Universidade de Aveiro Departamento de Matemática
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Reconhecimento de grafos com número de estabilidade quadrático convexo

Recognition of graphs with convex quadratic stability number

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Tese apresentada à Universidade de Aveiro para cumprimento dos requisitos necessários à obtenção do grau de Doutor em Matemática, realizada sob a orientação científica de Domingos Moreira Cardoso, Professor Catedrático do Departamento de Matemática da Universidade de Aveiro e co-orientação de Carlos Jorge da Silva Luz, membro do CIDMA - Centro de Investigação e Desenvolvimento em Matemática e Aplicações da Universidade de Aveiro.

Thesis submitted to the University of Aveiro in fulfillment of the requirements for the degree of Doctor of Philosophy in Mathematics, under the supervision of Domingos Moreira Cardoso, Full Professor at the Department of Mathematics of the University of Aveiro, and co-supervision of Carlos Jorge da Silva Luz, member of CIDMA - Center for Research Development in Mathematics and Applications (CIDMA) of the University of Aveiro.

O Júri

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Aos meus pais, que estão sempre bem-dispostos e que nunca nos falham.

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palavras-chave

Teoria espectral de grafos, programação quadrática convexa em grafos, conjuntos estáveis, matriz de adjacência, grafos com número de estabilidade quadrático convexo, conjuntos estrela, conjuntos (κ, τ)-regulares, grafos hamiltonianos.

resumo

Um conjunto estável máximo num grafo G é um conjunto estável com cardinalidade máxima. A cardinalidade de um conjunto estável máximo chama-se numero de estabilidade do grafo e denota-se $\alpha(G)$. O problema da determinação do número de estabilidade de um grafo arbitrário é um problema de optimização NP-completo e, como tal, não se conhecem algoritmos polinomiais capazes dessa determinação. O objectivo desta tese é a construção de algoritmos de reconhecimento para grafos com número de estabilidade quadrático convexo, que são grafos cujo número de estabilidade é igual ao valor óptimo de um programa quadrático convexo associado à respectiva matriz de adjacência. Com esse objectivo, apresentam-se resultados que relacionam os valores próprios da matriz de adjacência com a existência de estáveis máximos e descrevem-se algoritmos de reconhecimento baseados em tais resultados. Os algoritmos são posteriormente aplicados a vários problemas clássicos como o da dominação eficiente e da existência de emparelhamentos perfeitos e de ciclos de Hamilton.

keywords Spectral graph theory, convex quadratic programming in graphs, stable sets, adjacency matrix, graphs with convex-QP stability number, star sets, (κ, τ)-regular sets, Hamiltonian graphs.

abstract A maximum stable set is a stable set with the largest possible size, for a given graph G. This size is called the stability number of G, and it is denoted $\alpha(G)$. The problem of determining the stability number of an arbitrary graph, is a NP-complete optimization problem. As such, it is unlikely that there is a polynomial algorithm for finding a maximum stable set of a graph. The main purpose of this thesis is the achievement of recognition algorithms for graphs with convex quadratic stability number that are graphs whose stability number is equal to the optimal value of a convex quadratic program associated to the corresponding adjacency matrix . For that, results that relate the eigenvalues of the adjacency matrix and maximum stable sets are established and recognition algorithms are derived from those results. Such algorithms are applied to several well known problems such as efficient domination and the determination of graphs with perfect matchings and Hamiltonian cycles.

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List of Symbols

$\alpha(G)$	stability number of G
$\vert S\vert$	cardinality of the set S
uv	edge linking u and v
A_G	adjacency matrix of G
$\lambda_{min}(G)$	smallest eigenvalue of A_G
$m_G(\lambda)$	multiplicity of the eigenvalue λ
$\sigma(A_G)$	spectrum of A_G
$E(G)$	edge set of G
$P_G(\lambda)$	characteristic polynomial of G
$\mathcal{E}_G(\lambda)$	eigenspace associated to λ
$G[U]$	subgraph induced by the set U of vertices of G
$\overline{G}$	complement of G
$\omega(G)$	clique number of G
I_n	identity matrix of order n
$\mathbf{j}$	all-one vector
K_n	complete graph with n vertices
$K_{m,n}$	complete bipartite graph
$L(G)$	line graph of G
$N_G(v)$	set of the neighbours of v
$N_G[u]$	$N_G(u) \cup \{u\}$
$V(G)$	vertex set of G
$d_G(u)$	degree of vertex u
P_n	path with n vertices

C_n	Hamiltonian cycle with n vertices
$x(S)$	characteristic vector of the set S
B_G	incidence matrix of G
L_G	Laplacian matrix of G
$Main(G)$	vector space spanned by the main eigenvectors of G
(P_G)	quadratic program $\upsilon(G) = \max\left\{2\mathbf{j}^T x - x^T (H + I_n) x,\ \ x \geq 0\right\}$
$\upsilon(G)$	optimal value of (P_G)
Q	class of graphs with convex quadratic stability number
$\mathbf{g}_G(\kappa, \tau)$	(κ, τ) parametric vector of G
x^+	minimal least squares solution of $(A_G - (\kappa - \tau) I_n) x = \tau\mathbf{j}$

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Chapter 1

Introduction

The maximum stable set problem for a given graph G and a natural number k is the problem of deciding whether $\alpha(G) \geq k$ holds (where $\alpha(G)$ denotes the stability number of G). Karp proved that the maximum stable set problem or, in another formulation, the problem of determining the stability number of an arbitrary graph, is NP-complete: unless P=NP, exact algorithms are guaranteed to output a solution in a time that increases exponentially with the order of the graph [Kar72, GJ79].

Although the existence of an efficient algorithm for finding a maximum stable set of a graph is unlikely, there are classes of graphs for which it can be determined in polynomial time: perfect graphs [GLS84], claw-free graphs, which include line graphs, [Ber57, Min80, Sbi80] and particular subclasses of P_5-free graphs, including $(P_5, K_{1,m})$-free graphs, $(P_5, K_{2,3})$-free graphs and (P_6, C_4)-free graphs [Mos97, Mos99].

Among the many important applications of the maximum stable set problem, are, for instance, Economics [BBP03], Chemistry [GAW97, GAW00], Geometry [LS92], Telecommunications [APR99], Coding Theory [Slo89] and Computer Vision and Pattern Recognition [Har69, BBPP99]. Next to the Travelling Salesman, this is one of the most important problems in combinatorial optimization.

Following the equivalence between the maximum clique problem and the maximum stable set problem, the paper [BBPP99] contains a thorough survey about algorithms, complexity, and applications, as well as an extensive list of bibliographic references.

The maximum stable set problem can be formulated in several ways, either as an integer programming problem [NT75] or as a continuous global optimization problem: in 1965, Motzkin and Straus established a remarkable result about the clique number, proving that the size of the largest clique in a graph can be determined by solving a quadratic programming problem [MS65]. After that, several results that followed the same continuous line of action to the determination of the clique number or, equivalently, to the determination of the stability number of the complement, were published [Sho90, PP90, CP90]. Although the literature contains several different quadratic programming approaches to combinatorial problems in graphs (it is the case, for instance, of [AR01, Bom98, KFAR13, MS65]), in 1995, a new approach to the determination of the stability number, that also made use of the convex optimization techniques, was introduced in [Luz95], a paper where graphs whose stability number is equal to the optimal value of a convex quadratic program associated to the corresponding adjacency matrix were studied. Later, in [Car01], such graphs were named graphs with convex quadratic stability number or, abbreviating, graphs with convex-QP stability number. This approach has been ground to new results that have been obtained in the areas of Combinatorial Optimization and Spectral Graph Theory [CL98, Car01, Car03, CC06, CL16, CLLP16, Luz16].

Among the many other books and papers about the algebraic and combinatorial aspects of Graph Theory, we highlight [Cve71, Hae80, CDGT88, Sei89, Big93, God93, CDS95, CRS97, GR01].

The research described in this Ph.D. thesis is inscribed in the areas of Spectral Graph Theory and Combinatorial Optimization. Its goal is to establish results that relate the eigenvalues of the adjacency matrix and maximum stable sets and to derive recognition algorithms from those results. Although recognizing whether a given graph has convex-QP stability number is a problem that has resisted to all attempts to solve it and is currently still an open question - its difficulty is related to the need to recognize the so called adverse graphs, that are graphs without isolated vertices where both the optimal value of the convex quadratic program and the smallest eigenvalue are integer and remain unchanged if the neighbourhood of a vertex is deleted - families of graphs for which the recognition in polynomial time is possible are identified in this thesis.

The paper [CL16], where a simplex-like algorithm for recognizing Q-graphs as well as an innovative characterization of those graphs relying on star sets are described, provided strong motivation for a subsequent stage of this research, where recognition procedures based on star sets were developed. Star sets were initially introduced by Cvetković, Rowlinson and Simić [CRS93] as a tool to study eigenspaces of graphs and to deal withh the graph isomorphism problem. In [Ell93], published in the same year, Ellingham introduced the concept of star complement, under the designation μ-basis. The denomination *star complement* was introduced by Rowlinson in [Row98]. Star sets and star complements have since been the object of many papers and provide very useful techniques for the characterization of numerous families of graphs. Further ahead in this research, still motivated by the simplex-like recognition algorithm introduced in [CL16], a simplex-like algorithm for the determination of $(0,\tau)$-regular sets was developed and applied to the determination of efficient dominating sets.

A set S of vertices of G is dominating if every vertex of G outside S is adjacent to at least one vertex of S. A dominating set S is an efficient dominating set (or independent perfect dominating set) if each vertex of G is dominated by precisely one vertex of S. The *efficient dominating set problem* (or simply efficient domination) asks for the existence of an efficient dominating set in a given graph and, if it exists, finds such a set. In [BBS88], it was proved that such problem is NP-complete for general graphs and the same conclusion has been achieved for many particular families of graphs, such as bipartite graphs [YL96], chordal graphs [YL96], chordal bipartite graphs [LT02], planar graphs of maximum degree three [FH91], planar bipartite graphs [LT02] and many other special families. See e.g. [BMN13, LT02]. On the other hand, for graphs in several special classes, the efficient domination problem can be solved in polynomial-time (for a list of these special classes see e.g. [BMN13, CPRC95, LT97, LT02, Mil12]). A problem which is closely related to efficient domination is that of determining if G has an *efficient edge dominating set*, i.e., a set S of edges such that every edge of G shares a vertex with precisely one edge in S (assuming that an edge shares a vertex with itself). This problem is also NP-complete in general [GSSH93] and received considerable attention in the literature under several names, such as *efficient edge domination* or *dominating induced matching* (see e.g. [BHN10, BM14, CCDS08, CL09, CKL11, LKT02, LT98]). An instance of efficient edge domination can be transformed into an instance of efficient domination by associating to the input graph G its line graph $L(G)$. As a consequence, efficient domination is NP-complete for line graphs.

It is well known that the problem of deciding whether a graph has a Hamiltonian cycle is NP-complete. For a proof see, for instance, section 5.3.4 of the book [Ski90]; the only way to determine whether a given graph has a Hamiltonian cycle is to undertake an exhaustive search. Many results on the subject have been published but almost all of them have a handicap: either they are effective only for graphs of certain families or they provide conditions that, in most cases, are sufficient but not necessary (see [CSR08], [Har69]); it is the case of the well known theorems by Dirac ([Dir52]) and Ore ([Ore60]). The last stage of the current work is devoted to the implementation of a new procedure for the determination of Hamiltonian graphs, that relies on a result introduced in [ACS13] (characterizing line graphs of Hamiltonian graphs using (κ, τ)-regular sets) and imposes restrictions on the algebraic connectivity of the line graph.

The text is structured as follows.

In Chapter 2, several classical definitions of Graph Theory, notation and relevant fundamental results are introduced.

Chapter 3 introduces and characterizes the class of graphs with convex-QP stability number, first defined in [Luz95] with a different designation (the above designation was introduced in [Car01]), and the main properties of such graphs are enumerated. Known results for the recognition of graphs with convex quadratic stability number, also called Q-graphs, described in [Luz95], [Car01] and [Car03], are mentioned and new others are introduced. Algorithms for the polynomial recognition of Q-graphs that determine maximum stable sets are also presented and such algorithms efficiently solve the problem except when adverse graphs occur. Spectral and combinatorial characterizations of families of graphs where the polynomial-time recognition of Q-graphs is possible are also introduced in Chapter 3.

Chapter 4 begins with a result from [CL16] that relates properties of graphs for which the optimal solutions of (P_G) are critical points of the objective function with properties of adverse graphs; considering that one of the goals of this thesis is the recognition of adverse Q-graphs, such result, in Proposition 4.1, is of great relevance. Section 4.1 recalls the nullifying procedure described in [CL16] that is later generalized in Section 4.4. Section 4.2 contains a brief overview of fundamental facts about star sets and, in Section 4.3, results about the determination of (κ, τ)-regular sets are introduced; in Section 4.4, a simplex-like algorithm for the determination of $(0, \tau)$-regular sets, that relies on results about spectral properties and star complements, is introduced. In the subsequent section, such algorithm is applied to the determination of efficient dominating sets and to the determination, within certain families, of graphs with perfect matchings; an approach to the NP-complete problem of the determination of Hamiltonian cycles that relies on a result introduced in [ACS13] and on the algebraic connectivity of the graph is also contained in Chapter 4; the chapter ends with a new algorithmic approach to the determination of (κ, τ)-regular sets in general graphs.

This thesis ends with an appendix that was divided into two sections: Appendix A.1, where the equivalence between the results about the determination of (κ, τ)-regular sets introduced in Section 4.3 and the ones described in [CSZ10] is proved; Appendix A.2 summarizes the computational results that were obtained for Algorithm 3.

Chapter 2

Definitions and preliminary results

In this chapter, several definitions and notation will be introduced. Results from graph theory and connections between graphs and their adjacency matrices that are relevant for the forthcoming chapters will also be referred.

Throughout this text, $G = (V(G), E(G))$ will denote an undirected simple graph (which is a graph with no loops nor multiple edges) with n vertices, for which $V(G)$ and $E(G)$ denote, respectively, the (finite) set of the vertices and the set of the edges. The number of vertices of a graph is called the *order* of the graph and the number of edges is the *dimension* of the graph. Notice that each edge of G is a two element subset of $V(G)$. For the sake of simplicity, an edge linking vertices u and v of graph G will be denoted by uv. Vertex u is *adjacent* to vertex v if $uv \in E(G)$ and edge uv is said to be *incident* in vertices u and v. Two edges are adjacent if they share a common vertex . Given a graph G and a vertex $u \in V(G)$, the *neighbourhood* of u is the set of vertices that are adjacent to u and it is denoted by $N_G(u)$. Such vertices are the *neighbours* of u. Given a vertex $u, d_G(u) = |N_G(u)|$, the number of neighbours of u, is called the *degree* of u. A graph where all vertices have the same degree p is called a *p-regular graph.* A graph of order n in which all pairs of vertices are adjacent is a *complete graph*; the complete graph of order n is denoted by K_n. Every complete graph of order n is $(n-1)$-regular. The *complement* of a given graph G is the graph denoted by $\overline{G}$ and it is such that $\left|V(\overline{G})\right| = |V(G)|$ and $uv \in E(\overline{G})$ if and only if $uv \notin E(G)$. A graph of order n is a *null graph* if it is 0-regular or, in other words, if its complement is the complete graph K_n. Two simple graphs G and

H are *isomorphic* if there is a bijection $\phi : V(G) \to V(H)$ such that for any $u, v \in V(G)$, $uv \in E(G)$ if and only if $\phi(u)\phi(v) \in E(H)$. Given two graphs G and H, H is a *subgraph* of G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. If U is a subset of $V(G)$, the *subgraph of G induced by U* is the graph $G[U]$ such that $V(G[U]) = U$ and $E(G[U]) = \{uv : u, v \in U \text{ and } uv \in E(G)\}$. In other words, in order to obtain $G[U]$, the vertices of $V(G) \setminus U$ are ignored as well as the edges that incide in the elements of $V(G) \setminus U$.

If $G, H_1, H_2, ..., H_s$ are graphs, G is $(H_1, H_2, ..., H_s)$*-free* if, for $i = 1, ..., s$, H_i is not an induced subgraph of G. If $s = 1$ and $H = H_1$, G is a H*-free* graph.

For a given graph G, a *walk* on G, from vertex x to vertex y, is a non-empty sequence of vertices and edges of the form

$$x = v_0, v_0v_1, v_1, \dots, v_{k-1}, v_{k-1}v_k, v_k = y,$$

where there may be repetition of vertices and edges. A walk with no repeated vertices is a *path* and a walk with no repeated edges is a *trail*. A *circuit* is a closed trail, starting and ending at the same vertex, and a *cycle* is a closed trail in which the only coincident vertices are the initial and the last ones.

Walks, paths, trails are generally denoted by their sequence of vertices. Given a path P (respectively, cycle C) of a graph G, the *length* of P (respectively, C) is the number of edges it contains. The length of a path P is denoted by $l(P)$. A cycle of G such that $V(C) = V(G)$ is called a *Hamiltonian cycle*. A graph that has a Hamiltonian cycle is a *Hamiltonian graph*.

G is a *connected graph* if there is a path from any vertex to any other vertex of G. Otherwise, graph G is *disconnected*. A *connected component* (or simply component) of a disconnected graph G is a connected subgraph of G which is induced by a subset of vertices S such that $\forall u \in V(G) \setminus S$, the subgraph $G[S \cup \{u\}]$ is disconnected. A connected graph with $n \geq 2$ vertices such that $n-2$ of them have degree 2 and the remaining 2 vertices have degree 1 is a path and it is denoted by P_n. A connected 2-regular graph with order $k \geq 4$ is a *cordless cycle* and it is denoted by C_k. A 2-regular graph of order 3 is a *triangle* and it is denoted by C_3. Given two vertices u and v of a graph G and denoting by $\mathcal{P}_{u,v}$ the set of all paths linking u and v, the *distance* between vertices of G is the function $dist : V(G) \times V(G) \to \{0, ..., n-1, \infty\}$

such that

$$dist(u,v) = \begin{cases} min\{l(P) : P \in \mathcal{P}_{u,v}\} & \text{if } \mathcal{P}_{u,v} \neq \emptyset \\ \infty & \text{if } \mathcal{P}_{u,v} = \emptyset \end{cases}$$

The greatest distance among all pairs of vertices in a graph G is called the *diameter* of G and it is denoted by $diam(G)$. The length of the shortest cycle in G is the *girth* of G, denoted by $g(G)$. If G is disconnected, then $diam(G) = \infty$. If G has no cycles, then $g(G) = \infty$.

A graph G is *bipartite* if $V(G)$ is the disjoint union of two sets V_1 and V_2 such that $\forall uv \in E(G), |V_1 \cap \{u,v\}| = |\{u,v\} \cap V_2| = 1$ (each edge of the graph has an end point in V_1 and the other one in V_2). The partition (V_1, V_2) of the vertices of G is called a *bipartition*. In the particular case when $|V_1| = m, |V_2| = n$ and for all $u \in V_1$ and $v \in V_2$, $uv \in E(G)$, G is called *complete bipartite* and it is denoted by $K_{m,n}$. *Trees* are acyclic connected graphs and they form a special class of bipartite graphs.

