Universidade de Aveiro Departamento de Matemática
2011

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RESULTADOS ESPECTRAIS RELACIONADOS COM A ESTRUTURA DOS GRAFOS

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Ano 2011

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Resultados espectrais relacionados com a estrutura dos grafos

Tese apresentada à Universidade de Aveiro para cumprimento dos requisitos necessários à obtenção do grau de Doutor em Matemática, realizada sob a orientação científica dos doutores Domingos Moreira Cardoso, Professor Catedrático da Universidade de Aveiro e Slobodan Simić, Professor Catedrático do Insituto de Matemática da Academia de Ciências e Artes da Sérvia.

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agradecimentos

Aos meus orientadores Domingos M. Cardoso e Slobodan K. Simić por me introduzirem no maravilhoso campo da Teoria Espectral dos Grafos, por partilharem comigo os seus conhecimentos, pela paciência ilimitada e pelo tempo despendido durante o nosso trabalho.

A Domingos M. Cardoso a minha especial gratidão pelo seu contínuo apoio durante alguns dos tempos difíceis que passei no início da minha vinda para Portugal.

À FCT - Fundação para a Ciência e a Tecnologia pelo apoio financeiro prestado.

Ao CIDMA - Center for Research and Developments in Mathematics and Applications pelo apoio em algumas das minhas deslocações a conferências.

Aos meus colegas do Departamento de Matemática da Universidade de Aveiro por tornarem a minha estada em Aveiro numa bela experiência.

acknowledgments

My supervisors Domingos M. Cardoso and Slobodan K. Simić for introducing me into the wonderful field of Spectral graph theory, for sharing their knowledge, unlimited patience and all time spending on our work.

To Domingos M. Cardoso also my special gratitude for his continuous support during the many difficult times at the beginning of my stay in Portugal.

The FCT - Fundação para a Ciência e a Tecnologia for the financial support for participations in many important mathematical conferences.

The CIDMA - Center for Research and Developments in Mathematics and Applications for covering some travel expenses.

My colleagues from Department of Mathematics at University of Aveiro for making my stay in Aveiro an indeed wonderful experience.

palavras-chave

Teoria espectral dos grafos, matriz de adjacência e Laplaciana sem sinal, majorantes e minorantes espectrais, grafos separados em cliques e independentes, grafos duplamente separados em independentes, valores próprios principais e não principais, grafo estrela complementar, conjuntos (k,t)-regulares.

resumo

Nesta tese são estabelecidas novas propriedades espectrais de grafos com estruturas específicas, como sejam os grafos separados em cliques e independentes e grafos duplamente separados em independentes, ou ainda grafos com conjuntos (κ,τ)-regulares. Alguns invariantes dos grafos separados em cliques e independentes são estudados, tendo como objectivo limitar o maior valor próprio do espectro Laplaciano sem sinal. A técnica do valor próprio é aplicada para obter alguns majorantes e minorantes do índice do espectro Laplaciano sem sinal dos grafos separados em cliques e independentes bem como sobre o índice dos grafos duplamente separados em independentes. São fornecidos alguns resultados computacionais de modo a obter uma melhor percepção da qualidade desses mesmos extremos. Estudamos igualmente os grafos com um conjunto (κ,τ)-regular que induz uma estrela complementar para um valor próprio não-principal μ. Além disso, é mostrado que $\mu=\kappa-\tau$. Usando uma abordagem baseada nos grafos estrela complementares construímos, em alguns casos, os respectivos grafos maximais. Uma caracterização dos grafos separados em cliques e independentes que envolve o índice e as entradas do vector principal é apresentada tal como um majorante do número da estabilidade dum grafo conexo.

keywords

threshold graphs, adjacency matrix, signless Laplacian spectra, largest eigenvalue, bipartite graphs, spectral bounds, double nested graphs, non-main eigenvalue, star complement

abstract

In this thesis new spectral properties of graphs with a specific structure (as split graphs, nested split and double split graphs as well as graphs with (κ,τ)-regular sets) are deduced. Some invariants of nested split graphs are studied in order to bound the largest eigenvalue of signless Laplacian spectra. The eigenvalue technique is applied to obtain some lower and upper bounds on the index of signless Laplacian spectra of nested split graphs as well as on the index of double nested graphs. Computational results are provided in order to gain a better insight of quality of these bounds. The graphs having a (κ,τ)-regular set which induces a star complement for a non-main eigenvalue μ are studied. Furthermore, it is shown that μ= κ-τ. By the star complement technique, in some cases, maximal graphs with desired properties are constructed. A spectral characterization of families of split graphs involving its index and the entries of the principal eigenvector is given as well as an upper bound on the stability number of a connected graph.

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Chapter 1

Introduction

In this thesis we consider the spectral properties of graphs based on their specific structure. A significant part of the dissertation was motivated by conjectures on signless Laplacian spectra published in [29]. We first focused on Conjecture 7 from [29], that gives an upper bound on the largest eigenvalue of signless Laplacian spectra of a connected graph in terms of its number of vertices and number of edges. Since for connected graphs of fixed order and size, the graphs with maximal index and maximal largest eigenvalue of signless Laplacian are nested split graphs (see [30]) also known as threshold graphs we tried to prove the conjecture for this type of graphs what would have been sufficient. Unfortunately, using this approach we did not manage to prove the conjecture, but we got several interesting results concerning the vertex and edge degrees of nested split graphs. One part of the thesis is partially based on the results published in [4]. Meanwhile, this Conjecture was proven in [35]. Our approach gives a partial proof. Also, we give the simpler version of the proof presented in [35].

After this work we remained in the field of signless Laplacian spectra and nested split graphs. This time using the eigenvalue technique we established some new bounds on the index of signless Laplacian spectra. The specific structure of nested split graphs allows a successful use of this technique. The technique is based on estimations of coordinates of the principal eigenvector associated to the largest eigenvalue of signless Laplacian. Henceforth, we managed to approximate the principal eigenvector which led to an excellent application of Rayleigh quotient. The other bounds were mostly obtained by solving simple quadratic inequalities. Furthermore, we got several new bounds by solving cubic inequalities. All bounds were tested by *Mathematica* routines on various nested split graphs up to 41 000 vertices. Results obtained by this attractive technique take part of two papers. The first one, [5] has been submitted, while the second one, [6] has already been accepted for publication. At the end of this part of research we were slightly disappointed, since that in the most of the examples a pretty simple upper bound from Conjecture 7, [29] gave better approximation. Moreover, we found examples of nested split graphs where this bound is superior than all our upper bounds. However, there are graphs where our bounds are better. This fact is the highlight of our work, as well as some completely new lower bounds.

Our focus after the nested split graphs moved to the double split graphs. These are bipartite graphs and in the class of connected bipartite graphs play the same role as nested split graphs in the class of connected graphs, since in the class of bipartite graphs of fixed order and size those with largest index are double nested graphs. Moreover, this applies to the smallest least eigenvalue as well. In [9] it was shown that graphs whose least eigenvalue is minimal among the connected graphs of fixed order and size are either bipartite or are the graphs obtained from two disjoint nested split graphs, say G and H, not both totally disconnected by joining each vertex of G to each vertex in H. Then in [11] the structural details on related bipartite graphs were provided and there, for the first time, appears the notion of double nested graph. Almost simultaneously, these graphs were introduced in [14] under the name of chain graphs in the context of identifying bipartite graphs with the smallest least eigenvalue. The specific structure of double split graph is appropriate for the application of the eigenvalue technique. So, again we studied entries of the principal eigenvector and then we applied the new approximations to get some new bounds on the index of double split graphs. In this context, we improved one upper bound from [14]. We established the connection between nested split graphs and double nested graphs as well. By this approach, we benefit from some improvements on bounds on index of nested split graphs published in [42]. The new bounds on the index of double nested graph as well as on index of nested split graphs make part of paper [7] which has also been accepted for publication.

A part from research on graphs with nesting properties, we also studied graphs with a (κ, τ)-regular set inducing a star complement for some eigenvalue. We were attracted to this class of graphs by the fact that some properties of graphs, like whether a graph is Hamiltonian or whether a graph has a perfect matching, can be characterized at the same time by means of (κ, τ)-regular sets and the star complements as well. We have shown that if we restrict to a (κ, τ)-regular set inducing a star complement for a non-main eigenvalue μ, then μ has to be equal to $\kappa - \tau$, in comparasion to [21, Proposition 2.6] where another option was given. We point out that our initial conditions are stronger than those in the cited proposition. We also provided several examples where we illustrated that both options in [21, Proposition 2.6] can occur. Therefore it became more significant to determine some class of graphs where just one option holds. In several cases we applied a star complement technique to construct maximal graphs starting from a κ-regular graph H that would be a star complement for the eigenvalue $\kappa - \tau$ in final graph such that each vertex out of H has exactly τ neighbours in it. The results related with this subject are included in the submitted paper [2].

Recently in [23] an eigenvalue condition for a graph to be a bipartite was given as well as an upper bound for the sum of squares of entries of the principal eigenvector that correspond to the vertices of an independent set. We have managed to generalize these results in the sense that we have provided some similar characterizations for some other classes of graphs as well as a lower bound for the sum of squares of entries of the principal eigenvector that correspond to the vertices of an independent set. We have also obtained some further bounds on non-spectral invariants such as stability number and clique number in terms of entries of the principal eigenvector.

The thesis is organized as follows.

In Chapter 2 we give some basic definitions and some helpful results which will be used throughout the thesis in order to make it more self-contained. In the rest of the thesis all results are new.

In Chapter 3 we consider nested split graphs and investigate some invariants of these graphs such as vertex and edge degrees and average vertex and edge degrees, which can be of interest in bounding the largest eigenvalue of signless Laplacian spectra.

In Chapter 4 we study Q-index (or spectral radius) of a simple graph, i.e. the largest eigenvalue of its signless Laplacian. In the set of connected graphs with fixed order and size, the graphs with maximal Q-index are the nested split graphs. Therefore we focus our attention on this class of graphs. We use an eigenvector technique for getting some both lower and upper bounds on the Q-index of nested split graphs. In addition, we give some computational results in order to compare these bounds.

In Chapter 5 we first give a general observation about the structure of double nested graphs. Then we provide some new lower and upper bounds for the index of these graphs by the application of the eigenvalue technique. These new bounds have applications in bounding index of nested split graphs, by the formula connecting the index of double nested graphs and the nested split graphs. Some computational results are also included.

In Chapter 6 we study graphs with a (κ, τ)-regular set inducing a star complement for a non-main eigenvalue μ. It is proven that under these conditions, μ has to be equal to $\kappa - \tau$. Then by a star complement technique, in some cases, we construct maximal graphs with a κ-regular star complement H for the eigenvalue $\kappa - \tau$ such that H is a (κ, τ)-regular in the final graph.

In Chapter 7 an upper bound on the stability number of a connected graph is given. In some cases this bound gives a better approximation than the one obtained in [24]. Furthermore, for some connected graphs a lower bound for the sum of the squares of the entries of the principal eigenvector corresponding to the vertices of an independent set is established. Moreover we give a spectral characterization of some families of split graphs. In particular, the complete split graph case is presented.

Finally, in Chapter 8 we give some observations regarding our results as well as ideas and plans for the future research.

Chapter 2

Preliminary results

In this chapter we fix some notation and terminology. We also present some known results from spectral graph theory and linear algebra that will be used throughout this thesis.

We will consider only simple graphs, that is, finite undirected graphs without loops and multiple edges. Let G be such graph with vertex set $V(G)$ and edge set $E(G)$. If $|V(G)| = n$, we say that G is of order n. The number of edges will be usually denoted by m. If two vertices i and j are joined by an edge, we say that i and j are *adjacent* and write $i \sim j$. As usual, for $v \in V$ the set of neighbours of v is denoted by $N_G(v) = \{w \in V(G) : v \sim w\}$. Then $\deg(v) = |N_G(v)|$ (or d_v for short) is the degree of v. The least degree of vertices in G is denoted by $\delta(G)$, the largest by $\Delta(G)$. An edge that contains a vertex of degree 1 is called a *pendant* edge. The average degree of G ($= 1/n \sum_{v \in V} d_v$) is denoted by $\bar{d}$, while the average degree of the neighbors of v ($= 1/d_v \sum_{u \sim v} d_u$) is denoted by $\bar{d}_v$. If $e \in E(G)$, then $\deg^*(e)$ (or d_e^* for short) is the edge degree of e – it is the number of edges adjacent to e, or alternatively, the degree of e in $L(G)$, the line graph of G; clearly, $d_e^* = d_u + d_v - 2$. Recall, the *line graph* of a graph G, denoted by $L(G)$, has as the vertex set the edge set of G, and two vertices in $L(G)$ are adjacent if the corresponding edges in G are adjacent. The average edge degree of G ($= 1/m \sum_{e \in E} d_e^*$) is denoted by $\bar{d}^*$, while the average edge degree of the neighbours of e ($= 1/d_e^* \sum_{f \sim e} d_f^*$) is denoted by $\bar{d}_e^*$ (note, here $\sim$ denotes that the edges in question are adjacent).

A *p-regular* graph is a graph where each vertex has p number of neighbors . The *complete graph* K_n is a $(n-1)$-regular graph of order n. By C_n-*cycle* of order n we denote a connected 2-regular graph of order n. A connected graph with n vertices is said to be *unicyclic* if it has n edges i.e. if it contains an unique cycle. A complete subgraph of G is called a *clique* of G, while a *co-clique* is an induced subgraph without edges. The *stability number* (or *independence number*) of a graph G, denoted by $\alpha(G)$, is the number of vertices of largest co-clique of G. The *clique number* of G, denoted by $\omega(G)$, is the number of vertices in the largest clique of G.

A *subgraph* H of a graph G is graph such that $V(H) \subset V(G)$ and $E(H) \subset E(G)$. A subgraph of G *induced* by a subset S is denoted by $G[S]$ and it is obtained from G by deleting all vertices that are not in S and consequently all edges incident to them.

A graph G is H-free if it does not contain H as an induced subgraph.

The set of vertices (edges) is *independent* if all vertices (edges) in it are pairwise non-adjacent. Any set of independent edges in a graph G is called a *matching* of G. It is called *perfect* if each vertex of G is the end-vertex of an edge from the matching.

A *dominating set* in the graph G is a subset D of $V(G)$ such that each vertex of $V(G) \setminus D$ is adjacent to a vertex of D.

A *bipartite* graph is a graph whose set of vertices can be divided into two disjoint sets U and V such that every edge connects a vertex in U to one in V; that is, U and V are independent sets. A *complete bipartite* graph is a bipartite graph, which consists of an independent set V of k vertices completely joined to an independent set U of ℓ vertices. It is denoted by $K_{k,\ell}$. A graph of the form $K_{1,\ell}$ is called a *star*.

The *complement* of a graph G is denoted by $\bar{G}$ and as vertex set has $V(G)$, while $E(\bar{G}) = \{uv : u, v \in V(G), uv \notin E(G), u \neq v\}$. The graph consisting of k disjoint copies of G is denoted by kG. The *subdivision graph* $S(G)$ is obtained from G by inserting a vertex of degree 2 in each edge of G.

A cycle C with $V(C) = V(G)$ is called a *Hamiltonian* and a graph with such cycle is said to be *Hamiltonian*.

If u, v are vertices of a connected graph G then the *distance* between u and v, denoted by $d(u, v)$, is the length of the shortest $u - v$ path.

The *union* of disjoint graphs G and H is denoted by $G\dot{\cup}H$. The graph $K_1 \bigtriangledown H$ is called the *cone* over H and is obtained from $K_1\dot{\cup}H$ by joining vertex of K_1 to each vertex of H. Next, we consider a general graph operation called *NEPS - non-complete extended p-sum* of graphs. Let $\mathcal{B}$ be a set of non-zero binary n-tuples i.e. $\mathcal{B} \subset \{0,1\}^n \setminus \{(0,\ldots,0)\}$. The NEPS of graphs $G_1, \ldots, G_n$ with basis $\mathcal{B}$ is the graph with vertex set $V(G_1) \times \cdots \times V(G_n)$, in which two vertices, say $(x_1, \ldots, x_n)$ and $(y_1, \ldots, y_n)$, are adjacent if and only if there exists an n-tuple $\beta = (\beta_1, \ldots, \beta_n) \in \mathcal{B}$ such that $x_i = y_i$ whenever $\beta_i = 0$, and x_i is adjacent to y_i (in G_i) whenever $\beta_i = 1$. In particular, for n = 2 we have the following instances of NEPS:

- the *product* $G_1 \otimes G_2$, when $\mathcal{B} = \{(1,1)\}$;
- the *sum* $G_1 + G_2$, when $\mathcal{B} = \{(0,1),(1,0)\}$;
- the *strong sum* $G_1 \oplus G_2$, when $\mathcal{B} = \{(1,1),(0,1)\}$ and
- the *strong product* $G_1 * G_2$, when $\mathcal{B} = \{(0,1),(1,0),(1,1)\}$.

The $(0,1)$-adjacency matrix $A_G = (a_{ij})$ of G is defined as follows:

$$a_{ij} = \begin{cases} 1 & \text{if} \quad i \sim j \\ 0 & \text{otherwise.} \end{cases}$$

Since the eigenvalues of A_G are independent of the vertex-ordering they are called *eigenvalues* of G. Since A_G is symmetric matrix with real entries, these eigenvalues are real. We usually denote them by $\lambda_1, \lambda_2, \ldots, \lambda_n$ and we assume $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The largest eigenvalue $\lambda_1(G)$ is called the *index* of G. The *spectrum* of A_G, that is, the multiset of its eigenvalues (with multiplicities), is also called the spectrum of G and it is denoted $\sigma(G)$. Each non-zero vector $\mathbf{x} \in \mathbf{R}^n$ satisfying $A_G\mathbf{x} = \lambda\mathbf{x}$ is called an *eigenvector* of the matrix A_G (or of the graph G) corresponding to the eigenvalue λ. If $\mathbf{x} = (x_1, \ldots, x_n)$ then the relation $A_G\mathbf{x} = \lambda\mathbf{x}$ can be written in the following form:

$$\lambda x_u = \sum_{v \sim u} x_v \quad (u = 1, \ldots, n), \tag{2.1}$$

and these equations are called *eigenvalue equations* for G.

For an eigenvalue $\lambda \in \sigma(G)$, we denote by $\mathcal{E}_G(\lambda)$ the *eigenspace* of λ i.e. $\mathcal{E}_G(\lambda) = \{\mathbf{x} \in \mathbb{R}^n : A_G\mathbf{x} = \lambda\mathbf{x}\}$. Moreover, the dimension of $\mathcal{E}_G(\lambda)$ is equal to the multiplicity of λ. To denote the multiplicities, we will use exponential notation, for instant for distinct eigenvalues $\mu_1, \ldots, \mu_\ell$ with multiplicities $k_1, \ldots, k_\ell$ we write $\{[\mu_1]^{k_1}, \ldots, [\mu_\ell]^{k_\ell}\}$.

The eigenvalue μ of a graph G which has an associated eigenspace $\mathcal{E}_G(\mu)$ not orthogonal to the all-one vector $\mathbf{j}$ is said to be *main*, otherwise is called *non-main*.

The *signless Laplacian* of G is defined to be the matrix $Q = A + D$, where $A(= A_G)$ is the adjacency matrix of G, while $D(= D_G)$ is the diagonal matrix of its vertex degrees. The largest eigenvalue (or spectral radius) of Q is usually called the *Q-index* of G, and denoted by $\kappa(= \kappa(G))$.

A symmetric matrix M is *reducible* if there exists a permutation matrix P such that $P^{-1}MP = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix}$, where X, Y are square matrices. Otherwise, we say that M is *irreducible*. Here, we present an important theorem from linear algebra.

Theorem 2.1. *[27, Theorem 1.3.6] If M is an irreducible symmetric matrix with non-negative entries then the largest eigenvalue λ_1 of M is simple (i.e. is of multiplicity 1) with corresponding eigenvector whose entries are all positive.*

In the previous theorem M has unique positive unit eigenvector corresponding to λ_1 called *principal* eigenvector of M. In the case when M is the adjacency matrix of a connected graph G, we call this vector *principal eigenvector* of G.

The *Rayleigh quotient* for a symmetric matrix A of order n and a non-zero vector $\mathbf{y}$ in $\mathbb{R}^n$ is the scalar $\dfrac{\mathbf{y}^T A\mathbf{y}}{\mathbf{y^T y}}$. The supremum of the set of such scalars is the largest eigenvalue λ_1 of A i.e.

$$\lambda_1 = \sup\{\mathbf{x}^T A\mathbf{x} : x \in \mathbb{R}^n, \| x \| = 1\}. \tag{2.2}$$

Hence, for $\mathbf{y} \neq 0$, we have $\dfrac{\mathbf{y}^T A\mathbf{y}}{\mathbf{y^T y}} \leq \lambda_1$, with equality if and only if $A\mathbf{y} = \lambda_1\mathbf{y}$.

Next we give the Courant-Weyl inequalities.

Theorem 2.2. *[27, Theorem 1.3.15] Let A and B be $n \times n$ symmetric matrices. Then*

$$\lambda_i(A+B) \leq \lambda_j(A) + \lambda_{i-j+1}(B) \qquad (n \geq i \geq j \geq 1),$$
$$\lambda_i(A+B) \geq \lambda_j(A) + \lambda_{i-j+n}(B) \qquad (1 \leq i \leq j \leq n).$$

For a given graph G, the partition Π, $V(G) = V_1\dot{\cup}\cdots\dot{\cup}V_k$ is an *equitable partition* if every vertex in V_i has the same number of neighbours in V_j say b_{ij}, for all $i, j \in \{1, \ldots, k\}$. The directed multigraph graph D_Π with vertices $V_1, \ldots, V_k$ and b_{ij} arcs from V_i to V_j is called *divisor* of G with respect to Π. The matrix (b_{ij}) is called *divisor* matrix of Π. The following theorem plays an important role in spectral graph theory:

Theorem 2.3. *[27, Corollary 3.9.11] Any divisor of a graph G has the index of G as an eigenvalue.*

Chapter 3

Some properties of nested split graphs

Nested split graphs, also known as threshold graphs represent a well-studied class of graphs motivated from numerous directions. They were first introduced by Chvátal and Hammer in 1977 [22] (with motivation in integer linear programming) as graphs for which there exists a linear threshold function separating independent from non-independent (vertex) subsets. Since then, depending on pedigree, many different definitions and/or characterizations have been found. Here we will mention some.

- Constructive definition: Nested split graph is a graph that can be constructed from a one-vertex graph by repeated applications of the following two operations:
  - Addition of a single isolated vertex to the graph.
  - Addition of a single dominating vertex to the graph, i.e. a single vertex that is connected to all other vertices.
- Definition based on forbidden configurations: A graph is a nested split graph if and only if is $\{2K_2, P_4, C_4\}$–free graph.

From the definition which uses repeated addition of vertices, one can derive an alternative way of uniquely describing a nested split graph, by means of a string of symbols. The first character of the string is always a, and represents the first vertex of the graph. Every subsequent character is either b, which denotes the addition of an isolated vertex (or *union* vertex), or c, which denotes the addition of a dominating vertex (or *join* vertex).

Nested split graphs appear in studying graphical degree sequences, simplicial complexes, dynamical modeling of network formations etc. The importance of threshold graphs can be also seen through numerous of applications. A remarkable feature is that in some dynamic network formation process, at each period of time, the network is a threshold graph.

The detailed treatment of nested split graphs first appeared in the book by Golumbic [37]; the most complete reference on the topic is the book by Mahadev and Peled [40] (which includes nine different characterizations). Needless to say there are many different generalizations of nested split graphs. They can be viewed as special cases of some wider classes of graphs like cographs, split graphs, interval graphs, etc.

Our motivation for considering nested split graphs comes from the spectral graph theory. These graphs arise (within the graphs with fixed order and/or size) as graphs with the largest eigenvalue of the adjacency matrix. Brualdi and Hoffman [15] observed that they admit the stepwise form of the adjacency matrix, while later Hansen (see, for example, [8]) observed that they are split graphs distinguished by a nesting property imposed on vertices in the maximal co-clique, and hence called them the nested split graphs. As far as we know, it was first observed in [43], that they are $\{2K_2, P_4, C_4\}$-free graphs, and thus the threshold graphs. In [31] it was observed that they appear in the same role with respect to the signless Laplacian spectrum.

Recall, a *split graph* is a graph which admits a partition (or colouring) of its vertex set into two parts (say white and black) so that the vertices of the white part (say U) are independent (induce a co–clique), while the vertices of the black part (say V) are non-independent (induce a clique). All other edges, the *cross edges*, join a vertex in U to a vertex in V. To get a *nested split graph* (or NSG for short) we add cross edges in accordance to partitions of U and V into h cells (namely, $U = U_1 \cup U_2 \cup \cdots \cup U_h$ and $V = V_1 \cup V_2 \cup \cdots \cup V_h$) in the following way: each vertex $u \in U_i$ is adjacent to all vertices $v \in V_1 \cup V_2 \cup \cdots \cup V_i$ i.e. so if $u' \in U_i$ and $u'' \in U_{i+1}$ then $N_G(u') \subset N_G(u'')$, and this explains the nesting property in question (see Figure 3.1). The vertices $U_i \cup V_i$ form the i-th level of some NSG (h is the number of levels). The NSG as described can be denoted by $NSG(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)$, where $m_i = |U_i|$ and

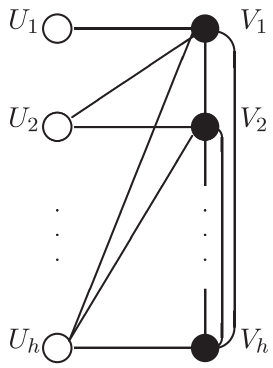

Figure 3.1: The structure of a nested split graph.

$n_i = |V_i|$ $(i = 1, 2, \ldots, h)$.

We now introduce some notation to be used later on (in Chapter 4 as well). First,

$$M_s = \sum_{i=1}^{s} m_i\,, \quad N_t = \sum_{j=1}^{t} n_j\,, \qquad \text{for } 1 \leq s, t \leq h.$$

Thus G is of order $n = M_h + N_h$, and size $m = \sum_{k=1}^{h} m_k N_k + \binom{N_h}{2}$.

We next define the following quantities:

$$\tilde{e}_s = m_s n_s$$

the number of cross edges between U_s and V_s;

$$\hat{e}_s = m_s N_s$$

the total number of cross edges with one end in U_s (so the other in $V_{1,s} = V_1 \cup \cdots \cup V_s$);

$$e_s = \sum_{i=1}^{s} m_i N_i$$

the total number of cross edges with one end in $U_{1,s} = U_1 \cup \cdots \cup U_s$ (so the other in $V_{1,s}$; note that $e_s = e_{s-1} + \hat{e}_s$);

$$\bar{e}_s = M_s N_s - e_s = \sum_{j=1}^{s} n_j M_{j-1}$$

the total number of non-edges between $U_{1,s}$ and $V_{1,s}$ (or, corresponding edges in $\bar{G}$). We also set

$$f_i = \sum_{t=1}^{i} n_t(n - 1 - M_{t-1}).$$

More generally, we can define

$$M_{st} = \sum_{i=s}^{t} m_i = M_t - M_{s-1}, \quad N_{st} = \sum_{j=s}^{t} n_j = N_t - N_{s-1}$$

$$e_{st} = e_t - e_{s-1} \quad \text{and} \quad f_{st} = f_t - f_s.$$

Note $1 \leq i \leq j \leq h$; we also assume that $m_0 = e_0 = 0$. We will also need the following parameters (defined for each $1 \leq i \leq h$):

- d_i $(= N_i)$, the degree of any (white) vertex in U_i;
- D_i $(= n - 1 - M_{i-1})$, the degree of any (black) vertex in V_i;
- $\bar{d}_i$ $(= \bar{d}_{u_i})$, the average degree of any (white) vertex in U_i;
- $\bar{D}_i$ $(= \bar{d}_{v_i})$, the average degree of any (black) vertex in V_i.

In the rest of this chapter we prove some inequalities for the quantities of NSG based on vertex or edge degrees and we give some considerations related to the spectral graph theory.

Remark 3.1. *The following constraints on h and N_h were obtained in [42]:*

$$1 \leq h \leq \min\left\{\frac{n}{2}, \sqrt{m}\right\}$$

and, for $h \geq 2$,

$$2n - 1 - \sqrt{(2n-1)^2 - 8\left(m + \binom{h}{2}\right)} \leq 2\,N_h \leq 1 + \sqrt{1 + 8\left(m - n + 1 - \binom{h-1}{2}\right)}.$$

3.1 Average vertex and edge degrees of nested split graphs

Let $G = (V, E)$ be a connected NSG of order $n \geq 5$. In this section we focus our attention on some questions related to average vertex (resp. edge) degrees of G.

