The graph bisection minimization problem

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Abstract

A method of determining a lower bound for the graph bisection minimization problem is described. The bound is valid for weigthed graphs with edge and node weights. The approach is based on Lagrangian relaxation and was previously used for determining an upper bound on the independence number of a graph. The determination of the lower bound is done by solving a quadratic programming problem. A characterization of the solutions of this problem is proved which allows to approximate the optimal solution of the graph bisection minimization problem. Some computational experiments are reported.

Keywords: Combinatorial Optimization, Graph Bisection Problem, Quadratic Programming

1 Introduction

The paper deals with the graph bisection minimization problem which is a particular case of the graph partitioning problem. This problem consists on partitioning the vertices of a weighted graph into a prescribed number of blocks so as to minimize (or maximize) the weight of crossing edges. If the required number of blocks is equal to two we obtain the so called graph bisection problem.

The graph partitioning problem is a well known NP-*hard* problem that has been successfully applied to many layout problems such as circuit board design, computer program segmentation and designing of hardware/software system architectures (see, for example, [5, 16, 20]).

Many heuristic algorithms have been considered for approximately solving the graph partitioning problem. Basically we can distinguish between spectral type methods [7, 8, 16, 25], local refinement type methods [9, 19], multilevel type methods [13, 18] and other optimization-based methods [1, 6, 15]. Very recently, following the remarkable paper of Goemans and Williamson on the max-cut problem [12] (see also [11]), approximation algorithms with performance guarantees have been developed for several variants of the graph partitioning problem, namely for the max bisection and the max k-cut (see [10, 28])

In [21] an upper bound on the independence number of a graph computable by quadratic programming was introduced (see also [22]). This bound was deduced by applying the theory of Lagrangian duality to a quadratic formulation of the independence set problem. This procedure is now applied to the graph bisection minimization problem which can be precisely described as follows.

Let $G = (V, E)$ represents a simple undirected graph where $V = \{1, \ldots, n\}$ denotes the vertex set and E is the edge set. To each edge $ij \in E$ a positive edge-weight $p = (p_{ij})_{ij \in E} \in \mathbb{R}_+^{n \times n}$ is associated. The weighted adjacency matrix of G, $A_p = [a_{ij}]$ is defined by setting

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

The weighted degree matrix of G is the diagonal matrix $D_p = \operatorname{diag}(d_1, \ldots, d_n)$, where $d_i = \sum_{j=1}^{n} p_{ij}$ is the weighted degree of a node $i \in V$ (in the sequel we will denote by $\operatorname{diag}(v)$ the diagonal matrix whose diagonal entries are the components of vector v). The matrix $L_p = D_p - A_p$ is called the weigthed Laplacian matrix of G. Note that L_p satisfies the following identity for every vector $x \in \mathbb{R}^n$:

$$x^T L_p x = \sum_{ij \in E} p_{ij} (x_i - x_j)^2 . \tag{1}$$

To each vertex $i \in V$ a positive node-weight, $w = (w_i)_{i \in V} \in \mathbb{R}_+^n$, is associated. For $S \subseteq V$, $w(S)$ denotes the weighted sum of the vertices belonging to S, i.e., $w(S) = \sum_{i \in S} w_i$. The notation $G_{p,w}$ represents the weigthed graph G with edge and node weights p and w.

Let $G_{p,w}$ be a weighted graph of order n. The graph bisection minimization problem on $G_{p,w}$ (GB for short) consists on determining two disjoint subsets V_1 and V_2 such that $V_1 \cup V_2 = V$ and $w(V_1) - w(V_2) = k$, so as the weighted sum of the edges connecting V_1 and V_2 is minimum. Assigning to each $i \in V$ variables x_i such that $x_i = 1$ (resp. $x_i = -1$) if $i \in V_1$ (resp. if $i \in V_2$), the total weight of edges between V_1 and V_2 is given by $\sum_{ij \in E} p_{ij} \left(\frac{x_i - x_j}{2}\right)^2$. Thus GB problem can be stated as the following binary quadratic programming problem:

$$\begin{array}{rll} \mathrm{GB}(G_{p,w}) = & \min & \frac{1}{4} \sum\limits_{ij \in E} p_{ij}(x_i - x_j)^2 \\ & \text{s. to} & w^T x = k \\ & & x \in \{-1, 1\}^n. \end{array}$$

Taking into account (1) the GB problem can be written as

$$\begin{array}{rll} \mathrm{GB}(G_{p,w}) = & \min & \frac{1}{4} x^T L_p x \\ & \text{s. to} & w^T x = k \\ & & x \in \{-1, 1\}^n, \end{array} \tag{2}$$

where $\mathrm{GB}(G_{p,w})$ denotes its optimum value. The GB problem has been intensively studied in the literature. The spectral type approach was developed in the seventies by Donath and Hoffman [3, 4] and Fiedler [7, 8]. Recently these methods have been recovered and developed [16, 26, 27] and others have been proposed [6, 15].

In this paper a lower bound for the GB problem valid for weigthed graphs with edge and node weights is proposed. The bound is easily computed by solving a quadratic programming

problem and, when $k = 0$ and all node weights are equal to 1, it coincides with the well known bound of Boppana [2] (see also [24, 27]).

It is also proved that always exist a solution of the quadratic programming problem that allows to obtain approximate solutions for the GB problem with at least a component equal to 1 or -1. These approximate solutions can be used in heuristics for approximating the GB problem optimal solution or in branch and bound algorithms for that problem.

The paper is organized as follows. In section 2 the lower bound for the graph bisection minimization problem is deduced and compared with the best known bound for the case where all node weights are equal to 1. Section 3 gives two alternative forms of computing the proposed bound. The section 4 shows how aproximate solutions of the GB problem with at least a component equal to 1 or -1 can be obtained. Based on this feature, a simple heuristic for the GB problem is described. Some computational experiments performed with this heuristic conclude the paper.