A set of mutually non adjacent vertices in a graph is called a *stable set* (or *independent set*) and a set of mutually adjacent vertices is called a *clique*. A stable set S is called *maximum stable set* if there is no other stable set with greater number of vertices. A clique is called *maximum clique* if there is no other clique with greater number of vertices. The number of vertices in a maximum stable set of graph G, is called the *stability number* (or *independence number*) of G and is denoted by $\alpha(G)$. The number of vertices in a maximum clique of G, is called the *clique number* of G and is denoted by $\omega(G)$. It can be concluded, from the previous definitions, that the problem of determining the stability number of a graph G is equivalent to the problem of determining the clique number of the complement of G because $\alpha(G) = \omega(\overline{G})$. The smallest number of cliques whose union is equal to $V(G)$ is denoted by $\theta(G)$ and a family of cliques with $\theta(G)$ elements so called a *minimum clique cover*. Since any clique cover of G has at least $\alpha(G)$ elements, it can be concluded that for any given graph $G, \alpha(G) \leq \theta(G)$.

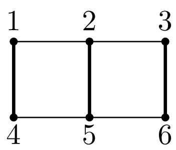
The problem of deciding if a given graph G of order n has a maximum stable set with cardinality $k \leq n$ is known to be NP-complete [Kar72][1]. There are, however, several families of graphs for which the stability number can be determined in polynomial time. It is the case of perfect graphs [Lov87], $K_{1,3}$-free graphs [Min80] and [Sbi80], (P_6, C_4)-free graphs [Mos99]

[1]For a formal definition of NP-completeness and other related concepts of the computational complexity theory see [GJ79] and [NW99].

and (P_5,banner)-free graphs [Loz00].

Given a graph G, the *line graph* of G, which is denoted by $L(G)$, is obtained by taking the edges of G as vertices of $L(G)$ and joining two vertices in $L(G)$ by an edge whenever the corresponding edges in G have a common vertex. A *matching* in G is a subset of edges, $M \subseteq E(G)$, no two of which have a common vertex. A *perfect matching* of G is a matching M such that every vertex $u \in V(G)$ is incident upon exactly one edge of M. A matching with maximum cardinality is a *maximum matching*. The problem of determining a maximum matching in G is equivalent to the problem of determining a maximum stable set in $L(G)$.

Graph G in Figure 2.1 has the maximum matching (which is also perfect) $\{\{14\},\{25\},\{36\}\}$ that corresponds to the maximum stable set $\{c,d,e\}$ of $L(G)$.



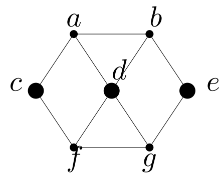


Figure 2.1: Graph G with the perfect matching $\{\{14\},\{25\},\{36\}\}$ and graph $L(G)$ with the maximum stable set $\{c,d,e\}$.

A matching M of a graph G is an *induced matching* if the subgraph induced by the set of vertices that correspond to edges of M is 1-regular. An induced matching of a graph G is maximal if there is no $M' \subseteq E(G)$ such that $M \subset M'$ and M' is an induced matching of G. A *perfect induced matching* M of G is an induced matching that covers all the edges of G, that is, every edge of $E(G) \setminus M$ is adjacent to exactly one edge of M.

Throughout the text, $\mathbf{j}$ will denote the all-one vector and I_n will denote the identity matrix of order n. All considered vectors are column vectors.

Given a subset of vertices S of graph G, the vector $x \in \mathbb{R}^n$ such that $x_v = 1$ if $v \in S$ and $x_v = 0$ if $v \notin S$ is the *characteristic vector* of S. Throughout the text, the characteristic vector of a set S will be denoted by $x(S)$.

Note that a set of vertices of a graph is (κ, τ)-regular if every vertex in the set has exactly

κ neighbours in the set and every vertex outside the set has exactly τ neighbours in it. The study of (κ, τ)-regular sets began with [Tho81] and [Neu82], with different designations in the context of regular and strongly regular graphs, respectively.

In [Neu82], such sets, in strongly regular graphs, are called regular sets with valency κ and nexus τ, and they are divided into positive regular sets, if $\kappa \geq \tau$ and negative regular sets, when $\kappa < \tau$. In [Tho81], subgraphs of regular graphs induced induced by (κ, τ)-regular sets are referred to as $\kappa - \tau$ eigengraphs. For arbitrary graphs, the study of (κ, τ)-regular sets was initiated in [CR04]. The thesis [Ram05] also contains a nice overview of the subject.

A_G denotes the *adjacency matrix* of G, that is, $A_G = (a_{ij})$ is such that

$$a_{ij} = \begin{cases} 1 & \text{if } ij \in E(G) \\ 0 & \text{if } ij \notin E(G) \end{cases}$$

A_G is a symmetric matrix so it has n real eigenvalues.

$$\lambda_{max}(A_G) = \lambda_1(A_G) \geq \lambda_2(A_G) \geq ... \geq \lambda_n(A_G) = \lambda_{min}(A_G)$$

denote the eigenvalues of A_G, sometimes referred to as eigenvalues of G. $\lambda_{max}(A_G) = \lambda_1$ is sometimes referred to as the *index* of G. The eigenspace of an eigenvalue λ is denoted by $\mathcal{E}_G(\lambda) = \ker(A_G - \lambda I_n)$ ($\ker(M)$ denotes the kernel or null space of a matrix M). The dimension of $\mathcal{E}_G(\lambda)$ coincides with the multiplicity of λ and, therefore, the algebraic and geometric multiplicities of each eigenvalue of A_G coincide and they will both be simply referred to as the *multiplicity* of the eigenvalue and denoted by $m(\lambda)$.

The characteristic polynomial of the adjacency matrix A_G of a graph G of order n is called the *characteristic polynomial of* G and it is denoted by $P_G(\lambda) = |A_G - \lambda I_n|$. Its roots are the eigenvalues of A_G whose set is called the *spectrum* of A_G and is denoted by $\sigma(A_G)$. For the sake of simplicity, we will use the notation $\sigma(G)$ for the set of the eigenvalues of the adjacency matrix A_G. Thus, if A_G has s real eigenvalues, its spectrum is $\sigma(G) = \{\lambda_1^{m_1}, ..., \lambda_s^{m_s}\}$ and m_i represents the multiplicity of the eigenvalue λ_i, with $i = 1, ..., s$. If G is a connected graph, its adjacency matrix is nonnegative so, by the Perron-Frobenius theorem, we conclude that the index of G, its largest eigenvalue, has multiplicity equal to one and an associated eigenvector with positive coordinates. It is well known (see [Doo82] and [CRS04]) that if G has at least one edge, then $\lambda_{min}(A_G) \leq -1$. Actually, $\lambda_{min}(A_G) = -1$ if and only if G has at least one edge and all its components are complete. Considering the line graph $L(G)$, $\lambda_{min}(A_{L(G)}) \leq -2$. A_G also has a positive eigenvalue not less than the average degree and not greater than the maximum degree in G [CDS95]. If G is the null graph, then all its eigenvalues are zero. In the particular case of a complete graph of order n, K_n, the characteristic polynomial is

$$P_{K_n}(\lambda) = \det\left(A_{K_n} - \lambda I_n\right) = \det \begin{pmatrix} -\lambda & 1 & \dots & 1 \\ 1 & -\lambda & \dots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \dots & -\lambda \end{pmatrix}.$$

Therefore, $-1 \in \sigma(K_n)$ and, since $A_{K_n}\mathbf{j} = (n-1)\mathbf{j}$, one can conclude that $(n-1) \in \sigma(K_n)$. These are the two unique eigenvalues of A_{K_n} and their multiplicities are $(n-1)$ and 1, respectively. If G is a line graph, $-2 \leq \lambda_{min}(A_G) \leq -1$ [CRS04].

We now introduce a collection of well known results that describe relations between the structure of a graph, the properties of its adjacency matrix and also the eigenvalues and eigenvectors of such matrix. The spectrum of a graph contains relevant information about the graph - analysing the spectrum, it is possible to find out if a given graph is bipartite, complete or regular, for instance, - but does not, in general, determine the graph.

The next theorem presents a lower bound for the number of distinct eigenvalues of the adjacency matrix of a graph G:

Theorem 2.1. *[Gan59] If G is a connected graph and A_G is its adjacency matrix, then A_G has at least $diam(G) + 1$ distinct eigenvalues.*

The next result states that it is possible to decide if a given graph G is bipartite from the analysis of the spectrum of A_G.

Theorem 2.2. *[CDS95] If G has at least one edge, then G is bipartite if and only if for any $\lambda \in \sigma(G), -\lambda \in \sigma(G)$.*

The following result introduces a property of the eigenvalues and eigenvectors of the adjacency matrix that describes a regular graph.

Theorem 2.3. *[CDS95] G is a regular graph if and only if $\mathbf{j}$ is an eigenvector of A_G. If G is p-regular, then p is an eigenvalue of A_G with corresponding eigenvector $\mathbf{j}$.*

A spectral property of line graphs will now be recalled:

Theorem 2.4. *[CRS04] For any given graph G, $\lambda_{min}\left(A_{L(G)}\right) \geq -2$. Equality is verified if and only if G has an odd cycle or two even cycles in the same connected component.*

The following upper bound on the stability number of a regular graph was obtained by Hoffman (unpublished) and presented by Lovász in [Lov79]:

Theorem 2.5. *If G is a p-regular graph of order n for which the spectra of the adjacency matrix is $p \geq \lambda_2 \geq \ldots \geq \lambda_n$, then*

$$\alpha(G) \leq n\frac{-\lambda_n}{p-\lambda_n}.$$

The *incidence matrix* of a simple graph G is the unsymmetrical (and, in general, not square) matrix $B_G = (b_{ij})$ with dimension $n \times m$ such that

$$b_{ij} = \begin{cases} 1, & \text{if} \quad e_j = v_i v_k \text{ with } k \neq i; \\ 0, & \text{if} \quad e_j = v_p v_q \text{ with } i \notin \{p, q\} \end{cases}.$$

The incidence matrix of a graph G and the adjacency matrices of G and of its line graph are related by (see [CDS95]),

$$B_G B_G^T = A_G + D_G, \quad B_G^T B_G = A_{L(G)} + 2I, \tag{2.1}$$

where D_G is a diagonal matrix with entries equal to the degrees of the vertices of G and $A_{L(G)}$ denotes the adjacency matrix of the line graph of G.

The Laplacian matrix of a graph G of order n is the $n \times n$ symmetric matrix defined by $L_G = D - A_G$, where $D = diag(d_1, \ldots, d_n)$ is the diagonal matrix formed from the vertex degrees and A_G is the adjacency matrix of G.

We will now recall a result from [Car01] about the existence of perfect matchings.

Theorem 2.6. *[Car01] A connected graph G of order $n > 1$, such that $L(G)$ is not complete, has a perfect matching if and only if $L(G) \in Q$.*

An eigenvalue of a graph G is *main* if its associated eigenspace is not orthogonal to the all-one vector $\mathbf{j}$. The vector space spanned by such eigenvectors of G is denoted $Main(G)$. The remaining (distinct) eigenvalues of G are referred to as *non-main.* The dimension of the eigenspace associated to each main eigenvalue λ_i of G, denoted by $\mathcal{E}_G(\lambda_i)$, is equal to the multiplicity of λ_i. For every graph G, the *index* of G, its largest eigenvalue, is main. The concepts of main and non-main eigenvalue were introduced in [CDS95] and an overview on the subject was published in [Row07]. If G has p distinct main eigenvalues $\mu_1, \ldots, \mu_p$, the *main characteristic polynomial* of G is

$$\begin{aligned} m_G(\lambda) &= \lambda^p - c_o\lambda^{p-1} - c_1\lambda^{p-2} - \cdots - c_{p-2}\lambda - c_{p-1} \\ &= \prod_{i=1}^{p}(\lambda - \mu_i). \end{aligned}$$

Theorem 2.7. *[Row07] If G is a graph with p main distinct eigenvalues $\mu_1, ..., \mu_p$, then the main characteristic polynomial of G, $m_G(\lambda)$, has integer coefficients.*

Chapter 3

Recognition of graphs with convex-QP stability number

The aim of this chapter is to introduce and characterize the class of graphs whose stability number can be determined by solving a convex quadratic program and to overview the main properties of such graphs; they were introduced in [Luz95] and are called graphs with convex-QP stability number or simply Q-graphs, where QP means quadratic programming.

In this chapter, several known results for the recognition of Q-graphs are overviewed, most of which were described in [Luz95], [Car01] and [Car03], and new others are introduced. Algorithms for the recognition, in polynomial time, of Q-graphs that simultaneously lead to the determination of maximum stable sets are also presented. Such algorithms efficiently solve the problem except when in the presence of the so called adverse graphs or of graphs with an adverse induced subgraph. Spectral and combinatorial characterizations of families of graphs where the polynomial-time recognition of Q-graphs is possible are also introduced.

3.1 Graphs with convex-QP stability number

Let G be a graph of order n with adjacency matrix A_G. Consider the quadratic programming problem,

$$\upsilon(G) = \max\left\{2\mathbf{j}^T x - x^T\left(H + I_n\right)x,\;\; x \geq 0\right\} \qquad (P_G)$$

where T stands for the transposition operation and

$$H = \begin{cases} \frac{1}{\tau}A_G & \text{if } E(G) \neq \emptyset \\ 0 & \text{otherwise} \end{cases},$$

with $\tau = -\lambda_{\min}(A_G)$. This program was introduced in [Luz95] in order to obtain an upper bound for the stability number of a graph G and it was analyzed in [CL98] where it was proved that its optimal value is the best upper bound among the optimal values of a family of quadratic programs. If G has at least one edge (i.e., $E(G) \neq \emptyset$), A_G is indefinite since its trace is zero. Hence $\lambda_{\min}(A_H) = -1$ and this guarantees the convexity of (P_G) because $H + I_n$ is positive semidefinite. Consequentely, $\upsilon(G)$ can be computed in polynomial time. On the other hand, if G has no edges, the value of $\upsilon(G) = \max\{2\mathbf{j}^T x - x^T x : x \geq 0\}$ coincides with $|V(G)|$ and both are equal to $\alpha(G)$.

It should be noted that, as Theorem 3.2 below states, the upper bound υ generalizes the well known upper bound for the stability number of a graph G of order n introduced by Hoffman in an unpublished paper (see [CDS95]).

Theorem 3.1. [*Hoffman, unpublished*]

$$\alpha(G) \leq \frac{-n\lambda_{min}(A_G)}{\lambda_{max}(A_G) - \lambda_{min}(A_G)}.$$

In fact, if G is a regular graph, the two bounds, Hoffman's and the quadratic programming bound υ, coincide:

Theorem 3.2. *[Luz95] If G is a regular graph,*

$$\upsilon(G) = \frac{-n\lambda_{min}(A_G)}{\lambda_{max}(A_G) - \lambda_{min}(A_G)}.$$

From the theory of convex optimization (see, for instance,[BSS06]), it is known that a vector $x \in \mathbb{R}^n$ is an optimal solution of program (P_G) if and only if it satisfies the Karush-Kuhn-Tucker optimality conditions, that is, if there is $y \geq 0$ such that

$$A_G x = \tau(\mathbf{j} - x) + y \tag{3.1}$$

$$y^T x = 0. \tag{3.2}$$

Therefore, provided that x is an optimal solution of (P_G), the above conditions guarantee the existence of vector $s \geq 0$ such that $2(H + I)x = 2\mathbf{j} + s$ and $x^T s = 0$. Such vector s is called the *complementary solution* associated to x and, as it was proved in [CL98], it is unique.

Theorem 3.3. *[CL98] Let G be a graph with at least one edge. If x_1^* and x_2^* are distinct optimal solutions for program (P_G) the difference $x_1^* - x_2^*$ belongs to $\mathcal{E}(\lambda_{\min}(A_G))$. Additionally, $s_1^* = s_2^*$, where s_1^* and s_2^* are the complementary solutions associated to x_1^* and x_2^*, respectively.*

Considering the objective function $f(x) = 2\mathbf{j}^T x - x^T (H + I)\, x$ of (P_G), any vector x, verifying $\nabla f(x) = 0$, is a critical point of $f(x)$. Since $\nabla f(x) = 2\mathbf{j} - 2\,(H + I)\,x$, an optimal solution x of (P_G) is a critical point of the objective function if and only if $(H + I)x = \mathbf{j}$. This is equivalent to saying that the complementary solution of x is the null vector. This way, we have the following consequence of Theorem 3.3:

Corollary 3.4. *If an optimal solution of (P_G) is a critical point of the objective function, then all optimal solutions of (P_G) are also critical points of that function.*

A graph G for which $\alpha(G) = \upsilon(G)$ is called a graph with *convex quadratic stability number* or a graph with *convex QP-stability number*, where QP stands for quadratic programming. The class of these graphs can also be denoted by $\mathcal{Q}$ and its elements called $\mathcal{Q}$*-graphs*.

The next result, from the original paper [Luz95], gives a criterion for a graph to have convex-QP stability number that was later extended by Cardoso and Cvetković.

Theorem 3.5. *[Luz95] If G has at least one edge, then $\alpha(G) = \upsilon(G)$ if and only if for a maximum stable set S of G (and then for all),*

$$-\lambda_{min}(A_G) \leq \min\left\{|N_G(u) \cap S| : u \notin S\right\}. \tag{3.3}$$

In their 2006 paper, Cardoso and Cvetković proved the following result:

Theorem 3.6. *[CC06] If G has at least one edge, then $\upsilon(G) = \alpha(G)$ if and only if there is a stable set verifying*

$$-\lambda_{min}(A_G) \leq \min\left\{|N_G(u) \cap S| : u \notin S\right\}.$$

There are several famous graphs that have convex-QP stability number. It is the case of the Petersen graph P in Figure 3.1, which is the strongly regular graph with parameters $(10, 3, 0, 1)$[1], for which $\lambda_{min}(A_P) = -2$ and $\{1, 3, 9, 10\}$ is a maximum stable set. P has convex-QP stability number because $\alpha(P) = \upsilon(P) = 4$. This is also the case of the Hoffman-Singleton graph HS, the strongly regular graph with parameters $(50, 7, 0, 1)$ for which $\lambda_{min}(A_{HS}) = -3$ and $\alpha(HS) = \upsilon(HS) = 15$. It is not yet known if the fourth graph of Moore M_4, the strongly regular graph with parameters $(3250, 57, 0, 1)$, exists. However, it was proved in [God93] that if M_4 exists, its stability number verifies $\alpha(M_4) \leq 400$. It was additionally proved by Cardoso, in an unpublished paper, that if $\alpha(M_4) = 400$, then M_4 has a $(0, 8)$-regular set (where $-8 = \lambda_{min}(A_{M_4})$) and, therefore, if M_4 exists, it has convex-QP stability number. Additionally, graphs defined by the disjoint union of complete subgraphs and complete bipartite graphs[2] are trivial examples of graphs with convex-QP stability number.

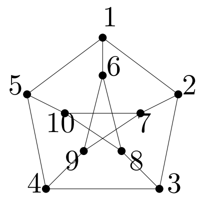


Figure 3.1: The Petersen graph P.