We first consider these quantities with respect to vertices. Recall first that for (distinct) vertex degrees the following holds:

$$d_1 < d_2 < \cdots < d_h \leq D_h < D_{h-1} < \cdots < D_1 = n-1. \quad (3.1)$$

In contrast, for average vertex degrees of neighbours in NSGs, we have another type of monotonicity (see Proposition 3.1). To prove this we first invoke the following fact:

($*$) for any strictly monotone sequence, say (s_n), the sequence of weighted arithmetic means (S_n) (so, $S_n = \frac{\sum_{i=1}^{n} w_i s_i}{\sum_{i=1}^{n} w_i}$, where (w_n) is a positive sequence of weights) is also a strictly monotone sequence.

Proposition 3.1. *If G is an NSG then:*

$$n-1 = \bar{d}_1 > \bar{d}_2 > \cdots > \bar{d}_h \geq \bar{D}_h > \bar{D}_{h-1} > \cdots > \bar{D}_1. \quad (3.2)$$

Proof. Note first that $\bar{d}_1 = n-1$. The monotonicity of $\bar{d}_i$'s easily follows from ($*$) (and (3.1)). Note next that $\bar{d}_h$ is an average degree of all black vertices (i.e. vertices from $V_1 \cup V_2 \cup \cdots \cup V_h$ of G). On the other hand $\bar{D}_h$ has a similar interpretation on the almost the same vertex set but with one black vertex from V_h removed while all white vertices from U_h added. So it follows at once that equality holds if U_h is a singleton (i.e. if $m_h = 1$). Finally, we prove that

$$\bar{D}_i < \bar{D}_{i+1} \quad (3.3)$$

for $1 \leq i \leq h-1$. Let $Q_i = \sum_{s=i}^{h} m_s d_s + \sum_{t=1}^{h} n_t D_t$, while $q_i = \sum_{s=i}^{h} m_s + \sum_{t=1}^{h} n_t - 1$. Then

$$\bar{D}_i = \frac{Q_i - D_i}{q_i}, \quad \bar{D}_{i+1} = \frac{Q_i - m_i d_i - D_{i+1}}{q_i - m_i},$$

and (3.3) is equivalent to $Q_i + \frac{q_i(D_i - D_{i+1})}{m_i} > q_i d_i + D_i$. Since $Q_i \geq q_i d_i + D_i$ (by (3.1)), we are done. This completes the proof. □

The next example (constructed ad hoc) shows that other graphs (like line graphs of NSGs) do not have such a nice property.

Example 3.1. *Let $G = NSG(1,2,1;1,1,1)$. Let the vertices of G be labelled so that $U_1 = \{1\}$, $U_2 = \{2,3\}$, $U_3 = \{4\}$, $V_3 = \{5\}$, $V_2 = \{6\}$ and $V_1 = \{7\}$. Consider the line graph of G,* *i.e. the graph* $H = L(G)$, *with* $V(H) = \{45, 17, 26, 36, 27, 37, 46, 56, 47, 57, 67\}$. *The degrees of the vertices of* H *(edges of* G*) are:* $\{4, 5, 5, 5, 5, 6, 6, 6, 7, 7, 9\}$, *respectively. It is now easy to see that* $d_u = 4$, $\bar{d}_u = 6.5$ $(u = 45)$ $d_v = 5$, $\bar{d}_v = 6.8$ $(v = 17)$ *and* $d_w = 6$, $\bar{d}_w = 6.0$ $(w = 46)$. *So* $d_u < d_v < d_w$, *but nothing analogous holds for* $\bar{d}_u, \bar{d}_v$ *and* $\bar{d}_w$.

We now consider the invariant $d_v + \bar{d}_v$ (v is a vertex of G, where G is not necessarily an NSG). It can be easily shown (as expected from (3.1) and (3.2)) that this invariant is not monotonic for NSGs in the sense of Proposition 3.1. On the other hand, this invariant was considered by Ch.K. Das (in [33]), where it was shown that $\max\{d_v + \bar{d}_v : v \in V(G)\} \leq \frac{2m}{n-1} + n - 2$, for any (connected) graph of order n and size m. Here, we give a short proof of this result, but only for NSGs.

Proposition 3.2. *If* G *is an NSG, then*

(i) $\max_{1 \leq i \leq h}\{d_i + \bar{d}_i\} \leq \dfrac{2m}{n-1} + n - 2$;

(ii) $\max_{1 \leq i \leq h}\{D_i + \bar{D}_i\} \leq \dfrac{2m}{n-1} + n - 2$;

The equality in (i) holds only for $G = K_n$, *while in (ii) only for* $i = 1$.

Proof. To prove (i) we have to show that

$$d_i + \frac{\sum_{t=1}^{i} n_t D_t}{d_i} \leq \frac{\sum_{t=1}^{i} n_t D_t + S_i}{n-1} + n - 2$$

holds for $i = 1, 2, \ldots, h$ (here $S_i = \sum_{t=i+1}^{h} n_t D_t + \sum_{s=1}^{h} m_s d_s$). The latter is equivalent to

$$d_i + (D_1 - d_i) \sum_{t=1}^{i} \frac{n_t D_t}{d_i D_1} \leq n - 2 + \frac{S_i}{D_1};$$

note $D_1 = n - 1$. Since $\frac{D_t}{D_1} \leq 1$ and $\sum_{t=1}^{i} n_t = d_i$, the left hand side is $\leq n - 1$. On the other hand $S_i \geq \sum_{s=1}^{h} m_s d_s \geq n - 1$; note, $\sum_{s=1}^{h} m_s d_s$ is the number of cross edges in G, and it is $\geq n - 1$ since the corresponding bipartite graph (on n vertices formed by the cross edges) is connected. So the right hand side is $\geq n - 1$, and we are done.

For (ii) we have to show that

$$D_i + \frac{\sum_{s=i}^{h} m_s d_s + \sum_{t=1}^{h} n_t D_t - D_i}{D_i} \leq \frac{\sum_{s=1}^{h} m_s d_s + \sum_{t=1}^{h} n_t D_t}{D_1} + n - 2,$$

holds for $i = 1, 2, \ldots, h$, or equivalently, that

$$D_i + (\frac{D_1 - D_i}{D_1 D_i})(D_i \bar{D}_i + D_i) \leq \frac{\sum_{s=1}^{i-1} m_s d_s}{D_1} + n - 1;$$

note, $\sum_{s=i}^{h} m_s d_s + \sum_{t=1}^{h} n_t D_t = D_i \bar{D}_i + D_i$. Since $\frac{\bar{D}_i}{D_1} \leq 1$, and since $D_1 - D_i = \sum_{s=1}^{i-1} m_s$, the left hand side is $\leq \dfrac{\sum_{s=1}^{i-1} m_s}{D_1} + n - 1$, and this is clearly $\leq \dfrac{\sum_{s=1}^{i-1} m_s d_s}{D_1} + n - 1$. So, we are again done.

This completes the proof. □

We now switch to the analogous quantities related to edges. We first note that the analogy of Proposition 3.1 now does not hold (see again Example 3.1). In sequel we will consider NSGs G for which the quantity $\max_{e \in E}\{\bar{d}_e^*\}$ (or equivalently, $\max\{\bar{d}_v : v \in V(L(G))\}$) is exceeding the value equal of $n - 3 + \bar{d}$. (Note, the quantity $\max_{v \in V}\{\bar{d}_v\}$ is always equal to $n - 1$ in NSGs, the maximal possible value by Proposition 3.1, and therefore is not interesting to be studied.)

Let $e = uv$ be an edge of any graph G (not necessarily an NSG). Then

$$\bar{d}_e^* = \frac{\sum_{f \sim u, f \neq e} \deg^*(f) + \sum_{f \sim v, f \neq e} \deg^*(f)}{\deg(u) + \deg(v) - 2},$$

where $f \sim u$ and $f \sim v$ mean that vertices u and v are incident to the edge f. Putting $p = \deg(u)$ and $q = \deg(v)$ we get

$$\bar{d}_e^* = \frac{\sum_{w \sim u, w \neq v}[p + d_w - 2] + \sum_{w \sim v, w \neq u}[q + d_w - 2]}{p + q - 2},$$

which yields

$$\bar{d}_e^* = \frac{p^2 + q^2 - 3p - 3q + 4}{p + q - 2} + \frac{\sum_{w \sim u, w \neq v} d_w + \sum_{w \sim v, w \neq u} d_w}{p + q - 2}.$$

Therefore, we get

$$\bar{d}_e^* = f(p, q) + \frac{S(u) + S(v)}{p + q - 2},$$

where

$$S(u) = \sum_{w \sim u, w \neq v} d_w, \quad S(v) = \sum_{w \sim v, w \neq u} d_w,$$

and

$$f(p, q) = p + q - 1 - 2\frac{pq - 1}{p + q - 2}.$$

In the sequel we assume that G is an NSG as depicted in Figure 3.1, other than a complete graph.

Lemma 3.1. *If $e = uv$, where $u \in V_i$ and $v \in V_j$ $(1 \le i \le j \le h)$, then*

$$\bar{d}^*_e < n - 3 + \bar{d}.$$

Proof. We have: $p = n-1-M_{i-1}$, $q = n-1-M_{j-1}$ $(= p - M_{i,j-1})$, $S(u) = 2m - e_{i-1} - p - q$ and $S(v) = 2m - e_{j-1} - p - q$ $(= S(u) - e_{i,j-1})$. So it follows that

$$f(p,q) = p - 2 - \frac{M_{i,j-1}}{2} + \frac{(\frac{M_{i,j-1}}{2})^2}{p - 1 - \frac{M_{i,j-1}}{2}},$$

$$\frac{S(u)+S(v)}{p+q-2} = -2 + \frac{2m - 2 - e_{i-1} - \frac{1}{2}e_{i,j-1}}{p - 1 - \frac{M_{i,j-1}}{2}}$$

and therefore

$$\bar{d}^*_e = p - 4 - \frac{M_{i,j-1}}{2} + \frac{2m - 2 - e_{i-1} - \frac{1}{2}e_{i,j-1} + (\frac{M_{i,j-1}}{2})^2}{p - 1 - \frac{M_{i,j-1}}{2}}.$$

So we will consider the following inequality:

$$n - M_{i-1} - 5 - \frac{M_{i,j-1}}{2} + \frac{2m - e_{i-1} - 2 - \frac{1}{2}e_{i,j-1} + (\frac{M_{i,j-1}}{2})^2}{n - M_{i-1} - 2 - \frac{M_{i,j-1}}{2}} \le n - 3 + \frac{2m}{n},$$

which is equivalent to

$$\frac{2m}{n - M_{i-1} - 2 - \frac{M_{i,j-1}}{2}} - \frac{2m}{n} \le 2 + M_{i-1} + \frac{M_{i,j-1}}{2} + \frac{e_{i-1} + 2 + \frac{1}{2}e_{i,j-1} - (\frac{M_{i,j-1}}{2})^2}{n - M_{i-1} - 2 - \frac{M_{i,j-1}}{2}}$$

and also to

$$2m \le n(n - 2 - M_{i-1} - \frac{M_{i,j-1}}{2}) + \frac{n\Big(2 + e_{i-1} + \frac{1}{2}e_{i,j-1} - (\frac{M_{i,j-1}}{2})^2\Big)}{2 + M_{i-1} + \frac{M_{i,j-1}}{2}}.$$

For $i = j = 1$ the latter inequality reduces to $m \le \binom{n}{2}$, and we are done. To prove it for $j > 1$, we first estimate the upper bound for m, in the case that G' (in the role of G) is an

NSG of order n having the first $j-1$ levels the same as G (namely, $U_1, V_1, \ldots, U_{j-1}, V_{j-1}$), and the remaining levels chosen so that the size of G' is maximal. It is next easy to see that the maximum (denoted by m') is attained when G' is *"the closest"* to the complete graph, i.e. when G' has exactly j levels, and the clique induced by the black vertices is the largest possible. This happens when U'_j has only one element, and $V_1 \cup \cdots \cup V_{j-1} \cup V'_j$ has $n - M_{j-1} - 1$ elements. Then $2m' = (n - M_{j-1})(n - M_{j-1} - 1) + 2e_{j-1}$. To complete the proof, it suffices to verify that

$$2m' < n(n - 2 - M_{i-1} - \frac{M_{i,j-1}}{2}) + \frac{n[2 + e_{i-1} + \frac{1}{2}e_{i,j-1} - (\frac{M_{i,j-1}}{2})^2]}{2 + M_{i-1} + \frac{M_{i,j-1}}{2}}.$$

We first observe that for every $s \in \{1, \ldots, i-1\}$

$$n - M_{j-1} - 1 + \frac{n(N_s - 1)}{2 + M_{i-1} + \frac{M_{i,j-1}}{2}} \geq N_j + m_j - 1 + \frac{n(N_s - 1)}{2 + M_{i-1} + \frac{M_{i,j-1}}{2}} \geq 2N_s,$$

since $n - M_{j-1} \geq N_j + m_j$ and $n \geq 2 + M_{i-1} + \frac{M_{i,j-1}}{2}$. Next, for every $s \in \{i, \ldots, j-1\}$ we have

$$n(N_s + M_{i-1} + 1) \geq (M_{i-1} + M_{i,j-1} + N_s + 2)(N_s + M_{i-1} + 1) \geq N_s(2M_{i-1} + M_{i,j-1} + 4),$$

since $n - M_{j-1} - 1 \geq N_s + 1$. Therefore we get

$$n - 1 - M_{j-1} + \frac{1}{2}\frac{n(N_s + M_{i-1} + 1)}{2 + M_{i-1} + \frac{M_{i,j-1}}{2}} \geq N_s + 1 + N_s > 2N_s.$$

Using the above inequalities, we obtain

$$
\begin{aligned}
& n(n-2-M_{i-1}-\frac{M_{i,j-1}}{2})+\frac{n[2+e_{i-1}+\frac{1}{2}e_{i,j-1}-(\frac{M_{i,j-1}}{2})^2]}{2+M_{i-1}+\frac{M_{i,j-1}}{2}} \\
& = n(n-M_{j-1}-1)+n(\frac{M_{i,j-1}}{2}-1)+\frac{n[2+e_{i-1}+\frac{1}{2}e_{i,j-1}-(\frac{M_{i,j-1}}{2})^2]}{2+M_{i-1}+\frac{M_{i,j-1}}{2}} \\
& = (n-M_{j-1})(n-M_{j-1}-1)+(M_{i-1}+M_{i,j-1})(n-M_{j-1}-1) \\
& +\frac{n}{2+M_{i-1}+\frac{M_{i,j-1}}{2}}[e_{i-1}-M_{i-1}+\tfrac{1}{2}(e_{i,j-1}+M_{i,j-1}(M_{i-1}+1))] \\
& = (n-M_{j-1})(n-M_{j-1}-1)+\textstyle\sum_{s=1}^{i-1} m_s[n-M_{j-1}-1+\frac{n(N_s-1)}{2+M_{i-1}+\frac{M_{i,j-1}}{2}}] \\
& +\textstyle\sum_{s=i}^{j-1} m_s[n-M_{j-1}-1+\frac{1}{2}\frac{n(N_s+M_{i-1}+1)}{2+M_{i-1}+\frac{M_{i,j-1}}{2}}] \\
& > (n-M_{j-1})(n-M_{j-1}-1)+2e_{j-1} \\
& = 2m'.
\end{aligned}
$$

This completes the proof. □

Lemma 3.2. *If $e=uv$, $u\in U_j$ and $v\in V_i$ $(1\le i\le j\le h)$, then*

$$\bar{d}^*_e \le n-3+\bar{d}$$

holds, unless $i=j=1$, $|V_1|=1$ and $\bar{d}>\frac{n}{2}$.

Proof. We now have: $p=N_j=N_i+N_{i+1,j}$, $q=n-1-M_{i-1}$, $S(u)=f_j-q=f_i+f_{ij}-q$ and $S(v)=2m-e_{i-1}-p-q$. So $S(u)+S(v)=2m-p-2q+R$, where $R=f_i+f_{ij}-e_{i-1}$. Let $C_{ij}=\sum_{s=i+1}^{j} n_sM_{i,s-1}$. It is a matter of routine calculations to show that $R=pq-C_{ij}$. But then $S(u)+S(v)=2m+pq-p-2q-C_{ij}$, and consequently we have that

$$\bar{d}^*_e = p+q-2+\frac{2m-pq-q-C_{ij}}{p+q-2},$$

or equivalently

$$\bar{d}^*_e = n-3-M_{i-1}+N_j+\frac{2m-(n-1-M_{i-1})(N_j+1)-C_{ij}}{n-3-M_{i-1}+N_j}.$$

So we have to prove the following inequality:

$$2m(M_{i-1}-N_j+3)\le n[(M_{i-1}-N_j)(n-3+N_j-M_{i-1})+(n-1-M_{i-1})(N_j+1)+C_{ij}].$$

We next consider the following two cases depending on the sign of $M_{i-1} - N_j + 3$.

Case 1: $M_{i-1} - N_j + 3 \geq 0$. If $M_{i-1} - N_j + 3 = 0$ then the above inequality reduces to $n(N_j - 2) + C_{ij} \geq (M_{i-1} + 1)(N_j + 1)$. Since $N_j - 2 = M_{i-1} + 1$ the latter inequality becomes $(n - N_j - 1)(N_j - 2) + C_{ij} \geq 0$, which holds since $n \geq M_{i-1} + N_j + 1$ and $N_j = M_{i-1} + 3 > 2$. So we next assume that $M_{i-1} - N_j + 3 > 0$. If $i = 1$ then $m_0 = 0$ and $N_j \leq 2$. If $N_j = 1$ (i.e. if $|V_1| = 1$) then we easily get that the above inequality reduces to $m \leq \frac{n^2}{4}$. So, if $|V_1| = 1$ and $\bar{d} > \frac{n}{2}$ we get that the inequality in question does not hold (an exceptional case from the lemma). Otherwise, if $N_j = 2$ then the above inequality reduces to $2m \leq n(n - 1 + C_{1j})$ which clearly holds. So we next assume that $i \geq 1$ and consequently we have to prove that

$$2m \leq \frac{n}{M_{i-1} - N_j + 3}[(M_{i-1} - N_j)(n - 3 + N_j - M_{i-1}) + (N_j + 1)(n - M_{i-1} - 1) + C_{ij}].$$

Assume now that G' is the graph with maximal number of edges obtained in the same way as in the proof of Lemma 3.1. Then $2m' = (n - M_{j-1})(n - M_{j-1} - 1) + 2e_{j-1}$. Therefore we have to prove that

$$2m' \leq \frac{n}{M_{i-1} - N_j + 3}[(M_{i-1} - N_j)(n - 3 + N_j - M_{i-1}) + (N_j + 1)(n - M_{i-1} - 1) + C_{ij}].$$

This can be done as follows:

$$\begin{aligned}
&\frac{n}{M_{i-1} - N_j + 3}[(M_{i-1} - N_j)(n - 3 + N_j - M_{i-1}) + (N_j + 1)(n - 1 - M_{i-1}) + C_{ij}] \\
&= (n - M_{j-1})(n - M_{j-1} - 1) + \frac{n}{M_{i-1} - N_j + 3}[(M_{i-1} - N_j)(n - 3 + N_j - M_{i-1}) + \\
&(N_j + 1)(n - 1 - M_{i-1}) - (n - 2M_{j-1} - 1)(M_{i-1} - N_j + 3) + C_{ij}] - M_{j-1}(M_{j-1} + 1) \\
&\geq (n - M_{j-1})(n - M_{j-1} - 1) + M_{j-1}(n - M_{j-1} - 1) + nM_{i,j-1} + \\
&\frac{n}{M_{i-1} - N_j + 3}[M_{j-1}(N_j - 2) + C_{ij}] \\
&\geq (n - M_{j-1})(n - M_{j-1} - 1) + M_{j-1}N_j + M_{j-1}(N_j - 2) \\
&\geq (n - M_{j-1})(n - M_{j-1} - 1) + 2M_{j-1}N_{j-1} \\
&\geq (n - M_{j-1})(n - M_{j-1} - 1) + 2e_{j-1} \\
&= 2m'.
\end{aligned}$$

Note that the first inequality in the chain follows since $n - M_{j-1} - N_j - 1 \geq 0$, while the second one is based on the following facts: $n > M_{i-1} - N_j + 3$, $n - M_{j-1} - 1 \geq N_j$, $M_{i,j-1} \geq 0$ and $C_{ij} \geq 0$. Finally, since the third one is self-evident, we are done in this case.

Case 2: $M_{i-1} - N_j + 3 < 0$. Now we have to verify that

$$2m > \frac{n}{M_{i-1} - N_j + 3}[(M_{i-1} - N_j)(n - 3 + N_j - M_{i-1}) + (N_j + 1)(n - M_{i-1} - 1) + C_{ij}].$$

In contrast to the previous case we will now have to minimize the number of edges in G'. For this aim we take that the first $j-1$ levels are the same as in G, while the remaining vertices are in the j-th level distributed so that V_j' is the same as V_j. Then $2m' = N_j(N_j - 1) + 2(n - M_{j-1} - N_j)N_j + 2e_{j-1}$. Therefore we have to prove that

$$2m' \geq \frac{n}{M_{i-1} - N_j + 3}[(M_{i-1} - N_j)(n - 3 + N_j - M_{i-1}) + (N_j + 1)(n - M_{i-1} - 1) + C_{ij}].$$

This can be done as follows:

$$\begin{aligned}
&\frac{n}{N_j - M_{i-1} - 3}[(N_j - M_{i-1})(n - 3 + N_j - M_{i-1}) - (N_j + 1)(n - M_{i-1} - 1) - C_{ij}] \\
&= N_j(N_j - 1) + 2(n - M_{j-1} - N_j)N_j + (2M_{j-1} + N_j + 1 - n)N_j \\
&+ \frac{n}{N_j - M_{i-1} - 3}(M_{i-1}^2 - nM_{i-1} + 4M_{i-1} + N_j + 1 - n - C_{ij}) \\
&\leq N_j(N_j - 1) + 2(n - M_{j-1} - N_j)N_j + M_{j-1}N_j - nM_{i-1} \\
&- \frac{n}{N_j - M_{i-1} - 3}[(n - N_j - 1)(M_{i-1} + 1) + C_{ij}] \\
&\leq N_j(N_j - 1) + 2(n - M_{j-1} - N_j)N_j + M_{j-1}N_j - nM_{i-1} - M_{j-1}(M_{i-1} + 1) - C_{ij} \\
&\leq N_j(N_j - 1) + 2(n - M_{j-1} - N_j)N_j + M_{i,j-1}N_j - C_{ij} \\
&\leq N_j(N_j - 1) + 2(n - M_{j-1} - N_j)N_j + 2e_{j-1} \\
&= 2m'.
\end{aligned}$$

Note that the first three inequalities in the chain follow since $n - M_{j-1} - N_j \geq 1$. On the other hand, the fourth one easily follows by observing that $e_{j-1} = e_{i-1} + e_{i,j-1}$ and $e_{i,j-1} + C_{ij} = M_{i,j-1}N_j$. So we are again done. This completes the proof. □

Collecting the above results we get that $\max_{e \in E}\{\bar{d}^*{}_e\} \leq n - 3 + \bar{d}$ for all NSGs G for which $n_1 > 1$, or $n_1 = 1$ and $\bar{d} \leq \frac{n}{2}$. In other words, if G has at least two vertices of degree $n-1$, or one vertex of degree $n-1$ and the average vertex degree $\bar{d} \leq \frac{n}{2}$ then $\max_{e \in E}\{\bar{d}_e^*\} \leq n - 3 + \bar{d}$ holds. We will say that these graphs are of type-I. In contrast, the graphs for which $\max_{e \in E}\{\bar{d}_e^*\} > n - 3 + \bar{d}$ are of type-II.

We will now consider in more details the graphs of type-II. Any such graph has a unique vertex of degree $n-1$ (thus $m_1 = k$ and $n_1 = 1$) and big average vertex degree ($> \frac{n}{2}$). The latter fact also implies that k cannot be too big. By a simple calculation we can get that $k < (1 - \frac{\sqrt{2}}{2})n < 0.3n$ (note, k is the largest if $G = NSG(k, 1; 1, n-k-2)$). Next, it is also reasonable to ask how large the quantity $\max_{e \in E}\{\bar{d}_e^*\}$ can be for a fixed k. But then, due to Lemmas 3.1 and 3.2, we have to take that $G = NSG(k, m_2, \ldots, m_h; 1, n_2, \ldots, n_h)$ for some choice of its parameters, and to consider an edge $e = uv$ with $u \in U_1$ and $v \in V_1$. By adding some edges if necessary (note, then the observed quantity cannot decrease) we arrive at the graph $G' = NSG(k, 1; 1, n-k-2)$. But then, by simple calculations, we get that that

$$\bar{d}_e^* \leq \frac{k^2 - (2n-3)k + (n-2)(2n-3)}{n-2},$$

with the largest possible value equal to $2n-5$ (attained for $G = NSG(1, 1; 1, n-3)$, if $k = 1$). Note, for the latter graph we have that

$$\max_{e \in E}\{\bar{d}_e^*\} = \max\{2n-6+\frac{1}{2n-5}, 2n-5, 2n-6+\frac{2}{2n-5}, 2n-6+\frac{5}{2n-5}\},$$

and so, as expected, for $n \geq 5$ the second value is the right one (note, the cases with $n < 5$ are excluded from considerations). Collecting the above results, we arrive at:

Proposition 3.3. *If G is an NSG then, depending on the type of G (I or II, respectively), we have:*

(i) $\max_{e \in E}\{\bar{d}_e^*\} \leq n - 3 + \bar{d}$, *or*

(ii) $n - 3 + \bar{d} < \max_{e \in E}\{\bar{d}_e^*\} \leq \dfrac{k^2 - (2n-3)k + (n-2)(2n-3)}{n-2}$, *where k is the number of vertices of degree one.*

3.2 An application in spectral graph theory

We will now use the above results to give some comments related to spectral graph theory. More precisely, we will highlight some phenomena related to Conjecture 7 from [29], the conjecture generated by the computer program AutoGraphiX (AGX). Let $\kappa(G)$ be the largest eigenvalue of the signless Laplacian of a graph G (not necessarily an NSG). Recall, $Q_G = D_G + A_G$, where A_G is the adjacency matrix of G, and D_G the diagonal matrix of its vertex degrees, is the signless Laplacian of G. According to [29], Conjecture 7 reads:

If G is a connected graph of order $n \geq 5$ and average vertex degree $\bar{d}(G)$, then $\kappa(G) \leq n-1+\bar{d}(G)$ with equality if and only if G is complete.

The next theorem covers some cases for which the above conjecture is true.

Theorem 3.1. *Let G is a connected graph of order n and size m, and average vertex degree $\bar{d}(G) \leq \frac{n}{2}$. Then $\kappa(G) < n-1+\bar{d}(G)$.*

Proof. Based on Theorem 5.4 from [29], it suffices to verify the conjecture only for NSGs. Since $\kappa(G) = \rho(L(G)) + 2$, where $\rho(G)$ is the largest eigenvalue of the adjacency matrix of a graph G (see, for example, Eq. (2) in [29]), we in fact have to prove that $\rho(L(G)) < n-3+\bar{d}(G)$. Due to Favaron et al. (cf. [34]), $\rho(L(G)) \leq \max_{e \in E}\{\bar{d}_e^*\}$. The final conclusion (for graphs in question) now follows by using Proposition 3.3. □

The following remark is worth mentioning:

Remark 3.2. *In particular, we immediately have that Conjecture 7 from [29] holds for all bipartite graphs G (including some non-bipartite graphs). On the other hand, it is true in general, as it was shown in [35], where the authors have made a short proof of the conjecture in question by proving first that $\kappa(G) \leq \max\{d_v + \bar{d}_v\}$ (see also [1]), and by using the sophisticated bound from [33] (see also Proposition 3.2).*

Chapter 4

Bounds on Q-index of nested split graphs

The Q-index of a graph is a very important spectral invariant, and also much studied in the literature since recently. Recall first that

$$\Delta + 1 \leq \kappa \leq 2(n-1)\,, \tag{4.1}$$

with equality for stars and complete graphs (for the lower and upper bound, respectively – cf. [28]); here Δ is the maximal vertex degree of a graph in question. The following bound was conjectured in [29], and later proved in [35] (cf. also [4]):

$$\kappa \leq n - 1 + \bar{d}\,, \tag{4.2}$$

where $\bar{d}$ is the average (vertex) degree of a graph. Many other bounds on Q-index for arbitrary graphs (usually connected ones) can be found in [27].

Here we will restrict ourselves only on connected graphs with maximal Q-index. These graphs, as already pointed in Chapter 3, are the nested split graphs. In [47, 48] one can find many nice results on the Q-index of NSGs.

