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Complementary spectrum of graphs

por

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Trabalho submetido como requisito parcial
para a obtenção do grau de

Doutora em Matemática Aplicada

Prof. Dr. Vilmar Trevisan
Orientador

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Trabalho submetido ao Programa de Pós-Graduação em Matemática Aplicada do Instituto de Matemática da Universidade Federal do Rio Grande do Sul, como requisito parcial para a obtenção do grau de

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LIST OF SYMBOLS

K_n	Complete graph with n vertices (clique with n vertices)
C_n	Cycle with n vertices
P_n	Path with n vertices
$K_{m,n}$	Complete bipartite graph, with m and n being the cardinality of its parts
S_n	Star with n vertices
$DS(p,q)$	Double-star with $p+q$ vertices
$LP(n,k)$	Lollipop with n vertices
$\|V\|$	Number of vertices
$\|E\|$	Number of edges
$\mathfrak{b}(G)$	Number of induced subgraphs of G that are not isomorphic to each other
$spect(G)$	Spectrum of the graph G with respect to its adjacency matrix
$spect_Q(G)$	Spectrum of the graph G with respect to its signless laplacian matrix
$spect_L(G)$	Spectrum of the graph G with respect to its laplacian matrix
$\ell(G)$	Line graph of the graph G
$\overline{G}$	Complementary graph of G
$\mathbb{I}_n$	Identity matrix of order n
$\lambda_1(G)$	Greatest eigenvalue of the adjacency matrix of the graph G (index of G)
$\lambda_n(G)$	n^{th} greatest eigenvalue of the adjacency matrix of the graph G
$\varrho(G)$	Greatest complementary eigenvalue of G
$\varrho_n(G)$	n^{th} greatest complementary eigenvalue of G

$G_1 \vee G_2$ Join between the graphs G_1 and G_2

$G_1 \cup G_2$ Union of the graphs G_1 and G_2

RESUMO

Neste trabalho, apresentaremos nosso estudo acerca de grafos coespectrais. Mostraremos construções de famílias de grafos coespectrais já conhecidas na literatura e também construções desenvolvidas durante nossa pesquisa envolvendo grafos thresholds e produto cartesiano. Iremos compartilhar com o leitor o processo histórico que envolve questionamentos acerca de grafos coespecrais. Por fim, apresentaremos nossa maior contribuição: sugerimos usar o espectro complementar de um grafo como alternativa para a representação espectral.

O espectro complementar não se trata de associar uma nova matriz a um grafo, mas sim de utilizar a já conhecida matriz de adjacências de uma forma diferente. Nesse viés, realizamos experimentos com famílias de grafos já conhecidas como as árvores, por exemplo. O espectro complementar, juntamente com os conceitos de raio espectral e entrelaçamento de grafos deram o suporte e embasamento para nosso estudo.

Por fim, estudamos o conceito de matróide e tentamos vincular com nosso problema de coespectralidade de grafos. Encontramos uma aplicação de um conhecido resultado de Teoria de Matróides na Teoria Espectral de Grafos, mais especificamente, na determinação de grafos.

ABSTRACT

In this work, we present our study around cospectral graphs. We display constructions of cospectral graphs already known in the literature, and also some constructions developed in our own research, which involve threshold graphs and cartesian product. Also, we share with the reader the historic process of raising questions about cospectral graphs. Finally, we then present our greatest contribution: we suggest use the complementary spectrum of a graph as an alternative to spectral representation.

The complementary spectrum is not about associating a new matrix to a graph, instead it is about utilizing the already known adjacency matrix in a different way. In this bias, we experiment with families of graphs that are well known, such as the trees, for example. The complementary spectrum, along with the concepts of spectral radius and graph interlacing, gave us the support and foundation to our study.

In the end, we study the concept of matroids and try to tie it with our problem of graph cospectrality. We find an application of a known result of the Matroid Theory on the Spectral Graph Theory, specifically, on graph determination.

RESUMO EXPANDIDO

Título: Espectro complementar de grafos

Um *grafo* é um par ordenado $G = (V, E)$, onde V é um conjunto finito cujos elementos são denominados *vértices* e E é um conjunto de subconjuntos de dois elementos pertencentes a V chamados de *arestas*. Os vértices são, comumente, representados por pontos e as arestas são representadas por ligações entre tais pontos.

Dado um grafo G, associamos a ele diferentes matrizes e o conjunto de seus autovalores formam o que chamamos de espectro de G. Podemos associar diferentes matrizes ao mesmo grafo G e isso significa diferentes espectros associados ao mesmo grafo, dependendo da matriz escolhida. A principal função da Teoria Espectral de Grafos é determinar características de um grafo a partir do espectro que associamos a ele. Entretanto, quando dois grafos possuem o mesmo espectro, nem sempre será possível determinar tais propriedades.

Quando dois grafos possuem características distintas, porém mesmo espectro, dizemos que esses grafos são coespectrais. Por outro lado, quando conseguimos associar um espectro unicamente a um dado grafo G, dizemos que esse grafo é determinado pelo seu espectro.

No Capítulo 2, explanamos a questão da coespectralidade de grafos. Ao longo dos anos, diversos matemáticos dedicaram-se ao estudo de grafos coespectrais. O problema de coespectralidade de grafos está ligado ao problema de isomorfismo, também clássico na Teoria de Grafos. Apresentamos a construção de Godsil [24] utilizando a operação Switching e, também, a construção de árvores coespectrais de Schwenk [41].

Inspirados nas construções de Godsil e Schwenk, dedicamos um tempo de nossa pesquisa ao estudo de construções de grafos coespectrais. Com a utilização do produto cartesiano, construímos grafos coespectrais em relação à matriz laplaciana sem sinal. Além disso, na família dos grafos thresholds, criamos uma família de tamanho exponencial de grafos coespectrais também em relação à matriz laplaciana sem sinal. O Capítulo 3 foi dedicado à apresentação desses artigos.

Muitos trabalhos foram feitos sobre coespectralidade de grafos ou, equivalentemente, sobre famílias que são determinadas pelo seu espectro. Uma questão que ainda não foi respondida é "Quais grafos são determinados pelo seu espectro?". Sabemos que esta é uma pergunta muito geral e respondê-la é difícil. Portanto, determinamos perguntas mais direcionadas, são elas:

1. Existem indícios de que alguma matriz determina um número maior de grafos do que outra?

2. Mudar a matriz associada ao grafo é, ou parece ser, a solução para o problema de coespectralidade?

3. Existe algum parâmetro que podemos associar unicamente a um grafo?

Uma questão natural seria: existe outro parâmetro que determina um família de grafos ou um grafo específico? Esta foi a questão que nos levou a estudar o espectro complementar. O espectro complementar de um grafo não é o conjunto de autovalores de uma nova matriz que iremos associar ao grafo. Trata-se de uma nova abordagem para a já conhecida matriz de adjacências.

Nosso estudo sobre espectro complementar nos apresenta indícios de uma resposta positiva para o problema de determinação de grafos. O espectro complementar de um grafo G pode ser visto como o conjunto dos índices (distintos) de todos os subgrafos induzidos de G. Os conceitos principais sobre espectro complementar estão no Capítulo 4.

Destacamos que, diferentemente da noção usual de espectro, a cardinalidade do espectro complementar não está exatamente bem difinida. Sabemos que ela é menor ou igual do que a quantidade de subgrafos induzidos do grafo inicial, já que não podemos garantir que todos os subgrafos induzidos terão índices distintos. Além disso, a cardinalidade desse conjunto será maior ou igual à quantidade de vértices do grafo inicial, pois, para cada subgrafo induzido retirando um vértice, teremos um índice distinto.

Dessa forma, alguns estudos estão sendo realizados acerca da cardinalidade do espectro complementar de um grafo G. Tais estudos também contribuem para nossa abordagem de coespectralidade de grafos, visto que a cardinalidade pode ser uma característica determinante em algumas famílias de grafos.

Encontramos, experimentalmente, o espectro complementar de famílias de grafos, como árvores, caminhos e ciclos, por exemplo e os resultados estão no Capítulo 5, no formato adaptado do artigo que publicamos.

Assim, podemos concluir que as contribuições desta tese são:

1. construção de uma família de grafos coespectrais em relação à matriz laplaciana sem sinal;
2. experimento para calcular o espectro complementar de famílias de grafos;
3. uma nova abordagem sobre espectro de grafos, utilizando a matriz de adjacências de forma não usual.

1 INTRODUCTION

Allegdly the first utilization of graphs have occured in 1736 by Leonard Euler (1707/1783) to solve the problem of the Seven Bridges of Königsberg [20] . This problem goes as follows: would it be possible to walk along the city of Königsberg passing by its seven bridges, without repetition, and return to the starting point? To solve this problem, Euler transformed the map of Königsberg into a graph, making use of the most elementary notion about graphs, which is defined below.

A *graph* is an ordered pair $G = G(V, E)$, where V is a finite set of elements that are known as *vertices*, and E is a collection of subsets composed of two vertices in V, which are called *edges*. The vertices are commonly represented by dots, while the edges are represented by lines connecting two of these dots.

In a graph $G = G(V, E)$, we say the edge $e = \{u, v\} \in E$ is incident to the vertices u and $v \in V$ and we also say the vertices u and v are adjacent, since there is an edge e incident to both u and v. To each vertex v_i we associate a natural number called *degree of the vertex* v_i, which represents the number of edges incident to v_i. We denote the degree of a vertex v_i by $d(v_i)$.

In Figure 1.1 we have a graph with 5 vertices and 4 edges where the vertices have degrees $d_{v_1} = 1$, $d_{v_2} = 3$, $d_{v_3} = 2$, $d_{v_4} = 2$ e $d_{v_5} = 0$.

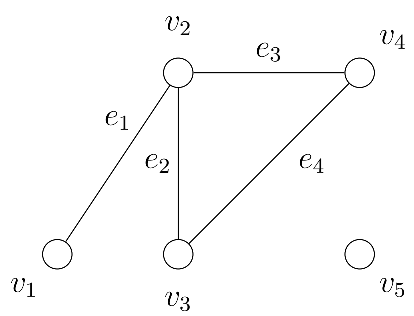


Figure 1.1: Graph represented by vertices and edges.

The graph used by Euler was that of the Figure 1.2, where each edge represents a bridge of Königsberg and the vertices are the islands formed by such bridges. The question now translates as: does a path that contains all the edges, with no repetitions, and that goes back to the starting point, exist?

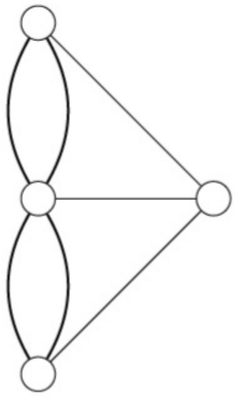


Figure 1.2: Graph that represents the problem of the Seven Bridges of Königsberg.

This kind of path has since being known as *Eulerian cycle* - or Eulerian circuit - thanks to the generalization given by Euler to solve the problem of the Seven Bridges of Königsberg. He proved that it's not possible to walk along all the bridges and return to the initial point without repeating any bridges, and the justification is very intuitive.

Suppose that such path exists and take a vertex v that belongs to the Eulerian cycle and that is not the initial vertex. The path can't repeat edges, so every time we use an edge to "enter" in v, we shall use another edge to "get out". This means we need an even number of edges incident to v, since if we did not have that, it would be impossible to "get out" of v without repeating an edge. The general result by Euler is that:

Theorem 1.1. *A connected graph G has an Eulerian cycle - or Eulerian circuit - if, and only if, all of its vertices have an even number of incident edges.*

Besides this, we can cite another classic problem in Graph Theory that is known as the Coloring Maps Problem. It deals with identifying how many colors are necessary for coloring a map in such a way that the neighbouring countries don't have the same color. Appel and Haken [5, 6] guaranteed that only four colors are enough, and their result became know as the Four Color Theorem. To the reader who wants to know more about Graph Theory, we indicate the following bibliography [8, 19].

Given a graph G, we associate it to different matrices, and the set of their eigenvalues make up what we call the spectrum of G. In 1931, Huckel [32] started what we nowadays know as the Spectral Graph Theory by representing molecules of hydrocarbon through a graph where the atoms of carbon are the vertices and their chemical bonds are the edges. He verified that the energy of the electrons associated to the molecule had a strong relation to the eigenvalues of the graph that represented it. Later, Cvetković [17] cemented this study with the publication of his thesis.

The matrices more developed in the bibliography are the adjacency (A), laplacian (L) and signless laplacian (Q) matrices. We recommend the bibliographies [9, 18, 45]. Each associated matrix will generate a different set of eigenvalues, which means we will have different spectra of the same graph depending on the kind of matrix we choose to associate it with.