2 The proposed lower bound

Let $l \in \mathbb{R}^n$ be a vector whose components sum is zero, i.e., such that $e^T l = 0$, where e is the all ones $n \times 1$ vector. As $x^T \operatorname{diag}(l) x = 0$ for $x \in \{-1, 1\}^n$, problem (2) is equivalent to the following perturbed problem

$$\begin{array}{rll} \mathrm{GB}(G_{p,w}) = & \min & \frac{1}{4}\left[x^T L_p x + x^T \operatorname{diag}(l) x\right] \\ & \text{s. to} & w^T x = k \\ & & x \in \{-1, 1\}^n \end{array}$$

or

$$\begin{array}{rll} \mathrm{GB}(G_{p,w}) = & \min & \frac{1}{2} x^T H x \\ & \text{s. to} & w^T x = k \\ & & x \in \{-1, 1\}^n, \end{array} \tag{3}$$

where $H = [L_p + \operatorname{diag}(l)]/2$. This problem is equivalent to the following continuous quadratic programming problem (e denotes, as before, the all ones $n \times 1$ vector):

$$\begin{array}{rll} \mathrm{GB}(G_{p,w}) = & \min & \frac{1}{2} x^T H x \\ & \text{s. to} & w^T x = k \\ & & x^T x = n \\ & & -e \leq x \leq e. \end{array}$$

Consider the restricted Lagrangian dual problem of this last problem, i.e.,

$$\begin{array}{ll} \max & \theta_0(v_1, v_2) \\ \text{s. to} & v_1, v_2 \geq 0, \end{array}$$

where

$$\begin{array}{rll} \theta_0(v_1, v_2) = & \min & v_1^T(-e + x) + v_2^T(-e - x) + \frac{1}{2} x^T H x \\ & \text{s. to} & w^T x = k \\ & & x^T x = n \end{array}$$

or

$$\theta_0(v_1, v_2) = -e^T(v_1 + v_2) + \theta_1(v_1, v_2) \tag{4}$$

with

$$\begin{array}{rll} \theta_1(v_1,v_2) = & \min & (v_1-v_2)^T x + \frac{1}{2}x^T H x \\ & \text{s. to} & w^T x = k \\ & & x^T x = n. \end{array} \tag{5}$$

Denote by $\bar{x}$ and $\bar{w}$ the vectors formed by the last $n-1$ components of $x = (x_1, x_2, \ldots, x_n)^T$ and $w = (w_1, w_2, \ldots, w_n)^T$, respectively. As

$$w^T x = k \Leftrightarrow x_1 = \frac{k - \bar{w}^T \bar{x}}{w_1}$$

and

$$x^T x = n \Leftrightarrow \bar{x}^T \bar{x} + \left(\frac{k - \bar{w}^T \bar{x}}{w_1}\right)^2 = n \Leftrightarrow$$

$$\bar{x}^T \bar{x} + \frac{k^2}{w_1^2} - 2\frac{k}{w_1^2}\bar{w}^T \bar{x} + \left(\bar{w}^T \bar{x}\right)^2 \Leftrightarrow \bar{x}^T \left(\bar{I} + \frac{\bar{w}\bar{w}^T}{w_1^2}\right)\bar{x} - 2\frac{k}{w_1^2}\bar{w}^T \bar{x} + \frac{k^2}{w_1^2} = n,$$

where $\bar{I}$ denotes the identity matrix of order $n-1$, we can substitute in (5) x_1 by $\left(k - \bar{w}^T \bar{x}\right)/w_1$ as follows

$$\begin{array}{rll} \theta_1(v_1,v_2) = & \min & (v_1-v_2)^T \begin{bmatrix} \frac{k-\bar{w}^T\bar{x}}{w_1} \\ \bar{x} \end{bmatrix} + \frac{1}{2}\begin{bmatrix} \frac{k-\bar{w}^T\bar{x}}{w_1} \\ \bar{x} \end{bmatrix}^T H \begin{bmatrix} \frac{k-\bar{w}^T\bar{x}}{w_1} \\ \bar{x} \end{bmatrix} \\ & \text{s. to} & \\ & & \bar{x}^T\left(\bar{I} + \frac{\bar{w}\bar{w}^T}{w_1^2}\right)\bar{x} - 2\frac{k}{w_1^2}\bar{w}^T\bar{x} + \frac{k^2}{w_1^2} = n \end{array} \tag{6}$$

Therefore, if

$$a = \begin{bmatrix} k/w_1 \\ \bar{0} \end{bmatrix} \quad \text{and} \quad W = \begin{bmatrix} -\bar{w}^T/w_1 \\ \bar{I} \end{bmatrix}, \tag{7}$$

where $\bar{0}$ represents the subvector of the null vector with exactly $n-1$ components, it follows that

$$\begin{bmatrix} \left(k - \bar{w}^T \bar{x}\right)/w_1 \\ \bar{x} \end{bmatrix} = a + W\bar{x}.$$

Thus, setting $M = W^T W = \bar{I} + \frac{\bar{w}\bar{w}^T}{w_1^2}$, problems (6) and (5) are equivalent to the next problem:

$$\begin{array}{rll} \theta_1(v_1,v_2) = & \min & (v_1-v_2)^T(a + W\bar{x}) + \frac{1}{2}(a + W\bar{x})^T H (a + W\bar{x}) \\ & \text{s. to} & \\ & & \bar{x}^T M \bar{x} - 2\frac{k}{w_1^2}\bar{w}^T\bar{x} + \frac{k^2}{w_1^2} = n. \end{array}$$

Consequently,

$$\theta_1(v_1,v_2) = (v_1-v_2)^T a + \frac{1}{2}a^T H a + \theta_2(v_1,v_2), \tag{8}$$

where

$$\begin{array}{rll} \theta_2(v_1,v_2) = & \min & (v_1 - v_2 + Ha)^T W\bar{x} + \frac{1}{2}\bar{x}^T W^T H W \bar{x} \\ & \text{s. to} & \\ & & \bar{x}^T M \bar{x} - 2\frac{k}{w_1^2}\bar{w}^T\bar{x} + \frac{k^2}{w_1^2} = n. \end{array}$$

Let $b = \frac{k}{w_1^2} M^{-1}\bar{w}$. Substituting $\bar{x}$ by $\bar{s} + b$ in the last problem we obtain

$$\theta_2(v_1, v_2) = (v_1 - v_2 + Ha)^T Wb + \frac{1}{2} b^T W^T HWb + \theta_3(v_1, v_2) \tag{9}$$

where

$$\begin{array}{rll} \theta_3(v_1, v_2) = & \min & [v_1 - v_2 + H(a + Wb)]^T Ws + \frac{1}{2}\bar{s}^T W^T HW\bar{s} \\ & \text{s. to} & \bar{s}^T M\bar{s} = \rho, \end{array} \tag{10}$$

with

$$\rho = n - \frac{k^2}{w_1^2} + b^T Mb = \left(n - \frac{k^2}{w^T w}\right), \tag{11}$$

taking into account that $M^{-1} = \bar{I} - \bar{w}\bar{w}^T / w^T w$.