The remainder of the chapter is organized as follows. In Section 4.1 we investigate the relation between the parameters of an NSG and the components of the eigenvector corresponding to the Q-index. In Section 4.2 we deduce only a few both lower and upper bounds for the index of NSGs in order to justify our previous investigations. In Section 4.3 we give some computational data to indicate the quality of our bounds. In Section 4.4 we provide several upper bounds obtained as solutions of cubic equations (in a contrast to quadratic ones in Section 4.2). In Section 4.5 these additional bounds are tested.

4.1 Q-eigenvectors of NSGs

We retain all settings from Chapter 3. Let G be a connected NSG graph of order n and size m, and let $\kappa = \kappa(G)$ be its Q-index; we also set

$$\kappa_t = \kappa - d_t\,, \quad \bar{\kappa}_t = \kappa - D_t + 1\,,$$

and

$$\mu_t = (\kappa - d_t)(\kappa - D_t + 1)\,, \quad \bar{\mu}_t = (\kappa - d_t)(\kappa - D_1 + 1)\,,$$

where $1 \leq t \leq h$. Observe that, according to (4.1), all these four quantities are positive. It is well known, since Q is a non-negative and irreducible matrix, that the eigenvector corresponding to the Q-index can be taken to be positive. In this section (and in the next one, if not told otherwise) we will assume that

$$\mathbf{x} = (x_1, \ldots, x_n)^T$$

is a Q-eigenvector of G, which is usually normalized, i.e.,

$$\sum_{i=1}^{n} x_i = 1\,.$$

The entries of $\mathbf{x}$ are also called the weights of the corresponding vertices. We first observe that all vertices within the sets U_s or V_t, for $1 \leq s, t \leq h$, have the same weights, since they belong to the same orbit of G. Let $x_u = a_s$ if $u \in U_s$, while $x_v = b_t$ if $v \in V_t$.

From the eigenvalue equations for κ (applied to any vertex from U_s, or V_t) we get

$$\kappa a_s = d_s a_s + \sum_{j=1}^{s} n_j b_j\,, \qquad \text{for } s = 1, \ldots, h, \tag{4.3}$$

and

$$\kappa b_t = D_t b_t + \sum_{i=t}^{h} m_i a_i + \sum_{j=1}^{h} n_j b_j - b_t\,, \qquad \text{for } t = 1, \ldots, h. \tag{4.4}$$

By normalization we have

$$\sum_{i=1}^{h} m_i a_i + \sum_{j=1}^{h} n_j b_j = 1\,, \tag{4.5}$$

and from (4.3) we easily get

$$a_s = \frac{1}{\kappa - d_s} \sum_{j=1}^{s} n_j b_j\,, \qquad \text{for } s = 1, \dots, h. \tag{4.6}$$

From (4.4) we have

$$b_t = \frac{1}{\kappa - D_t + 1} \left(\sum_{i=t}^{h} m_i a_i + \sum_{j=1}^{h} n_j b_j \right)\,, \qquad \text{for } t = 1, \dots, h,$$

and, therefore, using (4.5), we have

$$b_t = \frac{1}{\kappa - D_t + 1} \left(1 - \sum_{i=1}^{t-1} m_i a_i \right)\,, \qquad \text{for } t = 1, \dots, h, \tag{4.7}$$

or, using (4.3) for $s = h$,

$$b_t = \frac{1}{\kappa + 1 - D_t} \left(\sum_{i=t}^{h} m_i a_i + (\kappa - d_h) a_h \right)\,, \qquad \text{for } t = 1, \dots, h. \tag{4.8}$$

Setting $a_0 = b_0 = 0$, and $d_0 = 0$, from (4.6) and (4.7), together with (4.5), we get successively

$$(\kappa - d_s)(a_{s+1} - a_s) = n_{s+1}(a_{s+1} + b_{s+1})\,, \qquad \text{for } s = 0, \dots, h-1, \tag{4.9}$$

$$(\kappa - D_1 + 1)(b_1 - b_0) = 1\,, \qquad \text{for } t = 0, \tag{4.10}$$

and

$$(\kappa - D_{t+1} + 1)(b_{t+1} - b_t) = -m_t(a_t + b_t)\,, \qquad \text{for } t = 1, \dots, h-1\,, \tag{4.11}$$

bearing in mind the relations $d_{s+1} = d_s + n_s$ and $D_t = D_{t+1} + m_t$.

Since all components of $\mathbf{x}$ are positive and $\kappa \geq \Delta + 1$ (see (4.1)), it comes

$$a_{s+1} > a_s\,, \qquad \text{for } s = 1, \dots, h-1, \tag{4.12}$$

and

$$b_{t+1} < b_t\,, \qquad \text{for } t = 1, \dots, h-1. \tag{4.13}$$

Furthermore, setting $s = h$ in (4.6) and $t = h$ in (4.7), from (4.5), we obtain

$$(\kappa - D_h + 1) b_h = (\kappa - d_h + m_h) a_h\,.$$

Since $m_h \geq 1$ and $D_h = d_h + m_h - 1$, we also have

$$b_h \geq a_h \,,$$

with equality if and only if $m_h = 1$.

Remark 4.1. *We remark that*

$$a_1 = \frac{N_1}{\mu_1} \quad \textit{and} \quad b_1 = \frac{1}{\bar{\kappa}_1}, \tag{4.14}$$

(see (4.9) and (4.10)). Moreover, we also have

$$a_2 = \frac{1}{\mu_2}\left(N_2 - \frac{n_2 e_1}{\mu_1} + \frac{e_1}{\bar{\kappa}_1}\right) \quad \textit{and} \quad b_2 = \frac{1}{\bar{\kappa}_2}\left(1 - \frac{e_1}{\mu_1}\right), \tag{4.15}$$

and, in addition,

$$a_3 = \frac{1}{\mu_3}\left(N_3 - \left(\frac{(n_2+n_3)e_1}{\mu_1} + \frac{n_3\hat{e}_2}{\mu_2}\right) + \left(\frac{n_1 M_2}{\bar{\kappa}_1} + \frac{\tilde{e}_2}{\bar{\kappa}_2} + \frac{n_3\tilde{e}_1\tilde{e}_2}{\mu_1\mu_2}\right) - \left(\frac{\tilde{e}_1\tilde{e}_2}{\mu_1\bar{\kappa}_2} + \frac{m_2 n_3 e_1}{\mu_2\bar{\kappa}_1}\right)\right),$$

and

$$b_3 = \frac{1}{\bar{\kappa}_3}\left(1 - \left(\frac{\hat{e}_1}{\mu_1} + \frac{\hat{e}_2}{\mu_2}\right) - \frac{m_2\tilde{e}_1}{\mu_2\bar{\kappa}_1} + \frac{\tilde{e}_1\tilde{e}_2}{\mu_1\mu_2}\right).$$

Further on we will focus our attention on bounding a_i's and b_j's, since the exact expressions, as shown in the above remark, are becoming too messy. This will be done in the next sequence of lemmas.

Lemma 4.1. *For any $s = 1, \ldots, h$, we have*

$$\frac{N_s}{\kappa - N_s}\, b_s \leq a_s \leq \frac{N_s}{\kappa - N_s}\, b_1 \,. \tag{4.16}$$

Moreover, if $i = 0, \ldots, s-1$, then

$$\frac{N_s - N_i}{\kappa - N_i}\, b_s \leq a_s - a_i \leq \frac{\kappa}{\kappa - N_i}\,\frac{N_s - N_i}{\kappa - N_s}\, b_1. \tag{4.17}$$

Proof. From (4.6), we have

$$a_s = \frac{1}{\kappa - d_s}\sum_{j=1}^{s} n_j b_j \,.$$

Therefore, (4.16) immediately follows since b_j's are strictly decreasing (see (4.13)).

To prove (4.17), consider first the lower bound. By (4.6) we first get

$$a_s - a_i = \frac{1}{\kappa - d_s} \sum_{j=1}^{s} n_j b_j - \frac{1}{\kappa - d_i} \sum_{j=1}^{i} n_j b_j \,.$$

Since $d_s \geq d_i$, we have

$$a_s - a_i \geq \frac{1}{\kappa - d_i} \sum_{j=i+1}^{s} n_j b_j \;\geq \frac{b_s}{\kappa - d_i} (N_s - N_i) \,,$$

as required. Let us analyze now the upper bound. We have

$$a_s - a_i = \left(\frac{1}{\kappa - d_s} - \frac{1}{\kappa - d_i} \right) \sum_{j=1}^{i} n_j b_j + \frac{1}{\kappa - d_s} \sum_{j=i+1}^{s} n_j b_j .$$

Since b_j's are strictly decreasing, we have

$$a_s - a_i \leq \frac{N_i b_1 (d_s - d_i)}{(\kappa - d_s)(\kappa - d_i)} + \frac{N_s - N_i}{\kappa - d_s} b_1 = \frac{\kappa}{\kappa - d_i} \frac{N_s - N_i}{\kappa - d_s} b_1,$$

as required. □

Lemma 4.2. *For any* $t = 1, \ldots, h$*,*

$$\frac{1 - a_{t-1} M_{t-1}}{\kappa - n + 2 + M_{t-1}} \leq b_t \leq \frac{1 - a_1 M_{t-1}}{\kappa - n + 2 + M_{t-1}} \,, \tag{4.18}$$

and

$$\frac{(\kappa - N_h) a_h + M_{t,h} a_t}{\kappa - n + 2 + M_{t-1}} \leq b_t \leq \frac{\kappa - N_h + M_{t,h}}{\kappa - n + 2 + M_{t-1}} a_h. \tag{4.19}$$

Proof. Inequalities (4.18) follow from (4.7), since a_i's are strictly increasing; similarly, one gets (4.19) from (4.8). □

Lemma 4.3. *For any* $t = 1, \ldots, h$*,*

$$b_t \geq \frac{1}{\bar{\kappa}_t} \left(1 - \sum_{i=1}^{t-1} \frac{m_i N_i}{\bar{\mu}_i} \right) \,. \tag{4.20}$$

Proof. By induction on t. For $t = 1$, $b_1 = \frac{1}{\kappa - D_1 + 1}$ and thus (4.20) holds (see (4.14)). Assume next that $b_t \geq \frac{1}{\bar{\kappa}_t} \left(1 - \sum_{i=1}^{t-1} \frac{m_i N_i}{\bar{\mu}_i} \right)$, for some $t \geq 1$. From (4.11) and (4.16) we get

$$\begin{aligned} b_{t+1} &= b_t - \frac{m_t}{\bar{\kappa}_{t+1}} (a_t + b_t) \\ &\geq \left(1 - \frac{m_t}{\bar{\kappa}_{t+1}} \right) \frac{1}{\bar{\kappa}_t} \left(1 - \sum_{i=1}^{t-1} \frac{m_i N_i}{\bar{\mu}_i} \right) - \frac{m_t}{\bar{\kappa}_{t+1}} b_1 \frac{N_t}{\kappa - d_t} \\ &= \frac{1}{\bar{\kappa}_{t+1}} \left(1 - \sum_{i=1}^{t} \frac{m_i N_i}{\bar{\mu}_i} \right) , \end{aligned}$$

and the proof follows. □

Lemma 4.4. *For any $s = 1, \ldots, h$, we have*

$$a_s \leq \frac{1}{\bar{\mu}_s} \left(N_s - a_1 \bar{e}_s \right). \tag{4.21}$$

Proof. From (4.6) and (4.18), we have

$$\begin{aligned} a_s &= \frac{1}{\kappa - d_s} \sum_{j=1}^{s} n_j b_j \\ &\leq \frac{1}{\kappa - d_s} \sum_{j=1}^{s} n_j \frac{1}{\bar{\kappa}_1} (1 - a_1 M_{j-1}) \\ &= \frac{1}{\bar{\mu}_s} \left(N_s - a_1 \sum_{j=1}^{s} n_j M_{j-1} \right) \\ &= \frac{1}{\bar{\mu}_s} \left(N_s - a_1 \bar{e}_s \right) \end{aligned}$$

and the proof follows. □

Remark 4.2. *Clearly (4.21) is an improvement of the right hand side of (4.16). Yet another improvement is given in (4.25).*

Lemma 4.5. *For any $s = 1, \ldots, h$,*

$$a_s \geq \frac{N_s}{\bar{\mu}_s} \left(1 - \sum_{j=1}^{s} \frac{n_j}{N_s} \left(\sum_{i=1}^{j-1} \frac{m_i N_i}{\bar{\mu}_i} + \frac{M_{j-1}}{\bar{\kappa}_j} \right) \right). \tag{4.22}$$

Proof. For $s = 1$, the bound is true by (4.14). Otherwise, from (4.6) and (4.20) (with righthand side rearranged) we get

$$\begin{aligned} a_s &= \frac{1}{\kappa - d_s} \sum_{j=1}^{s} n_j b_j \\ &\geq \frac{1}{\kappa - d_s} \sum_{j=1}^{s} \frac{n_j}{\bar{\kappa}_1} \left(1 - \sum_{i=1}^{j-1} \frac{m_i N_i}{(\kappa - d_i)\bar{\kappa}_j} - \frac{M_{j-1}}{\bar{\kappa}_j} \right) \\ &\geq \frac{N_s}{\bar{\mu}_s} \left(1 - \sum_{j=1}^{s} \frac{n_j}{N_s} \left(\sum_{i=1}^{j-1} \frac{m_i N_i}{\bar{\mu}_i} + \frac{M_{j-1}}{\bar{\kappa}_j} \right) \right), \end{aligned}$$

and the proof follows. □

Remark 4.3. *From (4.22) we can easily deduce that*

$$a_s \geq \frac{1}{\bar{\mu}_s}\left(N_s - (N_s - N_1)\left(\frac{e_{s-1}}{\bar{\mu}_s} + \frac{M_{s-1}}{\bar{\kappa}_1}\right)\right),$$

or in addition that

$$a_s \geq \frac{N_s}{\bar{\mu}_s}\left(1 - \left(\frac{e_{s-1}}{\bar{\mu}_s} + \frac{M_{s-1}}{\bar{\kappa}_1}\right)\right). \tag{4.23}$$

Lemma 4.6. *For any $t = 1, \dots, h$ we have*

$$b_t \leq \frac{1}{\bar{\kappa}_t}\left(1 - \sum_{i=1}^{t-1}\frac{m_i N_i}{\bar{\mu}_i} + \sum_{i=1}^{t-1}\frac{m_i}{\bar{\mu}_i}\sum_{j=1}^{i} n_j\left(\sum_{k=1}^{j-1}\frac{m_k N_k}{\bar{\mu}_k} + \frac{M_{j-1}}{\bar{\kappa}_j}\right)\right). \tag{4.24}$$

Proof. For $t = 1$ the bound is true (4.14). From (4.7) and (4.22) we have

$$\begin{aligned} b_t &= \frac{1}{\bar{\kappa}_t}\left(1 - \sum_{i=1}^{t-1} m_i a_i\right) \\ &\leq \frac{1}{\bar{\kappa}_t}\left(1 - \sum_{i=1}^{t-1}\frac{m_i}{\bar{\mu}_i}\left(N_i - \sum_{j=1}^{i} n_j\left(\sum_{k=1}^{j-1}\frac{m_k N_k}{\bar{\mu}_k} + \frac{M_{j-1}}{\bar{\kappa}_j}\right)\right)\right) \\ &\leq \frac{1}{\bar{\kappa}_t}\left(1 - \sum_{i=1}^{t-1}\frac{m_i N_i}{\bar{\mu}_i} + \sum_{i=1}^{t-1}\frac{m_i}{\bar{\mu}_i}\sum_{j=1}^{i} n_j\left(\sum_{k=1}^{j-1}\frac{m_k N_k}{\bar{\mu}_k} + \frac{M_{j-1}}{\bar{\kappa}_j}\right)\right) \end{aligned}$$

and the proof follows. □

Remark 4.4. *From (4.24) we can easily deduce*

$$b_t \leq \frac{1}{\bar{\kappa}_t}\left(1 - \frac{e_{t-1}}{\bar{\mu}_1} + \frac{e_{t-1}e_{t-2}}{\bar{\mu}_{t-1}\bar{\mu}_{t-2}} + \frac{e_{t-1}M_{t-2}}{\bar{\kappa}_1\bar{\mu}_{t-1}}\right).$$

We shall now refine the upper bound for a_s (4.16).

Lemma 4.7. *For any s, with $1 \leq s \leq h$, we have*

$$\begin{aligned} a_s \leq \frac{N_s}{\bar{\mu}_s}\Bigg(1 &- \sum_{j=1}^{s}\frac{n_j}{N_s}\left(\sum_{i=1}^{j-1}\frac{m_i N_i}{\bar{\mu}_i} + \frac{M_{j-1}}{\bar{\kappa}_j}\right) + \\ &\sum_{j=1}^{s}\frac{n_j}{N_s}\sum_{i=1}^{j-1}\frac{m_i}{\bar{\mu}_i}\sum_{k=1}^{i} n_k\left(\sum_{\ell=1}^{k-1}\frac{m_\ell N_\ell}{\bar{\mu}_\ell} + \frac{M_{k-1}}{\bar{\kappa}_k}\right) + \\ &\sum_{j=1}^{s}\frac{n_j M_{j-1}}{N_s\bar{\kappa}_j}\sum_{i=1}^{j-1}\frac{m_i}{\bar{\mu}_i}\left(N_i - \sum_{k=1}^{i} n_k\left(\sum_{\ell=1}^{k-1}\frac{m_\ell N_\ell}{\bar{\mu}_\ell} + \frac{M_{k-1}}{\bar{\kappa}_k}\right)\right)\Bigg). \end{aligned} \tag{4.25}$$

Proof. The proof goes along the same lines as that of Lemma 4.1. Taking into account Lemma 4.6, we use here a better estimation for b_j's and proceed by induction on s. When $s = 1$, from (4.14), the bound is reduced to the equality. Assume now that the bound is verified for some $s \geq 1$. From (4.9), we get

$$a_{s+1} = \frac{\kappa - d_s}{\kappa - d_{s+1}}\, a_s + \frac{n_{s+1}}{\kappa - d_{s+1}}\, b_{s+1}\,.$$

Applying (4.25) and (4.24) in the previous equality, and bearing in mind that

$$\frac{\kappa - d_s}{(\kappa - d_{s+1})\bar{\mu}_s} = \frac{1}{\bar{\mu}_{s+1}} \quad \text{and} \quad 1 - \frac{M_s}{\bar{\kappa}_{s+1}} = \frac{\bar{\kappa}_1}{\bar{\kappa}_{s+1}}\,,$$

the proof easily follows. □

The results from the above lemmas can be summarized as follows:

Theorem 4.1. *For any s, t, with $1 \leq s, t \leq h$, let*

$$\alpha_s = \frac{N_s}{\bar{\mu}_s}\left(1 - \sum_{j=1}^{s} \frac{n_j}{N_s}\left(\sum_{i=1}^{j-1} \frac{m_i N_i}{\bar{\mu}_i} + \frac{M_{j-1}}{\bar{\kappa}_j}\right)\right)$$

and

$$\beta_t = \frac{1}{\bar{\kappa}_t}\left(1 - \sum_{i=1}^{t-1} \frac{m_i N_i}{\bar{\mu}_i}\right)\,.$$

Then

$$\alpha_s \leq a_s \leq \alpha_s + \frac{N_s}{\bar{\mu}_s}\left(\sum_{j=1}^{s} \frac{n_j}{N_s} \sum_{i=1}^{j-1} \frac{m_i}{\bar{\mu}_i} \sum_{k=1}^{i} n_k \left(\sum_{\ell=1}^{k-1} \frac{m_\ell N_\ell}{\bar{\mu}_\ell} + \frac{M_{k-1}}{\bar{\kappa}_k}\right) + \sum_{j=1}^{s} \frac{n_j M_{j-1}}{N_s \bar{\kappa}_j} \sum_{i=1}^{j-1} \frac{m_i}{\bar{\mu}_i}\left(N_i - \sum_{k=1}^{i} n_k \left(\sum_{\ell=1}^{k-1} \frac{m_\ell N_\ell}{\bar{\mu}_\ell} + \frac{M_{k-1}}{\bar{\kappa}_k}\right)\right)\right)$$

and

$$\beta_t \leq b_t \leq \beta_t + \frac{1}{\bar{\kappa}_t} \sum_{i=1}^{t-1} \sum_{j=1}^{i} \frac{n_j m_i}{\bar{\mu}_i}\left(\sum_{k=1}^{j-1} \frac{m_k N_k}{\bar{\mu}_k} + \frac{M_{j-1}}{\bar{\kappa}_j}\right).$$

Remark 4.5. *We point out that the previous bounds are very tight. In fact the estimated intervals, where a_s and b_t lie, are of lengths less than*

$$\frac{N_s e_{s-1} e_{s-2}}{\bar{\mu}_s \bar{\mu}_{s-1} \bar{\mu}_{s-2}} + \frac{\bar{e}_{s-1} \bar{e}_s}{\bar{\mu}_s \bar{\mu}_{s-1} \bar{\kappa}_1} + \frac{\bar{e}_s e_{s-1}}{\bar{\mu}_s \bar{\mu}_{s-1} \bar{\kappa}_1}$$

and

$$\frac{e_{t-1}e_{t-2}}{\bar{\kappa}_t\bar{\mu}_{t-1}\bar{\mu}_{t-2}} + \frac{e_{t-1}M_{t-2}}{\bar{\kappa}_1\bar{\kappa}_t\bar{\mu}_{t-1}}\,,$$

respectively. In particular, we have that the exact values are obtained for $s, t = 1$ (see Remark 4.1).

4.2 Some bounds on the Q-index of an NSG

In this section we will prove some bounds on the Q-index of NSGs. We start with lower ones.

Proposition 4.1. *If G is a connected NSG, then*

$$\kappa \geq \max_{1\leq k\leq h} \frac{1}{2}\left[2d_k + D_k - 1 + \sqrt{(2d_k + D_k - 1)^2 - 8(d_h - 1)d_k}\right].$$

Proof. On the one hand, from (4.8), we get

$$b_k = \frac{1}{\bar{\kappa}_k}\left(\sum_{i=k}^{h} m_i a_i + (\kappa - d_h)a_h\right) \geq a_k\frac{M_h - M_{k-1} + \kappa - N_h}{\bar{\kappa}_k},$$

since a_i's are increasing, from (4.12). On the other hand, from (4.3), we get

$$a_k = \frac{1}{\kappa - d_k}\sum_{j=1}^{k} n_j b_j \geq b_k\frac{N_k}{\kappa - d_k},$$

since b_j's are decreasing, from (4.13). From the last two inequalities we get

$$\mu_k \geq (\kappa - N_h + M_h - M_{k-1})N_k\,,$$

which is equivalent to

$$\kappa^2 - (2d_k + D_k - 1)\kappa + (2d_h - 2)d_k \geq 0$$

reaching the desired result. □

In particular, for $k = h$ and $k = 1$, we obtain the following corollary.

Corollary 4.1. *If G is a connected NSG, then*

$$\kappa \geq \frac{1}{2}\left[3N_h + m_h - 2 + \sqrt{(N_h + m_h - 2)^2 + 4\hat{e}_h}\right] \tag{4.26}$$

and

$$\kappa \geq \frac{1}{2}\left[2n_1 + n - 2 + \sqrt{(n-2)^2 + 4n_1(n_1 + M_h - N_h)}\right]. \tag{4.27}$$

Proposition 4.2. *If G is a connected NSG, then*

$$\kappa \geq \frac{1}{2}\left[\frac{\sum_{i=1}^{h} n_i D_i}{N_h} + N_h - 1 + t + \sqrt{\left(\frac{\sum_{i=1}^{h} n_i D_i}{N_h} + N_h - 1 - t\right)^2 + 4\hat{e}_h^*}\right],$$

where

$$t = \frac{\sum_{i=1}^{h} m_i N_i^3}{\sum_{i=1}^{h} m_i N_i^2} \quad \textit{and} \quad \hat{e}_h^* = \sum_{i=1}^{h} \frac{N_i}{N_h}\hat{e}_i\,.$$

Proof. Let $\mathbf{y} = (y_1, \ldots, y_n)^T$ be a vector whose components are indexed by the vertices of G, and let $y_u = N_i$ if $u \in U_i$, for some $i \in \{1, \ldots, h\}$, or, otherwise, $y_v = q = \kappa - t$, for some t if $v \in V_j$ for some $j \in \{1, \ldots, h\}$. Substituting $\mathbf{y}$ into the Rayleigh quotient we obtain

$$\kappa \geq \frac{2\sum_{i=1}^{h} m_i N_i^2 q + 2\binom{N_h}{2}q^2 + \sum_{i=1}^{h} m_i d_i N_i^2 + \sum_{i=1}^{h} n_i D_i q^2}{\sum_{i=1}^{h} m_i N_i^2 + N_h q^2}.$$

Since $q = \kappa - t$, we get

$$N_h q^3 + \left[N_h t - 2\binom{N_h}{2} - \sum_{i=1}^{h} n_i D_i\right] q^2 - \sum_{i=1}^{h} m_i N_i^2 q \geq \sum_{i=1}^{h} m_i N_i^3 - t\sum_{i=1}^{h} m_i N_i^2\,.$$

Choosing $t = \frac{\sum_{i=1}^{h} m_i N_i^3}{\sum_{i=1}^{h} m_i N_i^2}$ and taking into account that $N_1 \leq t \leq N_h$, we immediately get a quadratic inequality in q and the proof is concluded. □

Proposition 4.3. *If G is a connected NSG, then*

$$\kappa \leq \frac{1}{2}\left[2N_h + n - 2 + \sqrt{(n-2)^2 + 4e_h}\right]. \tag{4.28}$$

Proof. From (4.3), with $s = h$ and (4.5), we get $\sum_{s=1}^{h} m_s a_s + (\kappa - d_h)a_h = 1$. Using (4.16) we obtain

$$1 \leq \sum_{s=1}^{h} \frac{m_s N_s}{\bar{\mu}_s} + (\kappa - d_h)\frac{N_h}{\bar{\mu}_h},$$

and, therefore, $\bar{\mu}_h \leq (\kappa - N_h)N_h + e_h$ or, equivalently,

$$\kappa^2 - (n - 2 + 2N_h)\kappa - e_h + (n - 2 + N_h)N_h \leq 0\,,$$

and the proof follows. □

The following two bounds improve the bound (4.28). Recall that $\bar{d} = \frac{2m}{n}$.

Proposition 4.4. *If G is a connected NSG, then*

$$\kappa \leq \frac{1}{2}\left[2N_h + n - 2 + \sqrt{(n-2)^2 + 4e'_h}\right],$$

where

$$e'_h = e_h - n_1 \left[\frac{\sum_{s=1}^{h} m_s\bar{e}_s + (M_h + \bar{d} - 1)\bar{e}_h}{(\nu - 1 + \bar{d} - n_1)(\bar{d} + 1)}\right].$$

Proof. As in the proof of the previous proposition we have

$$\sum_{s=1}^{h} m_s a_s + (\kappa - d_h)a_h = 1\,.$$

Using (5.19), we get

$$1 \leq \sum_{s=1}^{h} \frac{m_s}{\bar{\mu}_s}(N_s - a_1\bar{e}_s) + \frac{(\kappa - d_h)}{\bar{\mu}_h}(N_h - a_1\bar{e}_h),$$

and, therefore,

$$\bar{\mu}_h \leq \sum_{s=1}^{h} m_s(N_s - a_1\bar{e}_s) + (\kappa - d_h)(N_h - a_1\bar{e}_h).$$

So

$$\kappa^2 - (2N_h + \nu - 2)\kappa + N_h(N_h + \nu - 2) - \left[e_h - a_1\sum_{s=1}^{h} m_s\bar{e}_s - a_1(\kappa - d_h)\bar{e}_h\right] \leq 0.$$

Since $a_1 = \frac{N_1}{\mu_1}$ (see (4.14)) and $\kappa \leq \nu - 1 + \bar{d}$, we have $a_1\sum_{s=1}^{h} m_s\bar{e}_s \geq n_1\frac{\sum_{s=1}^{h} m_s\bar{e}_s}{(\nu-1+\bar{d}-n_1)(\bar{d}+1)}$ and $a_1(\kappa - d_h)\bar{e}_h = n_1(\frac{\bar{e}_h}{\kappa - n_1} + \frac{(\nu-2-N_h)\bar{e}_h}{(\kappa-n_1)(\kappa-\nu+2)}) \geq n_1\frac{(M_h+\bar{d}-1)\bar{e}_h}{(\nu-1+\bar{d}-n_1)(\bar{d}+1)}$ and the proof easily follows. □

Proposition 4.5. *If G is a connected NSG, then*

$$\kappa \leq \frac{1}{2}\left[2N_h + n' - 2 + \sqrt{(n'-2)^2 + 4e'_h}\right],$$

where

$$n' = n - \frac{n_1\bar{e}_h}{(n - 1 + \bar{d} - n_1)(\bar{d} + 1)} \quad \textit{and} \quad e'_h = e_h - \frac{n_1\sum_{s=1}^{h} m_s\bar{e}_s}{(n - 1 + \bar{d} - n_1)(\bar{d} + 1)}.$$

Proof. As in the proof of Proposition 4.4 we have

$$\kappa^2 - (2N_h + n - 2)\kappa + N_h(N_h + n - 2) - \left(e_h - a_1\sum_{s=1}^{h} m_s\bar{e}_s - a_1(\kappa - d_h)\bar{e}_h\right) \leq 0.$$

or, equivalently,

$$\kappa^2 - (2N_h + n - 2 - a_1\bar{e}_h)\kappa + N_h(N_h + n - 2 - a_1\bar{e}_h) - \left(e_h - a_1 \sum_{s=1}^{h} m_s \bar{e}_s\right) \leq 0\,.$$

Again, substituting a_1 (4.14) and taking $\mu_1 \leq (n-1+\bar{d}-n_1)(\bar{d}+1)$, the proof follows. □

4.3 Computational results

In this section we give some selected computational results (generated with *Mathematica*) which will help us to gain a better insight into the quality of the bounds obtained in the previous section. All errors reported below are relative ones.