The main goal of the Spectral Graph Theory is to describe characteristics of graphs from their spectra. There was a belief that it would be possible to create an one-on-one relation between a graph and the spectrum of its adjacency matrix, and hence to determine a graph directly from its spectrum. This means that, given the spectrum of G, we would be able to say exactly how the graph G is, but, this is not possible.

When that happens, we say the graph is *determined by the spectrum* (DS). It was expected that, if two graphs had the same spectrum, they would be the same graph, just differing by nomenclature. By abusing the notation a little, we can say that isomorphic graphs are "the same graph with different label for the vertices". We will work with simple graphs, with no direction nor weights. The formal definition is given in the following [44]:

Definition 1.1. *Two graphs G_1 and G_2 are said to be isomorphic if there exists a bijection between the set of vertices of G_1 and G_2 given by $f : V(G_1) \to V(G_2)$ such that two vertices u and v of G_1 are adjacent if, and only if, $f(u)$ and $f(v)$ are adjacent in G_2.*

An example can be seen in Figure 1.3.

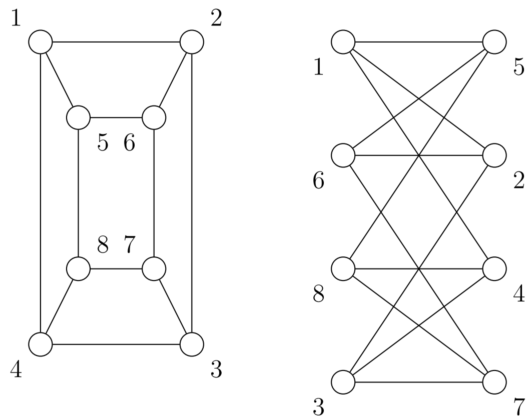


Figure 1.3: A pair of isomorphic graphs.

However, in 1957 [11], a pair of graphs that are not determined by the spectrum of their adjacency matrix was found. There were two graphs with distinct characteristics and with the same spectrum with respect to the adjacency matrix. They were a pair of non isomorphic graphs, but with the same spectrum. In this moment, we have the first idea of what we call cospectral pair of graphs.

Two graphs G_1 and G_2 are *cospectral* if the eigenvalues of the matrices associated with both graphs are the same, including multiplicities, and if G_1 and G_2 are not isomorphic. A classic example of a pair of cospectral graphs with respect to the adjacency matrix can be seen in Figure 1.4. This pair is called *Saltire pair*, was presented by Cvetković [17] and is the pair of cospectral graphs with respect to the adjacency matrix with the smallest number of vertices. All graphs with 4 vertices or less are determined by the spectrum of the adjacency matrix.

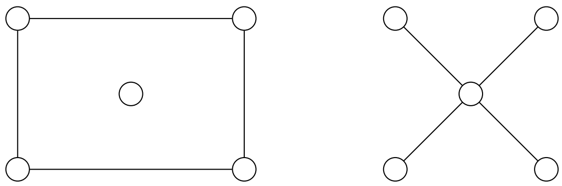


Figure 1.4: A pair of graphs with spectrum $\{-2, 0^{(3)}, 2\}$.

The graphs of Figure 1.4 are clearly not isomorphic, since one is disconnected and the other is not. By finding cospectral graphs, or family of cospectral graphs, we are at the same time finding families of graphs that are not determined by their spectrum. Therefore, we will be defining a class of graphs that are not DS.

There are a lot of works about cospectrality of graphs or, equivalently, families that are determined by their spectrum. A question which still has no answer is "What graphs are determined by their spectrum?". We know this is a very general question and answering it is hard. Thus, we ask the more specific questions listed below:

1. Are there indicatives that a particular matrix determines a greater number of graphs when we compare to another?
2. Does changing the matrix associated to the graph is, or seem to be, a solution to the problem of cospectrality?
3. Is there another parameter that we can associate to a graph and that ends up uniquely describing it?

In 1971, Schwenk [41] proved that almost all trees have a cospectral pair with respect to the spectrum of its adjacency matrix. This means that, given a tree T_1, there will almost always be another tree T_2 in such a way that both trees are not isomorphic, but both have the same spectrum with respect to the adjacency matrix. In 1977, Godsil and McKay [25] showed that this result also works for the laplacian matrix and the signless laplacian matrix.

In 1982, Godsil [24] presented an operation called switching, which was used to build pairs of cospectral graphs with respect to the adjacency matrix, but that also works with the signless laplacian matrix. In 2015, Souza and Trevisan [43] introduced a construction that generates pairs of cospectral graphs with respect to the signless laplacian matrix, utilizing the cartesian product operation between graphs. Recently, Carvalho et al. [10] came up with a construction that generates pairs of threshold graphs that are cospectral with respect to the signless laplacian matrix.

Although there exists constructions that generate pairs of cospectral graphs with respect to the three most used types of matrices, for a long time it was believed that modifying the associated matrix to the graph was a good way to lower the amount of existing cospectral graphs. In 2009, Cvetković [14, 16, 15] presented results that indicated the signless laplacian matrix as the possible solution to reduce the problem of cospectrality of graphs. The computational result given by Cvetković compares the quantity of cospectral graphs with respect to the adjacency, laplacian and signless laplacian matrices and points to the fact that, as the number of vertices increases, the number of cospectral graphs decreases.

This result, very well grounded, has been losing space, and even Cvetković himself already believes that whichever matrix is chosen, the quantity of cospectral graphs is essentially the same, if any, matrix determines a greater quantity of graphs. In this sense, we have the recent work of Haemers [27], that adresses several questions involving the matter, opening a range of possibilities to be studied. Initially, Haemers exhibit arguments in favour of the afirmative that cospectral graphs are rare, that is, in favour of the conjecture "Almost all graphs are DS". After that, he shows arguments that justify that cospectral graphs are abundant and can be constructed in a not so complicated way. These arguments will be presented further in the text.

Thereby, a natural question would be: is there another parameter that determines graphs? This was the question we asked at the start of our studies around the complementary spectrum. This new approach, that involves the adjacency matrix but does not use the usual spectrum, gives us hope that we have an affirmative answer.

During the research, we realized experiments and deeply studied the spectral theory applied to the complementary spectrum and our results were positive in several aspects. We introduce the complementary spectrum in detail in chapter 4, and our results are exhibited in chapter 5.

Chapter 2 is dedicated to the problematic on cospectrality. In this chapter, we bring recent results and conjectures on this subject, including for example classical constructions of cospectral graphs and, also, our article containing our original construction.

In chapter 3, we reproduce our paper on constructions of cospectral graphs. This is the result of our study involving the signless laplacian matrix.

2 COSPECTRALITY OF GRAPHS

In this chapter, we present the state-of-the-art about cospectrality of graphs, which is a subject that lately has been devoted a lot of attention. We show some ideas that have being deconstructed over time, and some new ideas that arise with the discovery of new tools.

2.1 Spectral Graph Theory

We will present some facts and results about Spectral Graph Theory. For more results, we indicate the following bibliographies [3, 9, 23, 30, 36]. Given a graph G, we associate to it different matrices which can represent from the adjacency between their vertices to the degree of each vertex. The matrices that will be discussed in this work are: adjacency matrix, laplacian matrix and signless laplacian matrix.

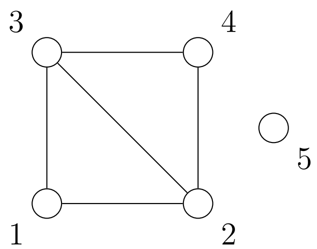
The *adjacency matrix* of a graph G, denoted by $A(G)$ is a square matrix of order equal to the number of vertices of G. The entries a_{ij} of this matrix will represent the adjacency between the vertices v_i and v_j of G. If v_i and v_j are adjacent, $a_{ij} = 1$. If not, $a_{ij} = 0$. Also, the diagonal of this matrix is made up only by zeroes.

The *degree matrix*, denoted by $D(G)$, is the matrix that shows only the information of the degree of each vertex. It will also be a square matrix of order equal to the number of vertices of G, but the entries will be $d_{ij} = 0$ when $i \neq j$ and, when $i = j$, $d_{ij} = d(v_i)$.

The *laplacian matrix* of a graph G, denoted by $L(G)$, is also a square matrix of order equal to the number of vertices of G, and is obtained by subtracting the adjacency matrix of G from the degree matrix of G. That is, $L(G) = D(G) - A(G)$.

The *signless laplacian matrix*, denoted by $Q(G)$, will be very similar to the laplacian matrix, except for the signs of the elements outside the diagonal. It is obtained by summing the adjacency matrix of G and the degree matrix of G. As such, we have $Q(G) = D(G) + A(G)$.

As it can be seen below, in Figure 2.1, we present a graph with 5 vertices and the adjacency, laplacian and signless laplacian matrices associated to it. Note that the only difference between the laplacian matrix and the signless laplacian matrix is the sign of the elements outside the diagonal. We do not explicit the degree matrix of G, though the same can be obtained just by looking at the diagonal of the laplacian or the signless laplacian matrices of G.



$$A(G) = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad L(G) = \begin{bmatrix} 2 & -1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 & 0 \\ -1 & -1 & 3 & -1 & 0 \\ 0 & -1 & -1 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$Q(G) = \begin{bmatrix} 2 & 1 & 1 & 0 & 0 \\ 1 & 3 & 1 & 1 & 0 \\ 1 & 1 & 3 & 1 & 0 \\ 0 & 1 & 1 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Figure 2.1: Graph G and the matrices $A(G)$, $L(G)$ and $Q(G)$.

In the same way we associate matrices to graphs, we can also associate a graph to their spectrum. If M is the representation matrix of the graph G, the M-

spectrum of G will be the set of eigenvalues of the matrix M. To find the eigenvalues of M, we define the *characteristic polynomial* $P(x)$ of an matrix M associated to the graph G as $P_G(x) = det(x\mathbb{I} - M)$. The roots of this polynomial are the eigenvalues of the matrix M.

More formally, we define the *eigenvalues* of M as being the numbers λ such that $Mv = \lambda v$ for some non-zero vector v. In that case, we say v is an *eigenvector* associated to the eigenvalue λ.

The *spectrum* of a graph G is denoted by $spect(G)$ and is defined as the matrix of order $2 \times s$ where the first line is constituted by the distinct eigenvalues of the adjacency matrix and the second line are their respective multiplicities. On the example of the Figure 2.1, $spect(G) = \begin{bmatrix} 0 & -1 & \frac{1}{2} - \frac{\sqrt{17}}{2} & \frac{1}{2} + \frac{\sqrt{17}}{2} \\ 2 & 1 & 1 & 1 \end{bmatrix}$.

To facilitate the reading, we will treat the spectrum of a graph as a set with its respective multiplicities indicated. For example, the matrix above will be represented by $spect(G) = \left\{ 0^{(2)}, -1, \frac{1}{2} - \frac{\sqrt{17}}{2}, \frac{1}{2} + \frac{\sqrt{17}}{2} \right\}$.

When we are treating with other kind of matrices, we will use the notation $spect_M$. Therefore, $spect_Q(G)$ will be the spectrum of the graph G with respect to the signless laplacian matrix and $spect_L(G)$ will denote the spectrum of G with respect to the laplacian matrix.

We define the *complementary graph* of G, denoted by $\overline{G}$, as the graph with the same set of vertices as G and with incident edges on the vertices v_i and v_j if, and only if, v_i and v_j are not adjacent in G.

We define the generalized spectrum of G, denoted by $spect_g(G)$, as the set formed by the union of the eigenvalues of $A(G)$ and of $A(\overline{G})$. As an example, set $F = C_4$, so that $\overline{G} = 2P_2$, as we can see in Figure 2.2. We will have $spect(G) = \{-2, 0^{(2)}, 2\}$ and $spect(\overline{G}) = \{-1^{(2)}, 1^{(2)}\}$. Thus, $spect_g(G) = \{-2, -1^{(2)}, 0^{(2)}, 1^{(2)}, 2\}$.

Figure 2.2: C_4 and $2P_2$.

Note that the matrices A, D, L and Q are simetric, so their eigenvalues are real and, consequently, the spectrum of the graph G will be a set of real numbers, no matter what of the associated matrices we're working with. The same will happen with the generalized spectrum. The spectrum of a graph is directly dependent of the matrix we use to find the characteristic polynomial. As such, the same graph may admit different sets as its spectrum.

The main goal of the Spectral Graph Theory is to determine characteristics of a graph from the spectrum we associate it with. However, when two graphs have the same spectrum, it's not always possible to determine this properties. And this is exactly the subject of our work: to analyse graphs, or even families of graphs, that can't have their characteristics determined by their spectrum.

Some very well known examples of informations that we can obtain from the matrices associated to a graph are the number of vertices, edges and the number of triangles, and those can be pointed out by just looking at the characteristic polynomial of the adjacency matrix.