There are are many other families of graphs with convex-QP stability number, several of which will be described in Section 3.4. Actually, as a consequence of the next two theorems, it is possible to conclude that the class of graphs with convex-QP stability number has an infinite number of elements.

[1]A graph G is strongly regular with parameters (n, p, a, c) if G has n vertices, G is $p-$regular, adjacent vertices have a neighbours in common and non-adjacent vertices have c neighbours in common.

[2]G is a complete bipartite graph if it is bipartite with $V = V_1 \cup V_2$ and $\forall u \in V_1, d_G(u) = |V_2|$ and $\forall v \in V_2, d_G(v) = |V_1|$.

Theorem 3.7. *[Car01] A connected graph G with at least one edge, which is nor a star*[3] *neither a triangle*[4]*, has a perfect matching if and only if its line graph $L(G)$ has convex-QP stability number.*

Corollary 3.8. *[Car01] If G is a connected graph with an even number of edges then $L(L(G))$ has convex-QP stability number.*

Proof. Since $L(G)$ is a connected and star-free graph of even order, by [LV75], $L(G)$ has a perfect matching. Therefore, by Theorem 3.7, $L(L(G)) \in Q$. □

Figure 3.2: Graph G and its subgraph G' induced by $V' = \{1, 2, 5, 6\}$.

It is also worth mentioning that the class of graphs with convex-QP stability number is not hereditary [CL12], in the sense that an induced subgraph of a graph with convex-QP stability number doesn't necessarilly have convex-QP stability number. Graph G in Figure 3.2, with maximum stable set $S = \{1, 3, 4, 5\}$, $\upsilon(G) = 4$ and $\lambda_{min}(A_G) = -2$, has convex-QP stability number, while its subgraph G' induced by $V' = \{1, 2, 5, 6\}$ for which $\lambda_{min}(A_{G'}) = -1.4812$ and $\upsilon(G') = 2,1939$ has not. It was shown in [CL12] that, although the chordless path on five vertices P_5 has convex-QP stability number, its induced subgraph P_4 does not. Nevertheless, as it was proved in [Car01], the class of graphs with convex-QP stability number is closed under the deletion of certain collections of vertices called α-*redundant* vertices. An α-redundant subset of vertices is $U \subseteq V(G)$ such that $\alpha(G) = \alpha(G - U)$.

[3]A star is a $K_{1,k}$ graph.

[4]Triangle means K_3.

In the examples in Figures 3.3 and 3.4, the highlighted sets A_1 and A_2 are *α-redundant* for the corresponding graphs G_1 and G_2 because the stability numbers of G_1 and G_2 remain the same after the removal of the vertices in A_1 and A_2, respectively.

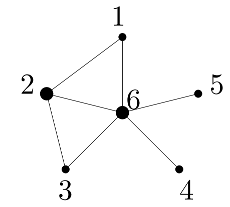


Figure 3.3: Graph G_1 for which $S_1 = \{1, 3, 4, 5\}$ is a maximum stable set, $\alpha(G) = 4$ and $A_1 = \{2, 6\}$ is an α-redundant set.

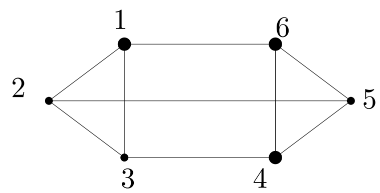


Figure 3.4: Graph G_2 with maximum stable set $S_2 = \{1, 4\}$ and α-redundant set $A_2 = \{1, 4, 6\}$.

It should be noted that the complement of a maximum stable set is always α-redundant.

3.2 Recognition results

In this section, several well known results for the recognition of Q-graphs are overviewed (see [Car01] and [Car03]) and new others are introduced. Algorithms for the recognition, in polynomial time, of Q-graphs that also determine maximum stable sets are also presented. Such algorithms efficiently solve the problem except when the considered graph is adverse or has an adverse induced subgraph, in the sense of Definition 3.9. Spectral and combinatorial characterizations of families of graphs in which the polynomial-time recognition of Q-graphs is possible are also introduced.

Theorem 3.10, included in [Car01], provides a process for the determination of a maximum stable set of a graph with convex quadratic stability number. Theorems 3.11 to 3.14, also proved in the same paper, give an algorithmic strategy for the recognition of Q-graphs unless the conditions $\upsilon(G) = \upsilon(G-u) = \upsilon(G-N_G(u))$ and $\lambda_{min}(A_G) = \lambda_{min}(A_{G-u}) = \lambda_{min}(A_{G-N_G(u)}), \forall u \in V$ are verified. When a graph verifies these conditions, the problem of being able to know whether or not it belongs to Q has resisted to all attempts of finding a solution, remaining an open question. Such difficulty has its origin in the recognition of the so called adverse graphs, defined as follows:

Definition 3.9. A graph G without isolated vertices such that

$\upsilon(G), \lambda_{min}(A_G) \in \mathbb{Z}$

$\forall u \in V, \upsilon(G) = \upsilon(G - N_G(u))$

$\forall u \in V, \lambda_{min}(A_G) = \lambda_{min}(A_{G-N_G(u)})$

is called an *adverse graph*.

Note that if G is adverse, equalities

$$\upsilon(G) = \upsilon(G-u) \tag{3.4}$$

and

$$\lambda_{min}(A_G) = \lambda_{min}(A_{G-u}) \tag{3.5}$$

are verified for all vertices $u \in V(G)$.

Since G has no isolated vertices,

$$\forall u \in V(G), \exists v \in V(G) : u \in N_G(v).$$

Considering that, for any vertex $u \in V(G)$, the conditions

$$\upsilon(G - N_G(v)) \leq \upsilon(G-u) \leq \upsilon(G), \forall u \in V(G)$$

and

$$\lambda_{\min}(A_G - N_G(v)) \geq \lambda_{\min}(A_{G-u}) \geq \lambda_{\min}(A_G)$$

hold, equalities (3.4) and (3.5) also hold.

Both the graph in Figure 3.5 below and the Petersen graph in Figure 3.1 on page 18 represent adverse graphs.

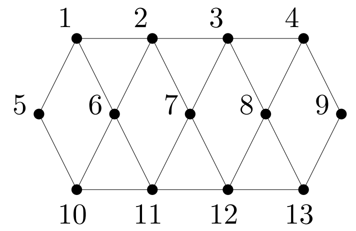


Figure 3.5: Adverse graph G.

Graph G in Figure 3.5 has $\{5, 6, 7, 8, 9\}$ (or $\{1, 3, 9, 10, 12\}$) as a maximum stable set. Since $\lambda_{min}(A_G) = -2$ and $\upsilon(P) = \alpha(P) = 5$, G has convex-QP stability number.

Next we will recall the sequence of results introduced in [Car01] that lead to an algorithm that decides if a given graph has convex-QP stability number or determines an adverse subgraph of it.

The following theorem provides a sufficient condition for a graph to have convex-QP stability number that leads to the determination of a maximum stable set.

Theorem 3.10. *[Car01] If $U \subseteq V(G)$ is such that $\upsilon(G - U) = \upsilon(G)$ and $\lambda_{min}(A_G) \neq \lambda_{min}(A_{G-U})$ then $G \in Q$ and, furthermore, any optimal solution of program (P_{G-U}) defines a characteristic vector of a maximum stable set of G.*

From the following theorem, it can be concluded that an induced subgraph of a graph with convex-QP stability number, obtained from the elimination of an α-redundant set of vertices, also has convex-QP stability number.

Theorem 3.11. *[Car01] If $G \in Q$ and $U \subseteq V(G)$ is such that $\alpha(G) = \alpha(G - U)$ then $G - U \in Q$.*

Theorem 3.12. *[Car01] If there exists $v \in V(G)$ such that*

$$\upsilon(G) \neq \max\{\upsilon(G - v), \upsilon(G - N_G(v))\}$$

then $G \notin Q$.

As a direct consequence of the previous result, if G has convex-QP stability number then

$$\forall v \in V(G), \upsilon(G) = \max\left\{\upsilon(G-v), \upsilon(G-N_G(v))\right\}. \tag{3.6}$$

Theorem 3.13. *[Car01] Consider that $\exists v \in V(G)$ such that $\upsilon(G-v) \neq \upsilon(G-N_G(v))$. Under this assumption:*

1. *If $\upsilon(G) = \upsilon(G-v)$ then $G \in Q \Leftrightarrow G-v \in Q$.*

2. *If $\upsilon(G) = \upsilon(G-N_G(v))$, then $G \in Q \Leftrightarrow G-N_G(v) \in Q$.*

Although neither Theorem 3.12 nor Theorem 3.13 can be applied to adverse graphs, Theorem 3.14 provides a branching strategy that is implementable for such graphs.

Theorem 3.14. *[Car01] If there is $v \in V(G)$ such that $\upsilon(G) = \upsilon(G-v) = \upsilon(G-N_G(v))$ then $G \in Q$ if and only if $G-N_G(v) \in Q$ or $G-v \in Q$.*

3.3 An algorithm for detecting Q-graphs

Based in Theorems 3.10 to 3.14, the next procedure recognizes if a graph has convex-QP stability number or determines one of its adverse subgraphs. Step 2 of the algorithm relies on Theorem 3.12; the conclusion in step 4 is a consequence of Theorem 3.10; Theorem 3.13 is the ground to step 5. The input of the procedure is graph G.

Algorithm 1 Determines if a given graph is a Q-graph or determines an adverse subgraph.

Require: Graph G with at least one edge.

Ensure: Induced subgraph H, x^*, CQP.

1: Set $H := G - Iso(G)$ and $\tau := -\lambda_{\min}(A_H)$ ($Iso(G)$ denotes the set of isolated nodes of G)

2: **If** $\exists v \in V(H)$ such that $\upsilon(G) \notin \{\upsilon(H-v), \upsilon(H-N_G(v))\}$ **then** $CQP = 0$ **STOP** $(G \notin Q)$.

3: **If** $\exists v \in V(H)$ such that $\tau \neq \min\left\{-\lambda_{min}(A_{H-v),-\lambda_{min}(A_{H-N_H(v)})}\right\}$ **then do**

4: **If** $\left(\tau \neq -\lambda_{min}(A_{H-N_H(v)}) \text{ and } \upsilon(H) = \upsilon(H-N_H(v))\right)$ **or** $\left(\tau \neq -\lambda_{min}(A_{H-v}) \text{ and } \upsilon(H) = \upsilon(H-v)\right)$ **then** $CQP = 1$ **STOP** $(G \in Q)$.

5: **If** $\exists v \in V(G)$ such that $\upsilon(H-v) \neq \upsilon(H-N_H(v))$ **then do**

6: **If** $\upsilon(H) = \upsilon(H-v)$ **then** $H \leftarrow H - v$

7: **If** $\upsilon(H) = \upsilon(H-N_H(v))$ **then** $H \leftarrow H - N_H(v)$

8: **Return** to step 2.

9: $CQP = -1$ **STOP** G contains the adverse subgraph H.

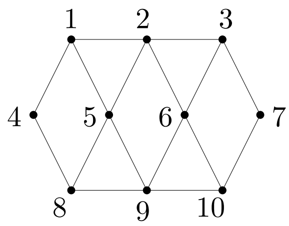


Figure 3.6: Graph B with 10 vertices.

Example 3.15. We will apply Algorithm 1 to graph B in Figure 3.6, in order to determine if it has convex quadratic stability number. It is easily checkable that

$$\forall v \in V(B), \upsilon(B) = \upsilon(B - N_B(v)) = 4.$$

Eliminating the neighbourhood of vertex 5, the following inequality is obtained:

$$-2 = \lambda_{min}(A_B) \neq \lambda_{min}(A_{B-N_B(5)}) = -1.8478.$$

Therefore, it can be concluded that graph B is a Q-graph.

The following results are also useful for the recognition of graphs with convex-QP stability number.

Theorem 3.18 was introduced in [Car03] (using different terminology) and it states that an adverse graph G is a Q-graph if and only if there is $S \subset V(G)$ which is $(0,\tau)$-regular, with $\tau = -\lambda_{min}(A_G)$. Therefore, the worst case complexity for the recognition of Q-graphs is the same as the worst case complexity for the recognition of $(0,\tau)$-regular sets, with $\tau = -\lambda_{min}(G)$, in adverse subgraphs. The proof of Theorem 3.18 is included for the sake of didatics.

It is worth to recall the following necessary and sufficient condition for graphs with (κ,τ) regular sets published in [CR04, Prop. 2.2].

Proposition 3.16. *A graph G has a (k,τ)-regular set S iff the characteristic vector of S is a solution of the linear system*

$$A_G x = k\boldsymbol{j}, \qquad \textit{when } k = \tau$$

or the system

$$\left(\frac{A_G}{\tau - k} + I_n\right)x = \frac{\tau}{\tau - k}\boldsymbol{j}, \qquad \textit{when } k \neq \tau,$$

where $\boldsymbol{j}$ denotes the all-ones n-vector and I_n the identity matrix of order n.

The following slight variation of of the above proposition appear in [CLLP16, Prop. 2.1].

Proposition 3.17. *A graph G of order n has a (κ,τ)-regular set S if and only if the system*

$$(A_G - (\kappa - \tau)I_n)x = \tau\mathbf{j}, \tag{3.7}$$

has a 0-1 solution. Furthermore, such a solution $x = (x_1,\ldots,x_n)^T$ is the characteristic vector of S (i.e., $x_i = 1$ if $i \in S$ and $x_i = 0$ otherwise).

Proof. Let us assume that G has a (k,τ)-regular set. Then, by Proposition 3.16 of [CR04], its characteristic vector is a solution of the system (3.7) and hence it has a 0-1 solution. Conversely, assuming that the system (3.7) has a 0-1 solution x and defining the vertex subset $S = \{v_i : x_i = 1\}$, from (3.7),

$$\sum_{j \in N_G(i)\cap S} x_j - (k-\tau)x_i = \tau \Leftrightarrow |N_G(i) \cap S| = (k-\tau)x_i + \tau, \text{ for } i = 1,\ldots,n,$$

and we may conclude that

$$|N_G(i) \cap S| = \begin{cases} k & \text{if } v_i \in S \\ \tau & \text{otherwise} \end{cases}.$$

Therefore S is a (k, τ)-regular set. □

Theorem 3.18. *[PC09] If G is adverse, $G \in Q$ if and only if there is $S \subseteq V(G)$ such that S is $(0, \tau)$-regular with $\tau = -\lambda_{min}(A_G)$.*

Proof. Since G is an adverse graph, it is immediate that every optimal solution x of (P_G) is such that $A_G x = -\lambda_{min}(A_G)(\mathbf{j} - x)$.

Supposing that $G \in Q$, the characteristic vector $\bar{x}$ of a maximum stable set S, is an optimal solution of (P_G) and, as $A_G\bar{x} = -\lambda_{min}(A_G)(\mathbf{j} - \bar{x})$, we have

$$\forall i \notin S, \sum_{j \in N(i)} \bar{x}_j = |N(i) \cap S| = -\lambda_{min}(A_G).$$

In order to prove the reciprocal condition, let $S \subset V(G)$ be a $(0, -\lambda_{min}(A_G))$-regular set, with characteristic vector $\bar{x}$. We have

$$(A_G\bar{x})_i = \sum_{j \in N(i)} \bar{x}_j = \begin{cases} 0 \text{ if } i \in S \\ -\lambda_{min}(A_G) \text{ if } i \notin S \end{cases}$$

As a consequence, $A_G\bar{x} = -\lambda_{min}(A_G)(\mathbf{j} - \bar{x})$ implies that $\bar{x}$ is an optimal solution for (P_G). Hence,

$$\alpha(G) \leq \upsilon(G) = \mathbf{j}^T\bar{x} = |S| \leq \alpha(G) \Rightarrow G \in Q.$$

□

As a consequence of the previous result, the recognition of Q-graphs can be done applying Algorithm 1 or recognizing a $(0, \tau)$-regular set, with $\tau = -\lambda_{min}(A_H)$, in an adverse subgraph H determined by the procedure.

3.4 Analysis of particular families of graphs

The results described in this section concern several particular families of graphs in which the recognition of Q-graphs can be obtained. Some of the results, as well as their proofs, were first introduced in [Car03] and others, later, in [PC09]. In order to make the examples that correspond to each class of graphs as clear as possible, the relevant results for each family of graphs as well as their proofs are included in the corresponding subsections.

3.4.1 Bipartite graphs

Recall that a graph is bipartite if $V(G)$ is the disjoint union of two sets V_1 and V_2 such that $\forall uv \in E(G), |V_1 \cap \{u, v\}| = |\{u, v\} \cap V_2| = 1$. Graph B in Figure 3.7 is a bipartite graph: the set of its vertices admits the bipartition $V_1 = \{1, 2\}, V_2 = \{3, 4, 5\}$.

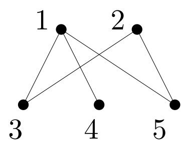


Figure 3.7: Bipartite graph B.

According to the Perron-Frobenius Theorem ([God93], Th. 6.1), every connected graph has a simple maximum eigenvalue. On the other hand, when the graph is bipartite, its eigenvalues are symmetric about the origin [CDS95]. Therefore, the minimum eigenvalue of a connected bipartite graph G is simple and then

$$\exists u \in V(G) : \lambda_{min}(A_G) < \lambda_{min}(A_{G-u}).$$

Hence, since $G \in Q$ if and only if each component is in Q, applying Algorithm 1 it can be recognized in polynomial-time if a bipartite graph is a Q-graph.

Theorem 3.19. *Bipartite graphs with convex-QP stability number can be recognized in polynomial time.*

3.4.2 Dismantlable graphs

Dismantlable graphs have the following recursive definition: the one-vertex graph is dismantlable and a graph G with two or more vertices is dismantlable if there are at least two vertices

u and v such that $N_G[u] \subseteq N_G[v]$[5] and $G - u$ is dismantlable.

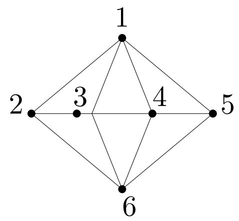


Figure 3.8: A dismantlable graph.

The next theorem states a neighbourhood inclusion condition that does not hold when a graph is adverse and, as a consequence, it may be concluded that there are no dismantlable adverse graphs.