Example 4.1. *We have $n = 20$, and assume that $m = 100$ and $N_h = 12$. There are 125 such NSGs, or $0, 1, 9, 30, 62, 22, 1, 0$ ones, for each $h = 1, 2, 3, 4, 5, 6, 7, 8$, respectively. In particular, for $h = 4$, we will take a sample graph (so one out of 30) with the following parameters:*

$$(m_1, m_2, m_3, m_4) = (4, 2, 1, 1) \quad \textit{and} \quad (n_1, n_2, n_3, n_4) = (2, 1, 5, 4)\,.$$

The exact value of the Q-index and the corresponding (lower and upper) bounds (together with errors) are given in the following table:

Prop. 4.1	*Prop. 4.2*	κ	*Prop. 4.5*	*Prop. 4.4*	*Prop. 4.3*
24.0000	*26.0594*	*26.8105*	*31.3072*	*31.3538*	*31.7238*
−10.5 %	−2.80 %	*0*	*16.8 %*	*16.9 %*	*18.3 %*

Example 4.2. *The NSGs given here will be derived from the NSG considered in the previous example. We first multiply each of its (basic) parameters by 10, 100, and 1000, respectively. Then we get:*

1. $NSG(40, 20, 10, 10; 20, 10, 50, 40)$

Prop. 4.1	*Prop. 4.2*	κ	*Prop. 4.5*	*Prop. 4.4*	*Prop. 4.3*
256.774	*277.454*	*284.920*	*329.782*	*330.250*	*333.896*
−9.88%	−2.62%	*0*	*16.7%*	*15.9%*	*17.2%*

2. $NSG(400, 200, 100, 100; 200, 100, 500, 400)$

Prop. 4.1	Prop. 4.2	κ	Prop. 4.5	Prop. 4.4	Prop. 4.3
2584.66	2791.51	2866.13	3314.63	3319.32	3355.72
−9.82%	−2.60%	0	15.6%	15.8%	17.1%

3. $NSG(4000, 2000, 1000, 1000; 2000, 1000, 5000, 4000)$

Prop. 4.1	Prop. 4.2	κ	Prop. 4.5	Prop. 4.4	Prop. 4.3
25863.6	27932.1	28678.3	33163.1	33210.0	33574.0
−9.81%	−2.60%	0	15.6%	15.8%	17.1%

The following sample graphs are obtained by multiplying only one of the parameters from the NSG of Example 4.1 by 10000. *Then we have:*

4. $NSG(40000, 2, 1, 1; 2, 1, 5, 4)$

Prop. 4.1	Prop. 4.2	κ	Prop. 4.5	Prop. 4.4	Prop. 4.3
40018.0	6692.83	40018.0	40024.0	40024.0	40028.0
$-2.5 \cdot 10^{-6}$%	−83.3%	0	0.015%	0.015%	0.025%

5. $NSG(4, 20000, 1, 1; 2, 1, 5, 4)$

Prop. 4.1	Prop. 4.2	κ	Prop. 4.5	Prop. 4.4	Prop. 4.3
20020.0	5027.32	20021.1	20028.4	20028.4	20031.0
$-5.6 \cdot 10^{-3}$%	−74.9%	0	0.037%	0.037%	0.049%

6. $NSG(4, 2, 10000, 1; 2, 1, 5, 4)$

Prop. 4.1	Prop. 4.2	κ	Prop. 4.5	Prop. 4.4	Prop. 4.3
10027.0	6698.81	10029.2	10036.5	10036.5	10037.0
−0.022%	−33.2%	0	0.073%	0.073%	0.078%

7. $NSG(4, 2, 1, 10000; 2, 1, 5, 4)$

Prop. 4.1	Prop. 4.2	κ	Prop. 4.5	Prop. 4.4	Prop. 4.3
10034.0	10035.8	10036.1	10041.0	10041.0	10041.0
−0.021 %	$-2.8 \cdot 10^{-3}$ %	0	0.049 %	0.049 %	0.049 %

8. $NSG(4, 2, 1, 1; 20000, 1, 5, 4)$

Prop. 4.1	Prop. 4.2	κ	Prop. 4.5	Prop. 4.4	Prop. 4.3
40020.0	40034.0	40034.0	40034.0	40034.0	40034.0
−0.03 %	$-1 \cdot 10^{-8}$ %	0	$1.5 \cdot 10^{-5}$ %	$1.5 \cdot 10^{-5}$ %	$2.3 \cdot 10^{-5}$ %

9. $NSG(4, 2, 1, 1; 2, 10000, 5, 4)$

Prop. 4.1	Prop. 4.2	κ	Prop. 4.5	Prop. 4.4	Prop. 4.3
20022.0	20028.0	20028.0	20032.0	20032.0	20032.0
−0.029 %	$-1.6 \cdot 10^{-8}$ %	0	0.02 %	0.02%	0.02 %

10. $NSG(4,2,1,1;2,1,50000,4)$

Prop. 4.1	*Prop. 4.2*	κ	*Prop. 4.5*	*Prop. 4.4*	*Prop. 4.3*
100014.0	*100016.0*	*100016.0*	*100022.0*	*100022.0*	*100022.0*
$-2 \cdot 10^{-3}$ %	$-4.7 \cdot 10^{-11}$ %	*0*	$6 \cdot 10^{-3}$ %	$6 \cdot 10^{-3}$ %	$6 \cdot 10^{-3}$ %

11. $NSG(4,2,1,1;2,1,5,40000)$

Prop. 4.1	*Prop. 4.2*	κ	*Prop. 4.5*	*Prop. 4.4*	*Prop. 4.3*
80016.0	*80016.0*	*80016.0*	*80023.0*	*80023.0*	*80023.0*
$-7 \cdot 10^{-7}$ %	$-1 \cdot 10^{-10}$ %	*0*	$8.7 \cdot 10^{-3}$ %	$8.7 \cdot 10^{-3}$ %	$8.7 \cdot 10^{-3}$ %

4.4 Some further bounds on Q-index of an NSG

In this section we give another two upper bounds on the Q-index of an NSG which are expressed as solutions of cubic equations. For this purpose we will need the following inequality.

Lemma 4.8. *If G is a connected NSG, then for any s $(1 \leq s \leq h)$*

$$\frac{1}{\kappa - d_s} \leq \frac{1}{\kappa} + \frac{2d_s}{\kappa^2}. \tag{4.29}$$

Proof. We have that $\kappa \geq 2d_h$ (see (4.26)). So $\kappa \geq 2d_s$ for any $s = 1, \dots, h$. On the other hand, (4.29) is equivalent to the latter inequality, and we are done. □

Proposition 4.6. *If G is a connected NSG, then κ is less than or equal to the only positive solution of the equation*

$$x^3 - (n - 2 + d_h)x^2 - e_h x - 2\sum_{i=1}^{h} m_s d_s^2 = 0$$

Proof. From the eigenvalue equation applied to any vertex from U_h we get that $\kappa a_h = d_h a_h + \sum_{t=1}^{h} n_t b_t$. Therefore, from (4.5) it follows that

$$\sum_{s=1}^{h} m_s a_s + (\kappa - d_h)a_h = 1.$$

Since, by (4.16)

$$a_s \leq \frac{d_s}{\bar{\mu}_s} \quad (s = 1, \dots, h),$$

where $\bar{\mu}_s = (\kappa - d_s)(\kappa - D_1 + 1)$, we easily get (making use of Lemma 4.8 above) that

$$\kappa^3 - (n - 2 + d_h)\kappa^2 - e_h\kappa - 2\sum_{i=1}^{h} m_s d_s^2 \leq 0,$$

as required.

For the rest, we analyze the properties of the function

$$f(x) = x^3 - (n - 2 + d_h)x^2 - e_h x - 2\sum_{s=1}^{h} m_s d_s^2.$$

Clearly, $f(x)$ has two local extrema, one positive x_1' and one negative x_2' . Since κ takes only positive values we assume that $x \geq 0$. Next, since $f(0) < 0$, x_1' is a local minimum. Therefore, the equation $f(x) = 0$ has only one positive solution, say x_1, and $f(x) \leq 0$ is equivalent to $x \leq x_1$.

This completes the proof. □

Using the similar arguments as in Proposition 4.6 we get:

Proposition 4.7. *If G is a connected NSG, then κ is less than or equal to the only positive solution of the equation*

$$x^3 - (n^{''} - 2 + d_h)x^2 - e_h^{''} x - 2(\sum_{i=1}^{h} m_s d_s^2 - \sigma') = 0,$$

where

$$n^{''} = n - \frac{d_1 \bar{e}_h}{(n - 1 + \bar{d} - d_1)(\bar{d} + 1)}, \quad e_h^{''} = e_h - \frac{d_1 \sum_{s=1}^{h} m_s \bar{e}_s}{(n - 1 + \bar{d} - d_1)(\bar{d} + 1)}$$

and

$$\sigma' = \frac{d_1 \sum_{s=1}^{h} m_s d_s \bar{e}_s}{(n - 1 + \bar{d} - d_1)(\bar{d} + 1)}.$$

Proof. As in the proof of the previous proposition we have

$$\sum_{s=1}^{h} m_s a_s + (\kappa - d_h)a_h = 1.$$

Now we will use a better estimate for a_s. As proved in (4.21), we have that

$$a_s \leq \frac{1}{\bar{\mu}_s}(d_s - a_1 \bar{e}_s) \quad (s = 1, \ldots, h).$$

Therefore we get

$$1 \leq \sum_{s=1}^{h} \frac{m_s}{\bar{\mu}_s}(d_s - a_1 \overline{e}_s) + \frac{(\kappa - d_h)}{\bar{\mu}_h}(d_h - a_1 \overline{e}_h),$$

or equivalently

$$\kappa^3-(n-2+d_h)\kappa^2-e_h\kappa-2\sum_{s=1}^{h}m_sd_s^2+a_1(\bar{e}_h\kappa^2+\sum_{s=1}^{h}m_s\bar{e}_s\kappa+2\sum_{s=1}^{h}m_sd_s\bar{e}_s)\leq 0.$$

Note first that $a_1=\frac{d_1}{\bar{\mu}_1}$. Applying the first inequality from Lemma 4.1 and the inequality $\kappa\leq n-1+\bar{d}$ we first get

$$a_1\geq\frac{d_1}{(n-1+\bar{d}-d_1)(\bar{d}+1)}.$$

Therefore

$$\kappa^3-(n''-2+d_h)\kappa^2-e''_h\kappa-2(\sum_{s=1}^{h}m_sd_s^2-\sigma')\leq 0,$$

as required. In the remainder we apply the same reasoning as in the proof of the previous proposition.

This completes the proof. □

4.5 More computational data

In this section we give some computational results (again generated with *Mathematica*). In the last column we have put the bound from Proposition 4.5 since it gives the best upper approximation in Section 4.2. Our main conclusion is that these bounds (except those which are the direct improvements of some others) are incomparable. All errors reported below are relative ones.

Example 4.3. *If we take, as in Example 4.1, that* $G=NSG(4,2,1,1;2,1,5,4)$ *then the exact value of the Q-index, and the corresponding upper bounds (together with errors) are given in the following table:*

Prop. 4.6	*Prop. 4.7*	κ	*Prop. 4.5*
31.563	*31.1367*	*26.8105*	*31.3072*
17.7 %	16.1 %	*0*	16.8%

So the bound from Proposition 4.7 is the best. It is noteworthy that in this situation the bound $\kappa\leq n-1+\bar{d}$ *is better then all from the above table (it gives* $\kappa\leq 29$*). But in general this does not hold. For example, if we take that* $G'=(1,2,12;3,1,1)$ *then* $\kappa=25.67$*, while the* *bound from Proposition 4.7 is* 26.55 *(relative error is* 3.44%*), while the value of* $n-1+\bar{d}$ *is* 27.10 *(relative error is* 5.57%*). Many NSGs such as* G' *can be constructed, but it turns that more frequently we encounter graphs for which the bound* $\kappa \leq n-1+\bar{d}$ *is superior.*

Example 4.4. *Now we will test the new bounds on the same NSGs as in the Example 4.2.*

1. $NSG(40, 20, 10, 10; 20, 10, 50, 40)$:

Prop. 4.6	*Prop. 4.7*	κ	*Prop. 4.5*
332.598	*328.406*	*284.920*	*329.782*
16.7 %	15.3%	*0*	16.7%

2. $NSG(400, 200, 100, 100; 200, 100, 500, 400)$

Prop. 4.6	*Prop. 4.7*	κ	*Prop. 4.5*
3343.01	*3301.16*	*2866.13*	*3314.63*
16.6%	15.2%	*0*	15.6%

3. $NSG(4000, 2000, 1000, 1000; 2000, 1000, 5000, 4000)$

Prop. 4.6	*Prop. 4.7*	κ	*Prop. 4.5*
33447.2	*33028.7*	*28678.3*	*33163.1*
16.6%	15.2%	*0*	15.6%

So we again have that the bound from Proposition 4.7 is the best.

4. $NSG(40000, 2, 1, 1; 2, 1, 5, 4)$

Prop. 4.6	*Prop. 4.7*	κ	*Prop. 4.5*
40028.0	*40024.0*	*40018.0*	*40024.0*
0.025%	0.015%	*0*	0.015%

5. $NSG(4, 20000, 1, 1; 2, 1, 5, 4)$

Prop. 4.6	*Prop. 4.7*	κ	*Prop. 4.5*
20031.0	*20028.4*	*20021.1*	*20028.4*
0.049%	0.036%	*0*	0.037%

6. $NSG(4, 2, 10000, 1; 2, 1, 5, 4)$

Prop. 4.6	*Prop. 4.7*	κ	*Prop. 4.5*
10037.0	*10036.5*	*10029.2*	*10036.5*
0.078%	0.073%	*0*	0.073%

7. $NSG(4, 2, 1, 10000; 2, 1, 5, 4)$

Prop. 4.6	*Prop. 4.7*	κ	*Prop. 4.5*
10041.0	*10041.0*	*10036.1*	*10041.0*
0.049 %	0.049 %	*0*	0.049%

8. $NSG(4, 2, 1, 1; 20000, 1, 5, 4)$

Prop. 4.6	*Prop. 4.7*	κ	*Prop. 4.5*
40034.0	*40034.0*	*40034.0*	*40034.0*
$2.3 \cdot 10^{-5}$ %	$1.5 \cdot 10^{-5}$ %	*0*	$1.5 \cdot 10^{-5}$%

9. $NSG(4, 2, 1, 1; 2, 10000, 5, 4)$

Prop. 4.6	*Prop. 4.7*	κ	*Prop. 4.5*
20032.0	*20032.0*	*20028.0*	*20032.0*
0.02 %	0.02 %	*0*	0.02%

10. $NSG(4, 2, 1, 1; 2, 1, 50000, 4)$

Prop. 4.6	*Prop. 4.7*	κ	*Prop. 4.5*
100022.0	*100022.0*	*100016.0*	*100022.0*
$6 \cdot 10^{-3}$ %	$6 \cdot 10^{-3}$ %	*0*	$6 \cdot 10^{-3}$%

11. $NSG(4, 2, 1, 1; 2, 1, 5, 40000)$

Prop. 4.6	*Prop. 4.7*	κ	*Prop. 4.5*
80023.0	*80023.0*	*80016.0*	*80023.0*
$8.7 \cdot 10^{-3}$ %	$8.7 \cdot 10^{-3}$ %	*0*	$8.7 \cdot 10^{-3}$%

The above results deserve some further comments. First, for all graphs except those from items 7. and 8. the bound $\kappa \leq n - 1 + \bar{d}$ is superior. On the other hand, as we proceed as above taking G' in the role of G, then the situation is changed, namely in most cases the bound $\kappa \leq n - 1 + \bar{d}$ is not superior (we will not go into these details because we insist that the graph G is randomly chosen).

We have made some further experiments by varying parameters of NSGs: say h was taken to be up to 30, while m_i's, and n_j's, were randomly chosen in ranges like $1-10$, $1-100$, $1-1000$ etc. In these examples it turns that the bound from Proposition 4.7 was, most frequently, superior than the bounds from Propositions 4.3 - 4.5, but usually not more than 1% better. On the other hand, we have also found, by an exhaustive search, some NSGs for which relative errors in all upper bounds were unexpectedly big, say around 40%. On the other hand, we have also found that the bound $\kappa \leq n - 1 + \bar{d}$ is superior than all our bounds from this chapter. One of the reason for this phenomena to hold is that the latter one is found by computer aided search by using a very power heuristics VNS (variable neighbourhood search) implemented into package AGX (see [29]).

Chapter 5

Bounds on the index of double nested graphs

As we have seen in Chapter 3 the class of NSGs is important because any graph with maximal index in the set of connected graphs of fixed order and size must be an NSG. So far, the connected graphs of fixed order and size, with maximal index have not been identified in the general case.

If we restrict ourselves to connected bipartite graphs, then the analogous question can be posed. Some results relevant to the latter problem can be found in [14, 16]. The structure of graphs which now arises is considered in [9, 11] and, independently, in [14]. According to [11], any such graph must be a *double nested graph* (or DNG for short) or, according to [14], a *chain graph* (more details will be given in the next section). We note here that DNGs appear in [9, 11] in studying graphs whose least eigenvalue is minimal among the connected graphs of fixed order and size.

There are not too many papers dealing with bounds for the index of bipartite graphs. Besides [14, 16], see, for example, [39]. If we restrict ourselves to DNGs, then the only relevant reference is [14]. In this chapter, we exploit the eigenvector technique for obtaining lower and upper bounds for the index of DNGs in the same spirit as in Chapter 4.

The rest of the chapter is organized as follows. In Section 5.1, we include some basic details

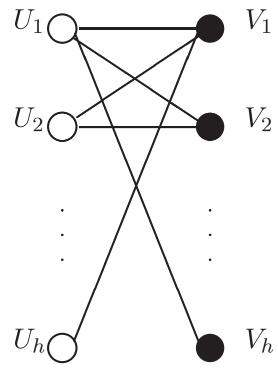

Figure 5.1: The structure of a double nested graph.

on the structure of DNGs. In Section 5.2, we investigate the relation between the parameters of a DNG and the components of an eigenvector corresponding to the index. In Section 5.3, we deduce the lower and upper bounds for the index of DNGs. In Section 5.4, we give some applications in bounding the index of NSGs. Finally, in Section 5.5, we give some computational results for attesting the quality of the new bounds.

5.1 Structure of double nested graphs

In this section, we describe the structure of connected DNGs (so isolated vertices are ignored). The vertex set of any such graph G consists of two colour classes (or co-cliques). To specify the nesting, both of them are partitioned into h non-empty cells $\bigcup_{i=1}^{h} U_i$ and $\bigcup_{i=1}^{h} V_i$, respectively; all vertices in U_s are joined (by cross edges) to all vertices in $\bigcup_{k=1}^{h+1-s} V_k$, for $s = 1, 2, \ldots, h$. Hence, if $u' \in U_{s+1}$ and $u'' \in U_s$, $v' \in V_{t+1}$ and $v'' \in V_t$ then $N_G(u') \subset N_G(u'')$ and $N_G(v') \subset N_G(v'')$, and this makes precise the double nesting property (here $1 \leq s, t \leq h$) (see Figure 5.1).

If $m_s = |U_s|$ and $n_s = |V_s|$ $(s = 1, 2, \ldots, h)$, then G is denoted by

$$DNG(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)\,.$$

We also write $m = (m_1, m_2, \ldots, m_h)$ and $n = (n_1, n_2, \ldots, n_h)$, and then, for short, $G = DNG(m; n)$.

We now introduce some notation to be used later on. Let

$$M_s = \sum_{i=1}^{s} m_i \quad \text{and} \quad N_t = \sum_{j=1}^{t} n_j\,, \quad \text{for } 1 \le s,t \le h.$$

Thus G is of order $\nu = M_h + N_h$, and size $\epsilon = \sum_{s=1}^{h} m_s N_{h+1-s}$. Observe that N_{h+1-s} is the degree of a vertex $u \in U_s$; the degree of a vertex $v \in V_t$ is equal to M_{h+1-t}. We will denote them by d'_s and d''_t, respectively.

We next define the following three quantities:

$$\hat{e}_s = m_s N_{h+1-s},$$

the number of cross edges with one end in U_s;

$$e_s = \sum_{i=1}^{s} \hat{e}_i = \sum_{i=1}^{s} m_i N_{h+1-i},$$

the total number of cross edges with one end in $U_{1,s} := \bigcup_{k=1}^{s} U_k$;

$$\bar{e}_s = M_s N_h - e_s = \sum_{j=1}^{s} m_j (N_h - N_{h+1-j}),$$

the total number of cross non-edges with one end in $U_{1,s}$.

More generally, setting $M_0 = N_0 = 0$, we define

$$M_{st} = \sum_{i=s}^{t} m_i = M_t - M_{s-1}\,, \quad N_{st} = \sum_{j=s}^{t} n_j = N_t - N_{s-1}\,;$$

on the other hand, not quite analogously, we define e_{st} as follows:

$$e_{st} = \sum_{i=s+1}^{t} m_i N_{h+1-i} \;= e_t - e_s.$$

Similarly, we can introduce further parameters if we exchange the roles of sets of $\cup_{i=1}^{h} U_i$ and $\cup_{j=1}^{h} V_j$. The parameters that arise in this way will be named by the letter f.

The following invariants for DNGs will be of interest in Section 5.3. If G is a DNG then

$$\sigma(G) = \sum_{s=1}^{h} m_s \sum_{j=1}^{h+1-s} n_j e_{h+1-j,h},$$

and analogously

$$\tau(G) = \sum_{t=1}^{h} n_t \sum_{i=1}^{h+1-t} m_i f_{h+1-i,h}.$$

We next prove:

Proposition 5.1. *If G is a DNG, then*

$$\sigma(G) = \tau(G) = \epsilon^2 - \sum_{(s,t)\in T_h} \hat{e}_s \hat{f}_t,$$

where $T_h = \{(s,t) : 1 \le s \le h, 1 \le t \le h, s+t \le h+1\}$.

Proof. Since $e_{s,h} = e_h - e_s$, we have

$$\sum_{s=1}^{h} m_s \sum_{j=1}^{h+1-s} n_j e_{h+1-j,h} = \epsilon^2 - \sum_{s=1}^{h} m_s \sum_{j=1}^{h+1-s} n_j e_{h+1-j}.$$

Exchanging the order of summation, we obtain

$$\sum_{s=1}^{h} m_s \sum_{j=1}^{h+1-s} n_j e_{h+1-j} = \sum_{(s,j)\in T_h} m_s n_j e_{h+1-j} = \sum_{j=1}^{h} \sum_{s=1}^{h+1-j} m_s n_j e_{h+1-j}.$$

Next, we have

$$\sum_{j=1}^{h} n_j M_{h+1-j} e_{h+1-j} = \sum_{j=1}^{h} \left(\hat{f}_j \sum_{s=1}^{h+1-j} \hat{e}_s \right) = \sum_{(s,j)\in T_h} \hat{e}_s \hat{f}_j.$$

Therefore $\sigma(G) = \epsilon^2 - \sum_{(s,t)\in T_h} \hat{e}_s \hat{f}_t$. The rest follows by symmetry. □

We now mention some general observations about the above parameters. First, we claim

$$1 \le h \le \min\left\{ \frac{\nu}{2}, \frac{-1+\sqrt{1+8\epsilon}}{2} \right\}.$$

The lower bound is attained whenever G is a complete bipartite graph. In this case, $h = 1$ and $M_1 = \frac{\nu+\sqrt{\nu^2-4\epsilon}}{2}$, and so a complete bipartite graph does not exist for every ν and ϵ.

To obtain the upper bound, note that h is largest if all m_i's and n_i's are equal to one. Thus in general we have that $h + (h-1) + \cdots + 1 \le \epsilon$, and consequently $\frac{h^2+h}{2} \le \epsilon$. On the other hand $h \le \frac{\nu}{2}$, which establishes our claim.

Next, for fixed ν and ϵ, we first note that when $h \ge 2$, we have

$$\epsilon + [(h-1) + (h-2) + \cdots + 1] \le M_h N_h,$$

where the second sum estimates the number of cross non-edges at each level. The equality holds if and only if $m_1 = M_h - (h-1)$, $m_2 = \cdots = m_h = 1$, or equivalently, $n_1 =$

$N_h-(h-1),\ n_2=\cdots=n_h=1$. Therefore, it follows easily that

$$\frac{1}{2}\left[\nu-\sqrt{\nu^2-4\left(\epsilon+\binom{h}{2}\right)}\right]\leq M_h,N_h\leq\frac{1}{2}\left[\nu+\sqrt{\nu^2-4\left(\epsilon+\binom{h}{2}\right)}\right].$$

Note that the argument of the square root is always positive.

Next we observe that

$$\epsilon\geq\binom{h+1}{2}+\max\{M_h-h,N_h-h\},$$

where the expression to the right counts guaranteed edges in the subgraph with all m_i's and n_j's equal to 1, and some of the remaining edges. Clearly, equality holds if and only if $m_h=M_h-(h-1)$, $n_h=N_h-(h-1)$, and $m_1=\cdots=m_{h-1}=n_1=\cdots=n_{h-1}=1$. Therefore

$$\max\{M_h,N_h\}\leq\epsilon-\binom{h}{2}.$$

We remark that the above bounds can be useful in generating DNGs of a given order and size.

In the remainder of this section we point out one interesting feature of DNGs. Let α,β be natural numbers, and let αm, βn be new h-tuples obtained by multiplying entries by α, β respectively.

Proposition 5.2. *If $G=DNG(m;n)$ and $G'=DNG(m';n')$, where $m'=\alpha m$ and $n'=\beta n$, then*

$$\rho(G')=\sqrt{\alpha\beta}\,\rho(G).$$

Proof. Clearly, $U_1\cup\cdots\cup U_h\cup V_1\cup\cdots\cup V_h$ is an equitable partition in G, and analogously, $U_1'\cup\cdots\cup U_h'\cup V_1'\cup\cdots\cup V_h'$ in G'. Then the adjacency matrices of divisors have the following form

$$\begin{bmatrix} O & B\\ C & O\end{bmatrix},\quad\begin{bmatrix} O & B'\\ C' & O\end{bmatrix},$$

where $B'=\beta B$ and $C'=\alpha C$. Considering the squares of these matrices, we easily get $\rho(G)^2=\rho(BC)$ and $\rho(G')^2=\rho(B'C')$, and the proof immediately follows. □

5.2 ρ-eigenvectors of DNGs

For a connected DNG G, of order ν and size ϵ, let $\rho = \rho(G)$ be its index. Since A is a non-negative and irreducible matrix, an eigenvector corresponding to the index can be taken to be positive. Unless stated otherwise, we will denote it by

$$\mathbf{x} = (x_1, x_2, \ldots, x_\nu)^T;$$

also we will usually take $\sum_{i=1}^{\nu} x_i = 1$. We will refer to x_i as the weight of a vertex v_i.

We first observe that all vertices within the sets U_s and V_t, for fixed s and t $(1 \leq s, t \leq h)$, have the same weight, since they belong to the same orbit of the automorphism group of G. Let $x_u = a_s$ if $u \in U_s$, while $x_v = b_t$ if $v \in V_t$.

In the rest of the section, due to symmetry, we will put focus mainly on relations involving a_i's (similar relations for b_i's are obtained by interchanging the roles of the m_i's and n_i's).