Theorem 2.1. *Let G be a graph with n vertices and m edges and let*

$$P_G(\lambda) = \lambda^n + a_1\lambda^{n-1} + a_2\lambda^{n-2} + \cdots + a_{n-1}\lambda + a_n$$

be the characteristic polynomial of G. Then the coefficients of $p_G(\lambda)$ satisfy:

(i) $a_1 = 0$*;*

(ii) $a_2 = -m$*;*

(iii) $a_3 = -2t$*, where t is the number of triangles of the graph G.*

Proof. Firstly, lets remember a fact from linear algebra of which the demonstration can be seen in [30], and that states that, for each i, $1 \leq i \leq n$, the sum of the principal minors of $A(G)$ with i rows and i columns is equal to $(-1)^i a_i$. The strategy of the demonstration of this Theorem is to calculate the sum of the principal minors of $A(G)$ of order 1, 2 and 3 to use the result of [30] and relate them with a_1, a_2 and a_3, respectively.

(i) We know that a_1 is going to be equal to the sum of all principal minors of $A(G)$ of order 1. This means we have to take out all the $n-1$ rows and their respective columns of $A(G)$, with the only remainder being a matrix of order 1 which the only element is a 0. We will have n such principal minors, so that:

$$(-1)^1 a_1 = n \cdot 0$$

$$a_1 = 0.$$

(ii) The principal minors of order 2 can either be zero or be of the type:

$$\begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} = -1$$

and for each pair of adjacent vertices in G, we will have a non-zero principal minor. So, by looking at all pairs of vertices of the graph, we see that for each existing edge in G, we will have a non-zero principal minor. Therefore,

$$(-1)^2 a_2 = (-1)m$$

$$a_2 = -m.$$

(iii) Now let's look at the principal minors of order 3. We have the following possibilities:

$$\begin{vmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{vmatrix} = 0, \begin{vmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{vmatrix} = 0, \begin{vmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{vmatrix} = 2$$

so we see the only non-zero possibility is when we have the three corresponding vertices adjacent to one another, that is, when we have a triangle.

Thus

$$(-1)^3 a_3 = 2t$$

$$a_3 = -2t.$$

□

Given a graph, we can associate several characteristics of it, as diameter, energy, algebraic connectivity, and so on. Initially it was believed that associating a graph with a matrix would be a good way to store informations about that graph. Furthermore, it was thought that the eigenvalues generated by the associated matrix would account for translating all these several characteristics in a way that it would be possible to identify the graph with the drawing that represents it.

As an example, we have the work of Kac [33] and Fisher [22] where the following question was proposed: "Can one hear the form of a drum?". Kac modelated a drum as a graph and the sound of the drum was characterized by the eigenvalues of the adjacency matrix of this graph. The question of Kac and Fisher is, essentially, "Are the graphs that characterize drums DS?". With the affirmative of this question, we would have an unique form to characterize the form of a drum (initial graph) through its sound (its eigenvalues).

It was only possible to think of the idea of graphs not being determined by their spectrum in 1957, after Collatz and Sinogowitz [11] presented the first pair of cospectral graphs that there's knowledge of: a pair of trees that can be seen in Figure 2.3. Until then, the belief was that all graphs were DS.

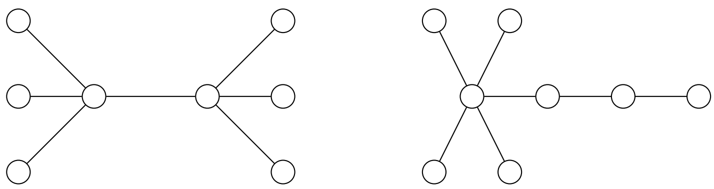


Figure 2.3: First pair of cospectral graphs.

What this meant was that, for example, graphs with different diameters could have the same set of eigenvalues. This being the case, it would be impossible to use this data bank generated via the spectrum of the adjacency matrix to "return" to the drawing of the graph. From this impossibility of uniquely defining a graph via spectrum of its adjacency matrix, it was born what is today one of the most recurring topics in Spectral Graph Theory: the cospectrality of graphs.

The isomorphism problem is a classic problem of the theory of complexity. It deals with determining the complexity to verify if two graphs are isomorphic and, up until these days, it's not known if this is a NP-complete problem. Although various specialists in the area believe that it is indeed a NP-complete problem, in 2015 Babai [31] announced in a series of talks that this problem is almost polynomial, with complexity bounded by

$$2^{O(log_n^c)}.$$

Though Babai's work still hasn't been published and is still being revised, the historic of Babai's excelent contributions to the area leads us to believe the result is correct, even it being an unexpected result.

The problem of cospectrality of graphs has a strong contribution to the problem of isomorphisms, since isomorphic graphs are, necessarily, cospectral with respect to all the matrices they may be associated with. In other words, when we determine a family of graphs DS with respect with some matrix (adjacency, laplacian or signless laplacian - to cite the matrices used on this work), we are actually claiming that there's no isomorphic graphs in that family with the same spectrum. Therefore, the quantity of possibly isomorphic graphs decreases and, consequently, the complexity to verify which pairs are isomorphic also does.

Hence, we see the importance of the matter, as well as some reasons that motivate the fact of this being such a recurrent topic and of great interest. And, indeed, the problem of cospectrality of graphs has been, for a long time, one of the greatest motivations to the study of different matrices in the search for new alternatives to describe graphs. We talked about pairs of cospectral graphs [1], although, we must note that there can be triples, quartets, etc.

In Figure 2.4, we have the example of a cospectral triple with respect to the adjacency matrix and of which the spectrum is

$$\{3.48929, 1.28917, 0^{(2)}, -1, -1.77846, -2\}.$$

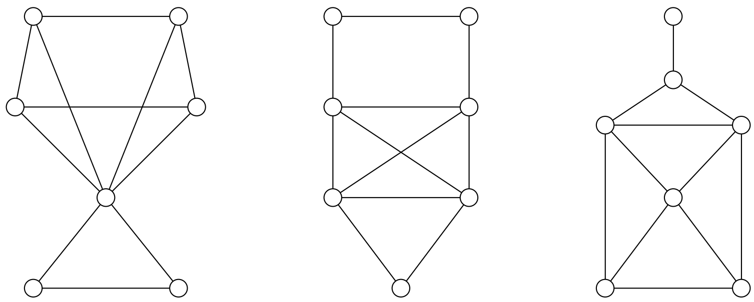


Figure 2.4: Triple of graphs which are cospectral with respect to the adjacency matrix.

It is already known that the adjacency matrix wasn't the best alternative to describe graphs via spectrum. Between the years of 2009 and 2010, Cvetković e Simić presented [14, 15, 16] a series of clues that lead to conclude that the signless laplacian was a better alternative to solve the cospectrality problem or, at least, to ease it. We will exhibit a concept called by this authors by cospectral uncertainty, that is determined by the ratio $\frac{|\mathfrak{G}'|}{|\mathfrak{G}|}$, where $\mathfrak{G}$ is the set of all graphs of n vertices and $\mathfrak{G}'$ is the set of all graphs with n vertices that have a cospectral pair.

The cospectral uncertainty is a parameter that depends on the type of matrix we associate to the graph, since the cospectral graphs in $\mathfrak{G}'$ will also depend on the associated matrix. The calculation is made in the following manner: fix the number of vertices n, $\mathfrak{G}$ represents the totality of graphs with n vertices and $\mathfrak{G}'$ are the graphs, inside the set $\mathfrak{G}$, that are cospectral with some other graph also in $\mathfrak{G}$.

[1]The original term is cospectral mate that does imply the possibility of having sets formed by more than two graphs.

The authors studied the cospectral uncertainties related to the adjacency, laplacian and signless laplacian matrices for graphs with up to 11 vertices. In Table 2.1, we have r_n, s_n and q_n, which are the cospectral uncertainties with relation to the adjacency, laplacian and signless laplacian matrices, respectively, and where n is the fixed number of vertices.

n	4	5	6	7	8	9	10	11
r_n	0	0,059	0,064	0,105	0,139	0,186	0,213	0,211
s_n	0	0	0,026	0,125	0,143	0,155	0,118	0,090
q_n	0,182	0,118	0,103	0,098	0,097	0,069	0,053	0,038

Table 2.1: Cospectral uncertainty introduced by Cvetković and Simić.

What supported the theory of Cvetković was the numerical result for q_n which, besides being the worst of the three for $n < 7$, seems to get increasingly better as n grows. Besides that, q_n forms a decreasing sequence for $n \leq 11$, thus suggesting that this sequence may continue to be decreasing even for $n > 11$.

For some time it was believed that finding pairs of cospectral graphs with respect to the signless laplacian matrix was something with a great degree of difficulty, even so that it turned this into a problem of interest for some authors. Indeed, the idea that some constructions of pairs of cospectral graphs with respect to the signless laplacian matrix were very difficult resulted on such constructions gaining room in the literature.

Recently, Haemers [27] came up with the following conjecture: "Almost all graphs are determined by the spectrum". Note that the term "almost all" means that, even though some graphs are not DS, as we increase the number of vertices, the proportion of cospectral graphs decreases. That is, the cospectral uncertainty goes to zero as the number of vertices goes to infinity.

Then, he presented arguments that either supported or contradicted the conjecture. Obviously this conjecture raises again the old question about determining graphs by their spectrum, and opens room for discussion, although now taking into account all the recent studies on the subject. But, first, we will present some special graphs.

Let $G = G(V, E)$ be a graph. We say that a *walk* of lenght n between two vertices v_i and $v_j \in V$ is a sequence $u_0e_1u_1e_2...u_{n-1}e_nu_n$ such that $u_0 = v_i$, $u_n = v_j$ and we have $u_1, ..., u_{n-1} \in V$ and $e_k = \{u_{k-1}, u_k\} \in E$, for all $k \in \{1, ..., n\}$. A *closed walk* is a walk that satisfies $v_i = v_j$. When there is no repetition of vertices of the walk and the initial vertex is different from the final vertex, we have a *path*. When the initial and final vertices of the walk are the same and no other vertex is repeated, we call that walk a cycle. A path with n vertices is denoted by P_n and a cycle with n vertices is denoted by C_n.

A graph is said *complete* if any two distinct vertices are adjacent. We denote by K_n a complete graph of n vertices. As follows in Figure **??**, we have an example of K_4.

A graph $G = (V, E)$ is said *k-partite* if there exists a partition of its vertices in k non-empty and two-by-two disjoint subsets in such a way that the vertices on each of the subsets are not adjacent between them. If $k = 2$, we say G is *bipartite* and if $k = 3$, we say G is *tripartite*.

We say a graph $G = (V, E)$ is *complete bipartite*, if G is bipartite ($V = V_1 \cup V_2$) and each vertex of the set V_1 is adjacent to all the vertices of V_2. Supposing $|V_1| = r$ and $|V_2| = s$, we write $G = K_{r,s}$. In Figure 2.5 we have an example of bipartite graph and of complete bipartite graph.

Figure 2.5: Bipartite graph and complete bipartite graph $K_{2,3}$.

A very well known and studied example of bipartite graph is the *tree*, that by definition is a connected and acyclic graph. In Figure 2.6 we have an example of a tree.

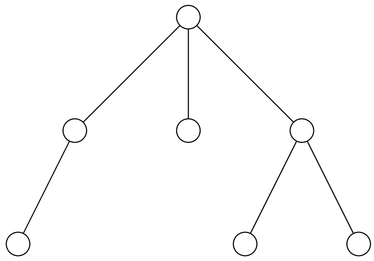


Figure 2.6: Example of a tree.

We say a graph is k*-regular* if all of its vertices have the same degree k. Let G be the regular graph with v vertices and degree k. The graph G will be called *strongly regular* if there are constants λ and μ such that: adjacent vertices in G have λ common neighbours, two by two; non-adjacent vertices in G have μ neighbours in common, two by two. We denote any such graph by $srg(v, k, \lambda, \mu)$. An example of strongly regular graph can be seen in Figure 2.7. This graph is known as *Paley graph* of order 9.

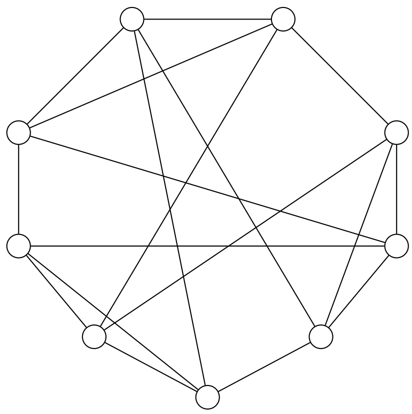


Figure 2.7: $srg(9, 4, 1, 2)$.

2.2 Arguments against the conjecture

Some arguments go in the direction of convincing us that almost all graphs have a cospectral pair, that is, they seem to contradict Haemers conjecture.

1. *Schwenk Trees [41]*: the first argument against the conjecture could not be another. Schwenk's construction is, without a doubt, the one with the most impact in Spectral Graph Theory. He proved that almost all trees are cospectral. This means that amongst the set of all trees, almost all of them have the necessary condition for the construction of a cospectral pair. We detail this construction in the next chapter.