Theorem 3.20. *[PC09] Let G be a graph, $\tau = -\lambda_{min}(A_G) > 1$ and $u, v \in V(G)$ such that $N_G[v] \subseteq N_G[u]$. Then $\upsilon(G) > \upsilon(G - N_G(u))$.*

Proof. Let x^* be an optimal solution of program (P_G), suppose that $\tau > 1$ and let y^* be the corresponding complementary solution. Then, considering the Karush-Kuhn-Tucker conditions and subtracting the v-th to the u-th row of condition 3.1, we obtain

$$\tau(x_u^* - x_v^*) + \sum_{j \in N_G(u)} x_j^* - \sum_{j \in N_G(v)} x_j^* = y_u^* - y_v^*$$

$$\Leftrightarrow (\tau - 1)(x_u^* - x_v^*) \sum_{j \in N_G[u]} x_j^* - \sum_{j \in N_G[v]} x_j^* = y_u^* - y_v^*$$

$$\Leftrightarrow (\tau - 1)(x_u^* - x_v^*) \sum_{j \in N_G[u] \setminus N_G[v]} x_j^* - \sum_{j \in N_G[v] \setminus N_G[u]} x_j^* = y_u^* - y_v^*.$$

Since we are supposing that $N_G[v] \subseteq N_G[u]$, then $N_G[v] \setminus N_G[u] = \emptyset$ and the last equality can be rewritten as

$$(\tau - 1)(x_u^* - x_v^*) + \sum_{j \in N_G[u] \setminus N_G[v]} x_j^* = y_u^* - y_v^*.$$

Therefore,

$$(\tau - 1)(x_u^* - x_v^*) \leq y_u^* - y_v^*.$$

[5] $N_G[x] = N_G(x) \cup \{x\}$.

If $\upsilon(G) = \upsilon(G - N_G(u))$ then there is an optimal solution x^{*u} of (P_G) with corresponding complementary solution y^* such that $x^{*u}_u = 1$. As a consequence, $y^*_u = 0$ and $x^{*u}_j = 0, \forall j \in N_G(u)$. Considering $x^* = x^{*u}$, $(\tau - 1)(x^*_u - x^*_v) \leq y^*_u - y^*_v$ is equivalent to

$$\tau - 1 \leq -y^*_v$$

which implies the contradiction

$$\tau \leq 1.$$

□

As an immediate consequence of Theorem 3.20, we have the following corollary:

Corollary 3.21. *Algorithm 1 recognizes dismantlable graphs with convex-QP stability number in polynomial time.*

3.4.3 Graphs with low Dilworth number

Given $u, v \in V(G)$ such that $N_G(u) \subseteq N_G(v)$, we say that vertices u and v are comparable. This binary relation is a preorder (that is, it is reflexive and transitive) and is called *vicinal preorder*. Therefore, graph $D(G)$ such that $V(D(G)) = V(G)$ and

$$E(D(G)) = \{uv \in E(G) : N_G(u) \subseteq N_G[v] \text{ or } N_G(v) \subseteq N_G[u]\}$$

is the comparability graph of the vicinal preorder of G. Considering the *Dilworth number* of a graph, which was introduced in [FH78] and is equal to its largest number of pairwise incomparable vertices, $dilw(G) = \alpha(D(G))$. As a consequence of the results introduced in the paper [Car03], we have the following theorem:

Theorem 3.22. *[PC09] Let G be a not complete graph. If $dilw(G) < \omega(G)$, then G is not adverse.*

Proof. Let G be a not complete adverse graph. Then

$$\forall uv \in E(G), \upsilon(G) = \upsilon(G - N_G(u)) = \upsilon(G - N_G(v)),$$

and, therefore, according to Theorem 3.20,

$$\forall uv \in E(G), N_G[u] \not\subseteq N_G[v] \wedge N_G[v] \not\subseteq N_G[u].$$

Thus, if $C \subseteq V(G)$ is a maximum clique, then $\forall u, v \in C$, u and v are not comparable with respect to the vicinal preorder. Consequently, $dilw(G) \geq |C| = \omega(G)$.

$\square$

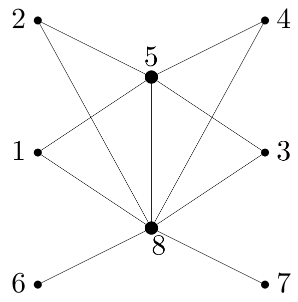


Figure 3.9: A threshold graph in which 1 is the first vertex of the construction process detailed next, $1, 2, 3, 4, 6$ and 7 are the isolated vertices and 5 and 8 are the dominating vertices (added in the order in which they are numbered).

As a consequence of Theorem 3.22, Algorithm 1 can be applied to recognize in polynomial-time if a graph with Dilworth number equal to 1 is a Q-graph. Note that a graph with Dilworth number equal to 1 is a *threshold graph* (see Figure 3.9), that is, a graph that can be constructed from a one vertex graph by successive applications of the following operations:

- adding a single isolated vertex to the graph.
- adding a single dominating vertex to the graph, that is, a single vertex that is connected to all other vertices.

From Theorem 3.22, taking into account that threshold graphs have Dilworth number equal to 1, we may conclude that:

Corollary 3.23. *Threshold graphs with convex-QP stability number can be recognized in polynomial time.*

3.4.4 (C_4,P_5)-free graphs

Supposing that the chordless path, P_4, is induced by the vertices x_1, x_2, x_3, x_4, the vertices x_2 and x_3 will be called (as usual) the midpoints of P_4.

Theorem 3.24. *Let G be a graph. If $\exists uv \in E(G)$ such that $\upsilon(G) = \upsilon(G - N_G(u)) = \upsilon(G - N_G(v))$, then uv belongs to a C_4 or u and v are the midpoints of a P_4.*

Proof. By Theorem 3.20, $N_G[v] \not\subseteq N_G[u]$ and $N_G[u] \not\subseteq N_G[v]$ and hence $\exists x \in N_G[u] \setminus N_G[v]$ and $\exists y \in N_G[v] \setminus N_G[u]$. Therefore, either uv belongs to a C_4 (if $uv \in E(G)$) or u and v are the midpoints of a P_4. □

Recalling that a banner is a graph isomorphic to the graph with vertices x_1, x_2, x_3, x_4, x_5 and edges $x_1x_2, x_2x_3, x_3x_4, x_4x_5$ and x_5x_2, from Theorem 3.24 and Corollary 1 in [BL01] (where it is stated that if G is a (banner,$P5$)-free graph, then any midpoint of a P_4, v, is such that $\alpha(G) = \alpha(G - v)$), we have the following.

Theorem 3.25. *Let G be an adverse graph for which*

$$\upsilon(G) = \upsilon(G - N_G(v)), \forall v \in V(G). \tag{3.8}$$

If G is (C_4, P_5)-free, then $\forall v \in V(G), \alpha(G) = \alpha(G - v)$.

Proof. Since G is a C_4-free graph, for which the equalities (3.8) hold and has no isolated vertices, by Theorem 3.24, any vertex is the midpoint of a P_4. Therefore, since any C_4-free graph is banner-free, from Corollary 1 in [BL01], we may conclude that $\forall v \in V(G), \alpha(G) = \alpha(G - v)$. □

Corollary 3.26. *There are no adverse (C_4, P_5)-free graphs and, consequently, (C_4, P_5)- free graphs with convex-QP stability number can be recognized in polynomial time.*

3.4.5 (Claw,P_4)-free and (Claw,P_5)-free graphs

Recall that a vertex in a graph is *α-critical* if its removal decreases the stability number and also that an edge is α-critical if its removal increases the stability number of the graph.

A claw-free graph is a $K_{1,3}$-free graph. Note that the line graph of any graph G is claw-free. Figure 3.10 shows a claw-free graph, G, for which $\upsilon(G) = 0.4805$. Then, G does not have convex-QP stability number.

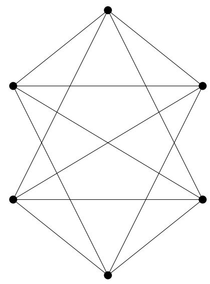


Figure 3.10: A claw-free graph without convex-QP stability number.

Theorem 3.27. *Let G be a claw-free graph. If $\exists uv \in E(G)$ such that $\upsilon(G) = \upsilon(G - N_G(u)) = \upsilon(G - N_G(v))$ and u and v are not the midpoints of a P_4, then neither u nor v are α-critical.*

Proof. According to Theorem 3.20, $N_G[u] \setminus N_G[v] \neq \emptyset$ and $N_G[v] \setminus N_G[u] \neq \emptyset$. Suppose that $u \in S$, where S is a maximum stable set of G.

- If the edge uv is α-critical, then it is well known that neither u nor v are α-critical and hence the result is proved.
- Suppose that uv is not α-critical. Then, since G is claw-free, $\exists' x \in (N_G(v) \cap S) \setminus \{u\}$ and, according to the hypothesis, $\exists y \in N_G[u] \setminus N_G[v]$. Since u and v are not the midpoints of a P_4, $xy \in E(G)$ and then the set of vertices $X = \{y, u, v, x\}$ induces a C_4 and is such that $u, x \in S$ and $v, y \notin S$. Furthermore, the neighbors of v and y in S are only u and x. Therefore, $S' = (S \setminus X) \cup (X \setminus S)$ is a maximum stable set of G, and thus neither u nor v are α-critical.

$\square$

Considering the chordless path P_5 defined by the sequence of vertices x_1, x_2, x_3, x_4, x_5, the vertex x_3 is called the midpoint of P_5 .

Theorem 3.28. *Let G be a claw-free graph without isolated vertices such that $\forall ij \in E(G)$, ij belongs to a C_4 or i and j are the midpoints of a P_4. Then, $\forall w \in V(G)$, w is the midpoint of a P_5, $uvwxy$, such that $u, w, y \in S$, where S is a maximum stable set of G, or $\alpha(G) = \alpha(G-w)$.*

Proof. Let S be a maximum stable set of G and w an arbitrary vertex. If $w \notin S$, then, obviously, $\alpha(G) = \alpha(G-w)$. Let us suppose that $w \in S$. Then, since w is not isolated, $\exists x \in V(G)$ such that $wx \in E(G)$.

- If wx is α-critical then $\alpha(G) = \alpha(G-w)$.
- Let us assume that wx is not α-critical. Then, $\exists y \in N_G(x) \cap (S \setminus \{w\})$. On the other hand, since wx belongs to a C_4 or w and x are the midpoints of a P_4, $\exists v \in N_G(w) \setminus N_G[x]$.
  - If $vy \in E(G)$ then, since G is claw-free, $(S \setminus \{w, y\}) \cup \{v, x\}$ is a maximum stable set of G and then $\alpha(G) = \alpha(G-w)$.
  - If $vy \notin E(G)$ then, either vw is α-critical (and thus $\alpha(G) = \alpha(G-w)$) or $\exists u \in N_G(v) \cap (S \setminus \{w\})$.

    Suppose that $\exists u \in N_G(v) \cap (S \setminus \{w\})$. If $ux \in E(G)$, then $\alpha(G) = \alpha(G-w)$, else $uvwxy$ is a P_5 with $u, w, y \in S$.

□

As immediate consequence, combining this theorem with Theorem 3.27, we may conclude the following Corollary.

Corollary 3.29. *Let G be a (claw, P_5)-free graph without isolated vertices. If G is adverse then, $\forall v \in V(G)$, $\alpha(G) = \alpha(G-v)$.*

The next theorem grants the recognition of α-redundant subsets of vertices in claw-free graphs with comparable non-adjacent vertices, in the sense of the vicinal preorder relation already defined. It is the case of the graph G in Figure 3.5.

Theorem 3.30. *[PC09] Let G be a claw-free graph and $u, v \in V(G)$ such that $uv \notin E(G)$. If $N_G(u) \subseteq N_G(v)$, then $N_G(u)$ is an α-redundant subset of vertices.*

Proof. Suppose G is a claw-free graph and u, v are two vertices of G that are not endpoints of the same edge. Additionaly assume that $\exists w \in N_G(u) : w \in S$ where S is a maximum stable set of G.

If $S \cap N_G(u) = \{w\}$, then the edge wu is α-critical and hence w is not an α-critical vertex and the conclusion follows.

If $|S \cap N_G(u)| > 1$ then, since G is claw-free, there is another vertex x such that $S \cap N_G(u) = \{w, x\}$. On the other hand, since $N_G(u) \subseteq N_G(v)$, it may be concluded that the set $A = \{u, w, v, x\}$ induces a C_4 such that $A \cap S = \{w, x\}$.

Therefore, $S' = (S \setminus A) \cup (A \setminus S)$ is also a maximum stable set of G and consequently $N_G(u)$ is an α-redundant subset of vertices. $\square$

Applying this result to each vertex x of degree 2 of the claw-free graph in Figure 3.5 and to each vertex w such that $N_G(x) \subseteq N_G(w)$ and successively deleting $N_G(x)$ while the above conditions remain true, a maximum stable set of G will be determined, as the following example illustrates.

Example 3.31. Consider the graph of Figure 3.5. It can easily be seen that the vertices of degree two, 5 and 9, verify

$$N_G(5) = \{1, 10\} \subseteq N_G(6) = \{1, 2, 10, 11\}$$

and

$$N_G(9) = \{4, 13\} \subseteq N_G(8) = \{3, 4, 12, 13\}\,.$$

According to Theorem 3.30, $N_G(5)$ and $N_G(9)$ are α-redundant and will be deleted. The obtained induced subgraph G_1 in Figure 3.11 has two vertices of degree two, which are 6 and

8, whose neighbourhoods verify the conditions below.

$$N_{G_1}(6) = \{2, 11\} \subseteq N_{G_1}(7) = \{2, 3, 11, 12\}$$

and also

$$N_{G_1}(8) = \{3, 12\} \subseteq N_{G_1}(7).$$

Then, the set of vertices $\{2, 3, 11, 12\}$ is α-redundant and will thus be deleted, leaving the maximum stable set of G

$$S = \{5, 6, 7, 8, 9\}.$$

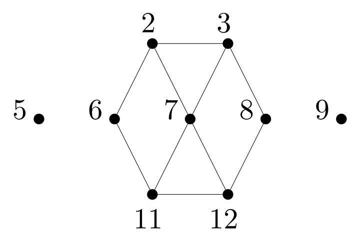


Figure 3.11: Adverse claw-free induced subgraph G_1.

As a direct consequence of Theorem 3.30, the following corollary can be stated.

Corollary 3.32. *There are no adverse (claw, P_4)-free nor (claw, P_5)-free graphs and, consequently, (claw, P_4)-free and (claw, P_5)-free graphs with convex-QP stability number can be recognized in polynomial time.*

Chapter 4

Determination of (κ, τ)-regular sets

The motivation for developing the contents of this chapter was the search for an answer to the question of recognizing, in the worst case scenario, $(0, \tau)$-regular graphs in adverse graphs. With that purpose in mind, the current chapter is devoted to the more general problem of determining (κ, τ)-sets.

The characteristic vectors of (κ, τ)-regular sets were studied in Proposition 4.1 and Corollary 4.3 of [CSZ10]. Based on different tools, namely the minimal least squares solution of a linear system, the result in Proposition 4.15 is equivalent to the above cited statements of [CSZ10]. The equivalence between the minimal least squares solution x^+ introduced in Proposition 4.15 and the parametric vector $g_G(\kappa, \tau)$ defined in [CSZ10] is proved in [CLLP16] and such proof is included in Appendix A.1.

Another significant source of motivation for developing the contents of this chapter was the paper [CL16], where the equivalence between a star solution and a basic feasible solution of a linear problem with certain constraints defined by a particular star set for $\lambda_{min}(A_G)$ was stated. A simplex-like algorithm for recognizing Q-graphs as well as an innovative characterization of those graphs that depends on star sets are also described in the mentioned paper and such characterization will be recalled in Section 4.2, being ground for the new recognition procedures described in this chapter. Star sets were first introduced by Cvetković, Rowlinson and Simić [CRS93] as a tool to study eigenspaces of graphs and to approach the graph isomorphism problem. In [Ell93], also published in 1993, Ellingham introduced the concept of star complement, under the designation μ-basis. The designation *star complement* was first introduced by Rowlinson in [Row98]. Star sets and star complements have since been the object of many papers and provide very useful techniques for the characterization of numerous families of graphs.

This chapter starts with a result from [CL16] that allows several properties of graphs for which the optimal solutions of (P_G) are critical points of the objective function to be regarded as properties of adverse graphs; The rest of this chapter is organized as follows: in Section 4.1, the nullifying procedure described in [CL16] is recalled and an example of its execution is described; Section 4.2 contains a brief overview of basic facts about star sets and star complements that lead to a new necessary and sufficient condition for a graph to have convex-QP stability number; in Section 4.3, results about the determination of (κ, τ)-regular sets are introduced (such results are equivalent to the ones introduced in [CSZ10] and the proof of such equivalence is included in Appendix A.1); in Section 4.4, a simplex-like algorithm for the determination of $(0, \tau)$-regular sets is introduced and, in Subsection 4.5.1, such algorithm, that relies on results about spectral properties and star complements, is applied to the determination of efficient dominating sets; Section 4.5.2 introduces several results that provide an efficient technique to detect the existence of perfect matchings in graphs of certain families of graphs; Section 4.5.3 describes an approach to the NP-complete problem of the determination of Hamiltonian cycles that relates a result introduced in [ACS13] with the algebraic connectivity of the graph; the chapter ends with Section 4.6, in which a new algorithmic approach for the detection of (κ, τ)-regular sets that relies on the multiplicity of $\kappa - \tau$ as an eigenvalue of the graph.

Proposition 4.1. *[CL16] If G is an adverse graph, then x^* is an optimal solution of (P_G) if and only if $x^* \geq 0$ and it is a critical point of the objective function, i.e., x^* is a nonnegative solution of $(A_G - \lambda_{min}(A_G)I_n)\, x = -\lambda_{min}(A_G)\boldsymbol{j}$.*

4.1 The *Nullifying Components* algorithm

The section will start with a result that assures the existence of an optimal solution of program (P_G), with a certain number of null components, for graphs where the optimal solutions of (P_G) are critical points of the objective function. The proof of such result is included in [CL16] and, being constructive, it provides an algorithm for the determination of the optimal solution. Such proof will not be replicated in this text, but the algorithm *Nullifying Components*, structured on that proof is included (see Algorithm 2), as well as an example of how it is executed.

Theorem 4.2. *[CL16, Th.11] Let G be a graph with n vertices and at least one edge. If the optimal solutions of (P_G) are critical points of the objective function, then there exists an optimal solution of (P_G), x^*, with at least k null coordinates, where $k = \dim(\mathcal{E}(\lambda_{\min}(A_G)))$. Furthermore, there is a basis of $\mathcal{E}(\lambda_{\min}(A_G))$ formed by k vectors $v_1, v_2, \ldots, v_k$ of $\mathbb{R}^n$ such that the submatrix of $[v_1 \ v_2 \ \cdots \ v_k]$ indexed by the rows corresponding to the k null components of x^* and by a certain permutation of columns $1, 2, \ldots, k$ coincides with the identity matrix of order k.*

Algorithm 2 Nullifying Components.

Require: A graph G with n vertices and at least one edge; an optimal solution x^* of (P_G).

Ensure: An optimal solution x^* of (P_G) with at least k null components; a basis for the null space of $H + I = \frac{A_G}{\lambda_{\min}(A_G)} + I$.

Compute a basis $\mathcal{B} = \{b_1, \ldots, b_k\}$ for the null space of $H + I$.

Set $j := 1$;

While $j \leq k$ **do**

  Compute $\frac{x_r^*}{b_{rj}} = \min\limits_{i=1,\ldots,n} \left\{ \frac{x_i^*}{b_{ij}} : b_{ij} > 0 \right\}$;

  Set $\tilde{x}^* := x^* - \frac{x_r^*}{b_{rj}} b_j$;

  While $1 \leq q \leq k$ and $q \neq j$ **do**

    $b_q := b_q - \frac{b_{rq}}{b_{rj}} b_j$;

  End While

  Set $b_j := \frac{1}{b_{rj}} b_j$;

  Set $x^* := \tilde{x}^*$ and $j := j + 1$;

End While

End

Graph G in Figure 4.1 will be used to clarify how the algorithm is executed.