As M is a positive definite matrix, a non singular J can be found such that $M = J^T J$ (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:

$$J = \bar{I} + \left(\frac{\sqrt{\bar{w}^T\bar{w} + 1} - 1}{\bar{w}^T\bar{w}}\right)\bar{w}\bar{w}^T.$$

This matrix J will be used in the sequel. Taking into account that $\bar{s}^T E^T E\bar{s} = (J\bar{s})^T J\bar{s}$, the substitution of $J\bar{s}$ by $\bar{r}$ allows to write (10) as a trust region problem,

$$\begin{array}{rll} \theta_3(v_1, v_2) = & \min & [v_1 - v_2 + H(a + Wb)]^T WJ^{-1}\bar{r} + \frac{1}{2}\bar{r}^T Q\bar{r} \\ & \text{s. to} & \bar{r}^T\bar{r} = \left(n - \frac{k^2}{w^T w}\right), \end{array} \tag{12}$$

where

$$Q = J^{-1} W^T HWJ^{-1}. \tag{13}$$

Let

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

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 $u_1 \ldots, u_m$, $u_{m+1}, \ldots, u_{n-1}$, where the first m vectors ($m \leq n-1$) correspond to $\lambda_{\min}(Q)$.

A lemma that gives a lower bound for $\theta_3(v_1, v_2)$ will be stated now. To facilitate the reading, the proof of this lemma is presented in the appendix.

Lemma 1 *Let*

$$\mathcal{V} = \left\{(v_1, v_2) : v_1, v_2 \geq 0 \wedge [v_1 - v_2 + H(a + Wb)]^T WJ^{-1}u_i = 0, \quad \forall i = 1, \ldots, m\right\}.$$

Then for any $(v_1, v_2) \in \mathcal{V}$ the following inequality is valid:

$$\theta_3(v_1, v_2) \geq \frac{1}{2}\lambda_{\min}(Q)\left(n - \frac{k^2}{w^T w}\right) - \frac{1}{2}\sum_{i=m+1}^{n-1} \frac{\left\{[v_1 - v_2 + H(a + Wb)]^T WJ^{-1}u_i\right\}^2}{\lambda_i(Q) - \lambda_{\min}(Q)}.$$

From this result it follows:

Theorem 1 *Consider the GB problem and let $\mathcal{V}$ be defined as in the lemma 1. Then*

$$\Phi(l) \leq GB(G_{p,w})$$

where

$$\Phi(l) = \frac{1}{2}\lambda_{\min}(Q)\left(n - \frac{k^2}{w^T w}\right) + \frac{1}{2}(a+Wb)^T H (a+Wb) + \phi^*$$

and ϕ^* is the optimal objective value of the following quadratic programming problem:

$$\begin{aligned}\phi^* = \max\Big\{ & -e^T(v_1+v_2) + (v_1-v_2)^T(a+Wb) \\ & -\frac{1}{2}\sum_{i=m+1}^{n-1} \frac{\left\{[v_1-v_2+H(a+Wb)]^T W J^{-1} u_i\right\}^2}{\lambda_i(Q)-\lambda_{\min}(Q)} : (v_1,v_2)\in\mathcal{V}\Big\}\end{aligned} \tag{14}$$

Proof. Taking into account (4), (8), (9) and (12) the proof follows immediately using Lagrangian duality and the lemma 1. ■

This theorem asserts that $\Phi(l) \leq \mathrm{GB}(G_{p,w})$, for all l such that $e^T l = 0$. Then

$$\max_{l\,:\,e^T l=0} \Phi(l) \tag{15}$$

constitutes a lower bound on $\mathrm{GB}(G_{p,w})$. The proposed lower bound is now related with the best well known upper bound for $\mathrm{GB}(G_{p,w})$ when $w = e$ (i.e., all node weights are equal to 1). This bound was proposed in [27] (see also [24]) and can be given in the form

$$\max_{l\,:\,e^T l=0} \Psi(l) \tag{16}$$

where

$$\begin{aligned}\Psi(l) = \quad & \min \quad \tfrac{n}{4}x^T\left[L_p + \mathrm{diag}(l)\right]x \\ & \text{s. to} \\ & \qquad x^T x = 1 \\ & \qquad e^T x = k/\sqrt{n}.\end{aligned}$$

When $k = 0$ (16) is precisely the bound proposed by Boppana [2].

Using the substitutions that lead from problem (5) to problem (12) it can be easily seen that the lower bound $\Psi(l)$ writes in the form

$$\begin{aligned}\Psi(l) = & \frac{1}{2}(a+Wb)^T H (a+Wb) + \\ + & \min \quad (a+Wb)^T H W J^{-1}\bar{r} + \tfrac{1}{2}\bar{r}^T Q \bar{r} \\ & \text{s. to} \quad \bar{r}^T\bar{r} = n - \tfrac{k^2}{n}.\end{aligned}$$

where $H = [L_p + \mathrm{diag}(l)]/2$ and Q is given in (13). If $k = 0$, $a + Wb = \frac{k}{n}e$ and then $\Psi(l) = \frac{n}{2}\lambda_{\min}(Q)$. On the other hand, $\Phi(l) = \frac{n}{2}\lambda_{\min}(Q)$ because the maximum in (14) is attained for $v_1 = v_2 = 0$. Thus $\Psi(l) = \Phi(l)$ and consequently the lower bound given in (16) coincides with (15) when $k = 0$.

When $k \neq 0$ it is not known whether the lower bounds (16) and (15) coincide or not. In fact, in all tested examples the equality was confirmed. However no proof of this equality can be done here and thus it remains an open question.

3 Other forms of the proposed bound

In the next lemma two equivalent forms for computing ϕ^* given in (14) are proposed. Its proof is presented in the appendix.