2. *Strongly regular graphs [45]*: The conjecture is not true for strongly regular graphs. The spectrum of a strongly regular graph G depends on three parameters: the number of vertices n, the number of triangles and the degree k of the graph. Since $0 \leq \lambda < k < n$, we have that n^3 is an upper bound for the number of different spectra we may have in the family of strongly regular graphs of n vertices. On the other hand, the number of graphs belonging to this family grows exponentially as n grows, hence the proportion of cospectral graphs among the family grows rapidly.

3. *Construction of cospectral graphs*: The construction of cospectral graphs is not extremely difficult. A famous example is the famous Godsil switching [24], which generates pairs of cospectral graphs with respect to the adjacency, the laplacian and also the signless laplacian matrices. This operation will be explained in the next chapter. Other examples can also be seen in recent works [10, 43] where we have the construction of pairs of cospectral graphs with respect to the signless laplacian matrix. The first reference presents a construction involving the cartesian product operation, and the second is about a construction for threshold graphs.

4. *There are just a few graphs known to be DS*: This argument is more subjective, although it has a strong bibliographic appeal. Only a few graphs have

been proved to be determined by their spectrum. And, when they are, it is because of some strong property, as an example we can cite the fact that paths and cycles are DS. But they account for a very little amount when compared to the immensity of graphs that are not known to be DS or not.

2.3 Arguments in favour of the conjecture

In the following, it can be observed that the arguments supporting the conjecture made by Haemers are more recent than those against the conjecture.

1. *Ratio of graphs that are DS*: Haemers presented a table with the results of the calculations of the ratio of graphs that are DS. For the graphs with up until 9 vertices, the reference is due to Godsil [24]. Haemers and Spence [2, 50] made the calculations for $n \geq 10$. The table shows the quantity of graphs that are DS decreases for graphs with up to 10 vertices, but it starts to increase from this point as we increase the number of vertices, what suggests that we have a greater quantity of graphs determined by the spectrum as long as we increase the number of vertices n.

n	number of graphs	ratio of graphs DS
1	1	1
2	2	1
3	4	1
4	11	1
5	34	0.941
6	156	0.936
7	1044	0.895
8	12346	0.861
9	274668	0.814
10	12005168	0.787
11	1018997864	0.789
12	165091172592	0.812

2. *Generalized Spectrum*: In [48], Wang e Xu present a method that, given a randomly generated graph G, finds all graphs with the same generalized spectrum of G. Some experiments showed us that a big part of this graphs is determined by its generalized spectrum. Besides that, [46, 47] also shows that the generalized spectrum determines a portion of graphs that satisfies some properties involving the path matrix.

Some constructions of cospectral graphs have been very important in the bibliography and will be presented below. The Godsil's switching, as well as the construction of the trees of Schwenk are, without a doubt, the best known constructions. Next, we exhibit a construction with threshold graphs that was made by us and is part of our original contribution. This construction has been published and the paper (with adaptations) will complement this section.

2.4 Godsil's Switching

The Godsil's switching is among the most important operations about cospectrality of graphs. This operation may be used to construct cospectral graphs with respect to the adjacency, laplacian or the signless laplacian matrix. Furthermore, this construction generalizes other constructions of cospectral graphs, such as for example the construction of cospectral trees of Schwenk.

Firstly, we exhibit an important result that is enough to show that Godsil's operation works for the adjacency, the laplacian and also the signless laplacian matrices.

One way to show the cospectrality between two graphs is to show that their matrices are similar. A matrix $B \in \mathbb{R}^{n\times n}$ is said to be *similar* to a matrix $A \in \mathbb{R}^{n\times n}$ if there exists a non-singular matrix $S \in \mathbb{R}^{n\times n}$ such that

$$B = S^{-1}AS.$$

Theorem 2.2. *Let A and $B \in \mathbb{R}^{n\times n}$. If B is similar to A, then the characteristic polynomials $P_A(x)$ of A and $P_B(x)$ of B are the same.*

Proof. We have that $P_B(x) = det(x\mathbb{I} - B)$. Since B is similar to A, there exists a matrix $S \in \mathbb{R}^{n\times n}$ such that $B = S^{-1}AS$. Rewriting $\mathbb{I} = S^{-1}S$ and $B = S^{-1}AS$, we obtain:

$$\begin{aligned} P_B(x) &= det\left[x(S^{-1}S) - S^{-1}AS\right] = det\left[S^{-1}(x\mathbb{I} - A)S\right] \\ &= det(S^{-1})det(x\mathbb{I} - A)det(S) = det(x\mathbb{I} - A) \\ &= P_A(x). \end{aligned}$$

□

Corollary 2.1. *If A and $B \in \mathbb{R}^{n\times n}$ are similar, then A and B have the same eigenvalues, counted with multiplicities.*

The operation *join*[2] between two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, denoted by $G_1 \vee G_2$, results in a graph in which the set of vertices is $V_1 \cup V_2$ and in which

[2]The operation join may also be known as the complete product.

the set of edges is obtained by keeping the existing edges in G_1 and G_2, and connecting each vertex of G_1 to all vertices of G_2. An example can be seen in Figure 2.8.

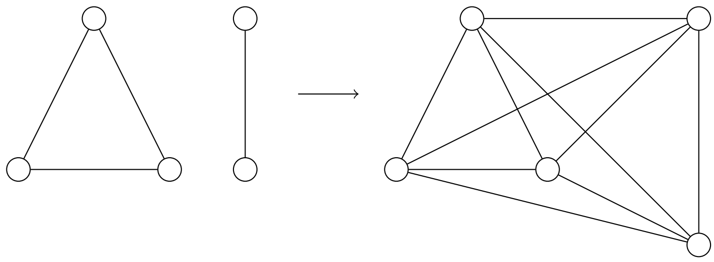


Figure 2.8: C_3, P_2 and $C_3 \vee P_2$.

Theorem 2.3. *[44] Let N be a matrix with only 0's and 1's as entries, and with size $b \times c$, such that the sum of its columns is either 0, b or $\frac{b}{2}$. Define $\tilde{N}$ obtained from N by exchanging each column v with $\frac{b}{2}$ entries equal to 1 by $1 - v$, where 1 represents the vector with all components equal to 1. Let B be a symmetric matrix of order $b \times b$ with constant sum of each of its rows and columns, and let C be a symmetric matrix of order $c \times c$. Take*

$$M = \begin{bmatrix} B & N \\ N^T & C \end{bmatrix} \tilde{M} = \begin{bmatrix} B & \tilde{N} \\ \tilde{N}^T & C \end{bmatrix}.$$

Then we have that M and $\tilde{M}$ are similar matrices and, thus, have the same eigenvalues.

Proof. The proof consists on finding a matrix Y such that $YMY^{-1} = \tilde{M}$. For doing so, we define $Y = \begin{bmatrix} \frac{2}{b}J - I_b & 0 \\ 0 & I_c \end{bmatrix}$ and, for means of nomenclature, we will call $Y_b = \frac{2}{b}J - I_b$.

CLAIM: $Y^{-1} = Y$.

Let's show that $Y^2 = I$.

$$YY = \begin{bmatrix} Y_b & 0 \\ 0 & I_c \end{bmatrix} \cdot \begin{bmatrix} Y_b & 0 \\ 0 & I_c \end{bmatrix} = \begin{bmatrix} Y_bY_b & 0 \\ 0 & I_cI_c \end{bmatrix} = \begin{bmatrix} Y_bY_b & 0 \\ 0 & I_c \end{bmatrix}.$$

Thus,

$$Y_bY_b = \begin{bmatrix} \frac{2}{b}-1 & \frac{2}{b} & \cdots & \frac{2}{b} \\ \frac{2}{b} & \frac{2}{b}-1 & \cdots & \frac{2}{b} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{2}{b} & \frac{2}{b} & \cdots & \frac{2}{b}-1 \end{bmatrix} \cdot \begin{bmatrix} \frac{2}{b}-1 & \frac{2}{b} & \cdots & \frac{2}{b} \\ \frac{2}{b} & \frac{2}{b}-1 & \cdots & \frac{2}{b} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{2}{b} & \frac{2}{b} & \cdots & \frac{2}{b}-1 \end{bmatrix}.$$

By taking $Y_bY_b = [y_{ij}]$, we will work with the cases $i = j$ and $i \neq j$.

(i) $i = j$:
we have $y_{ij} = \left(\frac{2}{b}-1\right)^2 + (b-1)\left(\frac{2}{b}\right)^2 = \frac{4}{b^2} - \frac{4}{b} + 1 + \frac{4b}{b^4} - \frac{4}{b^2} = 1.$

(ii) $i \neq j$:
we have $y_{ij} = 2\left[\frac{2}{b}\left(\frac{2}{b}-1\right)\right] + (b-2)\left(\frac{2}{b}\right)^2 = \frac{8}{b^2} - \frac{4}{b} + \frac{4b}{b^2} - \frac{8}{b^2} = 0.$

Hence $Y_bY_b = I_b$ and, consequently, $YY = I$. With that, we can conclude that $Y^{-1} = Y$ and we can continue with the proof of the Theorem 2.4.

See that:

$$YMY^{-1} = \begin{bmatrix} Y_b & 0 \\ 0 & I_c \end{bmatrix} \cdot \begin{bmatrix} B & N \\ N^T & C \end{bmatrix} \cdot \begin{bmatrix} Y_b & 0 \\ 0 & I_c \end{bmatrix} = \begin{bmatrix} Y_bB & Y_bN \\ I_cN^T & I_cC \end{bmatrix} \cdot \begin{bmatrix} Y_b & 0 \\ 0 & I_c \end{bmatrix}$$

$$= \begin{bmatrix} Y_bBY_b & Y_bNI_c \\ I_cN^TY_b & I_cCI_c \end{bmatrix} = \begin{bmatrix} Y_bBY_b & Y_bN \\ N^TY_b & C \end{bmatrix}.$$

Since we know B is a matrix with the sum of its rows and columns to be constant, it can be seen that $Y_bBY_b = B$. What needs to be demonstrated now is that the matrix Y_b transforms N in $\tilde{N}$.

To do that, we will verify the three types of columns possible to appear in N. We take $\vec{x}$ to be a column vector of N that has only zeroes, that has only ones or that has half of its entries being zeroes and the other half being ones.

(i) $\vec{x} = [1, 1, \cdots, 1]^T$: we have

$$Y_b\vec{x} = \begin{bmatrix} \left(\frac{2}{b} - 1\right) + \left(\frac{2}{b}\right)(b-1) \\ \vdots \\ \left(\frac{2}{b}\right)(b-1) + \left(\frac{2}{b} - 1\right) \end{bmatrix} = \begin{bmatrix} \frac{2}{b} - 1 + 2 - \frac{2}{b} \\ \vdots \\ \frac{2}{b} - 1 + 2 - \frac{2}{b} \end{bmatrix} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

(ii) $\vec{x} = \vec{0}$: it is easy to see that $Y_b\vec{x} = \vec{0}$.

(iii) $\vec{x}$ has $\frac{b}{2}$ zero entries and $\frac{b}{2}$ entries equal to 1: let's analyse the i^{th} line of $\vec{x}$, that is, the element $x_i \in \vec{x}$.

$$Y_b\vec{x} = \begin{bmatrix} \left(\frac{2}{b} - 1\right) x_1 + \left(\frac{2}{b}\right)(x_2 + x_3 + \cdots + x_b) \\ \left(\frac{2}{b} - 1\right) x_2 + \left(\frac{2}{b}\right)(x_1 + x_3 + \cdots + x_b) \\ \vdots \\ \left(\frac{2}{b} - 1\right) x_i + \left(\frac{2}{b}\right)(x_1 + x_2 + \cdots + x_{i-1} + x_{i+1} + \cdots + x_b) \\ \vdots \\ \left(\frac{2}{b} - 1\right) x_b + \left(\frac{2}{b}\right)(x_1 + x_2 + \cdots + x_{b-1}) \end{bmatrix}$$

▲ if $x_i = 0$, then:

$$\left(\frac{2}{b} - 1\right) \cdot 0 + \frac{2}{b} \cdot \frac{b}{2} = 1$$

▲ if $x_i = 1$, then:

$$\left(\frac{2}{b} - 1\right) \cdot 1 + \frac{2}{b} \cdot \left(\frac{b}{2} - 1\right) = \frac{2}{b} - 1 + 1 - \frac{2}{b} = 0$$

Hence, $Y_bN = \tilde{N}$ and consequently $YMY^{-1} = \tilde{M}$, that is, M and $\tilde{M}$ are similar. □

Now we introduce the switching operation defined by Godsil, and that is used to generate pairs of cospectral graphs with respect to each of the adjacency, laplacian and signless laplacian matrices.