Example 4.3. The execution of Algorithm 3 starts with the determination of an optimal solution of program (P_G) associated to the smallest eigenvalue of $G, \lambda_{\min}(A_G) = -2$.

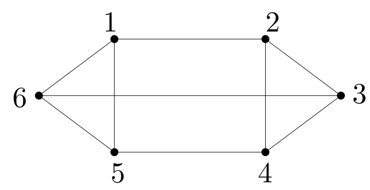


Figure 4.1: 3-regular graph G with 6 vertices.

Vector $x^* = \begin{bmatrix} 0.4 & 0.4 & 0.4 & 0.4 & 0.4 & 0.4 \end{bmatrix}^T$ is the desired optimal solution.
Note that $(H+I)\,x^* = \mathbf{j}$ and that the complementary solution associated to x^* is null.
Let $\mathcal{B} = \{b_1, b_2\}$ with

$$b_1 = \begin{bmatrix} 0.5459 & -0.5459 & 0.11 & 0.4358 & -0.4358 & -0.11 \end{bmatrix}^T,$$

$$b_2 = \begin{bmatrix} -0.1881 & 0.1881 & -0.5668 & 0.3787 & -0.3787 & 0.5668 \end{bmatrix}^T.$$

Any nonnegative vector of the form

$$x^* + \mu_1 b_1 + \mu_2 b_2 = \begin{bmatrix} 0.4 & 0.4 & 0.4 & 0.4 & 0.4 & 0.4 \end{bmatrix}^T + \mu_1 b_1 + \mu_2 b_2, \quad \mu_1, \mu_2 \in \mathbb{R}$$

is an optimal solution of (P_G).

After executing the algorithm, an optimal solution with two null components is obtained:

$$\tilde{x}^* = x^* - \frac{x_t^*}{b'_{t2}} b'_2 = \begin{bmatrix} 0 & 0.8 & 0.4 & 0 & 0.8 & 0.4 \end{bmatrix}^T.$$

Notice that the modified basis $\mathcal{B}''$ verifies the conditions of Theorem 4.2, taking into account that the entries corresponding to the null components of the obtained optimal solution correspond to the first and fourth rows of the following matrix:

$$\begin{bmatrix} \mathbf{1} & \mathbf{0} \\ -1 & 0 \\ 1 & -1 \\ \mathbf{0} & \mathbf{1} \\ 0 & -1 \\ 1 & 1 \end{bmatrix}.$$

4.2 Star sets, star complements and star solutions

The theory of star complements allows to relate the 0-1 solutions of program (P_G) with the concept of star set. Next some basic facts about such theory will be recalled (see [CDS95, pp. 136-140]).

Let μ be an eigenvalue[1] of a given graph G with n vertices and consider the eigenspace $\mathcal{E}(\mu)$ associated to μ. Let P represent the matrix of the orthogonal projection of $\mathbb{R}^n$ onto $\mathcal{E}(\mu)$ with respect to the standard orthonormal basis $\{e_1, e_2, \ldots, e_n\}$ of $\mathbb{R}^n$. The set of vectors Pe_j $(j = 1, \ldots, n)$ spans $\mathcal{E}(\mu)$ and, so, there is a set $X \subseteq V(G)$ such that the vectors Pe_j $(j \in X)$ form a basis for $\mathcal{E}(\mu)$. Such a subset X of $V(G)$ is called a *star set* for μ in G. Graph $G - X$, called the *star complement* for μ corresponding to X, is the subgraph of G induced by $\overline{X}$, the complement of X in $V(G)$. In addition, $\overline{X} = V(G) \setminus X$ is called a *μ-co-star-set*.

It should be noted that, from the definition of star set, it may be concluded that for every graph G and for every eigenvalue μ of G there is at least one star set associated to μ.

Proposition 4.4. *[CDS95] Let G be a graph with μ as an eigenvalue of multiplicity $k > 0$. The following conditions on a subset X of $V(G)$ are equivalent:*

1. *X is a star set for μ;*

2. *$\mathbb{R}^n = \mathcal{E}(\mu) \oplus V$, where $V = \langle e_i : i \notin X \rangle$;*

[1] Although the notation for eigenvalues used so far is λ, in the current chapter μ will be adopted for the eigenvalues.

3. $|X| = k$ *and* μ *is not an eigenvalue of* $G - X$.

It should be noted that the entries corresponding to the null components of the solution that Algorithm 2 outputs correspond to a star set of G, for the least eigenvalue, $\lambda_{min}(A_G)$.

Example 4.5. In Figure 4.2 below, the vertices of the graph already represented in Figure 4.1 were relabelled and now correspond to the eigenvalues of the graph in such a way that vertices labelled μ form a star set for eigenvalue μ.

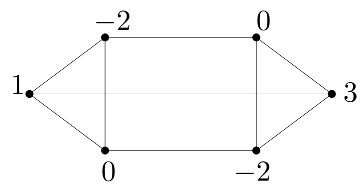


Figure 4.2: Star set partition of the graph in Figure 4.1.

For instance, -2 is an eigenvalue of multiplicity 2 and if the two vertices labelled -2 are eliminated, a graph that no longer has -2 as eigenvalue is obtained.

In the graph-theoretical context, the next result is known as the Reconstruction Theorem.

Theorem 4.6. *[CDS95] Let* X *be a set of* k *vertices in the graph* G *and supppose that* G *has adjacency matrix* $\begin{pmatrix} A_X & B^T \\ B & C \end{pmatrix}$, *where* A_X *is the adjacency matrix of the subgraph induced by* X. *Then* X *is a star set for* μ *in* G *if and only if* μ *is not an eigenvalue of* C *and*

$$\mu I - A_X = B^T(\mu I - C)^{-1}B.$$

In this situation, the eigenspace of μ *consists of the vectors*

$$\begin{pmatrix} x \\ (\mu I - C)^{-1}Bx \end{pmatrix}$$

where $x \in \mathbb{R}^k$.

Returning to problem (P_G), the following definition is introduced in [CL16]:

Definition 4.7. An optimal solution x of (P_G) is called a *star solution* for (P_G) if there is a star set X for $\lambda_{\min}(A_G)$ such that $x_i = 0$, for all $i \in X$. The star set X is said to be associated with the star solution x and vice-versa.

Based on this notion, Cardoso and Luz proved that the optimal solution of (P_G), given by the nullifying components procedure 2, is a star solution:

Theorem 4.8. *[CL16] Let G be a graph with n vertices and at least one edge. If the optimal solutions of problem (P_G) are critical points of the objective function, there is at least one star solution for (P_G).*

Example 4.9. Considering the graph in Example 4.3, if vertices 1 and 4, which correspond to the null components of the optimal solution determined by the algorithm, are removed from H, then -2 is no longer an eigenvalue of the resulting matrix. In fact, the optimal solution obtained at the end of the procedure is a star solution associated to the star set $X = \{1, 4\}$.

Theorem 4.10. *[CL16] Let G be a graph with n vertices and at least one edge. If x is a 0-1 optimal solution of (P_G) and $S = \{i \in V(G) : x_i = 1\}$, then there is a star complement for $\lambda_{\min}(A_G)$ containing the subgraph of G induced by S. Consequently, x is a star solution of (P_G).*

The next theorem introduces a necessary and sufficient condition for having convex-QP stability number that relies on the existence of a star set whose elimination does not affect the optimal value of (P_G).

Theorem 4.11. *[CL16] Let G be a graph with at least one edge. Then, $\alpha(G) = \upsilon(G)$ if and only if there is a star set X associated to the eigenvalue $\lambda_{\min}(A_G)$ such that $\upsilon(G-X) = \upsilon(G)$.*

Combining the previous result with Theorem 3.10, the following straightforward consequences are found:

Corollary 4.12. *If $\alpha(G) = \upsilon(G)$, there is a star set X associated to $\lambda_{min}(A_G)$ and $S \subseteq V(G - X)$ such that S is a maximum stable set of G. Furthermore, an optimal solution of program (P_{G-X}) is the characteristic vector of S.*

Corollary 4.13. *If $\alpha(G) = \upsilon(G)$, then*

$$|V(G)| - m(\lambda_{min}(A_G)) \geq \alpha(G).$$

Taking into account the results in this section, the following conclusion holds:

Theorem 4.14. *If G is an adverse graph, then a star solution of program (P_G) can be obtained in polynomial time.*

Unfortunately, there are adverse graphs for which not all star solutions are integer. So, given an adverse graph, the following question remains unanswered:

Considering an adverse graph G, is there a polynomial procedure to determine an integer star solution of (P_G) or to conclude that such solution does not exist?

4.3 (κ, τ)-regular sets

Most of the results included in this section were first published in the paper [CLLP16], where a simplex-like algorithm for the determination of $(0, \tau)$-regular sets was described. Recall that the problem of finding out if a graph G has convex-QP stability number and determining a maximum stable set is equivalent to the problem of finding a $(0, -\lambda_{min}(A_G))$-regular set of G.

According to Proposition 3.17, detecting a $(0, \tau)$-regular set in a graph G of order n is equivalent to search for a 0-1 solution of $(A_G + \tau I_n)\mathbf{x} = \tau\mathbf{j}$. Note that, if any solution x of this system is nonnegative, then $x \leq \mathbf{j}$. In fact, this system can be written in the form

$$\tau x_i + \sum_{k \in N_G(i)} x_k = \tau, \quad i = 1, \ldots, n;$$

thus, if $\mathbf{x} \geq 0$, we have, for all i, $\tau x_i \leq \tau$, and then $x_i \leq 1$ since $\tau > 0$. Therefore, the set of solutions of the system

$$\begin{cases} (A_G + \tau I_n)\mathbf{x} & = & \tau\mathbf{j} \\ \mathbf{x} & \geq & 0 \end{cases} \tag{4.1}$$

is included in the hypercube $[0, 1]^n$. Then, obtaining a $(0, \tau)$-regular set in G is equivalent to determining an extreme vertex of the convex polyhedron $[0, 1]^n$, satisfying the system (4.1).

The theory of star complements allows to link the 0-1 solutions of (4.1) and, more generally, its basic feasible solutions, with the star set concept. The books [PS98], [Dan63] and [NW99] convey nice overviews on the simplex method and the concept of basic feasible solution.

Next, an alternative result to the ones obtained in [CSZ10, Prop. 4.1 and Cor. 4.3] follows.

Proposition 4.15. *Let G be a graph of order n with at least one (k, τ)-regular set and denote by $\mathbf{x}^+$ the minimal least squares solution of system (3.7).*

Then a subset $S \subseteq V(G)$ is a (k, τ)-regular set in G if and only if its characteristic vector $\mathbf{x}$ is such that

$$\mathbf{x} = \mathbf{x}^+ + \mathbf{q}, \tag{4.2}$$

where $\mathbf{q} = \mathbf{0}$ if $(k - \tau) \notin \sigma(G)$ and $\mathbf{q} \in \mathcal{E}_G(k - \tau)$ otherwise. Moreover,

$$\mathbf{x}^+ = \begin{cases} (A_G - (k-\tau)I_n)^{-1}\,(\tau \mathbf{j}) & \text{if } (k-\tau) \notin \sigma(G) \\ \sum\limits_{i=1}^{n-t} \tau \dfrac{\mathbf{j}^T \mathbf{u}_i}{\lambda_i - (k-\tau)} \mathbf{u}_i & \text{if } (k-\tau) \in \sigma(G) \end{cases}, \tag{4.3}$$

where $t = \dim \mathcal{E}_G(k - \tau)$, $\lambda_1, \ldots, \lambda_{n-t}$ are the eigenvalues of A_G different from $k - \tau$ and $\mathbf{u}_1, \ldots, \mathbf{u}_{n-t}$ are corresponding mutually orthonormal eigenvectors.

Proof. First, notice that $\mathbf{x}^+$ is a solution of the system (3.7) and from Proposition 3.17 $S \subseteq V(G)$ is (k, τ)-regular if and only if its characteristic vector $\mathbf{x}$ is also a solution of the system (3.7), that is, if and only if $\exists \mathbf{q} \in \ker(A_G - (k - \tau)I_n)$ such that $\mathbf{x} = \mathbf{x}^+ + \mathbf{q}$. Saying that $\mathbf{q}$ belongs to the null space of the matrix $A_G - (k - \tau)I_n$ is equivalent to saying that $\mathbf{q}$ is an eigenvector of A_G associated to the eigenvalue $(k - \tau)$ when $(k - \tau) \in \sigma(G)$ and $\mathbf{q} = \mathbf{0}$ otherwise. Therefore, the first part of the proposition is proven.

It remains to prove that $\mathbf{x}^+ = \sum_{i=1}^{n-t} \tau \frac{\mathbf{j}^T \mathbf{u}_i}{\lambda_i - (k-\tau)} \mathbf{u}_i$ when $(k - \tau) \in \sigma(G)$. Let U_{n-t} be the matrix whose columns are the eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_{n-t}$ and let D_{n-t} be the diagonal matrix whose diagonal entries are $\lambda_i - (k - \tau)$, $i = 1, \ldots, n - t$. Since

$$A_G - (k - \tau)\, I = U_{n-t} D_{n-t} U_{n-t}^T,$$

considering the Moore-Penrose generalized inverse of $A_G - (k - \tau)\, I$ (see for instance [CM91]) which is usually denoted by $(A_G - (k-\tau)\, I)^\dagger$ it follows that

$$\begin{aligned}(A_G - (k-\tau)\, I)^\dagger &= \left(U_{n-t} D_{n-t} U_{n-t}^T\right)^\dagger \\ &= U_{n-t} D_{n-t}^{-1} U_{n-t}^T = \sum_{i=1}^{n-t} \frac{1}{\lambda_i - (k-\tau)} \mathbf{u}_i \mathbf{u}_i^T.\end{aligned}$$

Therefore, $\mathbf{x}^+ = (A_G - (k-\tau)\, I)^\dagger \;(\tau \mathbf{j}) = \sum\limits_{i=1}^{n-t} \tau \frac{\mathbf{j}^T \mathbf{u}_i}{\lambda_i - (k-\tau)} \mathbf{u}_i$, as required. □

The following corollary of Proposition 4.15 states that, if G has a (κ, τ)-regular set, its size can be determined.

Corollary 4.16. *If a graph G has a (k, τ)-regular set $S \subseteq V(G)$, then $|S| = \mathbf{j}^T \mathbf{x}^+$.*

Proof. If $S \subseteq V(G)$ is (k, τ)-regular set in G, then its characteristic vector $\mathbf{x}$ satisfies $\mathbf{x} = \mathbf{x}^+ + \mathbf{q}$. If $\mathbf{q} = \mathbf{0}$, $|S| = \mathbf{j}^T \mathbf{x} = \mathbf{j}^T \mathbf{x}^+$ and the corollary follows. Otherwise, $(A_G - (k-\tau) I_n)\, \mathbf{x} = \tau \mathbf{j}$ implies that $\mathbf{j}^T \mathbf{q} = 0$, i.e., $\mathbf{q}$ is orthogonal to the all-one vector $\mathbf{j}$. Therefore, $|S| = \mathbf{j}^T \mathbf{x} = \mathbf{j}^T \mathbf{x}^+ + \mathbf{j}^T \mathbf{q} = \mathbf{j}^T \mathbf{x}^+$. □

This corollary provides a straightforward sufficient condition for the non-existence of a (k, τ)-regular set.

Corollary 4.17. *If $\mathbf{j}^T \mathbf{x}^+$ is not a natural number, then G has no (k, τ)-regular sets.*

As a consequence of Propositions 3.17 and 4.15, we have the following result which allows the development of an algorithmic strategy for deciding whether a graph has a (κ, τ) regular set or not.

Proposition 4.18. *Let G be a graph of order n with a (κ, τ)-regular set S and let $\overline{x}$ be the minimal least squares solution of system (3.7). Considering that $\kappa - \tau$ is an eigenvalue of A_G with multiplicity t, if $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_t$ are t linearly independent associated eigenvectors, then there are t scalars δ_{i_j}, for $j = 1, \ldots, t$, such that $\delta_{i_j} \in \{-\overline{x}_{i_j}, 1 - \overline{x}_{i_j}\}$ and*

$$\mathbf{x} = \overline{x} + \sum_{j=1}^{t} \delta_{i_j} \boldsymbol{u}_j^{'} \tag{4.4}$$

is the characteristic vector of S.

Proof. Let U be a matrix whose columns are the eigenvectors $\mathbf{u}_1, \dots, \mathbf{u}_t$. Since these vectors are linearly independent, the matrix U has a subset of t rows indexed by $i_1, \dots, i_t$, defining a nonsingular $t \times t$ submatrix T of U. Then, we can replace each column of U by a linear combination of columns of U to obtain a matrix U' whose columns $\mathbf{u}_1^{'}, \dots, \mathbf{u}_t^{'}$ remain as linear independent eigenvectors of $\mathcal{E}_G(\kappa - \tau)$ and the corresponding $t \times t$ submatrix T' of U' defines the identity matrix. Therefore, considering that $\mathbf{x}$ is the characteristic of S, from system (4.2), where $\mathbf{q}$ is replaced by $\sum_{j=1}^{k} \delta_{i_j} \mathbf{u}_j^{'}$, it follows that

$$\begin{array}{rcl}
\mathbf{x}_{i_1} = \overline{x}_{i_1} + \delta_{i_1} & \Leftrightarrow & \delta_{i_1} = \mathbf{x}_{i_1} - \overline{x}_{i_1} \\
\mathbf{x}_{i_2} = \overline{x}_{i_2} + \delta_{i_2} & \Leftrightarrow & \delta_{i_2} = \mathbf{x}_{i_2} - \overline{x}_{i_2} \\
\vdots & \vdots & \vdots \\
\mathbf{x}_{i_t} = \overline{x}_{i_t} + \delta_{i_t} & \Leftrightarrow & \delta_{i_t} = \mathbf{x}_{i_t} - \overline{x}_{i_t}.
\end{array}$$

Since $\mathbf{x}_{i_j} \in \{0,1\}$, for $j = 1, \dots, t$, all possible values of δ_{i_j} can be determined. $\square$

4.4 A simplex-like algorithm to determine $(0,\tau)-$regular sets

In this section spectral results on (k,τ)-regular sets, as well as the theory of star complements will be applied, to introduce a simplex-like algorithm for detecting a $(0,\tau)$-regular set in an arbitrary graph. This approach will be applied to efficient domination in Section 4.5.1.

The simplex-like procedure for the determination of $(0,\tau)$-regular sets in a graph G when $\lambda = -\tau \in \sigma(G)$ will be described next. Note that, if $\lambda = -\tau$ is not an eigenvalue, determining the unique solution of $(A_G + \tau I_n)\mathbf{x} = \tau \mathbf{j}$ is sufficient to decide if G has a $(0,\tau)$-regular set.