Lemma 2 *The optimal solution of problem given in theorem 1 can be obtained by solving the problem (20) (see the appendix) or, alternatively, is given by*

$$\phi^* = \frac{1}{2}a^T Ha - \frac{1}{2}\left(a + Wb\right)^T H\left(a + Wb\right) - \frac{1}{2}\lambda_{\min}(Q)b^T Mb + \varphi^*$$

where

$$\begin{array}{rll} \varphi^* = & \min & \left[W^T Ha + \lambda_{\min}(Q)Mb\right]^T \bar{x} + \frac{1}{2}\bar{x}^T \hat{H}\bar{x} \\ & \text{s. to} & \\ & & -w_1 + k \leq \bar{w}^T \bar{x} \leq w_1 + k \\ & & -e \leq \bar{x} \leq \bar{e} \end{array} \tag{17}$$

with

$$\hat{H} = W^T HW - \lambda_{\min}(Q)\, M.$$

Using the above lemma we can now present an alternative form of computing the proposed lower bound for $\mathrm{GB}(G_{p,w})$ given in theorem 1.

Theorem 2 *Consider the GB problem given in (2). Then*

$$GB(G_{p,w}) \geq \Phi(l) = \frac{1}{2}\lambda_{\min}(Q)\left(n - \frac{k^2}{w_1^2}\right) + \frac{1}{2}a^T Ha + \varphi^*$$

where φ^* is given in (17).

Proof. By theorem 1

$$\Phi(l) = \frac{1}{2}\lambda_{\min}(Q)\left(n - \frac{k^2}{w^T w}\right) + \frac{1}{2}\left(a + Wb\right)^T H\left(a + Wb\right) + \phi^*.$$

Then using lemma 2,

$$\begin{aligned} \Phi(l) &= \frac{1}{2}\lambda_{\min}(Q)\left(n - \frac{k^2}{w^T w}\right) + \frac{1}{2}a^T Ha - \frac{1}{2}\lambda_{\min}(Q)b^T Mb + \varphi^* \\ &= \frac{1}{2}\lambda_{\min}(Q)\left(n - \frac{k^2}{w^T w} - b^T Mb\right) + \frac{1}{2}a^T Ha + \varphi^* \\ &= \frac{1}{2}\lambda_{\min}(Q)\left(n - \frac{k^2}{w_1^2}\right) + \frac{1}{2}a^T Ha + \varphi^*, \end{aligned}$$

where the last equality follows from (11). ■

4 A heuristic for the GB problem

To appraise the pratical value of the proposed bound some computational experiments were perfomed on a few graphs. In these tests a simple heuristic for approximately solving the GB problem was used. It is based on a characterization of the optimal solutions of problem (17) given in the next theorem (its proof is also postponed to the appendix).

Theorem 3 *Consider the problem (17) stated in theorem 2. Then there exists an optimal solution $\bar{x}$ of (17) such that the vector*

$$x = \begin{bmatrix} \frac{k-\bar{w}^T\bar{x}}{w_1} \\ \bar{x} \end{bmatrix}$$

with one more component that $\bar{x}$ is an approximate optimal solution of problem (2) and verifies:

(a) $w^T x = k$;

(b) *For some* $i \in \{1, 2, \ldots, n\}$, $x_i \in \{-1, 1\}$.

This theorem establishes that always exist a solution of the problem (17) that allows to obtain an approximate solution of the GB problem with at least a component equal to 1 or -1. This approximate solution can be used in heuristics for approximating the GB problem optimal solution or in branch and bound algorithms for that problem.

One of the possible heuristics is the following: for obtaining a bisection of a weighted graph $G_{p,w}$ into two disjoint subsets V_1 and V_2 such that $V_1 \cup V_2 = V$ and $w(V_1) - w(V_2) = k$ perform the steps:

1. Solve the problem (17) and apply the theorem 3 to obtain an approximate solution x of the GB problem with at least a component equal to 1 or -1;
2. Sort, in increasing order, the components of the approximated solution x;
3. Compute the $\left[\frac{w(V_1)}{w(V)}\right]^{th}$ weighted quantile (by the weights w_i) for the indices list corresponding to the sorted the components of x (in case $w(V_1) = w(V_2)$ this means to compute the weighted median of the components of x);
4. Include in V_1 the vertices that correspond to the components of x less or equal to the computed quantile; include the remaining nodes in V_2.

It should be noted the importance of theorem 3 in the context of this heuristic. For example, if $k = 0$ the null vector is an obvious solution of (17), taking into account that $W^T Ha + \lambda_{\min}(Q)Mb = 0$ (recall the definitions of a and b) and $\hat{H}$ is positive semidefinite. From the null vector we cannot extract any valuable information about the optimal solution of GB problem; but we can enrich our knowledge about this solution, by using the theorem 3 to pass to an alternative solution with at least a component 1 or -1.

The graph of figure 1 illustrates the above considerations. In fact, considering $w = e$, $k = 0$, $l = 0$ and A_p equal to the adjacency matrix of the graph, the null vector constitutes an optimal solution of problem (17). Aplying the procedure described in the proof of theorem 3, we obtain the alternative solution $x = (-1, -1, 1, 1, 1, -1)$ which is precisely an optimal solution of the GB problem. The optimal objective value in this case is 3 and the optimal partition is given by $V_1 = \{1, 2, 6\}$ and $V_2 = \{3, 4, 5\}$.

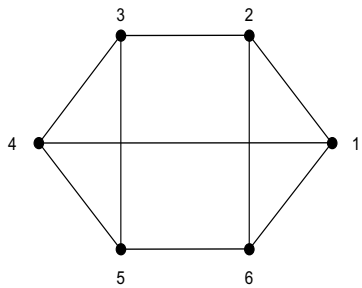

Figure 1: A graph that illustrates the usefulness of theorem 3.

			Edge Cuts	
Graph	nodes/edges	k	Heur.	Chaco
D&H	20/51	2	14	18
D&H	20/51	3	23	28
D&H	20/51	4	31	30
D&H	20/51	10	42	42
Col. HB	132/1758	2	304	304
Col. HB	132/1758	3	628	628
Col. HB	132/1758	4	896	853
Col. HB	132/1758	15	1403	1351
Col. HB	153/1135	2	92	98
Col. HB	153/1135	3	144	144
Col. HB	153/1135	4	261	260
Col. HB	153/1135	5	347	359
Col. HB	153/1135	10	638	611

Table 1: Some computational tests.

We now present the computational tests performed with the above heuristic. The tests were made on a 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 (17).