Definition 2.1. *Let $G = (V, E)$ be a graph and let S be a subset of $V(G)$. We say that H is a graph made from G by switching over S if H satisfies:*
$V(H) = V(G)$
$E(H) = \{xy \in E(G) | x, y \in S \text{ or } x, y \notin S\} \cup \{xy \notin E(G) | x \in S \text{ e } y \notin S\}$, *where x and y are vertices of G.*

Let G be a graph, and $\pi = (C_1, C_2, \cdots, C_k, D)$ be a partition of $V(G)$. Suppose that for all $1 \leq i, j \leq k$ and $v \in D$, we have:
(a) any two vertices in C_i have the same number of neighbours in C_j;
(b) v has 0, $\frac{n_i}{2}$ or n_i neighbours in C_i ($n_i = | C_i |$).

An example can be seen in Figure 2.9, where the vertex v is neighbour to all the vertices C_k, don't have neighbours in C_j and is neighbour of all the vertices of C_i.

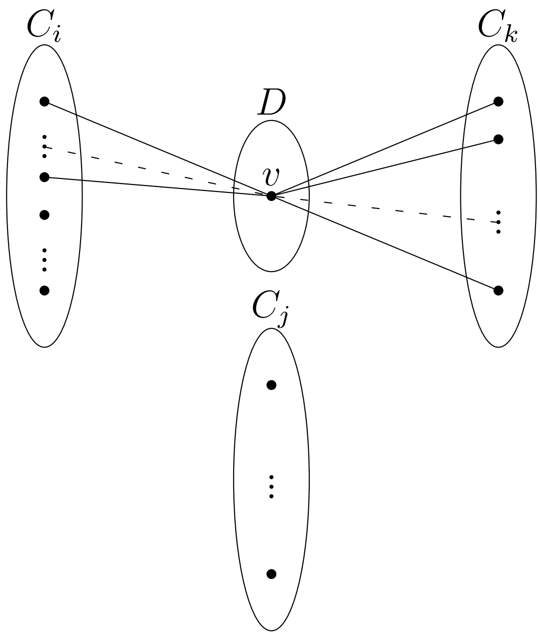
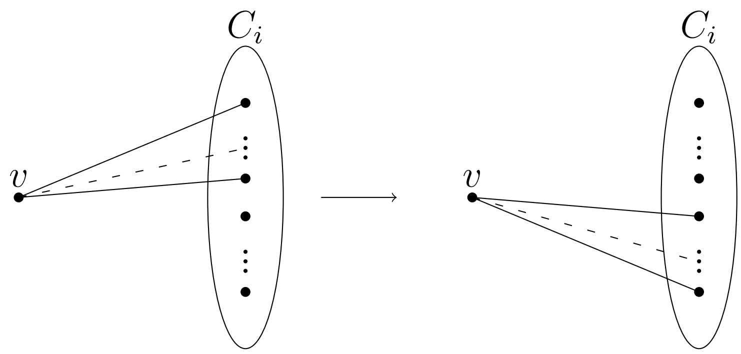


Figure 2.9: Example satisfying the conditions (a) and (b)

The graph $G^{(\pi)}$ is obtained by switching in G over π if $G^{(\pi)}$ is of the following kind:

(i) for each $v \in D$ and $1 \leq i \leq k$ such that v has $\frac{n_i}{2}$ neighbours in C_i, we delete this $\frac{n_i}{2}$ edges and use the join operation between v and the others $\frac{n_i}{2}$ vertices of C_i.



With the Theorem 2.4, we can prove the following Theorem directly.

Theorem 2.4. *Let G be a graph and π be a partition of $V(G)$ that satisfies conditions (a) and (b). Then $G^{(\pi)}$ and G are cospectral with respect to each of the adjacency, laplacian and signless laplacian matrices.*

Proof. The proof ends up being straightforward, since we can consider that the matrix M of Theorem 2.4 can be seen as the adjacency, the laplacian or the signless laplacian matrix of G, and the matrix $\tilde{M}$ then represents the adjacency, laplacian or signless laplacian of $G^{(\pi)}$. □

An example of this construction can be seen in Figure 2.10. On this case, all vertices of the cycle C_8 are in the same set C_1 and $v \in D$. The vertex v is adjacent to four vertices of the set C_1, which is half the cardinality of C_1. Therefore, we will take out all the edges existing between v and C_8 and add edges between v and the other vertices of C_8 that were not connected to v before.

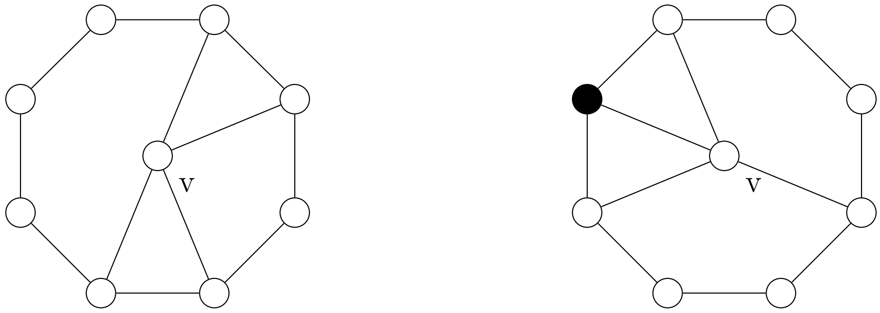


Figure 2.10: G and $G^{(\pi)}$, which are cospectral.

Note that the graphs are not isomorphic. Indeed, the second graph contains a vertex - which is painted in the figue - of degree 3 that is connected to two vertices which also have degree 3, and there's no such vertex on the first graph. The graph $G^{(\pi)}$ is made by the switching of G over the set $S = \{v\}$.

2.5 Schwenk's trees

Another classical construction is that of Schwenk [41] that was made, initially, for the adjacency matrix. Though, further on, Godsil and McKay[25] showed that the result is valid for all matrices: adjacency, laplacian and singless laplacian. To prove the result, we must first present some essential concepts. It is important to highlight that this result is a particular case of Godsil's swicthing. We start by showing the classical proof of the construction and, then, we make a brief explanation of how it can be seen as a particular case of the Godsil's switching.

Given a tree T, we define:

(i) *branch of T on v*: the maximal submatrix that has the vertex v;

(ii) the union of one or more branches on v will be called *limb on v*.

Given the tree T on Figure 2.11 with root on the vertex v, we show the branches and an example of limb in the Figure 2.12.

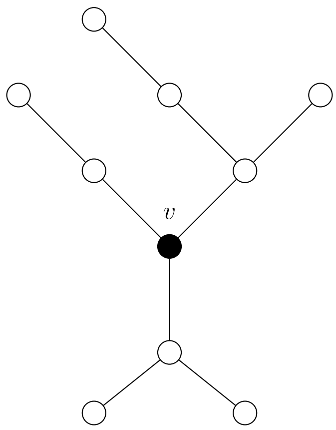


Figure 2.11: Tree T.

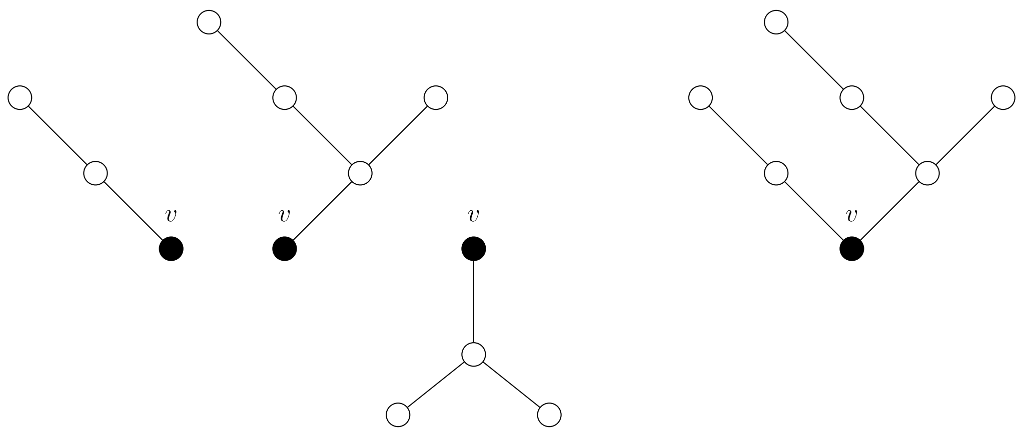


Figure 2.12: Branches of T and an example of limb.

Given two trees T_1 and T_2 with roots x_1 and x_2, respectively, we call coalescence, and denote by $T_1 \cdot T_2$, the union of the trees T_1 and T_2 through the identification of their roots x_1 and x_2. In Figure 2.13, we have an example of coalescence.

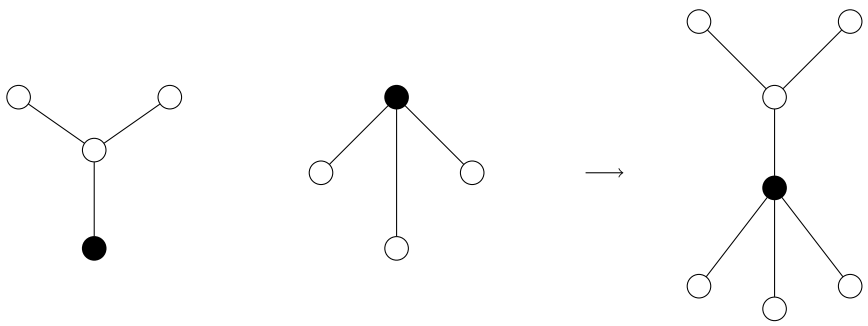


Figure 2.13: Example of coalescence.

The original result of Schwenk is the following:

Theorem 2.5. *Almost all trees are cospectral.*

The prove is given by the steps below:

(i) fix two limbs R and S (see Figure 2.14);

(ii) prove that, given a tree T, the graphs $T \cdot R$ and $T \cdot S$ obtained from the coalescence with the fixed limbs are not isomorphic;

(iii) show that $T \cdot R$ and $T \cdot S$ are cospectral;

(iv) demonstrate that, for sufficiently large number of vertices, almost all trees T have some of these limbs.

The limbs R and S given by Schwenk are actually isomorphic. Besides that, when we fix a root and join each of these limbs to a tree T by the operation of coalescence, we will be generating non isomorphic trees. It is enough to note that, after doing the coalescence operation between the limb S and a tree T, the vertex v will be a vertex of degree at least 3, connected with another vertex of degree 3 (the vertex w) and this will not occur with the graph generated by the coalescence between the limb R and the same tree T.

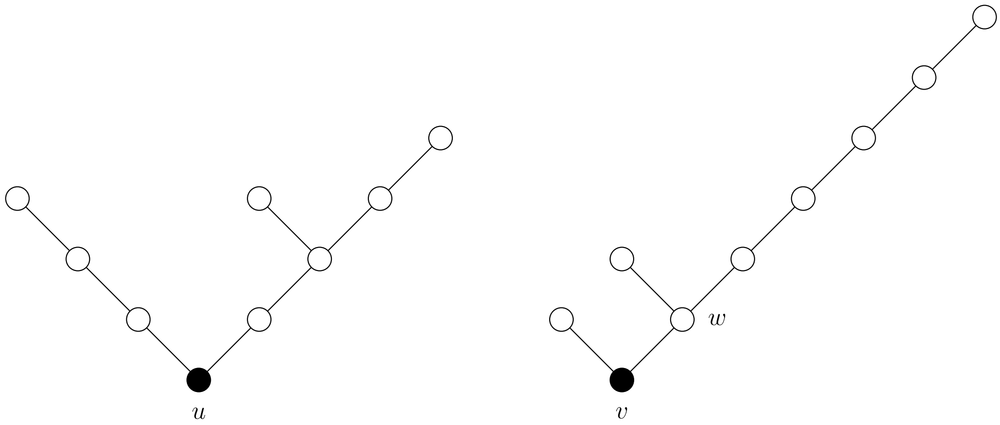


Figure 2.14: Limbs R and S.

In reality, Schwenk determines r_p and s_p as the number of trees with p vertices that do not have R and S as limbs, respectively, and proves that, on the limit, these numbers tend to zero. Thus, given a tree T_1, you may just identify if it has either R or S as a limb and, if it does, write it as $T_1 = X \cdot R$ (supposing without loss of generality it has R as a limb), where X is the tree composed by the branches of T_1 not belonging to R. Then, just take $T_2 = X \cdot S$ and you have two cospectral trees T_1 and T_2.

A more general result will be stated next.