From the Reconstruction Theorem 4.6, assuming that X is a star set for $\lambda = -\tau \in \sigma(G)$ in G it can be concluded that (4.1) is equivalent to the system:

$$\left\{ \begin{array}{rcl} \left[\begin{array}{cc} N & C_{\bar{X}} + \tau I_{|\bar{X}|} \end{array} \right] \mathbf{x} & = & \tau \mathbf{j}_{\bar{X}} \\ \mathbf{x} & \geq & 0 \end{array} \right. , \tag{4.5}$$

where $\mathbf{j}_{\bar{X}}$ is the all-one vector in $\mathbb{R}^{\bar{X}}$. Observe that (4.5) is a subsystem of (4.1) just formed by the equation associated to the indices in $\bar{X}$. The next result slightly generalizes Theorem

14 of [CL16].

Theorem 4.19. *Let G be a graph, $\lambda = -\tau \in \sigma(G)$ and X a star set for $\lambda = -\tau$ in G. Then, $\mathbf{x}$ is a star solution of (4.5) if and only if $\mathbf{x}$ is a basic feasible solution of this system.*

Proof. Theorem 14 of [CL16] proves the same assertion for system (4.5) when $\lambda = -\tau$ is the least eigenvalue of G. The same proof holds if any other eigenvalue $\lambda = -\tau \in \sigma(G)$ is considered. □

The last theorem ensures that every vertex subset $\bar{X}' \subset V(G)$ is a co-star set for the eigenvalue $\lambda = -\tau$ if and only if the columns of the matrix $\left[\begin{array}{cc} N & C_{\bar{X}} + \tau I_{|\bar{X}|} \end{array}\right]$ whose indices are in $\bar{X}'$ define a basic submatrix of (4.5). The next result guarantees that the search for a 0-1 solution of (4.5) can be limited to the set of its star solutions, i.e., to its basic feasible solutions, which is the same as saying that it is sufficient to search on some of the co-star sets for $\lambda = -\tau$.

Proposition 4.20. *Every 0-1 solution of the system* (4.5) *is a basic feasible solution.*

Proof. The polytope defined by (4.5) is included in the hypercube $[0, 1]^n$. Therefore, each 0-1 solution is an extreme vertex of this hypercube and thus a basic feasible solution. □

Based on the previous results, a simplex technique may be applied to system (4.5) in order to decide whether this system has or has not a 0-1 solution, i.e., for deciding if G has or has not a $(0, \tau)$-regular set.

We may start with the simplex tableau

$$\begin{array}{c|c|c} & x_N & \\ \hline x_B & \left(C_{\bar{X}'} + \tau I_{\bar{X}'}\right)^{-1} N & \tau \left(C_{\bar{X}'} + \tau I_{\bar{X}'}\right)^{-1} \mathbf{j}_{\bar{X}'} \\ \hline & & \end{array} \qquad (4.6)$$

where X' is some star set for $-\tau$ in G (which defines the indices of the nonbasic variables x_N) and $\bar{X}' = V(G) \setminus X'$ defines the indices of the basic variables x_B. It should be noted that the initial star solution (x_B, x_N) and the corresponding star set X' can be obtained by first computing a feasible solution of (4.5) and subsequently applying the nullifying procedure described in Theorem 4.2. Thus, if the right-hand side of (4.6) is nonnegative but not integer, we may apply the fractional dual algorithm for Integer Linear Programming (ILP) with Gomory cuts (described for example in [PS98] and [NW99]) until a 0-1 star solution is determined or the conclusion that such solution does not exist is obtained.

4.5 Applications

4.5.1 Efficient domination

Given a vertex v in a graph G, we say that v *dominates* all vertices in $N[v]$. A set S of vertices of G is *dominating* if every vertex of G outside S is adjacent to at least one vertex of S. The *domination number* of a graph G, denoted $\gamma(G)$, is the minimum size of a dominating set of vertices in G. A dominating set S is an *efficient dominating set* (or *independent perfect dominating set*) if each vertex of G is dominated by precisely one vertex of S or, equivalently, if the minimum length of a path between any two vertices of S is at least three. It is easy to deduce that not all graphs have an efficient dominating set: take, for instance, C_4, a cycle on four vertices.

The *efficient dominating set problem* (or simply efficient domination) is the problem of determining whether a given graph has an efficient dominating set and, if it exists, finding such a set.

In [BBS88], it was proved that $S = \{s_1, s_2, \ldots, s_k\}$ is an efficient dominating set of G if and only if $\{N[s_1], N[s_2], \ldots, N[s_k]\}$ is a partition of $V(G)$. It was also shown that, if G has an efficient dominating set then the cardinality of any efficient dominating set equals the domination number $\gamma(G)$ of G. As a consequence, all efficient dominating sets of G have the same cardinality.

An efficient dominating set of a graph G can also be defined as a set S of vertices that induces in G a regular graph of degree 0 (i.e., S is a stable set) such that every vertex of G outside S has precisely one neighbour in S, which is the same as saying that S is a $(0, 1)$-regular set.

Since an efficient dominating set can be regarded as a $(0, 1)$-regular set, efficient domination is a particular case of the general problem of determining whether a graph contains a $(0, \tau)$-regular set. Therefore, we will now consider $\tau = 1$ and apply the simplex-like approach for detecting $(0, \tau)$-regular sets (described in Section 4.4) to efficient domination.

Before proceeding to the algorithm, an upper bound for the size of an efficient dominating set using the star complement theory will be introduced.

Proposition 4.21. *Let G be a graph of order n. If G has an efficient dominating set S, then*

$$|S| \leq n - \max\{m(\lambda) : \lambda \in \sigma(G)\backslash\{0\}\}.$$

Proof. Recalling what has been said in the previous paragraphs, $|S| = \gamma(G)$. From a basic result from the theory of star complements introduced in [HHS98], any co-star set $\bar{X}$ for any eigenvalue $\lambda \neq 0$ is a dominating set for G. Since $\left|\bar{X}\right| = n - m(\lambda)$, the result follows. □

Now, applying the results of Section 4.3 to the particular case of efficient dominating sets the following proposition is obtained:

Proposition 4.22. *Let G be a graph of order n. Consider $k = 0$, $\tau = 1$ and $\mathbf{x}^+$ given by (4.3). Then:*

1. *If G has an efficient dominating set $S \subseteq V(G)$, then $|S| = \mathbf{j}^T\mathbf{x}^+$.*
2. *If $\mathbf{j}^T\mathbf{x}^+$ is not a natural number, then G has no efficient dominating set.*
3. *If $-1 \notin \sigma(G)$, G has an efficient dominating set if and only if the components of $\mathbf{x}^+$ are 0-1. Furthermore, if $\mathbf{x}^+$ is a 0-1 vector then it is the characteristic vector of the unique efficient dominating set of G.*

Proof. Proposition 4.15 and its corollaries imply facts 1, 2 and the first part of 3. To prove the last part of fact 3, assume that there are two distinct $(0, 1)$-regular sets S and S' with characteristic vectors $\mathbf{x}$ and $\mathbf{x}'$, respectively; then $\mathbf{q} = \mathbf{x} - \mathbf{x}' \in \ker(A_G + I_n)\backslash\{\mathbf{0}\}$, i.e., $-1 \in \sigma(G)$ which is a contradiction. □

Based on this proposition and taking into account Theorem 4.19 and Proposition 4.20, Algorithm 3 for the efficient domination problem follows.

Algorithm 3 EFFICIENT DOMINATION.

Require: The adjacency matrix of a graph G of order n.

Ensure: The characteristic vector of an efficient dominating set of G or the conclusion that such a vertex subset does not exists.

1: Determine the $\mathbf{x}^+$ vector given in (4.3);
2: **If** $\mathbf{j}^\mathbf{T}\mathbf{x}^+ \notin \mathbb{N}$ **then STOP** (G has no efficient dominating set) **End If**
3: **If** $-1 \notin \sigma(G)$ **then** return the output obtained from fact 3 of Proposition 4.22 and **STOP** **End If**
4: Determine a co-star set for the eigenvalue -1 and the associated simplex tableau (4.6);
5: **While** no conclusion about the existence of a 0-1 solution is obtained from the simplex tableau
6: Apply the fractional dual algorithm for ILP with Gomory cuts;
7: **End While**
8: **If** the fractional dual algorithm stopped with a 0-1 solution **then** return such solution as the characteristic vector of an efficient dominating set **else** return the conclusion that G has no efficient dominating set;
9: **End If**
10: **End**

Notice that the step 3 of Algorithm 3 ensures that it stops if $-1 \notin \sigma(G)$. It is clear that, in this case, the algorithm runs in polynomial time; otherwise, although there is no guarantee of polynomiality, Algorithm 3 is finite since the fractional dual algorithm for ILP with Gomory cuts (steps 5–7) is finite too. Since, by Proposition 4.20, all 0-1 solutions are basic, the correctness of the output produced by the algorithm in step 8 can be asserted.

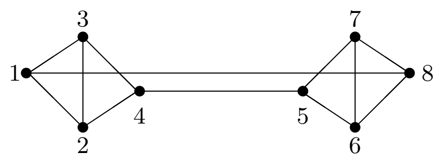


Figure 4.3: Graph G with $\sigma(G) = \{3, \sqrt{5}, 1, -1, -\sqrt{5}\}$, where $m(-1) = 4$.

Example 4.23. Algorithm 3 will now be applied to the graph G depicted in the Figure 4.3, in order to decide if G has or does not have a $(0,1)$-regular set.

Since the graph G is 3-regular, it is immediate that $\mathbf{x}^+ = \frac{1}{4}\mathbf{j}_8$, where $\mathbf{j}_8$ denotes an all-one vector with eight entries.

Since $\mathbf{j}^T\mathbf{x}^+ = 2 \in \mathbb{N}$, we proceed to the next step.

Since $m(-1) = 4$, we proceed to the next step.

Since the vertex subset $\bar{X} = \{4,5,7,8\}$ is a co-star set for the eigenvalue -1, then the matrix $\left[\begin{array}{cc} N & C_{\bar{X}} + \tau I_{|\bar{X}|} \end{array}\right]$ associated to this co-star set takes the form

$$\begin{array}{c} \\ \mathbf{4} \\ \mathbf{5} \\ \mathbf{7} \\ \mathbf{8} \end{array} \begin{array}{c} \begin{array}{cccccccc} 1 & 2 & 3 & 6 & \mathbf{4} & \mathbf{5} & \mathbf{7} & \mathbf{8} \end{array} \\ \begin{pmatrix} 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 \end{pmatrix} \end{array},$$

and the corresponding simplex tableau (4.6) is

$$\begin{array}{c|cccc|c} & x_1 & x_2 & x_3 & x_6 & \\ \hline x_4 & 1 & 1 & 1 & 0 & 1 \\ x_5 & -1 & 0 & 0 & 0 & 0 \\ x_7 & 0 & -1 & -1 & 1 & 0 \\ x_8 & 1 & 1 & 1 & 0 & 1 \\ \hline \end{array}\ .$$

The obtained solution is feasible and 0-1.

Therefore, $S = \{4,8\}$ is an efficient dominating set for G.

Notice that there are other efficient dominating sets that can be obtained from the above simplex tableau by pivoting operations.

Although this particular algorithm can be used to find an efficient dominating set in any given graph or to conclude that such a set doesn't exist, it is not polynomial in general. However, if -1 is not an eigenvalue of the adjacency matrix of the graph, it works in polynomial time.

Algorithm 3 has been tested on two classes of randomly generated graphs, namely a family of bipartite graphs and a set of graphs with eigenvalue -1 containing at least two efficient dominating sets. Notice that, for graphs without eigenvalue -1, the efficient domination problem is easily solved by Algorithm 3. For the sake of the fluency of this thesis, the results that were obtained in the performed computational experiments are included in Appendix A.2.

4.5.2 Recognition of graphs with perfect matchings

This section will rely on the notation introduced in Section 1.2 of the paper [CSZ10] that will be herein recalled and is, as has been mentioned in the beginning of this section, equivalent to the minimimal least squares notation, used so far in this section.

If G has p distinct main eigenvalues, the $n \times p$ walk matrix

$$W = W_p = (\mathbf{j}, A_G\mathbf{j}, A_G^2\mathbf{j}, \ldots, A_G^{p-1}\mathbf{j})$$

is referred to as the *walk matrix* of G.

Recalling the notation for the main characteristic polynomial and taking into account that

$$m_G(A_G) = 0 \Leftrightarrow A_G^p\mathbf{j} - c_0A_G^{p-1}\mathbf{j} - c_1A_G^{p-2}\mathbf{j} - \cdots - c_{p-2}A_G\mathbf{j} - c_{p-1}\mathbf{j} = 0,$$

the following result holds.

Theorem 4.24. *[CSZ10] If G has p main distinct eigenvalues, then*

$$W \begin{pmatrix} c_{p-1} \\ \vdots \\ c_1 \\ c_0 \end{pmatrix} = A^p\mathbf{j},$$

where c_j, with $0 \leq j \leq p-1$, are the coefficients of the main characteristic polynomial of G.

It follows from this theorem that the coefficients of the main characteristic polynomial of a graph can be determined solving the linear system

$$Wx = A^p\mathbf{j}.$$

The (κ,τ)-parametric vector $g_G(\kappa,\tau)$, defined below is equivalent to the the projection vector, x^+, corresponding to the minimal least squares solution of system (3.7) (see A.1).

$$\mathbf{g}_G(\kappa,\tau) = \sum_{j=0}^{p-1} \alpha_j A_G^j \mathbf{j},$$

where p is the number of distinct main eigenvalues of G and $\alpha_0,\ldots,\alpha_{p-1}$ is a solution of the linear system:

$$\begin{pmatrix} \kappa-\tau & 0 & \ldots & 0 & -c_{p-1} \\ -1 & \kappa-\tau & \ldots & 0 & -c_{p-2} \\ 0 & -1 & \ldots & 0 & -c_{p-3} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & -1 & \kappa-\tau-c_0 \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_{p-2} \\ \alpha_{p-1} \end{pmatrix} = -\tau \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}. \tag{4.7}$$

The following theorem is a slight variation of a result proven in [CSZ10].

Theorem 4.25. *[CSZ10] Let G be a graph with p distinct main eigenvalues $\mu_1,\ldots,\mu_p$. A vertex subset $S\subset V(G)$ is (κ,τ)-regular if and only if its characteristic vector $x(S)$ is such that*

$$x(S) = \boldsymbol{g} + \boldsymbol{q},$$

with

$$\boldsymbol{g} = \sum_{j=0}^{p-1} \alpha_j A^j \mathbf{j},$$

$(\alpha_0,\ldots,\alpha_{p-1})$ is the unique solution of the linear system (4.7) and if $(\kappa-\tau)\notin\sigma(G)$ then $\boldsymbol{q}=0$ else $\boldsymbol{q}\in\mathcal{E}_G(\kappa-\tau)$ and $\kappa-\tau$ is non-main.

Theorem 4.26. *If a graph G has a $(0,2)$-regular set S, then $|S| = \mathbf{j}^T\mathbf{g}_G(0,2)$.*

Proof. Supposing that $S\subset V(G)$ is a $(0,2)$-regular set, according to Theorem 4.1 in [CSZ10], its characteristic vector x_S verifies

$$x_S = \mathbf{g}_G(0,2) + \mathbf{q}.$$

Therefore,

$$|S| = \mathbf{j}^T x_S = \mathbf{j}^T\mathbf{g}_G(0,2) + \mathbf{j}^T\mathbf{q}.$$

Since $\mathbf{q} = 0$ or $\mathbf{q} \in \mathcal{E}_G(0-2)$ with -2 non-main, the conclusion follows.

$\square$

The following corollary provides a condition to decide when there are no $(0,2)$-regular sets in G.

Corollary 4.27. *If $\mathbf{j}^T \mathbf{g}_G(0,2)$ is not a natural number, then G has no $(0,2)$-regular set.*

Now let us consider the particular case of graphs where $m(-2) = 0$.

Theorem 4.28. *If G is a graph such that $m(-2) = 0$, then G has a $(0,2)$-regular set if and only if $\boldsymbol{g}_G(0,2) \in \{0,1\}^n$.*

Proof. According to Theorem 4.1 in [CSZ10], since -2 is not an eigenvalue of G, there is a $(0,2)$-regular set $S \subset V(G)$ if and only if $x_S = \mathbf{g}_G(0,2)$.

$\square$

It should be noticed that, according to Theorem 7 in [Car01], a graph G which is not a star neither a triangle has a perfect matching if and only if its line graph has a $(0,2)$-regular set. Therefore, Corollary 4.27 and Theorem 4.28 can be applied to the recognition of graphs with perfect matchings.

Example 4.29. Consider graphs G and $L(G)$ both depicted in Figure 4.4.

Figure 4.4: Graph G and its line graph $L(G)$.

Since -2 is not an eigenvalue of $L(G)$, the parametric vector $\mathbf{g}_{L(G)}(0,2)$ will be determined in order to find out if its coordinates are 0-1.

$L(G)$ has two main eigenvalues and its walk matrix is

$$W = \begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 2 \\ 1 & 1 \end{pmatrix}.$$

The coefficients of the main characteristic polynomial of $L(G)$, that are the solutions of system $Wx = A^2_{L(G)}\mathbf{j}$, are $c_0 = c_1 = 1$. The coefficients of $\mathbf{g}_{L(G)}(0,2)$, are $\alpha_0 = \frac{6}{5}$ and $\alpha_1 = -\frac{2}{5}$ (see [CSZ10] for details) Therefore,

$$\mathbf{g}_{L(G)}(0,2) = \alpha_0\mathbf{j} + \alpha_1 A_{L(G)}\mathbf{j} = \begin{pmatrix} 0.8 & 0.4 & 0.4 & 0.8 \end{pmatrix}^T.$$

It can be concluded that the graph $L(G)$ has no $(0,2)$-regular sets and, hence, the graph G does not have any perfect matching.

As a direct consequence of Theorem 3.5 in [Doo73], the multiplicity of the eigenvalue -2 of a graph G can be obtained as

$$m(-2) = \begin{cases} m - n & \\ m - n + 1 & \text{if } G \text{ is bipartite} \end{cases}$$

and a combination of this result with Theorem 4.28 provides an efficient technique to detect the existence of perfect matchings in graphs of certain families, namely trees and unicyclic graphs[2], where $m(-2) = 0$.

[2] A unicyclic graph is a connected graph with exactly one cycle [Har69].

Example 4.30. Consider graphs G and $L(G)$ both depicted in Figure 4.5.

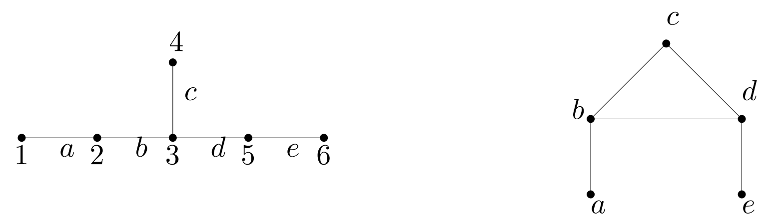


Figure 4.5: Tree G and its line graph $L(G)$.