For each of tested graphs, the problem (17) was solved for several values of k, considering $w = e$, $l = 0$ and A_p coincident with the adjacency matrix of the graph. Then, approximate solutions of the GB problem with at least a component equal to 1 or -1 were determined and the remaining steps of the above heuristic were performed. The table 1 presents the obtained results. The first graph (called D&H) appears in [4, 27]. The remaining graphs belong to the Harwell-Boeing collection. The obtained results were compared with the ones

produced by the well known package Chaco [14]. In spite of the limited number of performed computational tests the obtained results are encouraging as they are similar to those of Chaco, a very widespread software for graph partitioning. This is a positive fact but using local optimization and refinement techniques to the generated approximating solutions are necessary in order to have a competitive heuristic. On the other hand, better results can be expected if other more favorable vectors l are used. It is not known yet how to consistently update l to obtain more accurate lower bounds without using semidefinite programming.

To finalize, it seems desirable to investigate the classes of graphs for which the proposed bound and heuristic lead to the optimal solution. And, naturally, continuing to study the open question leaved in section 2 about the relationships between the proposed bound and the Rendl and Wolkowicz bound is a project for future work.

Appendix

Proof of Lemma 1. Let $(v_1, v_2) \in \mathcal{V}$ and suppose that the optimal value of problem (12), $\theta_3(v_1, v_2)$, is attained for $\bar{r}^* = \sum_{i=1}^{m} \beta_i u_i + \sum_{i=m+1}^{n-1} \gamma_i u_i$. Then, as $\bar{r}^{*T}\bar{r}^* = \left(n - \frac{k^2}{w^T w}\right)$, $\sum_{i=1}^{m} \beta_i^2 = \left(n - \frac{k^2}{w^T w}\right) - \sum_{i=m+1}^{n-1} \gamma_i^2$. Substituting $\bar{r}^*$ in the objective function for (12) and using the last equality yields,

$$\begin{aligned}
\theta_3(v_1, v_2) &= [v_1 - v_2 + H(a + Wb)]^T W J^{-1} \bar{r}^* + \frac{1}{2} \bar{r}^{*T} Q \bar{r}^* \\
&= [v_1 - v_2 + H(a + Wb)]^T W J^{-1} \sum_{i=1}^{n-1} (\bar{r}^{*T} u_i) u_i + \frac{1}{2} \sum_{i=1}^{n-1} \lambda_i(Q) (\bar{r}^{*T} u_i)^2 \\
&= \sum_{i=1}^{n-1} (\bar{r}^{*T} u_i) [v_1 - v_2 + H(a + Wb)]^T W J^{-1} u_i \\
&+ \frac{1}{2} \lambda_{\min}(Q) \sum_{i=1}^{m} \beta_i^2 + \frac{1}{2} \sum_{i=m+1}^{n-1} \lambda_i(Q) \gamma_i^2
\end{aligned}$$

$$\begin{aligned}
&= \sum_{i=m+1}^{n-1} \gamma_i [v_1 - v_2 + H(a + Wb)]^T W J^{-1} u_i + \frac{1}{2} \lambda_{\min}(Q) \left(n - \frac{k^2}{w^T w}\right) \\
&- \frac{1}{2} \lambda_{\min}(Q) \sum_{i=m+1}^{n} \gamma_i^2 + \frac{1}{2} \sum_{i=m+1}^{n} \lambda_i(Q) \gamma_i^2
\end{aligned}$$

or

$$\begin{aligned}\theta_3(v_1,v_2) = &\frac{1}{2}\lambda_{\min}(Q)\left(n-\frac{k^2}{w^Tw}\right)+\sum_{i=m+1}^{n-1}\gamma_i\left[v_1-v_2+H\left(a+Wb\right)\right]^T WJ^{-1}u_i\\ &+\frac{1}{2}\sum_{i=m+1}^{n-1}\left[\lambda_i(Q)-\lambda_{\min}(Q)\right]\gamma_i^2\\ &+\frac{1}{2}\sum_{i=m+1}^{n-1}\frac{\left\{\left[v_1-v_2+H\left(a+Wb\right)\right]^T WJ^{-1}u_i\right\}^2}{\lambda_i(Q)-\lambda_{\min}(Q)}\\ &-\frac{1}{2}\sum_{i=m+1}^{n-1}\frac{\left\{\left[v_1-v_2+H\left(a+Wb\right)\right]^T WJ^{-1}u_i\right\}^2}{\lambda_i(Q)-\lambda_{\min}(Q)}\end{aligned}$$

Thus,

$$\begin{aligned}\theta_3(v_1,v_2) = &\frac{1}{2}\lambda_{\min}(Q)\left(n-\frac{k^2}{w^Tw}\right)-\frac{1}{2}\sum_{i=m+1}^{n-1}\frac{\left\{\left[v_1-v_2+H\left(a+Wb\right)\right]^T WJ^{-1}u_i\right\}^2}{\lambda_i(Q)-\lambda_{\min}(Q)}\\ &+\frac{1}{2}\sum_{i=m+1}^{n-1}\left[\lambda_i(Q)-\lambda_{\min}(Q)\right]\left\{\gamma_i+\frac{\left[v_1-v_2+H\left(a+Wb\right)\right]^T WJ^{-1}u_i}{\lambda_i(Q)-\lambda_{\min}(Q)}\right\}^2.\end{aligned}$$

and

$$\theta_3(v_1,v_2) \geq \frac{1}{2}\lambda_{\min}(Q)\left(n-\frac{k^2}{w^Tw}\right)-\frac{1}{2}\sum_{i=m+1}^{n-1}\frac{\left\{\left[v_1-v_2+H\left(a+Wb\right)\right]^T WJ^{-1}u_i\right\}^2}{\lambda_i(Q)-\lambda_{\min}(Q)}$$

as required. ■

Proof of Lemma 2. To prove this lemma some additional notation is necessary. Let U be the matrix whose columns are the orthonormal eigenvectors u_i, $i=1,\ldots,n-1$ of Q. Denote by $V=[u_{m+1}\cdots u_{n-1}]$ the $(n-1)\times(n-1-k)$ matrix obtained from U by eliminating the m columns of the eigenvectors corresponding to the smallest eigenvalue $\lambda_{\min}(Q)$ of Q. In addition, the symbol Λ will denote the diagonal matrix whose entries are $1/[\lambda_i(Q)-\lambda_{\min}(Q)]$ with $i=m+1,\ldots,n-1$.