Theorem 2.6. *[44] Let G and G' be cospectral graphs and let x and x' vertices of G and G', respectively, such that $G - x$ and $G - x'$ are also cospectral. Also, let Γ be a graph with a fixed vertex y. The coalescence between the graph G and Γ with respect to x and y is cospectral to the coalescence between G' and Γ with respect to x' and y.*

Note that the limbs R and S are cospectral since, when isolated, they are isomorphic , and also that $R-u$ and $S-v$ are cospectral. So, the construction of Schwenk is a particular case of 2.5. In Figure 2.15, we have an example of this construction, where we take the limbs R and S and do the coalescence between them and the tree $T = P_3$.

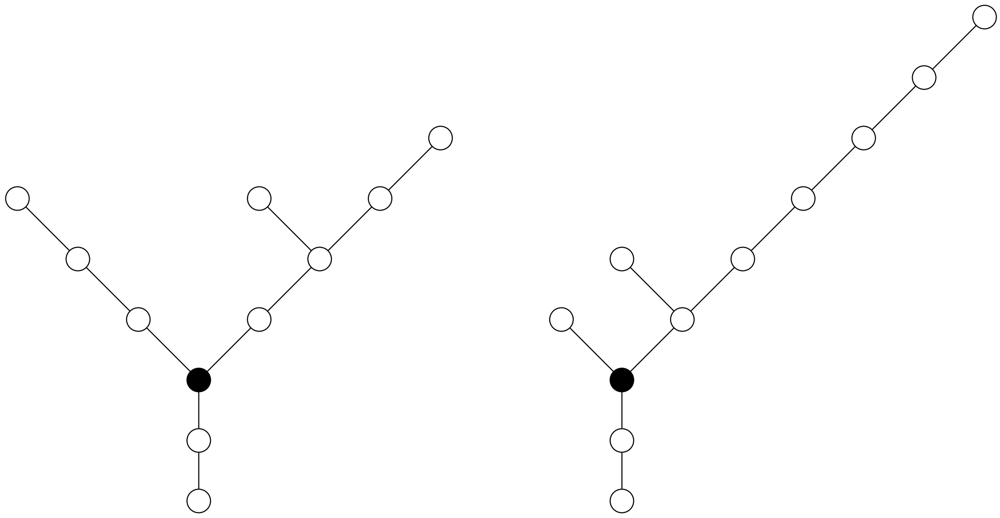


Figure 2.15: $T \cdot R$ and $T \cdot S$, which are cospectral.

3 EXPONENTIALLY MANY GRAPHS HAVE A Q-COSPECTRAL MATE

In this chapter, we bring an adapted version of our article entitled "Exponentially many graphs have a Q-cospectral mate", published on *Discrete Mathematics*. The editing was made so that there's no repetition with the chapter preliminary definitions.

Initially, at the start of the study of cospectral graphs, it was believed that finding pairs of cospectral graphs with respect to the signless laplacian matrix should be something very difficult to do. For that reason, we felt instigated to study the constructions exhibited in the previous chapter. With this concepts more comprehended, we experimented and, as a final result, developed the constructions that are introduced in the following. The second construction was presented in the Congress of Applied and Computational Mathematics of the Southeast, before it was turned into a part of our paper [10].

3.1 Abstract

We develop an algorithm for computing the characteristic polynomial of matrices related to threshold graphs. We use this as tool to exhibit, for any natural number $n \geq 4$, 2^{n-4} graphs with n vertices that have a non isomorphic pair with the same signless Laplacian spectrum. We also show how to construct infinite families of pairs of non isomorphic graphs having the same Q-spectrum.

3.2 Introduction

Are there other families with exponentially many graphs that are non-DS? We answer this question affirmatively, by exhibiting a family of 2^{n-4} threshold graphs with n vertices each one having a non isomorphic pair with the same signless Laplacian spectrum.

Our result may be unexpected for two reasons. Different from Schwenk's construction, that leads to a probabilistic result for trees, we actually find explicitly a family of 2^{n-4} threshold graphs with a Q-cospectral mate. We are not aware of any explicit construction of an exponential family of non-DS graphs. The second unexpected outcome is that the signless Laplacian matrix is believed to distinguish more graphs. Cvetković and Simić, in a series of papers, [14, 16, 15] (see also [13, 50, 4]), gathered reasons to argue that using the Q-spectrum is more advantageous than other matrices. In particular there is the belief that the ratio of non-DS graph over the total number of graphs (for a fixed number of vertices) tends to be smaller for the signless Laplacian matrix.

To corroborate this belief, one can consult the enumeration of all cospectral graphs of up to 11 vertices by Haemers and Spende [50] for several matrices. Also, it appears there are few constructions of families of graphs (of linear size) having a Q-cospectral mate. One such a construction is given by Omidi [38], where the author deals with the spectral characterization of T-shape trees. In this present note, we also show, given any initial pair of Q-cospectral graphs, how to build an infinite family of pairs of Q-cospectral mates. Our construction uses cartesian product of graphs and may produce different families as long as the initial pair is distinct.

3.2.1 Notation and preliminaries

Recall that the Cartesian product $G \Box H$ of two graphs $G = (V, E)$ and $H = (W, F)$ is the graph with vertex set $V \times W$ for which (v_1, w_1) and (v_2, w_2) are adjacent if and only if $v_1 = v_2$ and $\{w_1, w_2\} \in F$ or $w_1 = w_2$ and $\{v_1, v_2\} \in E$.

The following is a well known result about the spectrum of the cartesian product (see, for example, [28]).

Theorem 1. *Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be graphs and let M be a matrix associated a given graph G. If $\lambda_1, \ldots, \lambda_n$ are the M-eigenvalues of G_1 and $\mu_1, \ldots, \mu_m$ are the M-eigenvalues of G_2, then the M-eigenvalues of $G_1 \Box G_2$ are the numbers $\lambda_i + \mu_j$, with $1 \leq i \leq n$ and $1 \leq j \leq m$.*

We now review some facts about *threshold* graphs. This class of graphs has been discovered independently by several authors in many distinct contexts since the 1970's. They are an important class of graph because of their numerous application in diverse areas which include compute science, social science and psychology. See, for example, [34] for a more detailed account. A threshold graph can be characterized in many ways. We are going to define a threshold graphs through an iterative process which starts with an isolated vertex, and where, at each step, either a new isolated vertex is added, or a dominating vertex (adjacent to all previous vertices) is added. We can represent a threshold graph G on n vertices by a binary sequence $b_1, b_2, \ldots, b_n$. Here $b_i = 0$ if an isolated vertex v_i is added and $b_i = 1$ if v_i was added as a dominating vertex. We call this representation a *creation sequence*. The choice of b_1 is arbitrary and we use it as $b_1 = 0$. One can see, by ordering the vertices in the same way they are given in the creation sequence $(b_1, b_2, \ldots, b_n)$, that the adjacency matrix of G is

$$A = \begin{bmatrix} 0 & b_2 & b_3 & b_4 & \ldots & b_n \\ b_2 & 0 & b_3 & b_4 & \ldots & b_n \\ b_3 & b_3 & 0 & b_4 & \ldots & b_n \\ b_4 & b_4 & b_4 & 0 & \ldots & b_n \\ \ldots & \ldots & \ldots & & 0 & \ldots \\ b_n & b_n & b_n & b_n & \ldots & 0 \end{bmatrix},$$

where each b_i is either 0 or 1, depending whether the i-th vertex is isolated or dominant, respectively.

3.2.2 The characteristic polynomial of threshold-like matrices

In this section, we describe a method for the computation of the characteristic polynomial of matrices associated to threshold graphs. We observe that for a threshold graph G given by the sequence $b_1 b_2 \cdots b_n$, its Laplacian matrix is of the form

$$L = \begin{bmatrix} d_1 & -b_2 & -b_3 & -b_4 & \dots & -b_n \\ -b_2 & d_2 & -b_3 & -b_4 & \dots & -b_n \\ -b_3 & -b_3 & d_3 & -b_4 & \dots & -b_n \\ -b_4 & -b_4 & -b_4 & d_4 & \dots & -b_n \\ \dots & \dots & \dots & & d_i & \dots \\ -b_n & -b_n & -b_n & -b_n & \dots & d_n \end{bmatrix},$$

where $d_i, i = 1, 2, \dots, n$, are the vertex degrees. As for the signless Laplacian matrix Q, it has the form

$$Q = \begin{bmatrix} d_1 & b_2 & b_3 & b_4 & \dots & b_n \\ b_2 & d_2 & b_3 & b_4 & \dots & b_n \\ b_3 & b_3 & d_3 & b_4 & \dots & b_n \\ b_4 & b_4 & b_4 & d_4 & \dots & b_n \\ \dots & \dots & \dots & & d_i & \dots \\ b_n & b_n & b_n & b_n & \dots & d_n \end{bmatrix}.$$

To be more general, we discuss the computation of the characteristic polynomial of matrices having the following structure, that encompass the structure of several matrices associated with threshold graphs, including the adjacency, Laplacian and signless Laplacian.

$$M = \begin{bmatrix} \alpha_1 & \beta_2 & \beta_3 & \beta_4 & \dots & \beta_n \\ \beta_2 & \alpha_2 & \beta_3 & \beta_4 & \dots & \beta_n \\ \beta_3 & \beta_3 & \alpha_3 & \beta_4 & \dots & \beta_n \\ \beta_4 & \beta_4 & \beta_4 & \alpha_4 & \dots & \beta_n \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \beta_n & \beta_n & \beta_n & \beta_n & \dots & \alpha_n \end{bmatrix},$$

where $\alpha_i, \beta_i \in \mathbb{R}$, $i = 1, 2, \ldots, n$ are given numbers. We call those matrices *threshold-like matrices.*

For simplicity, we compute $\det(M - xI)$, that is, within a sign, the characteristic polynomial $\det(xI - M)$ of a threshold-like matrix M, and x is an indeterminate. The idea is to obtain a similar matrix T congruent to $M - xI$ using elementary operations in the rows and columns. Consider the matrix $M - xI$

$$\begin{bmatrix} \alpha_1 - x & \beta_2 & \beta_3 & \ldots & \beta_{n-1} & \beta_n \\ \beta_2 & \alpha_2 - x & \beta_3 & \ldots & \beta_{n-1} & \beta_n \\ \beta_3 & \beta_3 & \alpha_3 - x & \ldots & \beta_{n-1} & \beta_n \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ \beta_{n-1} & \beta_{n-1} & \beta_{n-1} & \ldots & \alpha_{n-1} - x & \beta_n \\ \beta_n & \beta_n & \beta_n & \ldots & \beta_n & \alpha_n - x \end{bmatrix}.$$

For each $i, 1 \leq i \leq n-2$, we perform the following operations

$$R_i \leftarrow R_i - R_{i+1},$$

$$C_i \leftarrow C_i - C_{i+1}$$

giving the tridiagonal matrix T:

$$\begin{bmatrix} \alpha_1+\alpha_2-2(x+\beta_2) & \beta_2-\alpha_2+x & 0 & \\ \beta_2-\alpha_2+x & \alpha_2+\alpha_3-2(x+\beta_3) & \beta_3-\alpha_3+x & 0 \\ 0 & \beta_3-\alpha_3+x & \ddots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \ldots \alpha_{n-1}+\alpha_n-2(x+\beta_n) & \beta_n-\alpha_n+x \\ 0 & 0 & \ldots \beta_n-\alpha_n+x & \alpha_n-x \end{bmatrix}.$$

The determinant of a tridiagonal matrix T may be easily computed, for example, by performing a Laplace expansion on the first row. From this we obtain a recursive formula for computing the characteristic polynomial of a threshold-like matrix, given by the Algorithm `CharPoly` shown in Figure 3.1.

INPUT: $(\alpha_1, \alpha_2, \ldots, \alpha_n)$ and $(\beta_1, \beta_2, \ldots, \beta_n)$

OUTPUT: $p(x)$

Algorithm CharPoly$(G, -x)$

initialize $p_0(x) \leftarrow 1$ and $p_1(x) \leftarrow \alpha_1 + \alpha_2 - 2(x+\beta_2)$

for $m = 2$ to n do

if $m \neq n$

$p_m(x) \leftarrow (\alpha_m + \alpha_{m+1} - 2(x+\beta_{m+1}))p_{m-1}(x) - (\beta_m - \alpha_m + x)^2 p_{m-2}(x)$

else if $m = n$

$p_m(x) \leftarrow (\alpha_m - x)p_{m-1}(x) - (\beta_m - \alpha_m + x)^2 p_{m-2}(x)$

end loop

$p(x) = (-1)^n p_m(x)$

Figure 3.1: Characteristic Polynomial.

Theorem 2. *For a threshold-like matrix M, and x an indeterminate,* `CharPoly(G,-x)` *computes the characteristic polynomial of M.*

Remark: This algorithm can certainly be executed in $O(n^2)$ multiplications in the field of the coefficients of $p(x)$, since there are $n-2$ steps and at each step $i = 3, \ldots, n$, the number of multiplication is $O(i)$. But this may be improved if one does a careful analysis.