In order to determine $g_{L(G)}(0,2)$, some calculations are required. Since

$$rank\,(\mathbf{j}) = 1$$

$$rank\,\begin{pmatrix}\mathbf{j} & A_{L(G)}\mathbf{j}\end{pmatrix} = 2$$

$$rank\,\begin{pmatrix}\mathbf{j} & A_{L(G)}\mathbf{j} & (A_{L(G)})^2\mathbf{j}\end{pmatrix} = 3$$

$$rank\,\begin{pmatrix}\mathbf{j} & A_{L(G)}\mathbf{j} & (A_{L(G)})^2\mathbf{j} & (A_{L(G)})^3\mathbf{j}\end{pmatrix} = 3,$$

$L(G)$ has 3 distinct main eigenvalues and

$$W = \begin{pmatrix}\mathbf{j} & A_{L(G)}\mathbf{j} & (A_{L(G)})^2\mathbf{j}\end{pmatrix} = \begin{pmatrix} 1 & 1 & 3 \\ 1 & 3 & 6 \\ 1 & 2 & 6 \\ 1 & 3 & 6 \\ 1 & 1 & 3 \end{pmatrix}.$$

The coefficients of the main characteristic polynomial of $A_{L(G)}$ are the solutions of the system $Wx = (A_{L(G)})^3\mathbf{j}$, $c_0 = 1, c_1 = 3$ and $c_2 = 0$. The coefficients of $\mathbf{g}_{L(G)}(0,2)$, are $\alpha_0 = 1, \alpha_1 = -1$ and $\alpha_2 = \frac{1}{3}$([CSZ10]). Therefore,

$$\mathbf{g}_{L(G)}(0,2) = \alpha_0\mathbf{j} + \alpha_1 A_{L(G)}\mathbf{j} + \alpha_2 (A_{L(G)})^2\mathbf{j} = \begin{pmatrix} 1 & 0 & 1 & 0 & 1 \end{pmatrix}^T$$

is the characteristic vector of a $(0,2)$-regular set of $L(G)$ that corresponds to the perfect matching $\{a, c, e\}$.

Example 4.31. The following calculations concern the unicyclic graph G depicted in Figure 4.6.

Figure 4.6: Unicyclic graph G and its line graph $L(G)$.

The line graph of the unicyclic graph G of Figure 4.6 has $p = 3$ distinct main eigenvalues and its walk matrix is

$$W = \begin{pmatrix} \mathbf{j} & A_{L(G)}\mathbf{j} & (A_{L(G)})^2\mathbf{j} \end{pmatrix} = \begin{pmatrix} 1 & 2 & 8 \\ 1 & 4 & 12 \\ 1 & 4 & 12 \\ 1 & 3 & 11 \\ 1 & 3 & 11 \end{pmatrix}.$$

The solution of $Wx = (A_{L(G)})^3\mathbf{j}$ is $c_0 = 2, c_1 = 5, c_2 = -2$ and the coefficients α_i in $g_{L(G)}(0,2) = \sum_{i=0}^{p-1} \alpha_i (A_{L(G)})^i \mathbf{j}$ are $\alpha_0 = \frac{3}{2}, \alpha_1 = -2, \alpha_2 = \frac{1}{2}$. Therefore,

$$g_{L(G)}(0,2) = \begin{pmatrix} 1.5 & \text{-0.5} & \text{-0.5} & 1 & 1 \end{pmatrix}^T$$

and the conclusion that G does not have a perfect matching follows.

4.5.3 Recognition of Hamiltonian graphs

Recall that a graph $G = (V, E)$ is Hamiltonian if it has a cycle containing all vertices. Such a cycle is called a Hamiltonian cycle.

Example 4.32. The following graph is Hamiltonian:

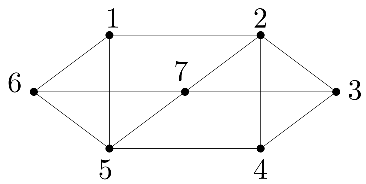


Figure 4.7: Hamiltonian graph G.

$\{\{16\}, \{67\}, \{72\}, \{23\}, \{34\}, \{45\}, \{51\}\}$ is a Hamiltonian cycle of G.

The determination of Hamiltonian cycles in arbitrary graphs is a NP-complete problem: no computationally efficient necessary and sufficient conditions for a general graph to be Hamiltonian are known. Many results on the subject have been obtained but almost all of them are effective either only for graphs of certain families or they provide conditions that are sufficient but not necessary (see [CSR08], [Har69]).

The very well known theorems by Dirac and Ore give sufficient conditions for a graph to be Hamiltonian and are recalled below.

Theorem 4.33. *[Dir52] A graph G of order $n \geq 3$ in which all vertices have degree $\geq \frac{n}{2}$ is Hamiltonian.*

Theorem 4.34. *[Ore60] If the sum of the degrees of each pair of nonadjacent vertices of a graph G with order n is $\geq n$, then G is Hamiltonian.*

The strategy described in this chapter to decide whether a graph is Hamiltonian is built upon the following characterization of line graphs of Hamiltonian graphs, using (κ, τ)-regular sets:

Theorem 4.35. *[ACS13] A graph G which is not a cycle is Hamiltonian if and only if its line graph $L(G)$ has a $(2, 4)$-regular set S inducing a connected subgraph of $L(G)$.*

Considering the previous theorem, the problem to be solved in order to determine if a given graph is Hamiltonian is the determination of a $(2,4)$-regular set inducing a connected subgraph of $L(G)$, given by the the solution of the linear programming program with bounded variables:

$$\min \left\{ \mathbf{j}'x : (A_{L(G)} + 2I_n)x = 4\mathbf{j}, 0 \leq x \leq \mathbf{j} \right\} \tag{4.8}$$

where G is a graph with n edges.

The application of the known results to the determination of Hamiltonian cycles was initially tested for line graphs of a family of graphs that were previously known to be Hamiltonian. The graphs of such family were obtained in the following way: for $6 \leq n \leq 100$, the cycle C_n was generated and aditional edges were randomly added to it, creating a new Hamiltonian graph. At least one integer feasible solution of (4.8) - corresponding to a $(2,4)$-regular set of $L(G)$ that induced a connected subgraph - was obtained for all instances. In order to test the connectivity of the subgraph of $L(G)$, G', induced by the $(2,4)$-regular set, the Laplacian matrix of G' was determined and the following result was applied:

Theorem 4.36. *[Fie73] The second smallest eigenvalue of the Laplacian matrix of a graph G is positive if and only if G is connected.*

Fiedler [Fie73] called the second smallest eigenvalue of the Laplacian matrix of a graph G, the *algebraic connectivity* of G and this is a good parameter to measure, to a certain extent, how well a graph is connected.

After determining a $(2,4)$-regular set in the line graph of a graph G, the positivity of the algebraic connectivity of the obtained induced subgraph is tested. If the algebraic connectivity is greater than zero, the initial graph is Hamiltonian and the question is answered; in the case where the algebraic connectivity is equal to zero, no conclusion can be made: the $(2,4)$-regular set that has been determined does not correspond to a Hamiltonian cycle of G but there may be another $(2,4)$-regular set inducing a connected subgraph of $L(G)$ and thus allowing the conclusion that the graph is Hamiltonian to be reached.

Algorithm 4 Detection of Hamiltonian graphs.

Require: A graph G of order n.

Ensure: The conclusion that G is/is not Hamiltonian.

Determine the line graph of G, $L(G)$;
Check if $L(G)$ has a $(2,4)$-regular set $S \subset V(L(G))$;
  If $\exists S \subset V(L(G))$ which is $(2,4)$-regular **then** determine the subgraph G' induced by S and its algebraic connectivity μ_{n-1};
    If $\mu_{n-1} > 0$ **then STOP** (G is Hamiltonian) **else STOP** (the algorithm is inconclusive);
    End If
  else
    STOP (G is not Hamiltonian);
  End If
End

The hard part of the described procedure is, of course, the determination of an adequate $(2,4)$-regular set; that is where the difficulty of the problem relies, making this recognition process not polynomial in general. In spite of this limitation - the complexity of the problem under consideration should be kept in mind - the strategy herein described and formalized in Algorithm 4 allows the identification of many Hamiltonian graphs that would not have been detected otherwise.

The procedure will now be clarified with a few examples.

Example 4.37. The line graph of the 3-cube[3] in Figure 4.8, $L(Q_3)$, has 12 vertices and $S = \{1,3,5,6,7,8,10,11\}$ as a $(2,4)$-regular set. The Laplacian matrix of the sugbraph of

[3] Recall that the hypercube Q_n is the graph whose 2^n vertices are the vectors with coordinates in $\{0,1\}^n$ where two vertices are connected if they differ in exactly one coordinate.

$L(Q_3)$ induced by S is

$$L = \begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & 0 & 0 & 0 & 0 & -1 & 0 \\ -1 & 0 & 2 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 2 & -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 2 & 0 & -1 \\ 0 & -1 & 0 & 0 & -1 & 0 & 2 & 0 \\ 0 & 0 & -1 & 0 & 0 & -1 & 0 & 2 \end{pmatrix}.$$

The eigenvalues of L are $\{0, 0.5858, 0.5858, 2, 2, 3.4142, 3.4142, 4\}$; therefore its algebraic connectivity is positive and the subgraph of $L(Q_3)$ induced by S is connected. The conclusion that the graph Q_3 is Hamiltonian then follows.

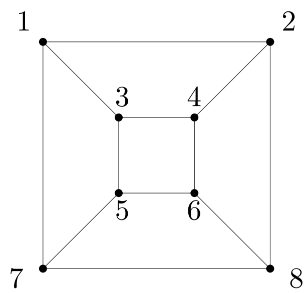


Figure 4.8: The 3-cube Q_3.

Example 4.38. In the case of Q_4, the cube with 16 vertices, the procedure is inconclusive: $S = \{1, 2, 5, 9, 11, 13, 14, 16, 22, 23, 24, 25, 27, 28, 30, 31\}$ is the $(2, 4)$-regular set of $L(Q_4)$ corresponding to the 0-1 solution determined when (4.8) is solved. S induces a subgraph whose Laplacian matrix has algebraic connectivity equal to zero. As mentioned before, the only assertion that can be derived is that the obtained $(2, 4)$-regular set does not induce a connected subgraph of $L(Q_4)$ but another unidentified $(2, 4)$-regular set inducing a connected subgraph may exist in $L(Q_4)$.

Example 4.39. A graph G is *hypohamiltonian* if G is not Hamiltonian, but $G - v$ is Hamiltonian for every $v \in V(G)$ (see [BM76]). The Petersen graph, P, well known to be nonhamiltonian, is the smallest hypohamiltonian graph.

In order to verify that P is hypohamiltonian, Algorithm 4 was executed with $P - v_i, i = 1, ..., 10$ as input. The obtained results are summarized in the table below, where a denotes the algebraic connectivity of the Laplacian matrix of the subgraph of $L(G)$ induced by each $(2, 4)$-regular set S.

i (deleted vertex)	$\lvert L(G)\rvert$	$(2, 4)$-regular set of $L(G)$	a	Hamiltonian
1	12	$\{1, 2, 4, 5, 6, 7, 8, 9, 11\}$	0.4679	Yes
2	12	$\{1, 2, 3, 4, 5, 9, 10, 11, 12\}$	0.4679	Yes
3	12	$\{1, 2, 4, 5, 6, 8, 9, 11, 12\}$	0.4679	Yes
4	12	$\{1, 2, 4, 6, 7, 8, 9, 10, 11\}$	0.4679	Yes
5	12	$\{1, 2, 4, 5, 6, 7, 9, 11, 12\}$	0.4679	Yes
6	12	$\{1, 2, 3, 6, 7, 8, 10, 11, 12\}$	0.4679	Yes
7	12	$\{1, 2, 4, 5, 8, 9, 10, 11, 12\}$	0.4679	Yes
8	12	$\{1, 3, 4, 6, 7, 9, 10, 11, 12\}$	0.4679	Yes
9	12	$\{1, 3, 5, 6, 7, 8, 9, 10, 11\}$	0.4679	Yes
10	12	$\{2, 3, 4, 5, 7, 8, 9, 10, 12\}$	0.4679	Yes

Table 4.1: The Petersen graph is hypohamiltonian.

4.5.3.1 A characterization of line graphs of Hamiltonian graphs by star complements

In a 1999 paper, Bell introduces a characterization of line graphs of Hamiltonian graphs with an odd number of vertices [Bel99, Corollary 2.5]. Such characterization depends on the existence of the cycle C_t in the set of the star complements for the eigenvalue -2.

Theorem 4.40. *[Bel99] Let t be an odd integer ≥ 3. A graph G is the line graph of a t-vertex Hamiltonian graph if and only if either $G = C_t$ or has C_t as a star complement for -2.*

A numerical example will now illustrate this strategy.

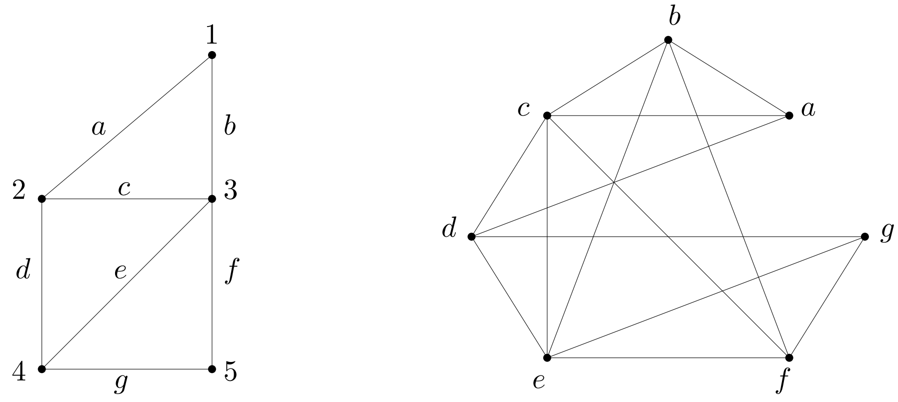


Figure 4.9: Graph H with an odd number of vertices and its line graph G.

Example 4.41. Since G is obviously not the cycle C_5, the set of all star complements for -2, $H_1, ..., H_7$, is determined, calculating all basic feasible solutions of the system (P_G), with $\lambda_{min}(A_G) = -2$:

$$V(H_1) = X_1 = \{a, d, e, f, g\}$$

$$V(H_2) = X_2 = \{a, c, e, f, g\}$$

$$V(H_3) = X_3 = \{a, b, e, f, g\}$$

$$V(H_4) = X_4 = \{a, b, d, f, g\}$$

$$V(H_5) = X_5 = \{a, b, c, f, g\}$$

$$V(H_6) = X_6 = \{a, b, c, e, g\}$$

$$V(H_7) = X_7 = \{a, b, c, d, g\}.$$

It is straightforward that $X_4 = \{a, b, d, f, g\}$ coincides with C_5 and the conclusion that the root graph H is Hamiltonian follows.

4.6 An algorithmic approach

As a consequence of the previous results, we have the following theorem which allows the development of an algorithmic strategy for deciding whether a graph has or not a (κ, τ) regular set.

Theorem 4.42. *Let G be a graph with a (κ,τ)-regular set $S \subset V(G)$ and let $\overline{\mathbf{x}}$ be a particular solution of the linear system (3.7). Assuming that $\kappa-\tau$ is an eigenvalue of G with multiplicity t, then the characteristic vector of S, $\mathbf{x}$, is determined by the equality*

$$\mathbf{x} = \overline{\mathbf{x}} + \sum_{j=1}^{t} \delta_{i_j} \hat{\mathbf{v}}_j, \tag{4.9}$$

where $\delta_{i_j} \in \{-\overline{\mathbf{x}}_{i_j}, 1-\overline{\mathbf{x}}_{i_j}\}$, for $j=1,\ldots,t$, and the vectors $\hat{v}_1,\ldots,\hat{v}_t \in \mathcal{E}_G(\kappa-\tau)$ are such that the matrix V whose columns are $\hat{\mathbf{v}}_1,\ldots,\hat{\mathbf{v}}_t$ has a $t\times t$ identity submatrix defined by the t rows of V with indices in $I=\{i_1,i_2,\ldots,i_t\} \subset V(G)$.

Proof. Let U be a matrix whose columns are t linear independent eigenvectors, $\hat{\mathbf{u}}_1,\ldots,\hat{\mathbf{u}}_t$, associated to the eigenvalue $\kappa-\tau$. Since these vectors are linearly independent, the matrix U has a subset of t rows indexed by $i_1,\ldots,i_t$, defining a nonsingular $t\times t$ submatrix T. Then, we can replace each column of U by a linear combination of columns of U to obtain a matrix V whose columns $\hat{\mathbf{v}}_1,\ldots,\hat{\mathbf{v}}_t$ remain as linearly independent eigenvectors associated to $\kappa-\tau$ and the corresponding $t\times t$ submatrix T' of V defines the identity matrix of order t. Therefore, considering that $\mathbf{x}$ is the characteristic vector of S, from the linear system (3.7), where $\mathbf{u}$ is replaced by $\sum_{j=1}^{t} \delta_{i_j}\mathbf{v}_j$, it follows

$$\begin{array}{rcl} \mathbf{x}_{i_1} = \overline{\mathbf{x}}_{i_1} + \delta_{i_1} & \Leftrightarrow & \delta_{i_1} = \mathbf{x}_{i_1} - \overline{\mathbf{x}}_{i_1} \\ \mathbf{x}_{i_2} = \overline{\mathbf{x}}_{i_2} + \delta_{i_2} & \Leftrightarrow & \delta_{i_2} = \mathbf{x}_{i_2} - \overline{\mathbf{x}}_{i_2} \\ \vdots \qquad \vdots & \vdots & \vdots \\ \mathbf{x}_{i_t} = \overline{\mathbf{x}}_{i_t} + \delta_{i_t} & \Leftrightarrow & \delta_{i_t} = \mathbf{x}_{i_t} - \overline{\mathbf{x}}_{i_t}. \end{array}$$

Since $\mathbf{x}_{i_j} \in \{0,1\}$, for $j=1,\ldots,t$, the result follows. $\square$

As immediate consequence of Theorem 4.42, Algorithm 5 decides in a finite number of steps if a graph G, having an eigenvalue $\lambda = \kappa - \tau$ with multiplicity t, has or not a (κ,τ)-regular set, determining such vertex subset when there exists.

Algorithm 5 Recognizes whether a graph G has a (κ,τ)-regular set and determines it when it exists.

Require: $\mathbf{A}_G$, κ, τ, t and the $n \times t$ matrix U whose columns are linearly independent vectors of $\mathcal{E}_G(\kappa-\tau)$.

Ensure: a (κ,τ)-regular set S or the conclusion that it does not exist.

COMPUTE a particular solution $\overline{\mathbf{x}}$ of the linear system (3.7).

SET $\mathbf{x} := \overline{\mathbf{x}}$.

DETERMINE the matrix V, with columns $\hat{\mathbf{v}}_1, \ldots, \hat{\mathbf{v}}_t$, obtained from U as in the proof of Theorem 4.42 and the index subset $I = \{i_1, \ldots i_t\} \subset \{1, \ldots, n\}$.