From the eigenvalue equations for ρ, applied to any vertex of U_s, we obtain

$$a_s = \frac{1}{\rho} \sum_{j=1}^{h+1-s} n_j b_j\,, \quad \text{for } s = 1, \ldots, h\,. \tag{5.1}$$

Similarly, we have

$$b_t = \frac{1}{\rho} \sum_{i=1}^{h+1-t} m_i a_i\,, \quad \text{for } t = 1, \ldots, h\,. \tag{5.2}$$

By normalization we have

$$\sum_{i=1}^{h} m_i a_i + \sum_{j=1}^{h} n_j b_j = 1. \tag{5.3}$$

Therefore we easily obtain

$$a_s = \frac{1}{\rho} \left(1 - \sum_{i=1}^{h} m_i a_i - \sum_{j=h+2-s}^{h} n_j b_j \right)\,, \quad \text{for } s = 1, \ldots, h\,. \tag{5.4}$$

Next, using (5.2) for $t = 1$, we obtain

$$a_s = \frac{1}{\rho} \left(1 - \rho b_1 - \sum_{j=h+2-s}^{h} n_j b_j \right)\,, \quad \text{for } s = 1, \ldots, h\,. \tag{5.5}$$

Similarly, we have

$$b_t = \frac{1}{\rho}\left(1 - \rho a_1 - \sum_{i=h+2-t}^{h} m_i a_i\right), \quad \text{for } t = 1, \ldots, h. \tag{5.6}$$

Setting $a_{h+1} = b_{h+1} = 0$, we next obtain

$$\rho(a_s - a_{s+1}) = n_{h+1-s} b_{h+1-s}, \quad \text{for } s = 1, \ldots, h-1, \tag{5.7}$$

and

$$\rho(a_h - a_{h+1}) = n_1 b_1, \quad \text{for } s = h. \tag{5.8}$$

Since all components of $\mathbf{x}$ are positive, we conclude that

$$a_{s+1} < a_s, \quad \text{for } s = 1, \ldots, h-1, \tag{5.9}$$

and similarly, that

$$b_{t+1} < b_t, \quad \text{for } t = 1, \ldots, h-1. \tag{5.10}$$

Note that from (5.8) we also have

$$a_h = \frac{n_1}{\rho} b_1 \quad \text{and} \quad b_h = \frac{m_1}{\rho} a_1. \tag{5.11}$$

In addition, putting $s = 1$ in (5.1) and $t = 1$ in (5.2), and using (5.3), we obtain

$$\rho(a_1 + b_1) = 1. \tag{5.12}$$

Therefore, from (5.5) and (5.6) we also have

$$a_s = a_1 - \frac{1}{\rho} \sum_{j=h+2-s}^{h} n_j b_j, \quad \text{for } s = 1, \ldots, h \tag{5.13}$$

and

$$b_t = b_1 - \frac{1}{\rho} \sum_{i=h+2-t}^{h} m_i a_i, \quad \text{for } t = 1, \ldots, h. \tag{5.14}$$

In the next seven lemmas we focus our attention on bounding the a_i's (and so also the b_j's in parallel).

Lemma 5.1. *For any $s = 1, \dots, h$, we have*

$$\frac{N_{h+1-s}}{\rho}\, b_{h+1-s} \leq a_s \leq \frac{N_{h+1-s}}{\rho}\, b_1. \tag{5.15}$$

Proof. From (5.1) we have

$$a_s = \frac{1}{\rho} \sum_{j=1}^{h+1-s} n_j b_j\,.$$

Therefore (5.15) follows immediately, since b_j's are strictly decreasing – see (5.10). □

Similarly we can prove: if $1 \leq j \leq i-1$ then for any $i \leq h$ we have

$$\frac{N_{h+2-i,h+1-j}}{\rho}\, b_{h+1-j} \leq a_j - a_i \leq \frac{N_{h+2-i,h+1-j}}{\rho}\, b_{h+2-i}. \tag{5.16}$$

In addition, we have:

Lemma 5.2. *For any $s = 1, \dots, h$ we have*

$$a_1 - \frac{b_{h+2-s}}{\rho}\, N_{h+2-s,h} \leq a_s \leq a_1 \left(1 - \frac{m_1}{\rho^2}\, N_{h+2-s,h}\right). \tag{5.17}$$

Proof. From (5.13) we have

$$a_s = a_1 - \frac{1}{\rho} \sum_{j=h+2-s}^{h} n_j b_j.$$

Therefore (5.17) follows, since the b_i's are strictly decreasing. For the upper bound we have used the fact that $b_h = \frac{m_1 a_1}{\rho}$; cf. (5.11). □

Lemma 5.3. *For any $s = 1, \dots, h$, we have*

$$a_s \geq a_1 \left(1 - \frac{1}{\rho^2} f_{h+1-s,h}\right). \tag{5.18}$$

Proof. We use induction on s. For $s = 1$, the inequality is reduced to $a_1 \geq a_1$. Next, let us assume that $a_s \geq a_1 \left(1 - \frac{1}{\rho^2} f_{h+1-s,h}\right)$, for some $s \geq 1$. From (5.7), using first (5.2), we obtain successively

$$\begin{aligned} a_{s+1} &= a_s - \frac{1}{\rho} n_{h+1-s} b_{h+1-s} \\ &= a_s - \frac{n_{h+1-s}}{\rho^2} \sum_{i=1}^{s} m_i a_i \\ &\geq a_1 \left(1 - \frac{1}{\rho^2} f_{h+1-s,h}\right) - \frac{n_{h+1-s}}{\rho^2} M_s a_1 \\ &= a_1 \left(1 - \frac{1}{\rho^2} f_{h-s,h}\right) \end{aligned}$$

and the proof is completed. □

Lemma 5.4. *For any $s = 1, \ldots, h$, we have*

$$a_s \leq \frac{b_1}{\rho} \left(N_{h+1-s} - \frac{n_1}{\rho^2} \bar{f}_{h+1-s} \right). \tag{5.19}$$

Proof. From (5.1), and the second inequality in (5.17) applied to b_j, we have

$$\begin{aligned} a_s &= \frac{1}{\rho} \sum_{j=1}^{h+1-s} n_j b_j \\ &\leq \frac{1}{\rho} \sum_{j=1}^{h+1-s} n_j b_1 \left(1 - \frac{n_1}{\rho^2} (M_h - M_{h+1-j})\right) \\ &= \frac{b_1}{\rho} \left(N_{h+1-s} - \frac{n_1}{\rho^2} \bar{f}_{h+1-s} \right) \end{aligned}$$

and the proof follows. □

Clearly, (5.19) is an improvement of the right hand side of (5.15). Yet another improvement is given later (see (5.24)).

Lemma 5.5. *For any $s = 1, \ldots, h$, we have*

$$a_s \geq \frac{b_1 N_{h+1-s}}{\rho} \left(1 - \frac{1}{\rho^2} \sum_{j=1}^{h+1-s} \frac{n_j e_{h+1-j,h}}{N_{h+1-s}} \right). \tag{5.20}$$

Proof. From (5.1) and (5.18) applied to b_j we obtain

$$\begin{aligned} a_s &= \frac{1}{\rho} \sum_{j=1}^{h+1-s} n_j b_j \\ &\geq \frac{1}{\rho} \sum_{j=1}^{h+1-s} n_j b_1 \left(1 - \frac{1}{\rho^2} e_{h+1-j,h}\right) \\ &= \frac{b_1 N_{h+1-s}}{\rho} \left(1 - \frac{1}{\rho^2} \sum_{j=1}^{h+1-s} \frac{n_j}{N_{h+1-s}} e_{h+1-j,h}\right). \end{aligned}$$

□

Note that from (5.20) we can deduce that

$$a_s \geq \frac{b_1 N_{h+1-s}}{\rho} \left(1 - \frac{e_{s,h}}{\rho^2}\right). \tag{5.21}$$

Lemma 5.6. *For any $s = 1, \ldots, h$, we have*

$$a_s \leq a_1 \left(1 - \frac{1}{\rho^2} f_{h+1-s,h} + \frac{1}{\rho^4} \sum_{i=h+2-s}^{h} n_i \sum_{j=1}^{h+1-i} m_j f_{h+1-j,h}\right). \tag{5.22}$$

Proof. From (5.13) and (5.20) we have

$$\begin{aligned} a_s &= \frac{1}{\rho} \left(\rho a_1 - \sum_{i=h+2-s}^{h} n_i b_i\right) \\ &\leq a_1 - \frac{1}{\rho} \sum_{i=h+2-s}^{h} n_i \frac{a_1 M_{h+1-i}}{\rho} \left(1 - \frac{1}{\rho^2} \sum_{j=1}^{h+1-i} \frac{m_j f_{h+1-j,h}}{M_{h+1-i}}\right) \\ &= a_1 \left(1 - \frac{1}{\rho^2} f_{h+1-s,h} + \frac{1}{\rho^4} \sum_{i=h+2-s}^{h} n_i \sum_{j=1}^{h+1-i} m_j f_{h+1-j,h}\right) \end{aligned}$$

and the proof follows. □

From (5.22) we can obtain

$$a_s \leq a_1 \left(1 - \frac{f_{h+1-s,h}}{\rho^2} + \left(\frac{f_{h+1-s,h}}{\rho^2}\right)^2\right). \tag{5.23}$$

We shall now refine the upper bound for a_s in (5.15).

Lemma 5.7. *For any $s = 1, \ldots, h$, we have*

$$a_s \le \frac{b_1 N_{h+1-s}}{\rho}\left(1 - \frac{1}{\rho^2}\sum_{j=1}^{h+1-s}\frac{n_j e_{h+1-j,h}}{N_{h+1-s}} + \frac{1}{\rho^4}\sum_{j=1}^{h+1-s}\frac{n_j}{N_{h+1-s}}\sum_{k=h+2-j}^{h} m_k \sum_{\ell=1}^{h+1-k} n_\ell e_{h+1-\ell,h}\right). \tag{5.24}$$

Proof. The proof is almost the same as the proof of Lemma 5.1. It differs only in better estimations for the b_j's, now taken from Lemma 5.6. □

The results from the above lemmas can be summarized as follows:

Theorem 5.1. *For any s, with $1 \le s \le h$, let*

$$\alpha_s = a_1\left(1 - \frac{1}{\rho^2} f_{h+1-s,h}\right) \qquad \text{and} \qquad \beta_s = \frac{b_1 N_{h+1-s}}{\rho}\left(1 - \frac{1}{\rho^2}\sum_{j=1}^{h+1-s}\frac{n_j e_{h+1-j,h}}{N_{h+1-s}}\right).$$

Then we have

$$\alpha_s \le a_s \le \alpha_s + \frac{a_1}{\rho^4}\sum_{i=h+2-s}^{h} n_i \sum_{j=1}^{h+1-i} m_j f_{h+1-j,h} \tag{5.25}$$

and

$$\beta_s \le a_s \le \beta_s + \frac{b_1}{\rho^5}\sum_{j=1}^{h+1-s} n_j \sum_{k=h+2-j}^{h} m_k \sum_{\ell=1}^{h+1-k} n_\ell e_{h+1-\ell,h}. \tag{5.26}$$

It is worth mentioning that the bounds in (5.25) and (5.26), for $s = 1$ and $s = h$ respectively, are reduced to the exact values. For other values of s, both of these bounds can be very tight, but there are also graphs for which if $s > 1$ (or $s < h$) the bounds in (5.25) (resp. (5.26)) are poor. These phenomena are then reflected in the bounds for the index (for more details, see Remark 5.4).

5.3 Some bounds on the index of a DNG

In this section we will make use of the results from Section 5.2 in order to establish some (lower and upper) bounds on the spectral radius of DNGs. For this purpose we will not exploit all the results from the previous section, only those which give rise to simpler forms of bounds, obtained by solving quadratic or biquadratic equations.

Proposition 5.3. *If G is a connected DNG, then*

$$\rho \geq \max_{1\leq k\leq h} \sqrt{d'_k d''_{h+1-k}}. \tag{5.27}$$

Proof. From (5.2) we obtain

$$b_k = \frac{1}{\rho}\sum_{i=1}^{h+1-k} m_i a_i \geq \frac{M_{h+1-k}a_{h+1-k}}{\rho},$$

since the a_i's are decreasing (by (5.9)). On the other hand, from (5.1) we obtain

$$a_{h+1-k} = \frac{1}{\rho}\sum_{j=1}^{k} n_j b_j \geq \frac{N_k b_k}{\rho},$$

since the b_j's are decreasing (by (5.10)). From the last two inequalities we find that $\rho^2 \geq M_{h+1-k}N_k$, and the proof follows easily. □

Proposition 5.4. *If G is a connected DNG, then*

$$\rho \geq \max\left\{\sqrt{\sum_{k=1}^{h}\frac{m_k}{N_h}(d'_k)^2}, \sqrt{\sum_{k=1}^{h}\frac{n_k}{M_h}(d''_k)^2}\right\}. \tag{5.28}$$

Proof. Let $\mathbf{y} = (y_1, y_2, \ldots, y_\nu)$ be a vector (whose components are indexed by the vertices of G), and let $y_u = d'_s$ if $u \in U_s$ for each s $(1 \leq s \leq h)$, or otherwise, if $v \in V_t$ then $y_v = \rho$ for all t $(1 \leq t \leq h)$. If we now use Rayleigh's principle and substitute in the Rayleigh quotient the vector $\mathbf{y}$ as defined above, we arrive easily at the required inequality. □

Remark 5.1. *The above proposition can be adapted to hold more generally, for any (connected) bipartite graph.*

Let $\phi = \sum_{(s,t)\in T_h} \hat{e}_s \hat{f}_t$ (see Section 5.1).

Proposition 5.5. *If G is a connected DNG for which $\phi \geq \frac{3}{4}\epsilon^2$, then*

$$\textit{either} \quad \rho \leq \sqrt{\frac{1}{2}(\epsilon - \sqrt{4\phi - 3\epsilon^2})}, \quad \textit{or} \quad \rho \geq \sqrt{\frac{1}{2}(\epsilon + \sqrt{4\phi - 3\epsilon^2})}. \tag{5.29}$$

Proof. From (5.2), with $t = 1$, we have $\rho b_1 = \sum_{s=1}^{h} m_s a_s$. Next, by using (5.20), we obtain

$$\rho b_1 \geq \sum_{s=1}^{h} m_s \frac{b_1}{\rho} \left(N_{h+1-s} - \frac{1}{\rho^2} \sum_{j=1}^{h+1-s} n_j e_{h+1-j,h} \right).$$

Therefore

$$\rho^4 - \epsilon\rho^2 + \sum_{s=1}^{h} m_s \sum_{j=1}^{h+1-s} n_j e_{h+1-j,h} \geq 0,$$

or equivalently $\rho^4 - \epsilon\rho^2 + \sigma \geq 0$. The rest of the proof follows easily from Proposition 5.1. □

Remark 5.2. *By a computer search we have found graphs for which* $\phi < \frac{3}{4}\epsilon^2$*. These graphs are less frequent, and deserve to be studied in more details.*

We first give a short proof of a well known upper bound from the literature (see, for example, [14]).

Proposition 5.6. *If G is a connected DNG, then*

$$\rho \leq \sqrt{\epsilon}. \tag{5.30}$$

Proof. As in the previous proposition we have $\rho b_1 = \sum_{s=1}^{h} m_s a_s$. Using (5.15) we deduce that $\rho b_1 \leq \sum_{s=1}^{h} m_s \frac{N_{h+1-s} b_1}{\rho}$. Therefore $\rho^2 \leq \sum_{s=1}^{h} m_s N_{h+1-s} = e_h$ $(= \epsilon)$, as required. □

The following two bounds improve the bound from (5.30).

Proposition 5.7. *If G is a connected DNG, then*

$$\rho \leq \min\left\{ \sqrt{\epsilon - n_1 \frac{\sum_{s=1}^{h} m_s \bar{f}_{h+1-s}}{\epsilon}}, \sqrt{\epsilon - m_1 \frac{\sum_{s=1}^{h} n_s \bar{e}_{h+1-s}}{\epsilon}} \right\}.$$

Proof. Again, as in the previous propositions, we have $\rho b_1 = \sum_{s=1}^{h} m_s a_s$. Using (5.19) we obtain

$$\rho b_1 \leq \sum_{s=1}^{h} \frac{m_s b_1}{\rho} \left(N_{h+1-s} - \frac{n_1 \bar{f}_{h+1-s}}{\rho^2} \right)$$

and therefore

$$\rho^2 \leq \sum_{s=1}^{h} m_s \left(N_{h+1-s} - \frac{n_1 \bar{f}_{h+1-s}}{\rho^2} \right).$$

Taking (5.30) into consideration, we have $\frac{n_1}{\rho^2} \geq \frac{n_1}{\epsilon}$, and we arrive easily at the result. □

Proposition 5.8. *If G is a connected DNG, then*

$$\sqrt{\frac{1}{2}(\epsilon - \sqrt{\epsilon^2 - 4\psi})} \leq \rho \leq \sqrt{\frac{1}{2}(\epsilon + \sqrt{\epsilon^2 - 4\psi})}.$$

where $\psi = \max\{m_1 \sum_{s=1}^{h}(n_s \bar{e}_{h+1-s}), n_1 \sum_{s=1}^{h}(m_s \bar{f}_{h+1-s})\}$.

Proof. As in the proof of the previous proposition, we have

$$\rho^2 \leq \sum_{s=1}^{h} m_s \left(N_{h+1-s} - \frac{n_1 \bar{f}_{h+1-s}}{\rho^2} \right)$$

or, equivalently,

$$\rho^4 - e_h \rho^2 + n_1 \sum_{s=1}^{h} m_s \bar{f}_{h+1-s} \leq 0.$$

Now the proof follows easily. □

5.4 Some new bounds on the index of an NSG

In this section we give some bounds on the index of an NSG deduced from the bounds of a DNG. For this purpose, we will need more notation. Let G be an NSG. As we have seen in Chapter 3 its vertex set consists of a co-clique and a clique whose vertex sets are partitioned into h cells $\cup_{i=1}^{h} U_i$ and $\cup_{j=1}^{h} V_j$, respectively. Assuming that $|U_i| = m_i$, $|V_j| = n_j$, $m = (m_1, \ldots, m_h)$ and $n = (n_1, \ldots, n_h)$ we write $G = NSG(m_1, m_2, \ldots, m_h; n_1, n_2 \ldots, n_h)$ (or $NSG(m; n)$ for short). We also denote by m^{-1} and n^{-1} the reverse h-tuples of m and n, respectively.

We will now consider two possibilities for transforming an NSG G into a bipartite graph. For this purpose we will make use of NEPS (non-complete extended p-sum; see Chapter 2). In both cases we will consider an NEPS between G and a copy of K_2. Then the vertex set of the resulting graph consists of the following two sets:

$$\left(\bigcup_{i=1}^{h} U_i' \right) \bigcup \left(\bigcup_{j=1}^{h} V_j' \right) \quad \text{and} \quad \left(\bigcup_{i=1}^{h} U_i'' \right) \bigcup \left(\bigcup_{j=1}^{h} V_j'' \right),$$

where $U_i' = U_i \times \{0\}$, $V_i' = V_i \times \{0\}$, $U_i'' = U_i \times \{1\}$, $V_i'' = V_i \times \{1\}$.

In the first case we take the basis for the NEPS to contain only one 2-tuple, namely $(1,1)$. Then the resulting graph is also called the product of G and K_2, and denoted by $G \otimes K_2$. Let $H = G \otimes K_2$, where $G = NSG(m;n)$. Now it is easy to see that H, together with edges joining vertices $(v,0)$ and $(v,1)$ for $v \in \cup_{j=1}^{h} V_j$, becomes equal to

$$B_G = DNG(n \cdot m^{-1}; n \cdot m^{-1}), \tag{5.31}$$

where $\cdot$ denotes the concatenation of the corresponding h-tuples. Thus

$$B_G = (G \otimes K_2) + pK_2,$$

where $+$ signifies here that $p\ (= |\cup_{j=1}^{h} V_j|)$ independent edges are being added to the latter graph; more precisely, by adding these edges we make the latter graph to be a DNG. Now, by the Courant-Weyl inequalities, with $i = j = 1$ we have

$$\rho(H) - 1 \leq \rho(B_G) \leq \rho(H) + 1.$$

Since $\rho(H) = \rho(G)$, we obtain

$$\rho(B_G) - 1 \leq \rho(G) \leq \rho(B_G) + 1.$$

In the second case we take the basis for the NEPS to contain two 2-tuples, namely $(1,1)$ and $(0,1)$. The corresponding bipartite graph operation will be denoted by $\oplus$. Then the resulting graph obtained with this basis consists of H as above and a perfect matching added to it. Thus it is equal to $H' = H + \nu K_2$, where ν is the order of G. Therefore, we have

$$B_G = (G \oplus K_2) - qK_2;$$

here the meaning of $-$ is clear from the context (notice also that $q = |\cup_{i=1}^{h} U_i|$). Using again as above the Courant-Weyl inequalities, we obtain

$$\rho(B_G) - 2 \leq \rho(G) \leq \rho(B_G).$$

Therefore we arrive at the following result:

Theorem 5.2. *Let $G = NSG(m;n)$, and B_G be the DNG defined in (5.31). Then*

$$\rho(B_G) - 1 \leq \rho(G) \leq \rho(B_G).$$

Needless to say, good (lower or upper) bounds for B_G give us good bounds for G. In the next section we shall confirm this fact by providing some computational results.

5.5 Some computational results

We will follow a strategy from Chapter 4 for presenting the computational results obtained by using *Mathematica*. For this aim we take a small DNG, say $G = DNG(1,2,3,2;2,1,3,1)$ (“ad hoc" chosen) with 15 vertices, 32 edges and of height $h = 4$. In the following table we summarize our computational results on bounds from Section 5.3 (in the bottom row we have relative errors):

Prop.5.3	Prop. 5.4	Prop. 5.5	ρ	Prop. 5.6	Prop. 5.7	Prop. 5.8
4.2426	4.8989	5.0484	5.0884	5.6568	5.2915	5.2262
−16.6 %	−3.72 %	−0.79 %	0	11.2 %	3.99 %	2.71 %

Example 5.1. *We will now consider graphs obtained from G by multiplying exactly one parameter by* 10 *and* 1000.

1. *a DNG with* $m = (10, 2, 3, 2)$, $n = (2, 1, 3, 1)$

Prop.5.3	*Prop. 5.4*	*Prop. 5.5*	ρ	*Prop. 5.6*	*Prop. 5.7*	*Prop. 5.8*
8.48528	*9.23503*	*9.2708*	*9.2822*	*9.74679*	*9.37241*	*9.3382*
−8.59 %	−0.508 %	−0.12 %	*0*	5.01 %	0.972 %	0.603 %

2. *a DNG with* $m = (1, 20, 3, 2)$, $n = (2, 1, 3, 1)$

Prop.5.3	*Prop. 5.4*	*Prop. 5.5*	ρ	*Prop. 5.6*	*Prop. 5.7*	*Prop. 5.8*
11.225	*11.1838*	*11.4919*	*11.4962*	*11.8322*	*11.5956*	*11.5853*
−2.36 %	−2.72 %	−0.037 %	*0*	2.92 %	0.864 %	0.774 %

3. *a DNG with* $m = (1, 2, 30, 2)$, $n = (2, 1, 3, 1)$

Prop.5.3	*Prop. 5.4*	*Prop. 5.5*	ρ	*Prop. 5.6*	*Prop. 5.7*	*Prop. 5.8*
9.94987	*10.0953*	*10.1201*	*10.1293*	*10.6301*	*10.3021*	*10.2789*
−1.77 %	−0.336 %	−0.091 %	*0*	4.94 %	1.71 %	1.48 %

4. *a DNG with* $m = (1, 2, 3, 20)$, $n = (2, 1, 3, 1)$

Prop.5.3	*Prop. 5.4*	*Prop. 5.5*	ρ	*Prop. 5.6*	*Prop. 5.7*	*Prop. 5.8*
7.2111	*7.37981*	*7.37204*	*7.41839*	*8.24621*	*7.59257*	*7.43373*
−2.79 %	−0.52 %	−0.62 %	*0*	11.2 %	2.35 %	0.207 %

5. *a DNG with* $m = (1, 2, 3, 2)$, $n = (20, 1, 3, 1)$

Prop.5.3	*Prop. 5.4*	*Prop. 5.5*	ρ	*Prop. 5.6*	*Prop. 5.7*	*Prop. 5.8*
12.6491	*12.9615*	*12.9677*	*12.9704*	*13.2665*	*12.9895*	*12.9769*
−2.48 %	−0.0691 %	−0.021 %	*0*	2.28 %	0.147 %	0.0495 %

6. *a DNG with* $m = (1, 2, 3, 2),\ n = (2, 10, 3, 1)$

Prop.5.3	*Prop. 5.4*	*Prop. 5.5*	ρ	*Prop. 5.6*	*Prop. 5.7*	*Prop. 5.8*
8.48528	*8.46316*	*8.79412*	*8.81015*	*9.27362*	*9.05539*	*9.04402*
−3.69 %	−3.94 %	−0.18 %	*0*	5.26 %	2.78 %	2.65 %

7. *a DNG with* $m = (1, 2, 3, 2),\ n = (2, 1, 30, 1)$

Prop.5.3	*Prop. 5.4*	*Prop. 5.5*	ρ	*Prop. 5.6*	*Prop. 5.7*	*Prop. 5.8*
9.94987	*9.95431*	*10.0155*	*10.026*	*10.6301*	*10.2323*	*10.197*
−0.76 %	−0.715 %	−0.11 %	*0*	6.03 %	2.06 %	1.71 %

8. *a DNG with* $m = (1, 2, 3, 2),\ n = (2, 1, 3, 10)$

Prop.5.3	*Prop. 5.4*	*Prop. 5.5*	ρ	*Prop. 5.6*	*Prop. 5.7*	*Prop. 5.8*
4.24264	*5.01248*	*5.0900*	*5.35218*	*6.40312*	*5.81839*	*5.63742*
−20.7 %	−6.35 %	−4.9 %	*0*	19.6 %	8.71 %	5.33 %

9. *a DNG with* $m = (1000, 2, 3, 2),\ n = (2, 1, 3, 1)$

Prop.5.3	*Prop. 5.4*	*Prop. 5.5*	ρ	*Prop. 5.6*	*Prop. 5.7*	*Prop. 5.8*
83.666	*83.7573*	*83.7573*	*83.7574*	*83.8153*	*83.7575*	*83.7574*
−0.109 %	$-7.08 \cdot 10^{-5}$ %	$-1.9 \cdot 10^{-5}$ %	*0*	0.0691 %	$1.76 \cdot 10^{-4}$ %	$8.03 \cdot 10^{-5}$ %

10. *a DNG with* $m = (1, 2000, 3, 2),\ n = (2, 1, 3, 1)$

Prop.5.3	*Prop. 5.4*	*Prop. 5.5*	ρ	*Prop. 5.6*	*Prop. 5.7*	*Prop. 5.8*
109.572	*109.554*	*109.599*	*109.599*	*109.636*	*109.608*	*109.608*
−0.0243 %	−0.0408 %	$-4.6 \cdot 10^{-6}$ %	*0*	0.034 %	$9.03 \cdot 10^{-3}$ %	$9.01 \cdot 10^{-3}$ %

11. *a DNG with* $m = (1, 2, 3000, 2),\ n = (2, 1, 3, 1)$

Prop.5.3	*Prop. 5.4*	*Prop. 5.5*	ρ	*Prop. 5.6*	*Prop. 5.7*	*Prop. 5.8*
94.9158	*94.9263*	*94.9298*	*94.9298*	*94.9895*	*94.9474*	*94.9474*
−0.0149 %	$-3.69 \cdot 10^{-3}$ %	$-1.2 \cdot 10^{-5}$ %	*0*	0.0628 %	0.0185 %	0.0185 %

12. *a DNG with* $m = (1, 2, 3, 2000),\ n = (2, 1, 3, 1)$

Prop.5.3	*Prop. 5.4*	*Prop. 5.5*	ρ	*Prop. 5.6*	*Prop. 5.7*	*Prop. 5.8*
63.3404	*63.3406*	*63.34.05*	*63.3406*	*63.4665*	*63.3411*	*63.3406*
$-3.99 \cdot 10^{-4}$ %	$-1.26 \cdot 10^{-6}$ %	$-1.2 \cdot 10^{-4}$ %	*0*	0.199 %	$7.89 \cdot 10^{-4}$ %	$3.27 \cdot 10^{-7}$ %

13. *a DNG with* $m = (1, 2, 3, 2),\ n = (2000, 1, 3, 1)$

Prop.5.3	*Prop. 5.4*	*Prop. 5.5*	ρ	*Prop. 5.6*	*Prop. 5.7*	*Prop. 5.8*
126.491	*126.523*	*126.523*	*126.523*	*126.554*	*126.523*	*126.523*
−0.025 %	$-7.37 \cdot 10^{-6}$ %	$-2.3 \cdot 10^{-6}$ %	*0*	0.025 %	$1.76 \cdot 10^{-5}$ %	$5.13 \cdot 10^{-6}$ %

14. *a DNG with* $m = (1, 2, 3, 2),\ n = (2, 1000, 3, 1)$

Prop.5.3	*Prop. 5.4*	*Prop. 5.5*	ρ	*Prop. 5.6*	*Prop. 5.7*	*Prop. 5.8*
77.5371	*77.5117*	*77.5672*	*77.5673*	*77.6273*	*77.6015*	*77.6015*
−0.0389 %	−0.0717 %	$-3.4 \cdot 10^{-5}$ %	*0*	0.0774 %	0.0442 %	0.0442 %

15. a DNG with $m = (1, 2, 3, 2)$, $n = (2, 1, 3000, 1)$

Prop.5.3	Prop. 5.4	Prop. 5.5	ρ	Prop. 5.6	Prop. 5.7	Prop. 5.8
94.9158	94.9105	94.9176	94.9176	94.9895	94.9369	94.9369
$-1.91 \cdot 10^{-3}$ %	$-7.4 \cdot 10^{-3}$ %	$-1.3 \cdot 10^{-5}$ %	0	0.0758 %	0.0204 %	0.0203 %

16. a DNG with $m = (1, 2, 3, 2)$, $n = (2, 1, 3, 1000)$

Prop.5.3	Prop. 5.4	Prop. 5.5	ρ	Prop. 5.6	Prop. 5.7	Prop. 5.8
31.7175	31.7192	31.7176	31.7192	32.1092	31.7287	31.7192
$-5.39 \cdot 10^{-3}$ %	$-1.06 \cdot 10^{-4}$ %	$-4.9 \cdot 10^{-3}$ %	0	1.23 %	0.0299 %	$2.83 \cdot 10^{-5}$ %

The lower bound from Proposition 5.8 is not included in the above table because it gives rise to the biggest errors (in the above sample of DNGs).