Let $(v_1,v_2)\in\mathcal{V}$. Then $\left[v_1-v_2+H\left(a+Wb\right)\right]^T WJ^{-1}u_i=0$, $i=1,\ldots,m$, and, bearing in mind the introduced notation, there exists $z\in\mathbb{R}^{n-1-m}$ such that

$$J^{-1}W^T\left[v_1-v_2+H\left(a+Wb\right)\right]=Vz \tag{18}$$

$$\Updownarrow$$

$$JVz+\frac{\bar{w}}{w_1}\left(v_{11}-v_{21}\right)+\bar{v}_2-W^TH\left(a+Wb\right)=\bar{v}_1 \tag{19}$$

where v_{11} and v_{21} are the first components of v_1 and v_2, and $\bar{v}_1$, $\bar{v}_2$ are, respectively, the subvectors containing the remaining components. Therefore

$$(v_1,v_2)\in\mathcal{V}\Longleftrightarrow\left\{\begin{array}{l}JVz+\frac{\bar{w}}{w_1}(v_{11}-v_{21})+\bar{v}_2-W^TH\left(a+Wb\right)\geq 0\\ \bar{v}_2,v_{11},v_{21}\geq 0\end{array}\right.$$

and taking into account (19),

$$-e^T(v_1+v_2) = -2\bar{e}^T\bar{v}_2 - \bar{e}^T JVz - \left(\frac{\bar{e}^T\bar{w}}{w_1}+1\right)v_{11} + \left(\frac{\bar{e}^T\bar{w}}{w_1}-1\right)v_{21} + \bar{e}^T W^T H\,(a+Wb)$$

where $\bar{e}$ is, as before, the all ones $(n-1)\times 1$ vector. Additionally from (18) it follows

$$W^T(v_1-v_2) = JVz - W^T H(a+Wb)$$

and then

$$(v_1-v_2)^T\,(a+Wb) = \frac{k}{w_1}\,(v_{11}-v_{21}) + b^T JVz - b^T W^T H(a+Wb).$$

Consequently, the problem giving ϕ^* in theorem 1 can be written in the following equivalent form

$$\begin{array}{rll} \phi^* = & \max & \bar{e}^T W^T H\,(a+Wb) - b^T W^T H(a+Wb) \\ & & -2\bar{e}^T\bar{v}_2 + (b-\bar{e})^T\,JVz - \left(\frac{\bar{e}^T\bar{w}}{w_1}+1-\frac{k}{w_1}\right)v_{11} \\ & & +\left(\frac{\bar{e}^T\bar{w}}{w_1}-1-\frac{k}{w_1}\right)v_{21} - \frac{1}{2}z^T\Lambda z \\ & \text{s. to} & \\ & & JVz + \frac{\bar{w}}{w_1}(v_{11}-v_{21}) + \bar{v}_2 - W^T H\,(a+Wb) \geq 0 \\ & & \bar{v}_2, v_{11}, v_{21} \geq 0 \end{array} \tag{20}$$

Consider the Lagrangian dual problem of (20), i.e.,

$$\begin{array}{ll} \min & h(x_1,x_2,x_3,x_4) \\ \text{s. to} & x_1,x_2,x_3,x_4 \geq 0, \end{array} \tag{21}$$

where $x_1, x_2 \in \mathbb{R}^{n-1}$, $x_3, x_4 \in \mathbb{R}$ and

$$\begin{aligned} h(x_1,x_2,x_3,x_4) = \max\big\{&\bar{e}^T W^T H\,(a+Wb) - b^T W^T H(a+Wb) \\ &-2\bar{e}^T\bar{v}_2 + (b-\bar{e})^T\,JVz - \left(\frac{\bar{e}^T\bar{w}}{w_1}+1-\frac{k}{w_1}\right)v_{11} \\ &+\left(\frac{\bar{e}^T\bar{w}}{w_1}-1-\frac{k}{w_1}\right)v_{21} - \frac{1}{2}z^T\Lambda z \\ &+x_1^T\left[JVz + \frac{\bar{w}}{w_1}(v_{11}-v_{21}) + \bar{v}_2 - W^T H\,(a+Wb)\right] \\ &+x_2^T\bar{v}_2 + x_3 v_{11} + x_4 v_{21} : z \in \mathbb{R}^{n-1-m}, \bar{v}_2 \in \mathbb{R}^{n-1}, v_{11}, v_{21} \in \mathbb{R}\big\} \end{aligned}$$

The function h is linear in $\bar{v}_2$, v_{11} and v_{21}, and convex quadratic in z. As $h(x_1,x_2,x_3,x_4)$ is finite only if the gradient with respect to $(z,\bar{v}_2,v_{11},v_{21})$ vanishes, i.e.,

$$V^T J\,(b-\bar{e}) - \Lambda z + V^T J x_1 = 0 \tag{22}$$

$$-2\bar{e} + x_1 + x_2 = 0 \tag{23}$$

$$-\left(\frac{\bar{e}^T\bar{w}}{w_1}+1-\frac{k}{w_1}\right) + \frac{x_1^T\bar{w}}{w_1} + x_3 = 0 \tag{24}$$

$$\left(\frac{\bar{e}^T\bar{w}}{w_1}-1-\frac{k}{w_1}\right) - \frac{x_1^T\bar{w}}{w_1} + x_4 = 0, \tag{25}$$

we have

$$\begin{aligned}
h(x_1,x_2,x_3,x_4) &= \bar{e}^T W^T H\,(a+Wb) - b^T W^T H(a+Wb)\\
&+ (-2\bar{e}+x_1+x_2)^T \bar{v}_2\\
&+ \left[-\left(\frac{\bar{e}^T\bar{w}}{w_1}+1-\frac{k}{w_1}\right)+\frac{x_1^T\bar{w}}{w_1}+x_3\right] v_{11}\\
&+ \left[\left(\frac{\bar{e}^T\bar{w}}{w_1}-1-\frac{k}{w_1}\right)-\frac{x_1^T\bar{w}}{w_1}+x_4\right] v_{21}\\
&+ (b-\bar{e})^T\, JV\Lambda^{-1}V^T J\,(x_1+b-\bar{e}) + x^T JV\Lambda^{-1}\,V^T J\,(x_1+b-\bar{e})\\
&- \frac{1}{2}\,(x_1+b-\bar{e})^T\, JV\Lambda^{-1}\Lambda\Lambda^{-1}V^T J\,(x_1+b-\bar{e}) - x^T W^T H\,(a+Wb)
\end{aligned}$$