SET $\Lambda := \{(\delta_{i_1}, \ldots, \delta_{i_t}) : \delta_{i_j} \in \{-\overline{\mathbf{x}}_{i_j}, 1 - \overline{\mathbf{x}}_{i_j}\}, i_j \in I\}$.

WHILE $\mathbf{x}$ is not $0-1$ and $\Lambda \neq \emptyset$

  CHOOSE $(\delta_{i_1}, \ldots, \delta_{i_t}) \in \Lambda$ and **SET** $\Lambda := \Lambda \setminus \{(\delta_{i_1}, \ldots, \delta_{i_t})\}$.

  IF $\overline{\mathbf{x}} + \sum_{j=1}^{t} \delta_{i_j} \hat{\mathbf{v}}_j$ is a $0-1$ vector **THEN SET** $\mathbf{x} := \overline{\mathbf{x}} + \sum_{j=1}^{t} \delta_{i_j} \hat{\mathbf{v}}_j$.

  END If

END WHILE

IF $\mathbf{x}$ is $0-1$ **THEN** return $\mathbf{x}$ as the characteristic vector of S.

  ELSE G has no (κ,τ)-regular sets.

END IF

Notice that in Algorithm 5, despite the set of possible tuples $(\delta_{i_1}, \delta_{i_2}, \ldots, \delta_{i_t})$ being finite, its cardinality is the exponential number 2^t. Therefore, when the multiplicity t of the eigenvalue $\kappa - \tau$ is larger, the determination of a tuple of scalars $(\delta_{i_1}, \delta_{i_2}, \ldots, \delta_{i_t})$ producing a $0-1$ solution in (4.9) or the recognition that it does not exist, can be not computationally effective by checking all possible tuples.

Example 4.43. Let us consider the graph G and its line graph H of Figure 4.9 which has

$-2 \in \sigma(H)$ with multiplicity 2, for which

$$U = \begin{array}{c} a \\ b \\ c \\ d \\ e \\ f \end{array} \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ -1 & 0 \\ \mathbf{0} & \mathbf{1} \\ 1 & 0 \\ 0 & -1 \\ 0 & 1 \end{pmatrix}$$

is a matrix whose columns are linearly independent eigenvectors from $\mathcal{E}_G(-2)$. As in the proof of Theorem 4.42, we can consider $V = U$, $i_1 = a$ and $i_2 = c$. On the other hand,

$$\overline{\mathbf{x}} = \begin{array}{c} a \\ b \\ c \\ d \\ e \\ f \end{array} \begin{pmatrix} 6/5 \\ 4/5 \\ 1/5 \\ 3/5 \\ 1/5 \\ 6/5 \end{pmatrix}.$$

is a particular solution of the linear system (3.7). Therefore, $\delta_a \in \{-\frac{6}{5}, 1 - \frac{6}{5}\}$ and $\delta_c \in \{-\frac{1}{5}, 1 - \frac{1}{5}\}$.

The next table summarizes, according to (4.9), the possible results obtained for $\overline{\mathbf{x}} + \delta_a \mathbf{u}_1 + \delta_c \mathbf{u}_2$, where $\mathbf{u}_j$, for $j = 1, 2$, are the columns of U (which is equal to V in this particular case).

δ_a δ_c	-6/5 -1/5	-6/5 4/5	-1/5 -1/5	-1/5 4/5
$(\overline{\mathbf{x}} + \delta_a \mathbf{u}_1 + \delta_c \mathbf{u}_2)_a$	0	0	**1**	1
$(\overline{\mathbf{x}} + \delta_a \mathbf{u}_1 + \delta_c \mathbf{u}_2)_b$	2	2	**1**	1
$(\overline{\mathbf{x}} + \delta_a \mathbf{u}_1 + \delta_c \mathbf{u}_2)_c$	0	1	**0**	1
$(\overline{\mathbf{x}} + \delta_a \mathbf{u}_1 + \delta_c \mathbf{u}_2)_d$	2	1	**1**	0
$(\overline{\mathbf{x}} + \delta_a \mathbf{u}_1 + \delta_c \mathbf{u}_2)_e$	-1	-1	**0**	0
$(\overline{\mathbf{x}} + \delta_a \mathbf{u}_1 + \delta_c \mathbf{u}_2)_f$	1	0	**1**	0
$(\overline{\mathbf{x}} + \delta_a \mathbf{u}_1 + \delta_c \mathbf{u}_2)_g$	1	2	**1**	2

Therefore, $\mathbf{x} = (1, 1, 0, 1, 0, 1, 1)^T$ is the characteristic vector of the unique $(2, 4)$-regular set in the line graph H. Since this $(2, 4)$-regular set induces a connected graph we may conclude that the corresponding edges form a Hamiltonian cycle.

Chapter 5

Conclusions and future work

In this thesis, necessary and sufficient conditions for the recognition of graphs with convex quadratic stability number that simultaneously provide maximum stable sets were established. Such conditions led to new recognition algorithms that were applied to several well known problems such as efficient domination and the determination of graphs with perfect matchings and Hamiltonian cycles.

In an initial phase of this project, a survey was made on the research about graphs with convex-QP stability number [Luz95] and adverse graphs [Car03] that had previously been published. Special attention was devoted to the results proved in [Car01] and [Car03] and other new ones were established. Based on those results, a recognition algorithm that also determined a maximum stable set was introduced and implemented. It was observed that the algorithm ran in polynomial time except when in the presence of adverse conditions - a graph is adverse if it is a non complete graph, without isolated vertices, such that the least eigenvalue of its adjacency matrix and the optimal value of (P_G) were both integer and none of them changed when the neighbourhood of any vertex was deleted - and families of graphs for which the algorithm is polynomial were also identified. At this point, the recognition problem was solved except when the graph was adverse and the question that kept unanswered was *do all adverse graphs have convex quadratic stability number?* Looking for evidence of the trueness or falseness of the conjecture *every adverse graphs has convex-QP stability number*, new results were established.

In the following stage, the research was directed to the attempt to prove the conjecture using the concepts of star complement, star set and star solution, in a new approach involving the introduction of a new necessary and sufficient condition for a graph to have a convex quadratic stability number related to the effect on the optimal value of (P_G) of the removal of the vertices of a star set. Motivated by the results in the papers [CSZ10] and [CL16], the research addressed the determination of (κ, τ)-regular sets. New conditions were introduced and a simplex-like algorithm for the determination of $(0, \tau)$-regular sets, relying on spectral properties and star complements, was introduced. Taking into account that a $(0, 1)$-regular set can be regarded as an efficient dominating set, the algorithm was applied to the determination of efficient dominating sets. The application of the algorithm to the determination of graphs with perfect matchings was also the object of special attention. The subsequent step of the research was devoted to a new procedure for the determination of Hamiltonian graphs, that applied a result introduced in [ACS13] and imposed restrictions on the algebraic connectivity of the line graph. The final stage of the research reported in this Ph.D. thesis consists of a new algorithmic strategy for the determination of (κ, τ)-regular sets.

This thesis was organized according to the chronological stages in which the results and algorithms were obtained. As mentioned previously, the main purpose of this research was the achievement of recognition algorithms for Q-graphs. The attempts that have been carried out in order to prove the conjecture *every adverse graph has convex-QP stability number* or to find a counterexample, conducted the research through somehow unexpected paths and new applications. Despite all efforts, the prove of the conjecture remains an open problem. An approach that relies on a combinatorial version of the simplex method is currently being explored but, due to the initial stage it is still at, no reference to it is made in this text.

Appendix A

A.1 Equivalence between Proposition 4.15 of Section 4.3 and Propositions 4.1 and 4.3 of [CSZ10]

In this appendix, the equivalence between Proposition 4.15 of Section 4.3 and the statements of Proposition 4.1 and Corollary 4.3 of [CSZ10] is proved. To make it possible, some more notation and terminology will be introduced.

In [CSZ10], the so called (k, τ)-parametric vector $\mathbf{g}$ was defined. If $(k - \tau) \in \sigma(G)$, this vector was characterized in Proposition 4.1 of [CSZ10] as follows:

$$\mathbf{g} = \sum_{i=1}^{p} \tau \frac{\mathbf{j}^T \mathbf{x}_i}{\mu_i - (k - \tau)} \mathbf{x}_i.$$

Here, $\mu_1, \ldots, \mu_p$ are the distinct main eigenvalues of G and $\{\mathbf{x}_1, \ldots, \mathbf{x}_p\}$ an orthonormal basis of the so called $\mathrm{Main}(G)$ which is the space spanned by the eigenvectors $\mathbf{v}_1, \ldots, \mathbf{v}_p$, such that $\mathbf{v}_i \in \mathcal{E}_G(\mu_i)$ and $\mathbf{v}_i^T \mathbf{j} \neq 0$ for each $i = 1, \ldots, p$.

It should be noted that, in view of Proposition 4.15, to assert that this statement and the statements of Proposition 4.1 and Corollary 4.3 of [CSZ10] are equivalent, it remains to show that, when $(k - \tau) \in \sigma(G)$, the minimal least squares solution $\mathbf{x}^+$ defined in (4.3) coincides with the parametric vector $\mathbf{g}$ given above. To see this, assume without loss of generality that the n eigenvalues of G in Proposition 4.15 can be grouped as follows: the first $r \geq p$ eigenvalues, say $\lambda_1, \ldots, \lambda_r$, are the main eigenvalues of G where each μ_i appears $m_G(\mu_i) = d_i$ times, $i = 1, \ldots, p$; the following eigenvalues $\lambda_{r+1}, \ldots, \lambda_{n-t}$ are non-main and the last t eigenvalues coincide with $k - \tau$ (which is non-main too). Using this grouping, $\mathbf{x}^+$ can be written as

$$\mathbf{x}^+ = \sum_{i=1}^{r} \tau \frac{\mathbf{j}^T \mathbf{u}_i}{\lambda_i - (k-\tau)} \mathbf{u}_i$$

since $\mathbf{j}^T\mathbf{u}_i = 0$ if $i = r+1, \ldots, n-t$. Additionally, for each main eigenvalue μ_i, denoting by P_i the orthogonal projection matrix of $\mathbb{R}^n$ onto $\mathcal{E}_G(\mu_i)$ with respect to the canonical orthonormal basis of $\mathbb{R}^n$ (i.e., $P_i = \mathbf{u}_1\mathbf{u}_1^T + \cdots + \mathbf{u}_{d_i}\mathbf{u}_{d_i}^T$ and $\{\mathbf{u}_1, \ldots, \mathbf{u}_{d_i}\}$ is an orthonormal basis of $\mathcal{E}_G(\mu_i)$), it can be written

$$\mathbf{x}^+ = \sum_{i=1}^{r} \tau \frac{\mathbf{j}^T \mathbf{u}_i}{\lambda_i - (k-\tau)} \mathbf{u}_i = \sum_{i=1}^{p} \frac{\tau}{\mu_i - (k-\tau)} P_i \mathbf{j} = \sum_{i=1}^{p} \tau \frac{||P_i\mathbf{j}||}{\mu_i - (k-\tau)} \frac{P_i\mathbf{j}}{||P_i\mathbf{j}||}.$$

Setting $\mathbf{x}_i = \frac{P_i\mathbf{j}}{||P_i\mathbf{j}||}$, $i = 1, \ldots, p$, we have that $\{\mathbf{x}_1, \ldots, \mathbf{x}_p\}$ is an orthonormal basis of $\mathrm{Main}(G)$ ([Row07, p. 463]); since $\mathbf{j}^T\mathbf{x}_i = \frac{\mathbf{j}^T P_i \mathbf{j}}{||P_i\mathbf{j}||} = \frac{||P_i\mathbf{j}||^2}{||P_i\mathbf{j}||} = ||P_i\mathbf{j}||$, it can finally be asserted that

$$\mathbf{x}^+ = \sum_{i=1}^{p} \tau \frac{\mathbf{j}^T \mathbf{x}_i}{\mu_i - (k-\tau)} \mathbf{x}_i = \mathbf{g}.$$

A.2 Computational results for Algorithm 3

As was mentioned in Section 4.5.1, Algorithm 3 has been tested on two classes of randomly generated graphs: a family of bipartite graphs and a set of graphs with eigenvalue -1 with at least two efficient dominating sets. The last set of graphs was generated taking into account Theorem 2.5 of [CDS95]:

Theorem A.1. *If the spectrum of the graph G contains an eigenvalue λ_0 with multiplicity $p > 1$, then the spectrum of the complementary graph $\bar{G}$ contains an eigenvalue $-\lambda_0 - 1$ with multiplicity q, where $p - 1 \leq q \leq p + 1$.*

Thus, starting with a null graph G_0 with a predefined number of vertices as well as a predefined cardinality, two different efficient dominating sets with this cardinality were randomly generated and implanted in G_0 giving rise to graph G_1; then, for a predefined density, a random graph G_2 was generated (see for instance [CL05, p. 376]) on the vertices of G_1 that do not belong to any of the two implanted efficient dominating sets. Next, 5 of these last vertices were duplicated in $\bar{G}_2$ allowing to obtain a graph, denoted by G_3, which necessarily has the eigenvalue $\lambda_0 = 0$ with multiplicity at least 5; the above cited Theorem 2.5 of [CDS95] ensures that the complementary graph $\bar{G}_3$ has -1 as an eigenvalue with multiplicity at least 4. Algorithm 3 was applied to the graphs $\bar{G}_3$ generated as described. Table A.1 summarizes some of the obtained results. Its first column, denoted by "n ", lists the twelve different graph orders considered, ranging from $n = 25$ until $n = 4005$ vertices. The second column, denoted by "$|S|$", presents three different cardinalities of the efficient dominating sets S generated for each considered value of n. The next three columns report on the densities of the generated graphs; it should be noted that, for each n and $|S|$, thirty instances were generated according to three predefined density levels (namely the 0.25, 0.5 and 0.75 densities); the density columns of the table show the minimum, median and maximum of the set of final densities reached by each of the thirty instances. Finally, the last column gives the average time (in seconds) spent by the algorithm on each set of thirty instances.

Note that Table A.1 reports on results of applying Algorithm 3 for a total of 1080 randomly generated graphs. The tests were carried out on a computer using an Intel(R) Core(TM) i7-3770K/3.50GHz processor with 16.0 Gb RAM and Windows 7 (64 bits) as the operating system. The overall procedure was implemented in MATLAB (version 7.6), where the built-in functions `randperm` and `rand` were respectively called to randomly generate the implanted efficient dominating sets and the graph induced by the remaining vertices.

As a first comment to the results presented in Table A.1 it has been observed that the graph density is apparently uncorrelated with the time spent by the algorithm to solve the efficient domination problem (the computed correlation coefficient is close to zero). Instead, the time spent by the algorithm is heavily dependent on the order of the graph, as expected. It should also be noted that tests with similar results have been run, considering several other values of $|S|$ and of the densities and with graphs where the eigenvalue -1 has high multiplicity. On the other hand, in all tested cases, the algorithm used no Gomory cuts; in fact, the determination of a co-star set associated to the eigenvalue -1 immediately yielded a 0-1 solution and consequently an efficient dominating set. Although this perhaps explains the low running times observed, trying to understand the reasons for this behaviour, can also be a motivation for future work. However, as a conclusion, we can say that Algorithm 3 is very suitable for solving the efficient domination problem in large graphs generated according to the foregoing procedure.

n	$\|S\|$	min dens	med dens	max dens	average time (s)
25	2	0.18	0.40	0.86	0.001
25	4	0.17	0.31	0.66	0.002
25	6	0.15	0.25	0.51	0.001
45	4	0.19	0.37	0.76	0.002
45	8	0.15	0.28	0.52	0.003
45	12	0.11	0.20	0.39	0.002
65	6	0.19	0.37	0.71	0.004
65	12	0.13	0.26	0.50	0.004
65	18	0.09	0.17	0.33	0.004
85	8	0.18	0.35	0.70	0.005
85	16	0.12	0.25	0.51	0.006
85	24	0.08	0.16	0.32	0.006
105	10	0.17	0.35	0.70	0.009
105	20	0.12	0.24	0.48	0.008
105	30	0.08	0.15	0.31	0.007
305	30	0.17	0.34	0.67	0.06
305	60	0.11	0.22	0.44	0.06
305	90	0.07	0.14	0.29	0.06
605	60	0.17	0.34	0.67	0.3
605	120	0.11	0.21	0.43	0.3
605	180	0.07	0.13	0.26	0.3
905	90	0.17	0.34	0.66	0.8
905	180	0.11	0.21	0.42	0.7
905	270	0.06	0.13	0.26	0.7

n	$\|S\|$	min dens	med dens	max dens	average time (s)
1005	50	0.21	0.41	0.82	0.9
1005	100	0.17	0.34	0.67	0.9
1005	300	0.07	0.13	0.27	0.9
2005	100	0.21	0.41	0.82	8.7
2005	200	0.17	0.33	0.66	8.7
2005	600	0.06	0.13	0.26	8.5
3005	150	0.21	0.41	0.81	29.3
3005	300	0.17	0.33	0.66	29.1
3005	900	0.06	0.13	0.25	28.0
4005	200	0.21	0.41	0.81	68.1
4005	400	0.17	0.33	0.66	67.8
4005	1200	0.06	0.13	0.25	65.9

Table A.1: Some computational results for randomly generated graphs with at least two efficient domination sets.

Using the same computer and Matlab environment as above, Algorithm 3 was also tested on some randomly generated bipartite graphs. As noted in Chapter 1, the efficient domination problem is NP-complete for bipartite graphs (this was proved in [YL96]). However, our tests reveal that this negative result does not prevent the successful use of Algorithm 3 for bipartite graphs. Table A.2 reports on the results that were obtained for 3600 randomly generated bipartite graphs. The first column, denoted by "n", gives the considered graphs' orders. Each row represents the results for 600 bipartite graphs of corresponding order. It should be noted that the bipartition of each vertex set of these graphs was also randomly generated. In addition, three density levels (200 graphs for each level) were considered in the generation of graphs corresponding to each row; the respective minimum, median and maximum of the final observed densities are shown in Table A.2. The remaining columns present, for each n, the number of graphs without and with efficient dominating set (eds) followed by the number of those with eigenvalue -1, respectively. Finally, the average time (in seconds) spent by the algorithm for each group of 600 bipartite graphs is reported.

Some similarities were observed between the tests with bipartite graphs and those first described in this section. In fact, in the present case, the graph density also seems to be uncorrelated with the time spent by the algorithm, which continues to be heavily dependent of graph order. In addition, the determination of a co-star set associated to the eigenvalue -1 immediately yielded an efficient dominating set, preventing the use of Gomory cuts. Finally, the low running times observed grants Algorithm 3 a promising practical value.

n	min dens	med dens	max dens	without eds	with $\lambda = -1$	with eds	with $\lambda = -1$	average time (s)
20	0.03	0.27	0.53	418	8	182	39	0.004
50	0.02	0.25	0.51	390	2	210	144	0.006
100	0.01	0.25	0.51	399	4	201	182	0.013
300	0.01	0.24	0.50	408	4	192	178	0.124
500	0.01	0.24	0.50	424	6	176	148	0.393
1000	0.01	0.25	0.50	586	23	14	4	4.352

Table A.2: Some computational results for randomly generated bipartite graphs.

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Keyword index