3.2.3 Examples

We illustrate algorithm `CharPoly` for the matrices $M = A, L$, and Q. We assume G is the threshold graph given by the sequence $(0, 1, 0, 1)$. We have that $b_2 = 1, b_3 = 0$ and $b_4 = 1$. After initialization, there are three steps, for $m = 2, 3, 4$.

For $M = A$, the initial values are $(\beta_1, \beta_2, \beta_3, \beta_4) = (0, 1, 0, 1)$ and $(\alpha_1, \alpha_2, \alpha_3, \alpha_4) = (0, 0, 0, 0)$, and $p_0(x) = 1, \quad p_1(x) = -2x - 2$, giving, for $m = 2$, $p_2(x) = (-2x - 2\beta_3)p_1 - (\beta_2 + x)^2 p_0 = 3x^2 + 2x - 1$. For $m = 3$, $p_3(x) = (-2x - 2\beta_4)p_2 - (\beta_3 + x)^2 p_1 = -4x^3 - 8x^2 - 2x + 2$. For $m = 4$ we have that the characteristic polynomial of A is

$$p_4(x) = -xp_3 - (\beta_4 + x)^2 p_2 = x^4 - 4x^2 - 2x + 1.$$

For the case $M = L$, the initial values are $(\beta_1, \beta_2, \beta_3, \beta_4) = (0, -1, 0, -1)$ and $(\alpha_1, \alpha_2, \alpha_3, \alpha_4) = (2, 2, 1, 3)$, and $p_0(x) = 1, \; p_1(x) = 4 - 2(x-1)$. After initialization, there are three steps, for $m = 2, 3, 4$. For $m = 2$ we have $p_2(x) = (-2x - 2\beta_3)p_1 - (\beta_2 + x)^2 p_0 = 3x^2 - 12x + 9$. For $m = 3$ we have $p_3(x) = (\alpha_3 + \alpha_4 - 2(x + \beta_4)p_2 - (\beta_3 - \alpha_3 + x)^2 p_1 = -4x^3 + 32x^2 - 76x + 48$. For $m = 4$ we have

$$p_4(x) = (\alpha_4 - x)p_3 - (\beta_4 - \alpha_4 + x)^2 p_2 = x^4 - 8x^3 + 19x^2 - 12x.$$

For the case $M = Q$, the initial values are $(\beta_1, \beta_2, \beta_3, \beta_4) = (0, 1, 0, 1)$ and $(\alpha_1, \alpha_2, \alpha_3, \alpha_4) = (2, 2, 1, 3)$, and $p_0(x) = 1, \quad p_1(x) = 4 - 2(x + 1)$. After initialization, the three steps, for $m = 2, 3, 4$ are as follows. For $m = 2$ we have $p_2(x) = (\alpha_2 + \alpha_3 - 2(x + \beta_3)p_1 - (\beta_2 - \alpha_2 + x)^2 p_0 = 3x^2 - 8x + 5$. For $m = 3$ we have $p_3(x) = (\alpha_3 + \alpha_4 - 2(x + \beta_4)p_2 - (\beta_3 - \alpha_3 + x)^2 p_1 = -4x^3 + 16x^2 - 20x + 8$. For $m = 4$, we have

$$p_4(x) = (\alpha_4 - x)p_3 - (\beta_4 - \alpha_4 + x)^2 p_2 = x^4 - 8x^3 + 19x^2 - 16x + 4.$$

3.2.4 Cospectral threshold graphs

In this section we present the exponential size family of threshold graph having a Q-cospectral mate.

Theorem 3. *Consider the threshold graphs G_1 and G_2 given by the binary sequences $S_1 = (0, 1, 1, 0, b_5, b_6, \ldots, b_n)$ and $S_2 = (0, 0, 0, 1, b_5, b_6, \ldots, b_n)$, for any $n \geq 4$. Then G_1 and G_2 are non isomorphic and Q-cospectral.*

G_1 and G_2 are clearly non isomorphic, since their degree sequence are distinct.

Let $p_n(x)$ be the characteristic polynomial of $Q(G_1)$ and $t_n(x)$ be the characteristic polynomial of $Q(G_2)$. Denote by $C = b_5 + b_6 + \cdots + b_n$. We determine $p_n(x)$ and $t_n(x)$ using the recursion given by the algorithm of Figure 3.1.

We notice that the elements $b_5, \ldots, b_n$ and $d_{b_5}, \ldots, d_{b_n}$ are equal in the recursions involving $p_n(x)$ and $t_n(x)$. Hence, in order to verify that $p_n(x) = t_n(x)$, we compute $p_5(x)$ and $t_5(x)$ which is the last equations involving $b_1, \ldots, b_4$ and $d_{b_1}, \ldots, d_{b_4}$ (that are different in both recursions).

For G_1, we have $b_1 = 0$, $b_2 = 1$, $b_3 = 1$ e $b_4 = 0$. The degrees are, $d_{b_1} = 2+C$, $d_{b_2} = 2 + C$, $d_{b_3} = 2 + C$ e $d_{b_4} = C$ We see that

$p_0(x) = 1$

$p_1(x) = 2 + 2\,C - 2\,x$

$p_2(x) = 3\,\left(1 + C - x\right)^2$

$p_3(x) = 4\,\left(1 + C - x\right)^3$

$p_4(x) = -\left(1 + C - x\right)^2 \left(-C^2 + 6\,Cx - 4\,d_{(b_5)}\,C + 8\,b_5\,C - 4\,C - 5\,x^2 + 4\,d_{(b_5)}\,x - 4\,d_{b)} - 8\,b_5\,x + 8\,x + 8\,b_5\right)$

$p_5(x) = -\left(1 + C - x\right)^2 (-12\,x^2 + 6\,d_{b_5}\,Cx + 6\,x^3 - 8\,b_5\,Cx + 8\,Cx + 2\,C^2x - 8\,Cx^2 - 4\,d_{b_5}\,C + 8\,d_{b_5}\,x - d_{b_5}\,C^2 - 5\,d_{b_5}\,x^2 - 8\,b_5\,x + 8\,b_5\,x^2 - 4\,d_{b_6}\,C + 8\,d_{b_6}\,x - d_{b_6}\,C^2 - 5\,d_{b_6}\,x^2 + 8\,b_6\,C - 16\,b_6\,x + 2\,b_6\,C^2 + 10\,b_6\,x^2 - 4\,d_{b_6}\,d_{b_5} + 8\,d_{b_6}\,b_5 + 6\,d_{b_6}\,Cx - 12\,b_6\,Cx - 4\,d_{b_6}\,d_{b_5}\,C + 8\,d_{b_6}\,b_5\,C + 4\,d_{b_6}\,d_{b_5}\,x - 8\,d_{b_6}\,b_5\,x + 8\,b_6\,d_{b_5}\,C - 16\,b_6\,b_5\,C - 8\,b_6\,d_{b_5}\,x + 16\,b_6\,b_5\,x + 8\,b_6\,d_{b_5} - 16\,b_6\,b_5 + 4\,{b_5}^2 + 4\,{b_5}^2C - 4\,{b_5}^2x)$

If one computes $t_1(x), t_2(x), t_3(x), t_4(x)$ and $t_5(x)$, it is easy to check that $t_i(x) = p_i(x)$ for $i = 1, \ldots, 5$. □

Corollary 1. *For any $n \geq 4$, there exist 2^{n-4} graphs having a Q-cospectral mate.*

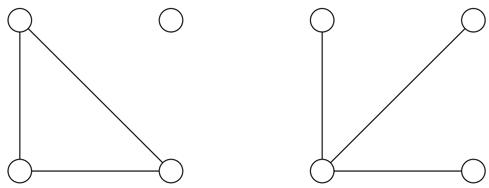
By Theorem 3, for $n \geq 4$, the binary sequence $0001b_5 \cdots b_n$ corresponds a threshold graph that have the Q-spectrum of the threshold graph represented by the sequence $0110b_5 \cdots b_n$. Both graphs are non isomorphic and therefore are cospectral mates. Since there exist 2^{n-4} binary sequences of the form $0001b_5 \cdots b_n$, there exists at least this number of Q-cospectral mates. □

Corollary 2. *Let $n \geq 4$ be an integer and G be a threshold graph with n vertices. The probability that G has threshold graph with the same Q-spectrum is at least $\frac{1}{8}$.*

There exist 2^{n-1} threshold graphs with n vertices and, by Corollary 1, 2^{n-4} have a Q-cospectral mate. □

3.3 Infinite families of Q-cospectral Pairs

The term "(unordered) pair of isospectral non-isomorphic graphs" denoted by PING [13] will be used here. The smallest Q-PING is the 4-vertex pair $K_{1,3}$ and $C_3 \cup K_1$ given in Figure 3.2. Other pairs with 5 vertices are given in the reference. Among them are $K_{1,3} \cup K_1$ and $K_3 \cup 2K_1$. 5 Q-PING on 6 vertices presented in [12] and a pair on 10 vertices is given in [50].



Q-spectrum: $0, 1^{(2)}, 4$

Figure 3.2: Q-PING on 4 vertices.

An infinite family of Q-PINGS is given by Omidi [38], where a T-shape tree with $4k$ vertices, for any $k > 0$, is shown to be Q-cospectral with a non bipartite graph. Here, by using the cartesian product operation, we provide the following construction, that finds an infinite family of Q-cospectral graphs with $n2^k$ vertices ($k = 0, 1, \ldots$), giving an initial pair of Q-cospectral graphs on n vertices.

Theorem 4. *Let H and G be two Q-cospectral graphs on n vertices. For all $k = 0, 1, 2, \ldots$ there are non-isomorphic graphs H_k and G_k with $2^k n$ vertices Q-cospectral graphs.*

For $k = 0$, let $H_0 = H$ and $G_0 = G$. Then, by the hypothesis, the Q-spectrum of H_0 and G_0 are the same. For any $k \geq 1$, define $H_k = H_{k-1} \Box P_2$ and $G_k = G_{k-1} \Box P_2$, where P_2 is the path on 2 vertices.

By induction, we suppose that q_i, the Q-eigenvalues of H_{k-1} are the same as those of G_{k-1}. By Theorem 1, the Q-spectrum of H_k is the (multi) set $\{q_i + 0, q_i + 2\}$, since the Q-eigenvalues of P_2 are 0 and 2. By the same reason, the Q-spectrum of G_k is the same.

The graphs are clearly non isomorphic, since H and G are not. It is easy to see that the number of vertices is $n2^k$, for all k. $\Box$

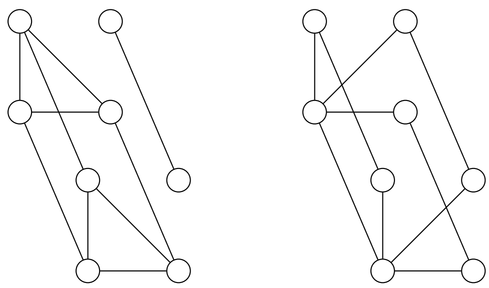


Figure 3.3: $G_1 \Box P_2$ and $G_2 \Box P_2$

Example. Figure 3.3 gives the first iteration given by the above result for the he Q-PING on 4 vertices given by Figure 3.2. The new spectrum of the graph is $\{0, 1^{(2)}, 2, 3^{(2)}, 4, 6\}$.

Figure 3.4 presents the second iteration given by Theorem 4. The new pair of Q-cospectral graphs has spectrum $\{0, 1^{(2)}, 2^{(2)}, 3^{(4)}, 4^{(2)}, 5^{(2)}, 6^{(2)}, 8\}$.

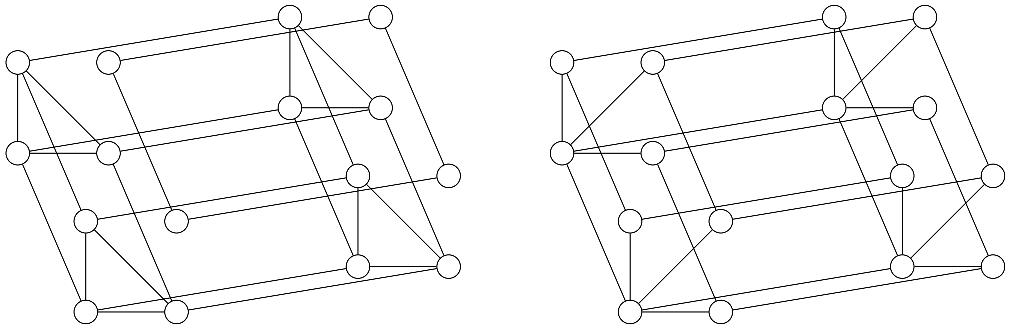


Figure 3.4: Second iteration

4 COMPLEMENTARY SPECTRUM

In this chapter, we introduce the concepts of complementary spectrum of graphs. The goal is to present the ideas that lead to the new representation of graphs by means of spectra.