or else $h(x_1,x_2,x_3,x_4)=+\infty$. Therefore, setting $x_1=-\bar{x}+\bar{e}$ and

$$\begin{aligned}
\hat{H} &= JV\Lambda^{-1}V^T J = J\left[Q-\lambda_{\min}(Q)\bar{I}\right] J\\
&= W^T HW - \lambda_{\min}(Q)W^T W = W^T HW - \lambda_{\min}(Q)M,
\end{aligned}$$

we can write $h(x_1,x_2,x_3,x_4)$ in the following form, taking into account (22)–(25):

$$\begin{aligned}
h(x_1,x_2,x_3,x_4) &= \bar{e}^T W^T H\,(a+Wb) - b^T W^T H(a+Wb)\\
&+ (b-\bar{e})^T \hat{H}\,(b-\bar{x}) + (\bar{e}-\bar{x})^T \hat{H}\,(b-\bar{x})\\
&- \frac{1}{2}(b-\bar{x})^T \hat{H}(b-\bar{x}) - (\bar{e}-\bar{x})^T W^T H\,(a+Wb)\\
&= -b^T W^T H(a+Wb) + \frac{1}{2}(b-\bar{x})^T \hat{H}(b-\bar{x}) + \bar{x}^T W^T H\,(a+Wb)
\end{aligned}$$

or

$$\begin{aligned}
h(x_1,x_2,x_3,x_4) &= -b^T W^T Ha - \frac{1}{2}b^T W^T HWb + \frac{1}{2}\bar{x}^T \hat{H}\bar{x} + \lambda_{\min}(Q)\bar{x}^T Mb\\
&- \frac{1}{2}\lambda_{\min}(Q)b^T Mb + \bar{x}^T W^T Ha.
\end{aligned}$$

Consequently, (21) can be written as

$$\begin{array}{ll}
\min & -b^T W^T Ha - \frac{1}{2}b^T W^T HWb - \frac{1}{2}\lambda_{\min}(Q)b^T Mb\\
& + \left[W^T Ha + \lambda_{\min}(Q)Mb\right]^T \bar{x} + \frac{1}{2}\bar{x}^T \hat{H}\bar{x}\\
\text{s. to} & \\
& -\bar{x}+x_2=\bar{e}\\
& -\left(\frac{\bar{e}^T\bar{w}}{w_1}+1-\frac{k}{w_1}\right)-\frac{\bar{x}^T\bar{w}}{w_1}+\frac{\bar{e}^T\bar{w}}{w_1}\le 0\\
& \left(\frac{\bar{e}^T\bar{w}}{w_1}-1-\frac{k}{w_1}\right)+\frac{\bar{x}^T\bar{w}}{w_1}-\frac{\bar{e}^T\bar{w}}{w_1}\le 0\\
& -\bar{x}+\bar{e}\ge 0\\
& x_2\ge 0
\end{array}$$

or, equivalently, taking into account that x_2 does not appear in the objective function,

$$\begin{array}{ll}
\min & -b^T W^T Ha - \frac{1}{2}b^T W^T HWb - \frac{1}{2}\lambda_{\min}(Q)b^T Mb\\
& + \left[W^T Ha + \lambda_{\min}(Q)Mb\right]^T \bar{x} + \frac{1}{2}\bar{x}^T \hat{H}\bar{x}\\
\text{s. to} & \\
& -w_1+k\le \bar{w}^T\bar{x}\le w_1+k\\
& -\bar{e}\le \bar{x}\le \bar{e}.
\end{array} \tag{26}$$

Note now that the problem (20) is a superconsistent convex program (see [23]). In fact $-\Lambda$ is negative definite and a Slater point for (20) can be easily obtained taking, for example, $z = 0$, v_{11} and v_{21} positive and equal, and $\bar{v}_2 = (C + \epsilon)\,\bar{e}$, where $\epsilon > 0$ and C is the greatest component of $W^T H(a + Wb)$. Consequently, the strong duality theorem holds, implying that the objective function values of problems (20) and (26) are both equal to ϕ^*. Finally, as

$$-b^T W^T Ha - \frac{1}{2} b^T W^T HWb = \frac{1}{2} a^T Ha - \frac{1}{2}\,(a + Wb)^T\, H\,(a + Wb)\,,$$

the above considerations and (26) imply that

$$\phi^* = \frac{1}{2} a^T Ha - \frac{1}{2}\,(a + Wb)^T\, H\,(a + Wb) - \frac{1}{2}\lambda_{\min}(Q) b^T Mb + \varphi^*,$$

where φ^* is given in (17), as required. ■

Proof of Theorem 3. Condition (a) follows immediately from the definition of x since

$$w^T x = w_1 \left(\frac{k - \bar{w}^T \bar{x}}{w_1} \right) + \bar{w}^T \bar{x} = k - \bar{w}^T \bar{x} + \bar{w}^T \bar{x} = k$$

and $\left(k - \bar{w}^T \bar{x}\right)/w_1$ belongs to $[-1, 1]$.

To prove (b) let $(z, \bar{v}_2, v_{11}, v_{21})$ and (x_1, x_2, x_3, x_4) be optimal solutions of the problems (20) and (21), respectively. As shown in the proof of lemma 2, these problems form a primal-dual pair with no duality gap. Thus, the above optimal solutions satisfy the Karush-Kunh-Tucker conditions. Four of them are given in (22)–(25) and the rest are the following:

$$JVz + \frac{\bar{w}}{w_1}(v_{21} - v_{11}) + \bar{v}_2 - W^T H\,(a + Wb) \geq 0 \tag{27}$$

$$\bar{v}_2, v_{11}, v_{21} \geq 0 \tag{28}$$

$$x_1, x_2, x_3, x_4 \geq 0 \tag{29}$$

$$x_1^T \left[JVz + \frac{\bar{w}}{w_1}(v_{21} - v_{11}) + \bar{v}_2 - W^T H\,(a + Wb) \right] = 0 \tag{30}$$

$$x_2^T \bar{v}_2 = 0 \tag{31}$$

$$x_3 v_{11} = 0 \tag{32}$$

$$x_4 v_{21} = 0. \tag{33}$$

Assume that $0 < x_1 < 2\bar{e}$, $x_3 > 0$ and $x_4 > 0$ for otherwise the theorem is true taking into account that:

