - x_1 = 0, \end{cases}$$

it follows that, considering $\widehat{H} = JVD^{-1}V^{\mathrm{T}}J$, we have

$$\begin{aligned}\rho(\bar{x},x_1) &= t(1-\bar{e}^{\mathrm{T}}\bar{x}-x_1)+\frac{1}{n}\bar{e}^{\mathrm{T}}JVD^{-1}V^{\mathrm{T}}J\left(\bar{x}-\frac{1}{n}\bar{e}\right)\\ &\quad+\frac{1}{2}\left(\bar{x}-\frac{1}{n}\bar{e}\right)^{\mathrm{T}}J^{\mathrm{T}}VD^{-1}DD^{-1}V^{\mathrm{T}}J\left(\bar{x}-\frac{1}{n}\bar{e}\right)\\ &\quad-\frac{1}{n}\bar{x}^{\mathrm{T}}F^{\mathrm{T}}He-\bar{x}^{\mathrm{T}}J^{\mathrm{T}}VD^{-1}V^{\mathrm{T}}J\left(\bar{x}-\frac{1}{n}\bar{e}\right)\\ &= -\frac{1}{2}\left(\bar{x}-\frac{1}{n}\bar{e}\right)^{\mathrm{T}}\widehat{H}\left(\bar{x}-\frac{1}{n}\bar{e}\right)-\frac{1}{n}\bar{x}^{\mathrm{T}}F^{\mathrm{T}}He\end{aligned}$$

or else $\rho(\bar{x},x_1)=-\infty$. Thus (26) can be written as

$$\begin{aligned}\max\quad & \rho(\bar{x},x_1)=-\frac{1}{2}\left(\bar{x}-\frac{1}{n}\bar{e}\right)^{\mathrm{T}}\widehat{H}\left(\bar{x}-\frac{1}{n}\bar{e}\right)-\frac{1}{n}\bar{x}^{\mathrm{T}}F^{\mathrm{T}}He\\ \text{s.t.}\quad & 1-\bar{e}^{\mathrm{T}}\bar{x}-x_1=0,\\ & \bar{x},x_1\geqslant 0.\end{aligned}\tag{27}$$

To give the final form to this problem we write $\rho(\bar{x},x_1)$ as follows:

$$\rho(\bar{x},x_1)=-\frac{1}{2n^2}\bar{e}^{\mathrm{T}}\widehat{H}\bar{e}-\frac{1}{n}e^{\mathrm{T}}HF\bar{x}+\frac{1}{n}\bar{e}^{\mathrm{T}}\widehat{H}\bar{x}-\frac{1}{2}\bar{x}^{\mathrm{T}}\widehat{H}\bar{x}.\tag{28}$$

On the other hand, noting that $VD^{-1}V^{\mathrm{T}}=Q-\lambda_{\min}(Q)\bar{I}$, we conclude by (9) that

$$\begin{aligned}\widehat{H}&=JVD^{-1}V^{\mathrm{T}}J=J[Q-\lambda_{\min}(Q)\bar{I}]J\\ &=JQJ-\lambda_{\min}(Q)JJ=F^{\mathrm{T}}HF-\lambda_{\min}(Q)F^{\mathrm{T}}F.\end{aligned}\tag{29}$$

Additionally, taking $\alpha=1$ in the left equality of (20) we obtain

$$e_1+\frac{1}{n}F\bar{e}=\frac{1}{n}e,$$

where e_1 is the unitary vector with all components null except the first one which is equal to 1. Using (29), the last equality and $e^{\mathrm{T}}F=0$ (which is the right equality of (20)), we obtain

$$\begin{aligned}\frac{1}{n}\bar{e}^{\mathrm{T}}\widehat{H}\bar{x}&=\frac{1}{n}\bar{e}^{\mathrm{T}}F^{\mathrm{T}}HF\bar{x}-\frac{1}{n}\lambda_{\min}(Q)\bar{e}^{\mathrm{T}}F^{\mathrm{T}}F\bar{x}\\ &=\left(\frac{1}{n}e-e_1\right)^{\mathrm{T}}HF\bar{x}-\lambda_{\min}(Q)\left(\frac{1}{n}e-e_1\right)^{\mathrm{T}}F\bar{x}\\ &=\frac{1}{n}e^{\mathrm{T}}HF\bar{x}-\bar{h}_{.1}^{\mathrm{T}}\bar{x}-\frac{1}{n}\lambda_{\min}(Q)e^{\mathrm{T}}F\bar{x}-\lambda_{\min}(Q)\bar{e}^{\mathrm{T}}\bar{x}\\ &=\frac{1}{n}e^{\mathrm{T}}HF\bar{x}-\bar{h}_{.1}^{\mathrm{T}}\bar{x}-\lambda_{\min}(Q)\bar{e}^{\mathrm{T}}\bar{x},\end{aligned}$$