Remark 5.3. *In Chapter 4 we have generated further instances by multiplying each entry from m and n by 10, 100 and 1000, respectively. We will not do this here in view of Proposition 5.2 since ρ, and each lower and upper bound from Section 5.3, is homogeneous with respect to m and/or n.*

Remark 5.4. *We have also compared our bounds with some general bounds from the literature. It turns that our bounds are better; this is not surprising since in general the other ones were not tailored for DNGs. In particular, it is also noteworthy that the upper bound from [39, Theorem 3] does not apply to DNGs, and so our upper bounds become more important. On the other hand, the only interesting bound from the literature concerning DNGs comes from [14, Theorem 4.1]. In our notation, if $G = DNG(m_1, \ldots, m_h, n_1, \ldots, n_h)$, then:*

$$\rho(G) \le \sqrt{\frac{1}{2}(\epsilon + \sqrt{\epsilon^2 - 4\varphi})}, \tag{5.32}$$

where

$$\varphi = \max\left\{ \frac{\sum_{1\le s<t\le h} m_s m_t N^2_{h+1-t} N^2_{h+2-t,h+1-s}}{\sum_{1\le s\le h-1} n_{h+1-s} N_{h-s}}, \frac{\sum_{1\le s<t\le h} n_s n_t M^2_{h+1-t} M^2_{h+2-t,h+1-s}}{\sum_{1\le s\le h-1} m_{h+1-s} M_{h-s}} \right\}.$$

Taking the graphs from Example 5.1 we found that bounds from Propositions 5.7 and 5.8 are usually slightly better than that from (5.32). For example, for the graph G of Example 5.1 the upper bound is equal to 5.3828 (our bounds from Propositions 5.7 and 5.8 are 5.2915 *and* 5.2226, *respectively).*

Next let us add that we have also found (by an extensive search) some examples in which the errors are not as small as those encountered with the graphs from Example 5.1. The strange *thing was that all bounds in those cases do not perform as expected (including the one from (5.32)), as follows from Monte Carlo simulations. The most important observation is that this situation occurs very rarely. On the other hand, if it does occur then the main reason is the poor quality of our estimates for eigenvector components. For example, because of this, it can happen that the bound from Proposition 5.5, can be not only extremely poor, but also empty, since the corresponding biquadratic equation (see the proof) has only complex roots.*

Finally we place some emphasis on the results from Section 5.4. In fact we show by an example that some bounds from [42] for NSGs can now be improved by making use of bounds for DNGs.

Example 5.2. *Let* $G = NSG(m, n)$*, where* $m = (40000, 2, 1, 1)$ *and* $n = (2, 1, 5, 4)$*. This is a graph already considered in [42, Exam.5.2]. The exact value for the index of* G *is* 283.394*. Let* $G' = DNG(n \cdot m^{-1}; n \cdot m^{-1})$*. The best upper bound for* $\rho(G)$ *(from [42]) is equal to* 285.891*. On the other hand the best upper bound for* $\rho(G')$ *based on Theorem 5.2 is given by Proposition 5.7, and is equal to* 284.027*. Thus we have some slight improvement, and this shows that we can have some benefits from the approach described in Section 5.4.*

Chapter 6

Relations between (κ, τ)-regular sets and star complements

In this chapter we investigate the graphs having a (κ, τ)-regular set inducing a star complement for some eigenvalue. First we give an overview of definitions and results that would be important throughout the chapter. Then in Section 6.1 we give several reasons why in our opinion this class of graphs deserve to be studied. In Section 6.2 the main result is given, followed by several remarks. Finally, in Section 6.3, the star complement technique is applied to construct maximal graphs with a given (κ, τ)-regular set inducing a star complement for a non-main eigenvalue.

Let P be the matrix of the orthogonal projection of $\mathbb{R}^n$ onto $\mathcal{E}_G(\mu) = \{\mathbf{x} \in \mathbb{R}^n : A_G\mathbf{x} = \mu\mathbf{x}\}$ with respect to the standard orthonormal basis $\{\mathbf{e}_1, \ldots, \mathbf{e}_n\}$ of $\mathbb{R}^n$. Then the set of vectors $P\mathbf{e}_j$ $(j = 1, \ldots n)$ spans $\mathcal{E}_G(\mu)$ and therefore exists $X \subseteq V(G)$ such that vectors $P\mathbf{e}_j$ $(j \in X)$ form a basis for $\mathcal{E}_G(\mu)$. Such a set X is called a *star set* for μ in G. The vectors $P\mathbf{e}_1, \ldots, P\mathbf{e}_n$ form an *eutactic star* which in general consists of vectors which are an orthogonal projection of pairwise orthogonal vectors of the same length.

We write $\bar{X}$ for the complement of X in $V(G)$. $G[X]$ denotes the subgraph of G induced by vertices from X, while $G \setminus X = G[\bar{X}]$. If X $(= X(\mu))$ is a star set for the eigenvalue μ then $\bar{X}$ $(= \bar{X}(\mu))$ is its *co-star set*, while $G \setminus X$ is said to be the *star complement* for μ in G. The following results are fundamental to the theory of star complements (see [26, pp. 136-140]).

Theorem 6.1. *Let G be a graph, let $X \subseteq V(G)$ and let μ be an eigenvalue of G with multiplicity k. Then the following statements are equivalent:*

(i) $\{P\mathbf{e}_j : j \in X\}$ *is a basis of* $\mathcal{E}_G(\mu)$*;*

(ii) $\mathbb{R}^n = \mathcal{E}_G(\mu) \oplus \mathcal{V}$*, where* $\mathcal{V} = \langle \mathbf{e}_j : j \in \bar{X} \rangle$*;*

(iii) $|X| = k$ *and* μ *is not an eigenvalue of* $G \setminus X$*.*

Theorem 6.2. *Let X be a set of k vertices in the graph G and suppose that G has the 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*

$$\mu I - A_X = B^T(\mu I - C)^{-1}B. \tag{6.1}$$

In this situation, $\mathcal{E}_G(\mu)$ *consists of the vectors* $\begin{pmatrix} \mathbf{x} \\ (\mu I - C)^{-1}B\mathbf{x} \end{pmatrix}$, $\mathbf{x} \in \mathbb{R}^k$.

The previous result is known as the *Reconstruction theorem*. The columns $\mathbf{b}_u$, $u \in X$ of the matrix B are the characteristic vectors of the H-neighbourhoods $N_H(u) = \{v \in V(H) : u \sim v\}$, where $u \in X$ and $H = G \setminus X$.

We write $t = |\bar{X}|(= n - k)$ and define a bilinear form on $\mathbb{R}^t$ by:

$$\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^T(\mu I - C)^{-1}\mathbf{y} \quad (\mathbf{x}, \mathbf{y} \in \mathbb{R}^t).$$

By equating entries in (6.1) we see that X is a star set for μ if and only if μ is not eigenvalue of $H = G \setminus X$ and the following hold:

$$\langle \mathbf{b}_u, \mathbf{b}_u \rangle = \mu \quad (u \in X), \tag{6.2}$$

and, for $u \neq v$

$$\langle \mathbf{b}_u, \mathbf{b}_v \rangle = -1 \text{ if } u \sim v, \qquad \langle \mathbf{b}_u, \mathbf{b}_v \rangle = 0 \text{ if } u \nsim v \quad (u, v \in X). \tag{6.3}$$

Following [12], we will fix some further notation and terminology. Given a graph H, a subset U of $V(H)$ and a vertex $u \notin V(H)$, denote by $H(U)$ the graph obtained from H by joining u

to all vertices of U. We will say that u is a *good vertex* for U (and U is a *good set* for u) with respect to μ, if μ is an eigenvalue of $H(U)$, but not of H. As we have seen, u is a good vertex for U with respect to μ if and only if $\langle \mathbf{b}_u, \mathbf{b}_u \rangle = \mu$, where $\mathbf{b}_u$ is the characteristic vector of U – see (6.2). Assume now that U_1 and U_2 are not necessarily good sets for vertices u_1 and u_2, with respect to μ. Let $H(U_1, U_2; 0)$ and $H(U_1, U_2; 1)$ denote graphs obtained from H by adding both vertices u_1 and u_2, where they are non-adjacent in the first, while adjacent in the second graph. We say that u_1 and u_2 are *good partners*, and that U_1 and U_2 are compatible sets if μ is of multiplicity two either in $H(U_1, U_2; 0)$ or in $H(U_1, U_2; 1)$. Again, by Theorem 6.2, two good vertices u_1 and u_2 are good partners if and only if $\langle \mathbf{b}_{u_1}, \mathbf{b}_{u_2} \rangle \in \{-1, 0\}$ – see (6.3). In addition, it follows that any vertex set X in which all vertices are good, both individually or in pairs, give rise to a good extension, say G, in which X can be viewed as a star set for μ with H as the corresponding star complement.

The above considerations describe in brief the star complement technique. In order to find *H-maximal* graphs for any $\mu \notin \{-1, 0\}$, i.e. those graphs which are not extendible any further, we form an *extendability graph* whose vertices are good vertices for a fixed μ and H. We add an edge between two good vertices whenever they are good partners. Therefore the search for maximal cliques in the extendability graph is equivalent to search for H-maximal extensions.

In case when $\mu = 0$ (or $\mu = -1$), we can have infinite series of extensions due to presence of *duplicate* (resp. *co-duplicate*) vertices. Recall that two vertices are *duplicate* (resp. *co-duplicate*) if they have the same open (closed) neighbourhood. So, if v and w are two distinct vertices then they are duplicate if $N_G(v) = N_G(w)$, or co-duplicate if $\overline{N_G(v)} = \overline{N_G(w)}$ (note that $\overline{N_G(u)} = N_G(u) \cup \{u\}$). If these two types of vertices are excluded in extensions, than any H-maximal extension of H (on t vertices), can have at most $\binom{t}{2}$ vertices, as it holds for all other values of μ (see [13]). A graph is called *reduced* (*co-reduced*) with respect to a fixed star complement if it has no duplicate (co-duplicate) vertices in the corresponding star set (for more details see [26, Chapter 7]).

A (κ, τ)-regular set is a subset of the vertices of a graph, inducing a κ-regular subgraph such that every vertex not in the subset has τ neighbors in it. The (κ, τ)-regular sets appeared first in [50] under the designation of eigengraphs and in [41], in both cases in the context of strongly regular graphs and designs. By convention, if G is a κ-regular graph then we say that $V(G)$ is a $(\kappa, 0)$-regular set. Also, (κ, τ)-regular sets were considered in [38, 49], related to the study of graphs with domination constrains, and later, in the general context of arbitrary graphs in [18, 19, 20].

Recall that μ is main eigenvalue of G if and only if $P\mathbf{j} \neq 0$ ([26, p. 46]). Recently, a nice survey paper on main (non-main) eigenvalues was published by Rowlinson [46].

A (κ, τ)-regular set in a graph G which is also a star set (co-star set) for some eigenvalue μ of G is called a (κ, τ)-*regular star set* (resp. (κ, τ)-*regular co-star set*). If H is a star complement for some eigenvalue μ of G, such that $V(H)$ is (κ, τ)-regular set then we say that H is (κ, τ)-*regular star complement.*

6.1 Motivation

Our motivation to consider graphs with (κ, τ)-regular star sets (or star complements) comes from several directions. Here we will mention some.

Domination sets. If X is (κ, τ)-regular set in graph G for $\tau \neq 0$ then X is dominating set in G. On the other hand, if X is a star set for $\mu \notin \{0, -1\}$, then $\bar{X}$ is a dominating set in G ([26, p. 172]).

Hamiltonian graphs. A *line graph* $L(G)$ of a graph G, has the edge set of G as its vertex set, where two vertices in $L(G)$ are adjacent if the corresponding edges in G have a common end-vertex. Having this in mind, the following necessary and sufficient condition for line graphs of Hamiltonian graphs was obtained in [10]:

Theorem 6.3. *A graph G is the line graph of a Hamiltonian graph of order t, where t is an odd integer greater than 2 if and only if either $G = C_t$ or G has C_t as a star complement for the eigenvalue -2.*

The class of line graphs of Hamiltonian graphs can be characterized using (κ, τ)-regular sets, as follows.

Theorem 6.4. *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 $S \subset V(L(G))$ inducing a connected subgraph of $L(G)$.*

Proof. Assume that G is Hamiltonian, that is, it contains a cycle C with all vertices of G. Then all edges not in C have each end-vertex in C and the corresponding vertices in $L(G)$ have 4 neighbors in $V(L(C))$. Since $V(L(C))$ induces a cycle in $L(G)$ then $S = V(L(C))$ is a $(2,4)$-regular set of $L(G)$, inducing a connected subgraph. Conversely, assume that $L(G)$ has a $(2,4)$-regular set S, inducing a connected subgraph. Then S corresponds to a cycle C in G and each edge not in C is connected to 4 edges in C. Therefore, each edge not in C has both end-vertices in C, which means that G is Hamiltonian. □

Perfect matching. Let G be a graph without isolated vertices for which X is a minimal dominating set, where X is the star set for the eigenvalue $\mu \notin \{-1, 0\}$. If $G \setminus X$ has no isolated vertices then the set of all edges between X and $\bar{X}$ is a perfect matching for G (see [26, p. 174]). Our motivation in this case comes from the fact that a connected graph with more than one edge has a perfect matching $M \subseteq E(G)$ if and only $V(L(M)) \subset V(L(G))$ is a (0,2)-regular set in $L(G)$ (see [17]). Notice that the line graph $L(M)$ has no edges.

6.2 (κ, τ)-regular sets and star complements

For a given vector $\mathbf{x} \in \mathbb{R}^n$ and a non-empty set $S \subset \{1, 2, \dots n\}$, let $\mathbf{x}_S$ denote the characteristic vector of S. The following result was proved in [21]:

Theorem 6.5. *Let G be a graph with a (κ, τ)-regular set $S \subset V(G)$, where $\tau > 0$. Then $\mu_i \in \sigma(G)$ is non-main if and only if*

(a) $\mu_i = \kappa - \tau$, or

(b) $\mathbf{x}_S$ is orthogonal to $\mathcal{E}_G(\mu_i)$, that is $P_i \mathbf{x}_S = 0$ holds.

The following facts deserve to be mentioned. Namely, we can have that only (a) or (b) holds, or that both (a) and (b) hold. We show this by the examples. Both of graphs being chosen are integral (so all eigenvalues are integers).

Let $G = S(K_{1,3})$. So G is a subdivision of a star $K_{1,3}$. We can label the vertices of G in breadth-first manner, starting from the vertex of degree 3, labelled 1; its neighbours are labelled 2, 3 and 4, and their neighbours respectively are labelled 5, 6 and 7. Let $S = V(G) \setminus \{1\}$. Then S is (1,3)-regular set in G. So $\kappa - \tau = -2$. Note first that $-2 \in \sigma(G)$. It is easy to show that $\mathcal{E}_G(-2)$ is generated by the vector $(3, -2, -2, -2, 1, 1, 1)^T$. So -2 is a non-main eigenvalue of G, but $\mathbf{x}_S$ is not orthogonal to $\mathcal{E}_G(-2)$. Therefore, (a) holds, but not (b). Next, it is easy to see that $1 \in \sigma(G)$ (so $1 \neq \kappa - \tau$). Moreover, 1 is a non-main eigenvalue of G. Namely, $\mathcal{E}_G(1)$ is spanned by vectors $(0, 1, -1, 0, 1, -1, 0)^T$ and $(0, 1, 0, -1, 1, 0, -1)^T$, and our claim holds. But now we have that $\mathbf{x}_S$ is orthogonal to $\mathcal{E}_G(1)$. Therefore, (a) does not hold, but (b) holds.

Let G be a graph which consists of a "central" edge with two pendant edges attached at its end-vertices (or it is a corona of K_2 and $2K_1$ – see [36]). We can label now the vertices of G as follows: one end-vertex of the central edge is labelled 1 and the other 4; vertices of degree one adjacent to 1 are labelled 2 and 3, while vertices of degree one adjacent to 4 are labelled 5 and 6. Let $S = \{1, 4\}$. Then S is a (1,1)-regular set. So $\kappa - \tau = 0$. Note first that $0 \in \sigma(G)$. Also, it is easy to see that $\mathcal{E}_G(0)$ is spanned by vectors $(0, 1, -1, 0, 0, 0)^T$ and $(0, 0, 0, 0, 1, -1)^T$. So 0 is a non-main eigenvalue of G. But now we have that $\mathbf{x}_S$ is orthogonal to $\mathcal{E}_G(1)$. Therefore, both (a) and (b) hold.

We now consider (κ, τ)-regular sets which are star (or co-star) sets, and we prove the following slightly different result.

Theorem 6.6. *Let G be a graph and $X_i \subset V(G)$ be a star set for the eigenvalue $\mu_i \in \sigma(G)$. If X_i or $\bar{X}_i$ is (κ, τ)-regular in G, with $\tau > 0$, then μ_i is non-main if and only if $\mu_i = \kappa - \tau$.*

Proof. Since A has spectral decomposition $A = \sum_{i=1}^{m} \mu_i P_i$ then each P_i commutes with A. Therefore, denoting the characteristic vector of X_i and $\bar{X}_i$, by $\mathbf{x} = \mathbf{x}_{X_i}$ and $\mathbf{x} = \mathbf{x}_{\bar{X}_i}$, respectively, we have:

$$P_i A\mathbf{x} = \begin{cases} P_i A\mathbf{x}_{X_i} = \sum_{u \in X_i} P_i A\mathbf{e}_u = \sum_{u \in X_i} \mu_i P_i \mathbf{e}_u = \mu_i P_i \mathbf{x}_{X_i} & \text{if } \mathbf{x} = \mathbf{x}_{X_i}, \\ P_i A\mathbf{x}_{\bar{X}_i} = \sum_{u \in \bar{X}_i} P_i A\mathbf{e}_u = \sum_{u \in \bar{X}_i} \mu_i P_i \mathbf{e}_u = \mu_i P_i \mathbf{x}_{\bar{X}_i} & \text{if } \mathbf{x} = \mathbf{x}_{\bar{X}_i}. \end{cases}$$

Furthermore, according to the hypothesis, one of the characteristic vectors $\mathbf{x} = \mathbf{x}_{X_i}$ or $\mathbf{x} = \mathbf{x}_{\bar{X}_i}$ satisfies $A\mathbf{x} = (\kappa - \tau)\mathbf{x} + \tau\mathbf{j}$. After the multiplication of both sides of this equality by P_i on the left, it follows

$$\mu_i P_i\mathbf{x} = (\kappa-\tau)P_i\mathbf{x} + \tau P_i\mathbf{j} \quad \Leftrightarrow \quad (\mu_i - (\kappa-\tau))P_i\mathbf{x} = \tau P_i\mathbf{j}. \tag{6.4}$$

1. If $\mathbf{x} = \mathbf{x}_{X_i}$, since the vectors $P_i\mathbf{e}_u$, $(u \in X_i)$ are linearly independent then $P_i\mathbf{x}_{X_i} \neq \mathbf{0}$. Therefore, from (7.17), $\mu_i = \kappa - \tau \Leftrightarrow P_i\mathbf{j} = 0$.

2. Assume that $\mathbf{x} = \mathbf{x}_{\bar{X}_i}$. If $\mu_i = \kappa - \tau$ then from (7.17), $P_i\mathbf{j} = 0$ and therefore μ_i is non-main. Conversely, if μ_i is non-main then $P_i\mathbf{j} = 0$ implies $P_i\mathbf{x}_{\bar{X}_i} = -P_i\mathbf{x}_{X_i}$. Therefore, $P_i\mathbf{x}_{X_i} \neq 0 \Leftrightarrow P_i\mathbf{x}_{\bar{X}_i} \neq 0$ and, from (7.17), it follows $\mu_i = \kappa - \tau$.

Therefore, in both cases, $P_i\mathbf{x} \neq \mathbf{0}$ and thus $\mu_i = \kappa - \tau \Leftrightarrow P_i\mathbf{j} = 0$. □

Remark 6.1. *Note that, under the assumptions of Theorem 6.6, when X_i or $\bar{X}_i$ is (κ,τ)-regular, nor $\mathbf{x}_{X_i}$ neither $\mathbf{x}_{\bar{X}_i}$ are orthogonal to $\mathcal{E}_G(\kappa-\tau)$. In fact, according to the proof of Theorem 6.6, $P_i\mathbf{x}_{X_i} \neq \mathbf{0}$ and $P_i\mathbf{x}_{\bar{X}_i} \neq \mathbf{0}$.*

Notice that if X_i ($\bar{X}_i$) is a (κ,τ)-regular star set (co-star set), with $\tau > 0$, and the eigenvalue $\mu_i \in \sigma(G)$ is main then $P_i\mathbf{x}_{X_i}$ (resp. $P_i\mathbf{x}_{\bar{X}_i}$) is a scalar multiple of $P_i\mathbf{j}$. In fact, in a such case,

$$\frac{\mu_i - (\kappa-\tau)}{\tau}P_i\mathbf{x}_{X_i} = P_i\mathbf{j} \qquad \left(\frac{\mu_i - (\kappa-\tau)}{\tau}P_i\mathbf{x}_{\bar{X}_i} = P_i\mathbf{j}\right).$$

As immediate consequence, we have the following corollary.

Corollary 6.1. *If X_i ($\bar{X}_i$) is a (κ,τ)-regular star set (resp. co-star set) for the main eigenvalue μ_i of a graph G, with $\tau > 0$, then $\mu_i \neq \kappa - \tau$ and the vector*

$$\frac{\mu_i - (\kappa-\tau)}{\tau}\mathbf{x}_{X_i} - \mathbf{j} \qquad \left(\frac{\mu_i - (\kappa-\tau)}{\tau}\mathbf{x}_{\bar{X}_i} - \mathbf{j}\right) \tag{6.5}$$

is orthogonal to $\mathcal{E}_G(\mu_i)$.

Remark 6.2. *Let G be a graph with a (κ,τ)-regular set S, such that $\kappa - \tau \in \sigma(G)$. Then we have:*

- *If $\kappa - \tau \in \sigma(G[S])$ then we may say that $G[S]$ is not a star complement for $\kappa - \tau$ and that S need not be a star set as well. For instance, the graph G depicted in*

Figure 6.1, which is an octahedron, or a cocktail party graph $CP(6)$, has the spectrum $\sigma(G) = \{[-2]^2, [0]^3, [4]^1\}$, and the set $S = \{1, 2, 4, 5\}$ as a $(2, 4)$-regular set. (Recall, $CP(2k)$ is a $(2k-2)$-regular graph on $2k$ vertices.) Furthermore, $-2 \in \sigma(G[S])$, S is not a star set and $G[S]$ is not a star complement for the eigenvalue $-2 \in \sigma(G)$. On the other hand, if $G = K_3$ then any set S with $|S| = 2$ is $(1, 2)$-regular, $-1 \in \sigma(G[S])$ and S is a star set.

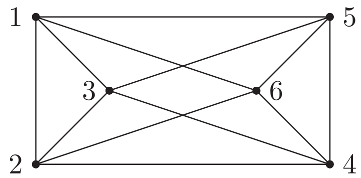

Figure 6.1: Graph with the $(2, 2)$-regular star set (co-star set) $\{1, 3, 5\}$ for the eigenvalue $\mu = 0$.

- *If $\kappa - \tau \notin \sigma(G[S])$ then it is obvious that S can be a co-star set, or it can be shown that the cardinality of $\bar{S}$ is greater than the multiplicity of $\kappa - \tau$. In the former case, S can be both, the star set and the co-star set for $\mu = \kappa - \tau$ (see Figure 6.1)*

We conclude this section with the following example:

Example 6.1. *Let H be a κ-regular connected graph of order n. Consider a vertex $u \notin V(H)$ and let $U = V(H)$ then $H(U) = K_1 \nabla H$. (Here ∇ stands for a join of two graphs). Then*

$$A_{H(U)} = \begin{pmatrix} 0 & \mathbf{j}^T \\ \mathbf{j} & A_H \end{pmatrix},$$

where $\mathbf{j}$ is an all-one vector. It is immediate that U is a (κ, n)-regular set in $H(U)$. Since all eigenvalues of H but κ are non-main then for every $\mu_i \in \sigma(H) \setminus \{\kappa\}$

$$\hat{\mathbf{u}} \in \mathcal{E}_H(\mu_i) \Rightarrow \begin{pmatrix} 0 \\ \hat{\mathbf{u}} \end{pmatrix} \in \mathcal{E}_{H(U)}(\mu_i).$$

Therefore, $\sigma(H(U)) = (\sigma(H) \setminus \{\kappa\}) \cup \{\lambda_1, \lambda_2\}$, where λ_1 and λ_2 are both main eigenvalues of $H(U)$ (since the all other ones remain non-main and $H(U)$ is non-regular). On the other hand, since the trace of $A_{H(U)}$ remains zero then $\lambda_1 = \kappa + \delta$ and $\lambda_2 = -\delta$, with $\delta > 0$. Thus,

U is a (κ, n)-regular co-star set for λ_1 and also for λ_2. Then, applying Corollary 6.1, the vectors

$$\frac{\kappa+\delta-(\kappa-n)}{n}\begin{pmatrix} 0 \\ \mathbf{j} \end{pmatrix} - \begin{pmatrix} 1 \\ \mathbf{j} \end{pmatrix} = \frac{\delta}{n}\begin{pmatrix} -\frac{n}{\delta} \\ \mathbf{j} \end{pmatrix},$$

$$\frac{-\delta-(\kappa-n)}{n}\begin{pmatrix} 0 \\ \mathbf{j} \end{pmatrix} - \begin{pmatrix} 1 \\ \mathbf{j} \end{pmatrix} = -\frac{\kappa+\delta}{n}\begin{pmatrix} \frac{n}{\kappa+\delta} \\ \mathbf{j} \end{pmatrix},$$

where $\mathbf{j}$ is the all-one vector, are orthogonal to $\mathcal{E}_{H(U)}(\kappa+\delta)$ and $\mathcal{E}_{H(U)}(-\delta)$, respectively. Since this eigenspaces are also orthogonal to the eingenspaces $\mathcal{E}_{H(U)}(\mu_i)$ it follows that $\mathcal{E}_{H(U)}(\kappa+\delta)$ is spanned by $\begin{pmatrix} \delta \\ \mathbf{j} \end{pmatrix}$ and $\mathcal{E}_{H(U)}(-\delta)$ is spanned by $\begin{pmatrix} -(\kappa+\delta) \\ \mathbf{j} \end{pmatrix}$. Hence, it is immediate that $\delta = \frac{-\kappa+\sqrt{\kappa^2+4n}}{2}$, $\lambda_1 = \frac{\kappa+\sqrt{\kappa^2+4n}}{2}$ and $\lambda_2 = \frac{\kappa-\sqrt{\kappa^2+4n}}{2}$. The same result can be obtained by formula (2.8) *in [27, p. 27].*

6.3 Some examples

From now on, G is a graph having a vertex subset S ($\emptyset \subseteq S \subseteq V(G)$) such that:

1^o S is (κ, τ)-regular in G, with $\tau > 0$;

2^o $G[S]$ is a star complement for $\mu = \kappa - \tau$.