- If there exists a component j of x_1 such that $x_{1j} = 0$ or $x_{1j} = 2$, then $\bar{x}_j = 1$ or $\bar{x}_j = -1$ in problem (17), thus proving the theorem (note that (17) and (26) have the same feasible solutions; remember the correspondence $x_1 = -\bar{x} + \bar{e}$, between the solutions of the problems (21) and (26), established in the proof of lemma 2);
- If $x_3 = 0$, it follows from (24) that $x_1^T \bar{w} - \bar{e}^T \bar{w} = w_1 - k$ and then $\bar{w}^T \bar{x} = -w_1 + k$ in (17) which implies $\left(k - \bar{w}^T \bar{x}\right)/w_1 = 1$, i.e., the first component of x belongs to $\{-1, 1\}$ as required in the theorem;

- Analogously the theorem is also true if $x_4 = 0$ as, in this case, it follows from (25) that $x_1^T \bar{w} - \bar{e}^T \bar{w} = -w_1 - k$ and consequently, $\bar{w}^T \bar{x} = w_1 + k$ and $\left(k - \bar{w}^T \bar{x}\right)/w_1 = -1$, i.e., the first component of x belongs to $\{-1, 1\}$.

Under the above assumptions we proceed with the proof.

The definition of the matrix V entails that the rows of $V^T J$ are linearly dependent. Consequently, there exist a vector $q = (q_1, q_2, \ldots, q_{n-1})^T$, with at least a non null component, such that $V^T J q = 0$. Let

$$\lambda = \min\{\lambda_1, \lambda_2, \lambda_3\}$$

where

$$\begin{aligned}
\lambda_1 &= \min_j \left\{ \frac{x_{1j}}{q_j} : q_j > 0 \right\} \\
\lambda_2 &= \min_j \left\{ \frac{x_{1j} - 2}{q_j} : q_j < 0 \right\} \\
\lambda_3 &= \begin{cases} \left(w_1 + k + x_1^T \bar{w} - \bar{e}^T \bar{w}\right)/\bar{w}^T q, & \text{if } \bar{w}^T q < 0 \\ \left(w_1 - k - x_1^T \bar{w} + \bar{e}^T \bar{w}\right)/\bar{w}^T q, & \text{if } \bar{w}^T q > 0 \end{cases} .
\end{aligned}$$

As $V^T J q = 0$, the vectors $\hat{x}_1 = x_1 - \lambda q$ (whose components are $\hat{x}_{1j} = x_{1j} - \lambda q_j$) and z satisfy the condition (22) because

$$\begin{aligned}
V^T J\left(b - \bar{e}\right) - \Lambda z + V^T J \hat{x}_1 &= V^T J\left(b - \bar{e}\right) - \Lambda z + V^T J x_1 - \lambda V^T J q \\
&= V^T J\left(b - \bar{e}\right) - \Lambda z + V^T J x_1 = 0.
\end{aligned}$$

Also, the new variables $\hat{x}_{1j}$ belong to the interval $[0, 2]$ as follows from the definitions of λ, λ_1 and λ_2 (note that $\hat{x}_{1j} = 0$ if $\lambda = \lambda_1$ and $\hat{x}_{1j} = 2$ if $\lambda = \lambda_2$). Thus if we substitute $\hat{x}_2 = 2\bar{e} - \hat{x}_1$ for x_2, the condition (23) is satisfied and the inequality $\hat{x}_2 \geq 0$ is also true.

On the other hand, let $\hat{x}_3 = x_3 - \lambda \bar{w}^T q / w_1$ and $\hat{x}_4 = x_4 + \lambda \bar{w}^T q / w_1$. Using some algebra, the definition of λ and λ_3 and the conditions (24) and (25), it can be seen that $\hat{x}_3, \hat{x}_4 \geq 0$ (we have $\hat{x}_3 = 0$ if $\lambda = \lambda_3$ and $\bar{w}^T q > 0$, and $\hat{x}_4 = 0$ if $\lambda = \lambda_3$ and $\bar{w}^T q < 0$). In addition, it can be easily checked that $\hat{x}_1$, $\hat{x}_3$ and $\hat{x}_4$ satisfy the conditions (24) and (25).

As results from above, the condition (29) is also satisfied by the new variables $\hat{x}_1, \hat{x}_2, \hat{x}_3$ and $\hat{x}_4$.

Finally, taking into account that the complementary conditions (30)–(33) remain true (as all the components of $JVz + \frac{\bar{w}}{w_1}(v_{21} - v_{11}) + \bar{v}_2 - W^T H\left(a + Wb\right)$ and $\bar{v}_1, v_{11}$ and v_{21} are null because the old variables x_1, x_2, x_3 and x_4 are strictly positive), we conclude that (27) and (28) are also true and that $\hat{x}_1$, $\hat{x}_3$ and $\hat{x}_4$ are optimal solutions of problem (21) which verify at least one of the following:

- There exists a component j of $\hat{x}_1$ such that $\hat{x}_{1j} = 0$ (if $\lambda = \lambda_1$);
- There exists a component j of $\hat{x}_1$ such that $\hat{x}_{1j} = 2$ (if $\lambda = \lambda_2$);
- One of the equalities $\hat{x}_3 = 0$ or $\hat{x}_4 = 0$ are true (if $\lambda = \lambda_3$ and $\bar{w}^T q > 0$ or if $\lambda = \lambda_3$ and $\bar{w}^T q < 0$, respectively); thus $\left(k - \bar{w}^T \bar{x}\right)/w_1 = 1$ or $\left(k - \bar{w}^T \bar{x}\right)/w_1 = -1$, respectively.

Consequently, $\bar{x} = -\hat{x}_1 + e$ is an optimal solution of (17) and the vector $x = \left(\frac{k-\bar{w}^T\bar{x}}{w_1}, \bar{x}^T\right)^T$ satisfy the condition (b) of the theorem, as required. ■

Acknowledgements The author is grateful to the referee for the comments, suggestions and corrections, which definitively improved the paper. Gratefulness for the support given to this research is also due to the UID Matemática e Aplicações of Aveiro University.

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