where $\bar{h}_{.1}$, as defined in (22), is the vector formed by the last $n-1$ components of the first column of H. Therefore, substituting in (28),

$$\rho(\bar{x}, x_1) = -\frac{1}{2n^2}\bar{e}^{\mathrm{T}}\widehat{H}\bar{e} - [\bar{h}_{.1} + \lambda_{\min}(Q)\bar{e}]^{\mathrm{T}}\bar{x} - \frac{1}{2}\bar{x}^{\mathrm{T}}\widehat{H}\bar{x}$$

and thus (27) can be written as

$$\begin{aligned} \max \quad & -\frac{1}{2n^2}\bar{e}^{\mathrm{T}}\widehat{H}\bar{e} - [\bar{h}_{.1} + \lambda_{\min}(Q)\bar{e}]^{\mathrm{T}}\bar{x} - \frac{1}{2}\bar{x}^{\mathrm{T}}\widehat{H}\bar{x} \\ \text{s.t.} \quad & 1 - \bar{e}^{\mathrm{T}}\bar{x} - x_1 = 0, \\ & \bar{x}, x_1 \geqslant 0, \end{aligned}$$

or, equivalently, taking into account that x_1 does not appear in the objective function,

$$\begin{aligned} \max \quad & -\frac{1}{2n^2}\bar{e}^{\mathrm{T}}\widehat{H}\bar{e} - [\bar{h}_{.1} + \lambda_{\min}(Q)\bar{e}]^{\mathrm{T}}\bar{x} - \frac{1}{2}\bar{x}^{\mathrm{T}}\widehat{H}\bar{x} \\ \text{s.t.} \quad & \bar{e}^{\mathrm{T}}\bar{x} \leqslant 1, \\ & \bar{x} \geqslant 0. \end{aligned}$$

Note now that the problem in (25) is a superconsistent convex program (see [20]). In fact D is positive definite and a Slater point for the problem in (25) can be easily obtained taking, for example, $z = 0$ and $t = L + \epsilon$, where L is the greatest component of $-\frac{1}{n}F^{\mathrm{T}}He$ and $\epsilon > 0$. Consequently, the strong duality theorem holds, implying that the objective function values of problem in (25) and problem (26) are equal.

Finally, using this equality and the definition of $\widehat{H}$, we have

$$\begin{aligned} \eta &= \frac{\alpha^2}{n^2}\bar{e}^{\mathrm{T}}F^{\mathrm{T}}He + \alpha^2\left(-\frac{1}{2n^2}\bar{e}^{\mathrm{T}}\widehat{H}\bar{e} + \phi^*\right) \\ &= \frac{\alpha^2}{n^2}\bar{e}^{\mathrm{T}}F^{\mathrm{T}}He - \frac{\alpha^2}{2n^2}\bar{e}^{\mathrm{T}}F^{\mathrm{T}}HF\bar{e} + \frac{1}{2}\alpha^2\frac{n-1}{n}\lambda_{\min}(Q) + \alpha^2\phi^* \\ &= \frac{1}{2}\frac{\alpha^2}{n^2}e^{\mathrm{T}}He + \frac{1}{2}\alpha^2\frac{n-1}{n}\lambda_{\min}(Q) + \alpha^2\phi^*, \end{aligned}$$

where

$$\begin{aligned} \phi^* = \max \quad & -[\bar{h}_{.1} + \lambda_{\min}(Q)\bar{e}]^{\mathrm{T}}\bar{x} - \frac{1}{2}\bar{x}^{\mathrm{T}}\widehat{H}\bar{x} \\ \text{s.t.} \quad & \bar{e}^{\mathrm{T}}\bar{x} \leqslant 1, \\ & \bar{x} \geqslant 0. \end{aligned}$$

The third equality can be easily checked using (20) and thus the lemma is proved. □

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