It is noteworthy that μ (defined in 2^o) is a non-main eigenvalue (by Theorem 6.6). The graph $G[S]$ is denoted by H, that is, $H = G[S]$. Then a graph is S-*maximal* if it is H-maximal for μ with respect to good vertices u with good sets $U \subseteq S$, such that $|U| = \tau$. So, if G is S-maximal then for any $u \notin V(G)$, with good set $U \subseteq S$ such that $|U| = \tau$, S is not a co-star set in $G + u$.

In this section we study S-maximal graphs G for which $G[S]$ is κ-regular with $\kappa \in \{0, 1, 2, s-2, s-1\}$, with $s = |S|$.

We first show that S-maximal graphs for $\kappa = k$ and $\kappa = s-k-1$ are complementary graphs.

Theorem 6.7. *Let S be a non-empty set in G. Then S is a (κ, τ)-regular co-star set for the non-main eigenvalue $\mu = \kappa - \tau$ if and only if S is a $(|S| - \kappa - 1, |S| - \tau)$-regular co-star set in $\bar{G}$ for the non-main eigenvalue $-\mu - 1$.*

Proof. First, if S is a (κ, τ)-regular in G then in its complement, $\bar{G}$, S is $(|S|-\kappa-1, |S|-\tau)$-regular. For any $\mathbf{x} \in \mathcal{E}_G(\kappa-\tau)$ we have $A_{\bar{G}}\mathbf{x} = (J - I - A_G)\mathbf{x} = (-1-\kappa+\tau)\mathbf{x}$ since $J\mathbf{x} = 0$. By this we have proved that $\mathbf{x} \in \mathcal{E}_G(\kappa - \tau)$ if and only if $\mathbf{x} \in \mathcal{E}_{\bar{G}}(-1 - \kappa + \tau)$. Note, eutactic stars of both eigenvalues are same and therefore all star sets (co-star sets) coincide (see [26, Chapter 7]). Hence S is the star complement for the eigenvalue $-1 - \kappa + \tau$ in $\bar{G}$. □

6.3.1 Case $\kappa \in \{0, s - 1\}$

Assume first that $\kappa = 0$. Then $H = sK_1$, $\mu = -\tau$; note since $\tau > 0$, $-\tau \notin \sigma(H)$. Now, we can obtain the following result (since we can easily get that $\tau = 1$).

Proposition 6.1. *If G is an S-maximal graph with $\kappa = 0$ then $\tau = 1$ and $G = sK_2$.*

Next we assume $\kappa = s - 1$. By Theorem 6.7 and Proposition 6.1 we also have:

Proposition 6.2. *If G is an S-maximal graph with $\kappa = s - 1$ then $\tau = s - 1$ and $G = \overline{sK_2}$.*

6.3.2 Case $\kappa \in \{1, s - 2\}$

Assume first $\kappa = 1$. In this case $H = hK_2$, where $h = \frac{s}{2}$, $\mu = 1 - \tau$ $(\tau \notin \{0, 2\}$ since $\mu \notin \sigma(H))$. So, $\tau \in \{0, 1, \ldots, 2h\} \setminus \{0, 2\}$. Following the notation of Theorem 6.2, the submatrix C is block-diagonal with h blocks $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and exactly τ nonzero entries in each column of B. Therefore $\langle \mathbf{b}_u, \mathbf{b}_u \rangle = 1 - \tau$ if and only if

$$\mu \sum_{i=1}^{2h} b_i^2 + 2 \sum_{i=1}^{h} b_{2i-1} b_{2i} = \mu(\mu^2 - 1),$$

where $\mathbf{b}_u = (b_1, \ldots, b_{2h})^T$. Since $\sum_{i=1}^{2h} b_i^2 = \tau$ then

$$2 \sum_{i=1}^{h} b_{2i-1} b_{2i} = \tau(1 - \tau)(\tau - 3). \tag{6.6}$$

The nonnegativity of the left hand side implies $\tau \in \{1, 3\}$.

Subcase $\tau = 1$: Now $\mu = 0$, and we immediately obtain:

Proposition 6.3. *If G is an S-maximal graph with $\kappa = 1$ and $\tau = 1$ then $G = hC_4$ $(|S| = 2h)$.*

Remark 6.3. *Note $G = hC_4$ has duplicate vertices, but not in the star set consisting of two adjacent vertices.*

Subcase $\tau = 3$: Now $\mu = -2$. Then, by (6.6) $\sum_{i=1}^{h} b_{2i-1}b_{2i} = 0$ if and only if $(b_{2i-1}, b_{2i}) \neq (1,1)$ for any $i \in \{1, \ldots, h\}$. There are exactly three i's such that (b_{2i-1}, b_{2i}) is equal either to $(1,0)$ or to $(0,1)$. Consequently, there are exactly $8\binom{h}{3}$ good vertices. Two good vertices with $\mathbf{b}_u = (a_1, \ldots, a_{2h})^T$ and $\mathbf{b}_v = (b_1, \ldots, b_{2h})^T$ are good partners if and only if

$$\langle \mathbf{b}_u, \mathbf{b}_v \rangle = \frac{1}{3} \sum_{i=1}^{h} (-2a_{2i-1}b_{2i-1} + a_{2i}b_{2i-1} + a_{2i-1}b_{2i} - 2a_{2i}b_{2i}).$$

This sum can be reduced to the sum of three terms of the form $(-2a_{2i-1}b_{2i-1} + a_{2i}b_{2i-1} + a_{2i-1}b_{2i} - 2a_{2i}b_{2i})$. Each of them (for a good vertex) is equal to -2, 0 or 1:

- -2, if and only if $\begin{cases} (a_{2i-1}, a_{2i}) = (b_{2i-1}, b_{2i}) = (1,0), & \text{or} \\ (a_{2i-1}, a_{2i}) = (b_{2i-1}, b_{2i}) = (0,1) \end{cases}$

- 1, if and only if $\begin{cases} (a_{2i-1}, a_{2i}) = (1,0), \ (b_{2i-1}, b_{2i}) = (0,1), & \text{or} \\ (a_{2i-1}, a_{2i}) = (0,1), \ (b_{2i-1}, b_{2i}) = (1,0) \end{cases}$

- 0, if and only if $\begin{cases} (a_{2i-1}, a_{2i}) = (0,0), & \text{or} \\ (b_{2i-1}, b_{2i}) = (0,0) \end{cases}$

Therefore $\langle \mathbf{b}_u, \mathbf{b}_v \rangle = -1$ if and only if there are exactly two terms equal to -2 and one equal to 1. On the other hand $\langle \mathbf{b}_u, \mathbf{b}_v \rangle = 0$ if and only if one term is -2 and two are equal to 1 or all three are 0. Now, we can reformulate the obtained results as follows. Two good vertices u and v with corresponding good sets U and V of hK_2 are good partners in the following three cases:

- If U and V have only one vertex in common then the remaining two are end-vertices of two copies of K_2 and u and v are non-adjacent.

- If U and V are disjoint then it does not exist a copy of K_2 having one end-vertex in U and the other in V and u and v are non-adjacent.

- If U and V have exactly two vertices in common then the remaining ones are different end-vertices of the same copy of K_2, and u and v are adjacent.

Note that H has at least 6 vertices. In the following example we will discuss what happens when $H = 3K_2$.

Example 6.2. *Let $H = 3K_2$, such that $V(H) = \{1, \ldots, 6\}$, and consider good vertices $u_1, \ldots, u_8$, such that $U_1 = \{1, 3, 5\}$, $U_2 = \{1, 4, 6\}$, $U_3 = \{2, 3, 6\}$, $U_4 = \{2, 4, 5\}$, $U_5 = \{1, 3, 6\}$, $U_6 = \{1, 4, 5\}$, $U_7 = \{2, 3, 5\}$, $U_8 = \{2, 4, 6\}$. The maximal number of those which are compatible is 4 (for $U_i \cap U_j = \emptyset$, u_i and u_j are not good partners). Up to isomorphism we can add:*

- u_1, u_2, u_3, u_4;

- u_1, u_2, u_3, u_5;

- u_1, u_2, u_5, u_6.

This leads to three connected maximal graphs G_1, G_2, G_3, with the $(1, 3)$-regular co-star set $H = 3K_2$ for the eigenvalue $\mu = -2$ (see Figures 7.3-6.4, where dark edges belong to a star complement).

Proposition 6.4. *If G is an S-maximal graph, with $\kappa = 1$ and $\tau = 3$, then $G = n_1G_1\dot{\cup}n_2G_2\dot{\cup}n_3G_3\dot{\cup}n_4K_2$, where the graphs G_1, G_2, G_3 are depicted in Figures 7.3-6.4.*

Moreover we can conclude that it does not exist a graph with $(1, 3)$-regular co-star set H if $|V(H)| < 6$. Graphs G_1, G_2, G_3 are the only connected graphs in this class (graphs with $(1, 3)$-regular co-star set).

Now, we switch to the complementary case.

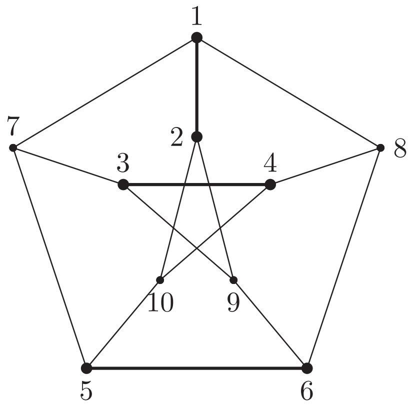

Figure 6.2: The Petersen graph G_1.

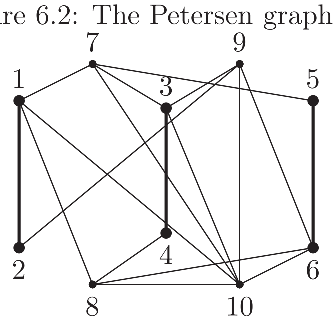

Figure 6.3: Graph G_2.

Proposition 6.5. *If G is an S-maximal graph, with $\kappa = s-2$, then $\tau \in \{s-1, s-3\}$ and $G = \overline{\frac{s}{2}C_4}$ for $\tau = s-1$ and $\overline{n_1G_1\dot{\cup}n_2G_2\dot{\cup}n_3G_3\dot{\cup}n_4K_2}$ for $\tau = s-2$, where the graphs G_1, G_2, G_3 are depicted in Figures 7.3-6.4.*

6.3.3 Case $\kappa = 2$

Now H is a disjoint union of cycles. For simplicity, here we will assume that H is connected. So let $H = C_h$, and $\mu = 2-\tau$, $C = \text{circul}(0,1,0,\ldots,0,1)$, where circul denotes the circular matrix (in this case of order h). Recall that (see [51, p. 107])

$$\text{circul}(a_1,\ldots,a_h)^{-1} = \frac{1}{h}\overline{F}D^{-1}F,$$

where F is $h\times h$ matrix with $f_{ij} = \omega^{(i-1)(j-1)}$, $\omega = e^{\frac{2\pi}{h}i}$ is a prime h-th root of 1 and $D = \text{diag}(\lambda_1,\ldots,\lambda_h)$ is such that $\lambda_i = f(\omega^{(i-1)})$ for $f(\lambda) = \sum_{i=1}^{h} a_i\lambda^{i-1}$. Then

$$\langle \mathbf{b}_u, \mathbf{b}_u\rangle = \mathbf{b}_u{}^T\,\text{circul}(\mu,-1,0,\ldots,0,-1)^{-1}\mathbf{b}_u = \mu$$

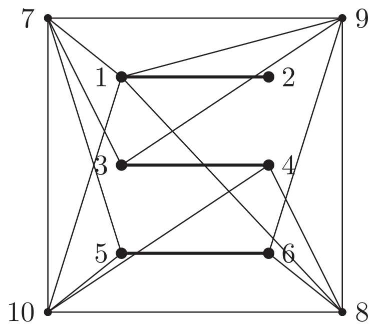

Figure 6.4: Graph G_3.

if and only if

$$\sum_{i=1}^{h} \lambda_i^{-1} |x_i|^2 = \mu h, \tag{6.7}$$

where $x_i = \sum_{j=1}^{h} b_j \omega^{(i-1)(j-1)}$. Since $\mathbf{b}_u$ has exactly τ nonzero entries then $x_1 = \tau$. It is well known (cf. [51, p. 107]) that $\lambda_i = \mu - \omega^{(i-1)} - \omega^{-(i-1)} = \mu - 2\cos\frac{2(i-1)\pi}{h}$ which implies $\mu - 2 \le \lambda_i \le \mu + 2$, that is, $-\tau \le \lambda_i \le 4 - \tau$. Suppose $\tau > 4$. Hence, $\frac{1}{4-\tau} \le \frac{1}{\lambda_i} \le -\frac{1}{\tau}$ and consequently $\sum_{i=2}^{h} \lambda_i^{-1} |x_i|^2 \le -\frac{(h-1)\tau^2}{\tau}$, since $|x_i|^2 \le \tau^2$. Moreover, $\lambda_1^{-1}|x_1|^2 = \frac{\tau^2}{\mu-2}$. Summing up all these observations, from (6.7) we obtain:

$$\frac{\tau^2}{\mu - 2} + (-\frac{(h-1)\tau^2}{\tau}) \ge \mu h,$$

an obvious contradiction. Therefore $\tau \in \{1, 2, 3, 4\}$. Since all eigenvalues of C_h are different from $2 - \tau$, we conclude the following:

1. If $h \equiv 0 (\text{mod } 12)$ then there is no option for τ;
2. If $h \equiv 6 (\text{mod } 12)$ then $\tau = 2$;
3. If $h \equiv x (\text{mod } 12)$, with $x \in \{1, 5, 7, 11\}$, then $\tau \in \{1, 2, 3, 4\}$;
4. If $n \equiv x (\text{mod } 12)$, with $x \in \{2, 10\}$, then $\tau \in \{1, 2, 3\}$;
5. If $n \equiv x (\text{mod } 12)$, with $x \in \{3, 9\}$, then $\tau \in \{1, 2, 4\}$;
6. If $n \equiv x (\text{mod } 12)$, with $x \in \{4, 8\}$, then $\tau \in \{1, 3\}$.

Subcase $\tau = 1$: Now $\mu = 1$. To determine all good vertices we will determine all unicyclic graphs with one pendant edge having 1 as an eigenvalue. These graphs are characterized in the next lemma.

Lemma 6.1. *Let G be a graph of order $h+1$ having the cycle C_h as a star complement. Then $1 \in \sigma(G)$ if and only if $h = 6k-1$ for some $k \in \mathbb{N}$.*

Proof. Note that $h(\mathrm{mod}\ 6) \neq 0$ since $1 \in \sigma(C_{6k})$ for any $k \in \mathbb{N}$. Let $\mathbf{x} = (x_0, x_1, \dots x_h)$ be the eigenvector for $\mu = 1$ (the pendent vertex is labelled by 0). We may set $x_0 = 1$ since 0 is in the star set. From the eigenvalue equations it follows

$$\mathbf{x} = (1, \underbrace{1, a, a-1, -1, -a, 1-a}, \dots, \underbrace{1, a, a-1, -1, -a, 1-a}, \dots, -a)^T,$$

for some $a \in \mathbb{R}$. The coordinates of $\mathbf{x}$ (starting from x_1) will periodically repeat with period 6. Depending on remainder of h modulo 6, $x_h = -a$ takes one of the values $1, a, a-1, -1, -a$ and $1-a$. Except for $h = 6k-1$ for some $k \in \mathbb{N}$, this argument leads to a contradiction. $\square$

For $C = A_{C_{6k-1}}$,

$$(I-C)^{-1} = \mathrm{circul}(1, \underbrace{\underbrace{0,-1,-1}, \underbrace{0,1,1}, \dots, \underbrace{0,-1,-1}}_{2k-1}, 0).$$

Good sets are singletons and hence the corresponding characteristic vectors can be labelled by e_i, $1 \leq i \leq 6k-1$ and good vertices by u_i. From

$$e_i^T (I-C)^{-1} e_j = \begin{cases} a_{6k-i+j}, & j \leq i-1 \\ a_{j-i+1}, & j > i-1 \end{cases},$$

where $(a_1, \dots, a_{6k-1})^T = (1, 0, -1, -1, 0, 1, 1, \dots, 0, -1, -1, 0)^T$, we obtain

- $a_1 = a_{6p} = a_{6p+1} = 1$ for $1 \leq p \leq k-1$;
- $a_{3p+2} = 0$ for $0 \leq p \leq 2k-1$;
- $a_{6p+3} = a_{6p+4} = -1$ for $0 \leq p \leq k-1$.

Therefore $u_i \sim u_j$, $i < j$ if and only if $j - i \equiv 2, 3 (\mathrm{mod}\ \ 6)$; $u_i \nsim u_j$, $i < j$ if and only if $j - i \equiv 1, 4 (\mathrm{mod}\ \ 6)$ while u_i and u_j are not good partners if and only if $j - i \equiv 0, 5 (\mathrm{mod}$

6). Hence, we can add at most 5 vertices. Moreover, by each rotation around u_i from i to any $6l+i$ the cycle C_{6k-1} remains $(2,1)$-regular co-star set for $\mu=1$. Hence:

Theorem 6.8. *Let G be a maximal graph having the cycle C_h as a $(2,1)$-regular co-star set for the non-main eigenvalue μ. Then $\mu=1$ and $h \equiv 5(mod \quad 6)$ and G is a graph depicted in Figure 5, where*

$$\{d(0,p), d(0,q), d(0,r), d(0,s)\} = \{1,2,3,4\},$$

and $d(0,v)$ is the reduced modulo 6 clockwise distance between 0 and v. In particular, if $h=5$ then G is the Petersen graph.

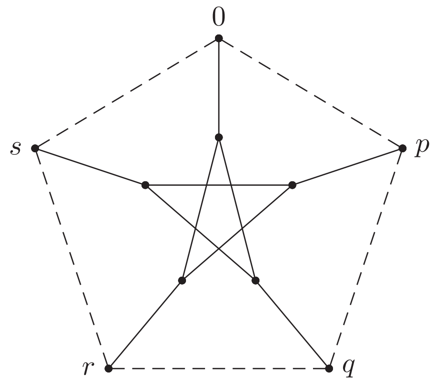

Figure 6.5: Graph with a $(2,1)$-regular co-star set C_{6k-1}.

<u>Subcase $\tau=2$:</u> Then $\mu=0$. Let $C=\text{circul}(0,1,0,0,\dots,0,1)$ of size h, with $h \not\equiv 0(\text{mod} \quad 4)$ and let $D=2C^{-1}$. Here we only consider the case $h \equiv 1(\quad \text{mod } 4)$; other two cases are quite analogous. Then

$$D = \text{circul}(1,1,-1,-1;1,1,-1,-1;\dots;1,1,-1,-1;1).$$

For $\mathbf{b}=(b_1,b_2,\dots,b_h)^T$ in view of the equation (6.2) we get

$$\langle \mathbf{b},\mathbf{b}\rangle = \sum_{i=1}^{h} b_i^2 + 2 \sum_{\substack{1\le i<j\le h \\ j-i\equiv 0(mod\ 4) \\ j-i\equiv 1(mod\ 4)}} b_ib_j - 2 \sum_{\substack{1\le i<j\le h \\ j-i\equiv 2(mod\ 4) \\ j-i\equiv 3(mod\ 4)}} b_ib_j,$$

which is equal to 0 if and only if

$$b_k = \begin{cases} 0, & k \neq i,j \\ 1, & k=i,j, \text{ where } j-i\equiv 2(mod\ 4) \text{ or } j-i \equiv 3(mod\ 4). \end{cases}$$

Since $h = 4l + 1$ then we have

$$4l - 1 + 4l - 5 + \cdots + 3 + 4l - 2 + 4l - 6 + \cdots + 2 = l(4l + 1) = hl$$

good vertices u_{ij} arising from $U = \{i, j\}$ where (i, j), $i < j$ corresponds to the position of -1 in the matrix D. Good vertices correspond to the sets:

$$\{i, 4k + 2 + i\},\ 1 \le i \le 4(l - k) - 1 \text{ and } \{i, 4k + 3 + i\},\ 1 \le i \le 4(l - k) - 2.$$

There are to many different types of vertices and therefore a question which of them are compatible becomes too messy. Therefore we restrict ourselves to some easier cases. First, it is easy to see that vertices of C_h at distance two are compatible with all. If we add all h vertices that arise in this way we get 4-regular graph G which is equal to NEPS (non-complete extended p-sum) of graphs C_h and K_2 with basis $\mathfrak{B} = \{(1, 1), (1, 0)\}$. For $h = 9$ this graph is depicted in the Figure 6.6.

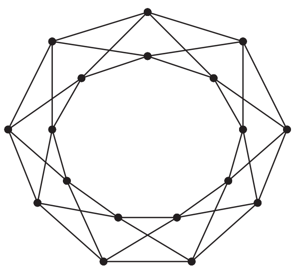

Figure 6.6: 4-regular graph with a (2,2)-regular co-star set.

The similar procedure can be applied when $h \equiv 2, 3 \pmod 4$. Thus we have:

Proposition 6.6. *NEPS of graphs C_h ($h \not\equiv 0 (mod\ 4)$) and K_2 with basis $\mathfrak{B} = \{(1, 1), (0, 1)\}$ is a 4-regular graph having C_h as a $(2, 2)$-regular co-star set for the eigenvalue 0.*

In the following example, we take $h = 9$ and in this particular case we determine all maximal graphs having C_h as $(2, 2)$-regular co-star set for the eigenvalue $\mu = 0$.

Example 6.3. *In this situation we divide good sets into two sets:*

$$S = \{\{1, 3\}, \{2, 4\}, \{3, 5\}, \{4, 6\}, \{5, 7\}, \{6, 8\}, \{7, 9\}, \{1, 8\}, \{2, 9\}\} \quad \textit{and}$$

$$T = \{\{1,4\},\{2,5\},\{3,6\},\{4,7\},\{5,8\},\{6,9\},\{1,7\},\{2,8\},\{3,9\}\}.$$

The vertices associated to subsets of S are compatible with all other subsets, while each vertex associated to a subset in T is not compatible with two vertices. More precisely, vertices arising from each of subsets $T_1 = \{\{1,4\},\{4,7\},\{1,7\}\}$, $T_2 = \{\{2,5\},\{5,8\},\{2,8\}\}$ and $T_3 = \{\{3,6\},\{6,9\},\{3,9\}\}$ are not compatible. So, we have 3^3 possibilities. However, some give rise to isomorphic graphs. Thus we get that there are three maximal reduced non-isomorphic graphs with desired properties. Their star sets correspond to the following three sets: $S \cup \{\{1,4\},\{2,5\},\{3,6\}\}$, $S \cup \{\{1,4\},\{2,5\},\{6,9\}\}$ and $S \cup \{\{1,4\},\{5,8\},\{3,6\}\}$. Here we depict the graph that arise in the first case.

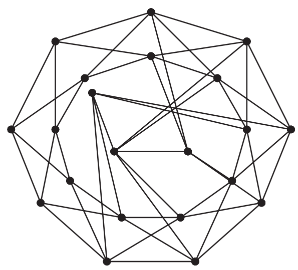

Figure 6.7: Non-regular graph with a $(2,2)$-regular co-star set C_9.

Subcase $\tau = 3$: Now $\mu = -1$. Again, by similar calculations, it follows that all good vertices which correspond to the three consecutive vertices of the cycle C_h are compatible with all. If we include all such h vertices we get 5-regular graph, bearing in mind that $h \not\equiv 0 (\text{mod } 3)$. Moreover:

Proposition 6.7. *NEPS of graphs C_h ($h \not\equiv 0 (mod\, 3)$) and K_2 with basis $\mathfrak{B} = \{(1,1),(0,1),(1,0)\}$ is a 5-regular graph having C_h as a $(2,3)$-regular co-star set for the eigenvalue -1.*

Subcase $\tau = 4$: Now $\mu = -2$. Graphs with $(2,4)$-regular co-star set are determined in [12] as graphs whose star complement for -2 is a cycle. The maximal graph is the line graph of K_h. The construction is possible only for odd cycles. It turns out that the good sets are the end-vertices of two non-adjacent edges of C_h.

We conclude this section with the following remarks. Besides the motivation given in Section 6.1, we have also in mind to consider star complement technique in presence of some regular-

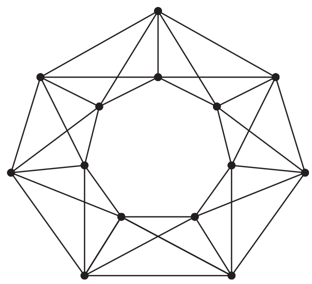

Figure 6.8: 5-regular graph with a (2,3)-regular co-star set.

ities (here (κ, τ)-regular sets) in order to see which maximal extensions can be characterized (by a simple subgraph and the star complement of some eigenvalue, see [44, 45]).

Considering the above examples, it turns that the Petersen graph (see Theorem 6.8) appears in this context; but also, in the same theorem, we found some non-regular graphs as its unusual "generalizations". So far we have tackled only some simpler cases for which analytical considerations were possible. It will be interesting to apply this technique to other cases. For instance, we believe that some strongly regular graphs, besides the Petersen graph, can be also constructed. But for this aim, computer aided approach must be used.

Chapter 7

Spectral characterization of families of split graphs

In this chapter we give an upper bound on the stability number of a connected graph. Also, for some connected graphs we establish a lower bound for the sum of the squares of the entries of the principal eigenvector corresponding to the vertices of an independent set. A spectral characterization of families of split graphs, involving its index and the entries of its principal eigenvector corresponding to the vertices of the maximum independent set of G is given.

The chapter is organized as follows. First we give an overview of the result from [23]. Then in Section 7.1 we apply this result to obtain an upper bound on stability number of a connected graph. In Section 7.2 a lower bound on the sum of squares of the entries of the principal eigenvector which correspond to the vertices of an independent set is given. In Section 7.3 we analyze when this lower bound reduces to equality, and by this we obtain a spectral characterization of some split graphs. In Section 7.4 on several examples we illustrate our results.

We start by recalling that a *split graph* is a graph whose vertex set can be divided into two subsets, one being a co-clique, the other being a clique, and all other edges (the cross-edges) join two vertices belonging to different subsets. If each vertex in co-clique is adjacent to all vertices in clique then G is called a *complete split graph.*

The eigenvector corresponding to the index of A_G can be taken to be positive. Unless stated otherwise, we will denote such vector by

$$\mathbf{x} = (x_1, x_2, \ldots, x_\nu)^T, \quad \nu = |V(G)|,$$

and assume that $\sum_{i=1}^{\nu} x_i^2 = 1$, i.e., $\mathbf{x}$ is a unit vector known as the *principal eigenvector* of G [26, p.16]. The results of this chapter are stated in terms of this eigenvector.

In [23] the following result was shown.

Theorem 7.1. *[23] Let G be a connected graph. If $S \subset V(G)$ is an independent set, then*

$$\sum_{i \in S} {x_i}^2 \leq \frac{1}{2}.$$

Moreover, G is bipartite with S as one color class if and only if $\sum_{i\in S} {x_i}^2 = \frac{1}{2}$.

For convenience we give the proof of this result. Here the set of edges with just one end vertex in S is denoted by $\partial(S)$.

Proof. Let $A_G = \begin{pmatrix} A_{G[S]} & B \\ B^T & A_{G[\bar{S}]} \end{pmatrix}$, λ_1 the index of G and $\mathbf{x}$ its corresponding eigenvector as introduced above, such that $\mathbf{x} = \begin{pmatrix} x \\ y \end{pmatrix}$, where the entries of $x = (x_1, \ldots, x_m)^T$ correspond to the vertices in S and the entries in $y = (y_1, \ldots, y_n)^T = (x_{m+1}, \ldots, x_\nu)^T$ correspond to the vertices in $\bar{S}$. Since $\lambda_1 x_i = \sum_{j\sim i} x_j$, then $\lambda_1 x_i^2 = \sum_{j \sim i} x_i x_j$. Therefore, it follows

$$\begin{aligned}
\lambda_1 \sum_{i \in S} x_i^2 &= \sum_{ij \in \partial(S)} x_i x_j \\
&= \sum_{pq \in E(G)} x_p x_q - \sum_{rs \in E(G[\bar{S}])} x_r x_s \\
&= \frac{\mathbf{x}^T A_G \mathbf{x}}{2} - \frac{1}{2} y^T A_{G[\bar{S}]} y \\
&= \frac{\lambda_1}{2} - \frac{1}{2} y^T A_{G[\bar{S}]} y.
\end{aligned}$$

Thus, we may conclude that

$$\lambda_1 (\frac{1}{2} - \sum_{i \in S} x_i^2) = \frac{1}{2} y^T A_{G[\bar{S}]} y. \tag{7.1}$$

Therefore, $y^T A_{G[\bar{S}]} y \geq 0 \Leftrightarrow \frac{1}{2} - \sum_{i \in S} x_i^2 \geq 0$, with equality if and only if $y^T A_{G[\bar{S}]} y = 0$, that is, if and only if $\bar{S}$ is also an independent set. □

However, there are bipartite graphs G with color classes V_1 and V_2 such that non of them are maximum independent sets, that is, there exists $S \subset V(G)$ such that $|S| > \max\{|V_1|, |V_2|\}$. As consequence, even for bipartite graphs G (as it is the case of the graph depicted in the next figure), there are maximum independent sets $S \subset V(G)$ such that

$$\sum_{i \in S} x_i^2 < \frac{1}{2}.$$

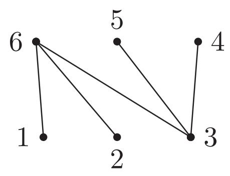

Figure 7.1: A bipartite graph where none of the color classes $V_1 = \{1, 2, 3\}$ and $V_2 = \{4, 5, 6\}$ is a maximum independent set and the maximum independent set $S = \{1, 2, 4, 5\}$ is such that $\sum_{i \in S} x_i^2 < 1/2$.

7.1 Upper bound on the stability number of connected graphs

From now on, assuming that $\mathbf{x}$ is the principal eigenvector of the connected graph G, $\underline{x}$ and $\bar{x}$ denote the minimum and the maximum, respectively, of the entries of $\mathbf{x}$.

As a consequence of Theorem 7.1, we deduce the following corollary.

Corollary 7.1. *If G is a connected graph of order ν, with index λ_1 and principal eigenvector $\mathbf{x}$, then*

$$\alpha(G) \leq \min\{\lfloor \frac{1}{2\underline{x}^2} \rfloor, \lfloor \nu - \frac{1}{2\bar{x}^2} \rfloor\}. \tag{7.2}$$

Proof. Let $S \subset V(G)$ be a maximum independent set for G. From (7.1), since $\frac{1}{2} - \sum_{i \in S} x_i^2 \geq 0$, it follows

$$\frac{1}{2} \geq \sum_{i \in S} x_i^2 \geq \alpha(G)\underline{x}^2 \Rightarrow \alpha(G) \leq \frac{1}{2\underline{x}^2}.$$

On the other hand, $\sum_{j\in\bar{S}} x_j^2 \geq \frac{1}{2} \Rightarrow (\nu-\alpha(G))\bar{x}^2 \geq \frac{1}{2} \Rightarrow \alpha(G) \leq \nu - \frac{1}{2\bar{x}^2}$. □

As immediate consequence of Corollary 7.1, if G is a connected regular graph of order ν, then

$$\alpha(G) \leq \frac{\nu}{2}.$$

7.2 A lower bound on $\sum_{i\in S} x_i^2$

Throughout this section, we consider a connected graph G with a vertex subset $S \subset V(G)$, such that $A_G = \begin{pmatrix} A_{G[S]} & B \\ B^T & A_{G[\bar{S}]} \end{pmatrix}$. Then

$$\lambda_1 = x^T A_{G[S]} x + 2\, x^T B y + y^T A_{G[\bar{S}]} y, \tag{7.3}$$

where $x = (x_1, x_2, \ldots, x_m)^T$ is such that x_j is the coordinate of $\mathbf{x}$ corresponding to the vertex $j \in S$ and $y = (y_1, y_2, \ldots, y_n)^T$ is such that y_i is the coordinate of $\mathbf{x}$ corresponding to the vertex $i \in \bar{S}$.

If S is an independent set, then $x^T A_{G[S]} x = 0$ and, since

$$\lambda_1 \sum_{i\in S} {x_i}^2 = \sum_{ij\in\partial(S)} x_i y_j = x^T B y\,,$$

from (7.3), it follows that

$$\lambda_1 = 2\lambda_1 \sum_{i\in S} {x_i}^2 + y^T A_{G[\bar{S}]} y. \tag{7.4}$$

For any $i \in \bar{S}$, by Cauchy-Schwartz inequality, we have

$$\sum_{j\in N_G(i)\cap\bar{S}} y_j \leq \sqrt{{d_i}'} \sqrt{\sum_{j\in N_G(i)\cap\bar{S}} {y_j}^2} \leq \sqrt{{d_i}'} \sqrt{1 - \sum_{j\in S} {x_j}^2 - {y_i}^2}, \tag{7.5}$$

where ${d_i}' = |N_G(i) \cap \bar{S}|$. Hence,

$$\sum_{j\in N_G(i)\cap\bar{S}} y_j \leq \sqrt{{d_i}'} \sqrt{1 - \sum_{j\in S} {x_j}^2 - {y_i}^2} \leq \sqrt{\Delta'} \sqrt{1 - \sum_{j\in S} {x_j}^2 - {y_i}^2} \tag{7.6}$$

where $\Delta' = \max_{i\notin S} {d_i}'$. Then,

$$y^T A_{G[\bar{S}]} y = (\sum_{j\in N_{G[\bar{S}]}(1)} y_j) y_1 + \ldots + (\sum_{j\in N_{G[\bar{S}]}(n)} y_j) y_n \leq \sqrt{\Delta'} \sum_{i\in\bar{S}} \left(\sqrt{1 - \sum_{j\in S} {x_j}^2 - {y_i}^2} \right) y_i. \tag{7.7}$$

Now, we look for the maximum of the function

$$F(y_1,\ldots,y_n)=\sqrt{\Delta'}\sum_{i\in\bar{S}}\left(\sqrt{1-\sum_{j\in S}{x_j}^2-{y_i}^2}\right)\ y_i \tag{7.8}$$

under the constraint

$$\sum_{i=1}^{n}{y_i}^2=1-\sum_{j\in S}{x_j}^2. \tag{7.9}$$

For this purpose we introduce the *Lagrangian* associated with constrained problem:

$$G(y_1,\ldots,y_n,\mu)=F(y_1,\ldots,y_n)-\mu\left(\sum_{i=1}^{n}{y_i}^2-(1-\sum_{j\in S}{x_j}^2)\right). \tag{7.10}$$

The stationary points of the function $G(y_1,\ldots,y_n,\mu)$ are the solutions of the following system of the equations:

$$\frac{\partial G}{\partial y_i} = \sqrt{\Delta'}\left(\frac{-{y_i}^2}{\sqrt{1-\sum_{j\in S}x_j^2-y_i^2}}+\sqrt{1-\sum_{j\in S}x_j^2-y_i^2}\right)-2\mu y_i=0,\ \text{ for } i=1,\ldots,n, \tag{7.11}$$

$$\frac{\partial G}{\partial \mu} = \sum_{i=1}^{n}y_i^2-\left(1-\sum_{j\in S}x_j^2\right)=0. \tag{7.12}$$

From (7.11) we obtain

$$y_i^2=\left(1-\sum_{j\in S}x_j^2\right)\left(\frac{1}{2}\pm\frac{\mu}{2\sqrt{\mu^2+\Delta'}}\right),\qquad \text{for } i=1,\ldots,n. \tag{7.13}$$

Let us first determine the entries y_i such that $y_i^2=\left(1-\sum_{j\in S}x_j^2\right)\left(\frac{1}{2}+\frac{\mu}{2\sqrt{\mu^2+\Delta'}}\right)$.

Assuming that there are p such entries y_i, with $0\le p\le n$, it follows that

$$p\left(1-\sum_{j\in S}x_j^2\right)\left(\frac{1}{2}+\frac{\mu}{2\sqrt{\mu^2+\Delta'}}\right)\le 1-\sum_{j\in S}{x_j}^2 \ \Leftrightarrow\ p\left(\frac{1}{2}+\frac{\mu}{2\sqrt{\mu^2+\Delta'}}\right)\le 1 \tag{7.14}$$

and then $p\le 2$. Otherwise, we get a contradiction.

Therefore, $p\in\{0,1,2\}$.

- If $p = 2$, then $\mu = 0$ and $n = 2$. Thus we get the stationary point of $G(y_1, \ldots, y_n, \mu)$:

$$(y_1^*, y_2^*, \mu^*) = (\sqrt{\frac{1 - \sum_{j\in S} x_j^2}{2}}, \sqrt{\frac{1 - \sum_{j\in S} x_j^2}{2}}, 0).$$

- If $p = 1$, then

$$\left(1 - \sum_{j\in S} x_j^2\right)\left(\frac{1}{2} + \frac{\mu}{2\sqrt{\mu^2 + \Delta'}}\right) + (n-1)\left(1 - \sum_{j\in S} x_j^2\right)\left(\frac{1}{2} - \frac{\mu}{2\sqrt{\mu^2 + \Delta'}}\right) = 1 - \sum_{j\in S} x_j^2,$$

which is equivalent to

$$\frac{n-2}{2}\left(1 - \frac{\mu}{\sqrt{\Delta' + \mu^2}}\right) = 0.$$

Therefore, $n = 2$ or $\Delta' = 0$.

1. If $\Delta' = 0$, then G is bipartite, with S as one of the two color classes and we obtain the stationary points of the function $G(y_1, \ldots, y_n, \mu)$:

$$(y_1^*, \ldots, y_n^*, \mu^*) \in \{(\sqrt{1 - \sum_{j\in S} x_j^2}, 0, \ldots, 0, \mu), \ldots, (0, 0, \ldots, \sqrt{1 - \sum_{j\in S} x_j^2}, \mu)\}$$

   where μ is arbitrary. But for any of these points $F(y_1^*, \ldots, y_n^*) = 0$.

2. If $\Delta' \neq 0$, then $n = 2$ and we obtain the following two stationary points of the function $G(y_1, \ldots, y_n, \mu)$:

$$\begin{aligned} (y_1^*, y_2^*, \mu^*) &= (\sqrt{1 - \sum_{j\in S} {x_j}^2}\sqrt{\frac{1}{2} - \frac{\mu}{2\sqrt{\mu^2 + \Delta'}}}, \sqrt{1 - \sum_{j\in S} {x_j}^2}\sqrt{\frac{1}{2} + \frac{\mu}{2\sqrt{\mu^2 + \Delta'}}}, \mu) \\ &\text{or} \\ &= (\sqrt{1 - \sum_{j\in S} {x_j}^2}\sqrt{\frac{1}{2} + \frac{\mu}{2\sqrt{\mu^2 + \Delta'}}}, \sqrt{1 - \sum_{j\in S} {x_j}^2}\sqrt{\frac{1}{2} - \frac{\mu}{2\sqrt{\mu^2 + \Delta'}}}, \mu) \end{aligned}$$

- If $p = 0$, then

$$n\left(1 - \sum_{j\in S} x_j^2\right)\left(\frac{1}{2} - \frac{\mu}{2\sqrt{\mu^2 + \Delta'}}\right) = 1 - \sum_{j\in S} x_j^2,$$

which is equivalent to $\mu^2 = \frac{(n-2)^2}{4(n-1)}\Delta'$. Therefore, we obtain the following stationary point of the function $G(y_1, \ldots, y_n, \mu)$:

$$(y_1^*, \ldots, y_n^*, \mu^*) = (\sqrt{\frac{1 - \sum_{j\in S} {x_j}^2}{n}}, \ldots, \sqrt{\frac{1 - \sum_{j\in S} {x_j}^2}{n}}, \frac{n-2}{2}\sqrt{\frac{\Delta'}{n-1}}).$$

According to the above analysis, we may say that the maximum of the function $F(y_1, \ldots, y_n)$, with $n \geq 2$, under the constraint (7.12), is attained at the point

$$(y_1^*, \ldots, y_n^*) \quad = \quad (\sqrt{\frac{1-\sum_{j\in S} {x_j}^2}{n}}, \ldots, \sqrt{\frac{1-\sum_{j\in S} {x_j}^2}{n}}) \tag{7.15}$$

and therefore

$$F(y_1, \ldots, y_n) \leq F(y_1^*, \ldots, y_n^*) = \sqrt{\Delta'}\sqrt{n-1}(1-\sum_{j\in S} x_j^2). \tag{7.16}$$

In case when $n = 1$ the graph in question is a star S_{m+1} and therefore bipartite with $\Delta' = 0$, which leads to $F(y_1, \ldots, y_n) = 0$, for any $(y_1, \ldots, y_n) \in \mathbb{R}^n$.

Now, taking into account (7.4) and (7.16), we obtain:

$$\lambda_1 \quad \leq \quad 2\lambda_1 \sum_{j\in S} {x_j}^2 + \sqrt{\Delta'}\sqrt{n-1}(1-\sum_{j\in S} {x_j}^2) \tag{7.17}$$

$$\Updownarrow$$

$$\lambda_1 - \sqrt{\Delta'}\sqrt{n-1} \quad \leq \quad (2\lambda_1 - \sqrt{\Delta'}\sqrt{n-1})\sum_{j\in S} {x_j}^2. \tag{7.18}$$

As immediate consequence, we have the main result of this section.

Theorem 7.2. *Let G be a connected graph with index λ_1 and let $S \subset V(G)$ be an independent set. Let us assume also that Δ' is the maximum degree of the subgraph of G induced by $\bar{S} = V(G) \setminus S$, $n = |\bar{S}|$ and $2\lambda_1 - \sqrt{\Delta'}\sqrt{n-1} > 0$. Then*

$$\sum_{j\in S} {x_j}^2 \geq \frac{\lambda_1 - \sqrt{\Delta'}\sqrt{n-1}}{2\lambda_1 - \sqrt{\Delta'}\sqrt{n-1}}. \tag{7.19}$$

7.3 Characterization of some split graphs

Based on the results obtained in the previous section, we are in conditions to introduce the following result.

Theorem 7.3. *Let G be a connected graph with index λ_1 and an independent set $S \subset V(G)$ such that $|\bar{S}| = n > 2$. Then G is a split graph such that $\sum_{k\in N_G(i)\cap S} d_k$ is constant for every $i \in \bar{S}$ if and only if*

$$\sum_{i\in S} x_i^2 = \frac{\lambda_1 - n + 1}{2\lambda_1 - n + 1} \tag{7.20}$$

with $\lambda_1 > \frac{n-1}{2}$.

Proof. Using the results obtained in the previous section, we may conclude the following.

1. The inequality (7.19) with $\lambda_1 > \frac{n-1}{2}$ holds as equality if and only if (7.17) with $\lambda_1 > \frac{n-1}{2}$ holds as equality.

2. The inequality (7.17) with $\lambda_1 > \frac{n-1}{2}$ holds as equality if and only if the principal eigenvector of G, $\mathbf{x} = \begin{pmatrix} x \\ y \end{pmatrix}$, is such that $y = (y_1^*, \ldots, y_n^*)^T$, $y^T A_{G[\bar{S}]} y = F(y_1^*, \ldots, y_n^*)$ and $\lambda_1 > \frac{n-1}{2}$.

3. The equality $y^T A_{G[\bar{S}]} y = F(y_1^*, \ldots, y_n^*)$ with $y = (y_1^*, \ldots, y_n^*)^T$ and $\lambda_1 > \frac{n-1}{2}$ holds if and only if both inequalities in (7.5) hold as equality with $y = y^*$ and $\lambda_1 > \frac{n-1}{2}$.

4. Both inequalities in (7.5) with $y = y^*$ hold as equality and $\lambda_1 > \frac{n-1}{2}$ if and only if the entries y_j^* are all equal for $j \in N_G(i) \cap \bar{S}$ (as it is the case, by (7.15)) and $N_G(i) \cap \bar{S} = \bar{S} \setminus \{i\}$, for every $i \in \bar{S}$, i.e., each vertex in $\bar{S}$ is adjacent to all vertices in $\bar{S}$ and $\lambda_1 > \frac{n-1}{2}$.

5. The previous statement is equivalent to say that both inequalities in (7.5) with $y = y^*$ hold as equality and $\lambda_1 > \frac{n-1}{2}$ if and only if the entries y_j^* are all equal for $j \in N_G(i) \cap \bar{S}$ (the point defined in (7.15)), each vertex in $\bar{S}$ is adjacent to all vertices in $\bar{S}$, i.e., $\bar{S}$ induces a complete subgraph, and $\lambda_1 > \frac{n-1}{2}$.

6. The entries y_j^* are all equal for $j \in N_G(i) \cap \bar{S}$, each vertex in $\bar{S}$ is adjacent to all vertices in $\bar{S}$ and $\lambda_1 > \frac{n-1}{2}$ if and only if y^*, defined in (7.15), is the subvector of the principal eigenvector of G with entries corresponding to the vertices in $\bar{S}$ and $\bar{S}$ induces a complete subgraph (then $\Delta' = n - 1$ and, as will see later, $\lambda_1 > \frac{n-1}{2}$).

7. The vector $y = y^*$ is the subvector of the principal eigenvector of G with entries corresponding to the vertices in $\bar{S}$ and $\bar{S}$ induces a complete subgraph if and only if G is a split graph such that $\sum_{k \in N_G(i) \cap S} d_k$ is constant for every $i \in \bar{S}$. In fact, let us prove this equivalence.

(a) Assume that $y = y^*$ (as defined in (7.15)) is the subvector of the principal eigenvector of G with entries corresponding to the vertices in $\bar{S}$ and $\bar{S}$ induces a complete subgraph. Therefore, G is a split graph. Furthermore, since $y_i^* = \sqrt{\frac{1-\sum_{j\in S} x_j^2}{n}}$, for $i = 1, \ldots, n$, by the eigenvalue equations, $\forall i \in S$

$$\lambda_1 x_i = d_i \sqrt{\frac{1-\sum_{j\in S} {x_j}^2}{n}} \quad \Leftrightarrow \quad x_i = \frac{d_i}{\lambda_1}\sqrt{\frac{1-\sum_{j\in S} x_j^2}{n}} \tag{7.21}$$

and $\forall i \in \bar{S}$

$$\lambda_1 \sqrt{\frac{1-\sum_{j\in S} x_j^2}{n}} = (n-1)\sqrt{\frac{1-\sum_{j\in S} x_j^2}{n}} + \sum_{k\in N_G(i)\cap S} \frac{d_k}{\lambda_1}\sqrt{\frac{1-\sum_{j\in S} {x_j}^2}{n}} \tag{7.22}$$

$$\Updownarrow$$

$$\lambda_1 = n-1+\sum_{k\in N_G(i)\cap S}\frac{d_k}{\lambda_1}. \tag{7.23}$$

The equality (7.23) means that $\sum_{k\in N_G(i)\cap S} d_k$ is constant for every $i \in \bar{S}$ and also that $\lambda_1 > n-1$.

(b) Conversely, if G is a split graph such that $\sum_{k\in N_G(i)\cap S} d_k$ is constant for every $i \in \bar{S}$, setting $y = y^*$, the eigenvalue equations (7.21) and (7.22) hold, and then the vector $\mathbf{x}$ became defined as an eigenvector of A_G. Since its entries are all positive components, then $\mathbf{x}$ is the principal eigenvector of G associated to the eigenvalue λ_1 which is the positive root of the quadratic polynomial

$$p(\lambda) = \lambda^2 - (n-1)\lambda - \sum_{k\in N_G(i)\cap S} d_k, \tag{7.24}$$

where i is chosen arbitrarily from $\bar{S}$ and then $\lambda_1 > n-1$.

8. Finally, since (7.19) (with $\lambda_1 > \frac{n-1}{2}$) holds as equality if and only if G is a split graph (therefore, $\Delta' = n-1$ and $\lambda_1 > n-1$) such that $\sum_{k\in N_G(i)\cap S} d_k$ is constant for every $i \in \bar{S}$, the result follows.

□

Computing the positive root of the quadratic polynomial (7.24), it follows that $\forall i \in \bar{S}$

$$\lambda_1 = \frac{1}{2}\left(n-1+\sqrt{(n-1)^2+4\sum_{k\in N_G(i)\cap S} d_k}\right).$$

For the particular case of a complete split graph, denoting the independence number of G by $\alpha(G)$ and its clique number by $\omega(G)$, we may conclude the following corollary.

Corollary 7.2. *Let G be a graph such that $\alpha = \alpha(G)$ and $\omega = \omega(G) > 2$ and let $S \subset V(G)$ be a maximum independent set. Then G is a complete split graph if and only if*

$$\sum_{j \in S} x_j^2 = \frac{1}{2} - \frac{\omega - 1}{2\sqrt{(\omega-1)^2 + 4\omega\alpha}},$$

where the x_j's are the entries of the principal eigenvector of G corresponding to the vertices of S.

Proof. Since the index of a complete split graph G is $\lambda_1 = \frac{\omega-1}{2} + \frac{1}{2}\sqrt{(\omega-1)^2 + 4\omega\alpha}$, applying Theorem 7.3, the result follows. □

7.4 Numerical examples

The graph of order $\nu = 9$ depicted in the Figure 7.2 has as principal eigenvector:

$$\mathbf{x}^T = [0.33610, 0.18607, 0.24307, 0.33610, 0.24307, 0.42779, 0.42779, 0.25191, 0.43797]$$

and its spectrum is

$$\sigma(G) = \{-3.11742, -1.65855, -1.61803, 0.00000, 0.00000, 0.00000, 0.61803, 1.17772, 4.59825\}.$$

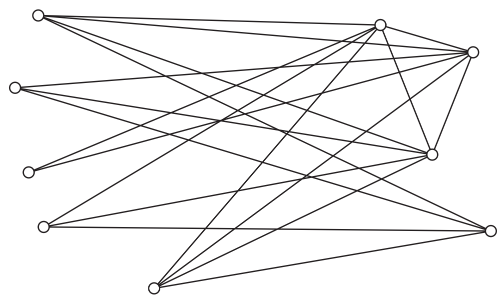

Figure 7.2: A connected graph G with independence number $\alpha(G) = 5$

Applying Corollary 7.1, since $\underline{x} = 0.18607$ and $\bar{x} = 0.43797$ it follows

$$\begin{aligned} \alpha(G) &\leq \min\{\lfloor \frac{1}{2\underline{x}^2} \rfloor, \lfloor \nu - \frac{1}{2\bar{x}^2} \rfloor\} \\ &= \min\{\lfloor 14.44167 \rfloor, \lfloor 6.39336 \rfloor\} \\ &= 6. \end{aligned}$$

Considering the maximum independent set of G, S, since $n = \nu - \alpha(G) = 4$ and $\Delta' = 2$, then $4.59825 = \lambda_1 > \frac{\sqrt{\Delta'(n-1)}}{2} = \frac{\sqrt{2\times 3}}{2} = 1.22474$. Therefore, taking into account that the entries of the principal eigenvector, $\mathbf{x}$ of G, corresponding to the maximal independent set are the first 5 (below denote by $x_1, \ldots, x_5$), applying Theorem 7.3, we obtain

$$\begin{aligned} 0.378715 = \sum_{j=1}^{5} x_j^2 &\geq \frac{\lambda_1 - \sqrt{\Delta'(n-1)}}{2\lambda_1 - \sqrt{\Delta'(n-1)}} \\ &= \frac{4.59825 - \sqrt{2\times 3}}{2 \times 4.59825 - \sqrt{2 \times 3}} \\ &= 0.318476. \end{aligned}$$

The graph H depicted in the Figure 7.3 has order $\nu = 6$ and principal eigenvector:

$$\mathbf{x}^T = [0.35877, 0.35877, 0.35877, 0.42099, 0.42099, 0.50931].$$

The spectrum of this graph is

$$\sigma(H) = \{-2.48361, -1.28282, 0, 0, 0, 3.76644\}.$$

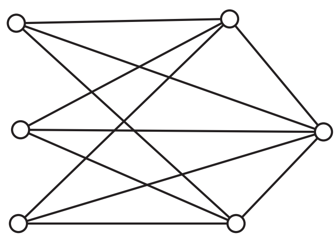

Figure 7.3: A connected graph H with independence number $\alpha(H) = 3$

Applying Corollary 7.1, since $\underline{x} = 0.35877$ and $\bar{x} = 0.50931$ it follows

$$\begin{aligned} \alpha(H) &\leq \min\{\lfloor \frac{1}{2\underline{x}^2} \rfloor, \lfloor \nu - \frac{1}{2\bar{x}^2} \rfloor\} \\ &= \min\{\lfloor 3.88452 \rfloor, \lfloor 4.07245 \rfloor\} \\ &= 3. \end{aligned}$$

It is worth mentioning that, in this case, this upper bound on the stability number is better than the one obtained by Cvetković in [24] (see also [26, Theorem 3.10.1.]), where $\alpha(G) \leq \min\{\nu-\nu^+, \nu-\nu^-\}$, with ν^+ and ν^- denoting the number of positive and negative eigenvalues of G respectively. In this particular case, the bound obtained by Cvetković gives $\alpha(H) \leq 4$.

Considering the maximum independent set of G, S, since $n = \nu - \alpha(H) = 3$ and $\Delta' = 2$, then $3.76644 = \lambda_1 > \frac{\sqrt{\Delta'(n-1)}}{2} = \frac{\sqrt{2\times 2}}{2} = 1$. Therefore, taking into account that the entries of the principal eigenvector $\mathbf{x}$ of H, corresponding to the maximal independent set are the first 3 (below denote by x_1, x_2, x_3), applying Theorem 7.3, we obtain

$$\begin{aligned} 0.38615 = \sum_{j=1}^{3} x_j^2 &\geq \frac{\lambda_1 - \sqrt{\Delta'(n-1)}}{2\lambda_1 - \sqrt{\Delta'(n-1)}} \\ &= 0.31926. \end{aligned}$$

Chapter 8

Conclusions and future work

With this work we managed to establish several spectral results on graphs with specific structure. Most of them give lower and upper bounds on the index of graphs (adjacency or signless Laplacian). Some parts of investigations gave side-effects as well. For example, the attempt to resolve the conjecture related with the largest eigenvalue of signless Laplacian led to the discovery of some properties of average edge (vertex) degrees of nested split graphs. In the end, these results have more merit since, by the initial approach, we gave only a partial proof of the conjecture mentioned above.

New bounds on the signless Laplacian index of nested split graphs offer also a better insight into the behaviour of Q-index of NSGs. Although our results, based on eigenvalue technique, include all relevant parameters and information on structure of nested split graphs, it turns out that in much of the cases a pretty simple bound that can be applied to any connected graph gives superior approximation. This phenomenon deserve to be studied more.

Regarding the approximations of the index of double split graphs, besides new bounds which are pretty good, we also benefit from the relation established between NSGs and DNGs, which gives a better upper bound on the index of NSGs than the known bounds. We have also found (by an extensive search) some examples in which the errors are not as small as those encountered with the graphs from Example 5.1. Fortunately this occurs very rarely. If it does occur then the main reason is the poor quality of our estimates for eigenvector components.

All these phenomena make part of our future interest. Also, it seems that regarding signless Laplacian spectra DNGs play similar role as in the case of adjacency spectra i.e. among all connected bipartite graphs of fixed order and size those whose signless Laplacian index is maximal, we suppose, are DNGs. If this conjecture is true, then it would be interesting to observe bounds regarding signless Laplacian spectra and see if the same phenomenon appears as in the case of NSGs. Another direction for the continuation of this work is to try to obtain bounds of DNGs using divisor matrix and the already existing bounds on the index of non-negative matrices. As it was mentioned in Remark 5.2 another interesting task can be a study of DNGs such that $\phi < \frac{3}{4}\epsilon^2$. These graphs are less frequent and therefore becomes more appealing to identify them.

Considering (κ, τ)-regular sets and star complements we give a better insight into Theorem 6.5 published in [21], providing several examples. We show that under the condition of Theorem 6.5 both mentioned options can hold as well just one. Moreover, we have showed that under the conditions that we posed just one option holds. Based on this result and star complement technique in several cases (where analytical approach was possible) we have constructed maximal graphs with a (κ, τ)-regular set inducing a star complement for a non-main eigenvalue μ, which has to be equal to $\kappa - \tau$. Here it will be interesting to apply this technique to other cases. For instance, we believe that some strongly regular graphs, besides the Petersen graph, can be also constructed. But for this aim, computer aided approach must be used. What appears as one more possibility for future work in this field is to observe the behaviour of star complements and (κ, τ)-regular sets under the generalized graph product NEPS.

So far, we have several ideas how to proceed work presented in Chapter 7. It would be interesting to see if the similar spectral characterizations can be obtained for nested split and double split graphs as well as some lower bounds on stability and clique number for any connected graph.

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