The goal of the Spectral Graph Theory is to describe properties of graphs through their spectrum. A big problem that arises is that there are non isomorphic graphs with the same set of eigenvalues, the cospectral pairs. Different types of matrices have already been studied in order to minimize the problem of cospectrality of graphs, but all of them present a big number of pairs of cospectral graphs when we consider the set of graphs with fixed number of vertices. In this work, we will introduce a new approach to the spectrum of graphs using the adjacency matrix related to the graph. We have evidence to believe that this new approach determines better a greater class of graphs.

4.1 The problem of complementary eigenvalue

Initially, let us introduce the problem of complementary eigenvalue (EiCP) that is defined as follows:

Definition 4.1. *Given a real matrix A of order n, the problem of complementary eigenvalue (EiCP) consists in finding a scalar $\lambda \in \mathbb{R}$ and a vector $x \in \mathbb{R}^n - \{0\}$ such that*

$$\begin{aligned} w &= Ax - \lambda x \\ x \geq 0&, w \geq 0 \\ x^T w &= 0 \end{aligned} \tag{4.1}$$

where $w \in \mathbb{R}^n$. If (λ, x) satisfy the conditions given in (4.1), λ is called complementary eigenvalue and x is a complementary eigenvector associated.

Note that, if $w = 0$ and we don't consider the condition that x be non-negative, we have the already known eigenvalue problem (EiP).

$$Ax = \lambda x.$$

The problem of complementary eigenvalues has several applications, we can cite [21] as an example. If we consider a matrix A that is the adjacency matrix of a given graph G and λ satisfies the EiCP, we say λ is a complementary eigenvalue of the graph G. More formally, we have:

Definition 4.2. *Given a graph G and A the adjacency matrix of G. If λ satisfies the EiCP, then λ is a complementary eigenvalue of G. The set of all distinct complementary eigenvalues of G is the complementary spectrum of G, and we will denote it by $\mathcal{CS}(G)$.*

In this chapter, we will present results about the complementary spectrum of a graph G, such as the cardinality of $\mathcal{CS}(G)$, graphs with the same complementary spectrum, graphs determined by their complementary spectrum, and more. Our main goal is to stablish families of graphs that are determined by their complementary spectrum (DCS). For such, we need to take care of some preliminary results.

4.2 Initial concepts about complementary eigenvalues

When we consider A the adjacency matrix of a given graph G, we will obtain some properties that will also be listed as a Lemma.

Lemma 4.1. *[21] Let A be a matrix of order n and λ be the solution to the EiCP* (4.1). *Then λ is an eigenvalue of a principal submatrix of A.*

Lemma 4.2. *[21] Let G be a connected graph, $A(G)$ be its adjacency matrix and λ be the greatest eigenvalue of A, that is, λ is the index of G. Then*

(i) λ is a complementary eigenvalue of G;

(ii) λ *is the only eigenvalue of* A *that is a complementary eigenvalue of* G*;*

(iii) all the complementary eigenvalues of G *are non-negative;*

(iv) the complementary eigenvalues of G *are the greatest eigenvalues of the principal submatrices of* A*.*

A graph $H = (W, F)$ is said *subgraph* of $G(V, E)$ if $W \subseteq V$ and $F \subseteq E$. In the case that $F = \{e = \{u, v\} \in E, u, v \in W\}$, we say H is an *induced subgraph* of G. In Figure 4.1 we have a graph G, to the left a subgraph of G and to the right an induced subgraph of G.

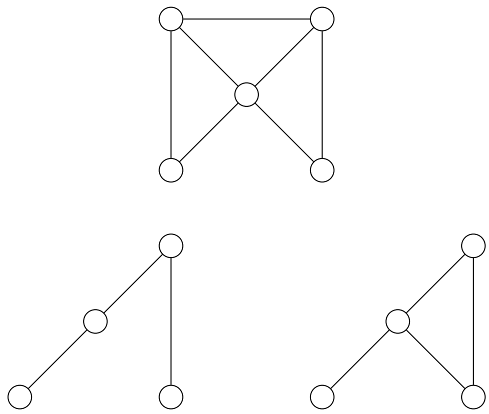


Figure 4.1: G, a subgraph of G and an induced subgraph of G.

A graph G is said to be *connected* if there's always a path connecting any two distinct vertices. If there is no such path between any pair of distinct vertices, we say G is *disconnected*. We call C_i a *connected component* of G if C_i is a maximal connected subgraph of G. A disconnected graph is composed by connected components C_i. In Figure 4.2 we have a connected graph and a disconnected graph with two connected components.

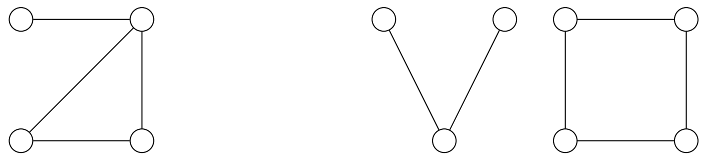


Figure 4.2: Connected graph and disconnected graph with 2 connected components.

Given a matrix M of order n, we say M' is a principal submatrix of M of order $n-k$ if M' is obtained from M by taking out k rows and their respective k columns. A principal minor of a matrix M is the determinant of any principal submatrix of M, that is, it is the determinant of one matrices M' obtained by the removal of k rows and k columns of M.

We say that a matrix P is a permutation matrix if P is obtained through simultaneous permutations of both rows and columns of the identity matrix. Given a matrix A, if there is not a permutation matrix P that transforms A into a matrix A' of the following kind

$$A' = \begin{bmatrix} X & Y \\ 0 & Z \end{bmatrix}$$

where X and Y are square matrices, we say A is irreducible. If there is such permutation matrix P, A is said to be reducible.

A classical result of the Spectral Graph Theory that is related with irreducible matrices states the following: a graph G is connected if, and only if, its adjacency matrix $A(G)$ is irreducible. The demonstration is quite simple if we look at the configuration of the matrix $A'(G)$. That is, suppose that $A(G)$ is reducible, so that the matrix $A'(G)$ obtained via a permutation matrix P exists. Note that turning $A(G)$ into $A'(G)$ with a permutation matrix means to reorder the vertices of G. Then, the matrix $A'(G)$ will also be an adjacency matrix of the graph G and, consequently, it will also be simetric. Thus we have

$$A' = \begin{bmatrix} X_{r\times r} & 0 \\ 0 & Z_{s\times s} \end{bmatrix}.$$

If we think that the vertices of G were reordered in such a way that $V(G) = V_1 \cup V_2$, where $V_1 = \{1, ..., r\}$ and $V_2 = \{1, ..., s\}$, the null blocks mean that the r vertices of V_1 are not adjacent to the s vertices of V_2. So, G possesses two connected components, one with r vertices and other one with s vertices. We then conclude that G is disconnected.

A matrix A is said to be non-negative, positive or negative if all the entries of A are non-negative, positive or negative, respectively.

Theorem 4.1. *(Perron-Frobenius) [3] Let A be a non-negative, symmetric and irreducible matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Then:*

(i) $\lambda_1 > 0$ *and there exists a positive associated eigenvector;*

(ii) $\lambda_2 < \lambda_1$*;*

(iii) $|\lambda_i| \leq \lambda_1$ *for all* $i \in \{1, ..., n\}$.

We know the principal submatrices of $A(G)$ correspond to the adjacency matrix of the induced subgraphs of G. That is, the complementary spectrum of G is composed by the set of all of the greatest eigenvalues of the principal submatrices of $A(G)$. Hence, we can determine the complementary spectrum of G by calculating the index of all induced subgraphs of G.

Furthermore, the index of a disconnected subgraph is given by the greatest index of its connected components, being enough to consider only graphs G that are connected as well as their induced subgraphs. Another important observation is the fact we do not consider the multiplicity of the complementary eigenvalues, that is, the complementary spectrum of G only accounts for the distinct indexes of the induced subgraphs. With this we have the following results.

Corollary 4.1. *Let G be a connected graph of n vertices. The complementary spectrum of G is composed of the index of all induced subgraphs of G, without repetition.*

Corollary 4.2. *Let G be a connected graph with n vertices and $\mathfrak{b}(G)$ the number of connected induced subgraphs not isomorphic to each other, then*

$$|\mathcal{CS}(G)| \leq \mathfrak{b}(G).$$

The equality on Corollary 4.2 will only occur when all of the connected induced subgraphs of G that are not isomorphic have distinct indexes. Besides that, there's a big difference between the cardinality of the complementary spectrum and the other spectra we are used to work with. When we consider the adjacency, laplacian or signless laplacian matrices, the number of eigenvalues (counting multiplicities) of a certain graph G is equal to the number of its vertices.

When we work with complementary spectrum, we don't have the same relation with the number of vertices of G, since two induced connected subgraphs that are not isomorphic may still have the same index. We can only guarantee that we'll have no more than $\mathfrak{b}(G)$ complementary eigenvalues for G. However, a lower bound can also be given if we consider the following result that is a direct consequence of the eigenvalues' interlacing.

Lemma 4.3. *Let G be a graph, H be a proper subgraph of G, $\lambda(G)$ the index of G and $\lambda(H)$ the index of H. Then*

$$\lambda(H) < \lambda(G).$$

Note that, given a graph G with n vertices, the graph must have at least n induced connected subgraphs that are not isomorphic to each other if we think of taking out a vertex at a time, that is, if we think in a family of proper subgraphs. This means we can calculate a lower bound for the number of complementary eigenvalues .

Theorem 4.2. *[42] Let G be a connected graph, then*

$$n \leq |\mathcal{CS}(G)|.$$

The equality will happen whenever G is an elementary graph, that is, a cycle, a path, a complete graph or a star. We now prove the following:

Theorem 4.3. *Let G be a graph with n vertices and $\mathcal{CS}(G)$ the complementary spectrum of G, we then have that $|\mathcal{CS}(G)| = n \Leftrightarrow G$ is an elementary graph.*

Proof. One of the implications is very simple, it is enough to calculate the complementary spectrum of the elementary graphs (this will be done later) and note that the cardinality of the set of complementary eigenvalues will be equal to the number of vertices. So, if G is an elementary graph with n vertices, its complementary spectrum is composed of n elements.

The direct implication will be shown by induction over the number of vertices. The strategy is to show that, given a connected graph G with n vertices, if the only connected induced subgraph of G with $n-1$ vertices is an elementary graph, then G will also be an elementary graph.

Given the set $\Delta_n = \{P_n, C_n, K_n, S_n\}$, we affirm that

$$\{F \in \mathbf{C_n} : |\mathcal{CS}(F)| = n\} \subseteq \Delta_n, n \geq 6.$$

This affirmative is true for $n = 6$, since you can just calculate the complementary spectrum of all 112 connected graphs of 6 vertices and note that, if F is a graph with n complementary eigenvalues, then it is an elementary subgraph.

Now, suppose the affirmative is true for n, and lets show it is also true for $n+1$. This means we have to show that, taking $G \in \mathbf{C_{n+1}}$ such that $|\mathcal{CS}(G)| = n+1$, we must have $G \in \Delta_{n+1}$.

Let $\{F_1, F_2, ..., F_r\}$ be a family of graphs F_i that are connected induced subgraphs of G (we will denote that by $F_i \lhd G$) of n vertices. We have that

$$\mathcal{CS}(F_i) \cup \{\varrho(G)\} \subseteq \mathcal{CS}(G) \Rightarrow |\mathcal{CS}(F_i)| + 1 \leq |\mathcal{CS}(G)| = n+1.$$

But, since F_i is a graph with n vertices, we know it possesses at least n complementary eigenvalues, hence

$$|\mathcal{CS}(F_i)| + 1 \geq n+1$$

So, we have

$$n+1 \leq |\mathcal{CS}(F_i)| + 1 \leq n+1.$$

And with that, $|\mathcal{CS}(F_i)| = n$ and we can conclude that $F_i \in \Delta_n$, that is, $\{F_1, F_2, ..., F_r\}$ are elementary graphs. We have already shown that all induced subgraphs of G with $n-1$ vertices are all elementary. Now it's enough to show that $r = 1$, that is, that the connected induced subgraph of G (which we already know is elementary) is unique, as this guarantees G is itself an elementary graph.

Let's suppose, by contradiction, that $r \geq 2$. The index of all elementary graphs are different, except for S_5 and C_5, but we're working with $n \geq 6$. As we already know all the F_i are elementary graphs of different indexes, we can sort them by their indexes, which is also their greatest eigenvalue. Take the ordering $\varrho(F_1) > \varrho(F_2) > ... > \varrho(F_r)$.

The complementary spectrum of G will contain the complementary eigenvalues of F_2, the greatest complementary eigenvalue of F_1 (which is different from the greatest complementary eigenvalue of F_2) and, also, its own index (that will be the greatest complementary eigenvalue of G). That is, we must have

$$\mathcal{CS}(F_2) \cup \{\varrho(F_1), \varrho(G)\} \subseteq \mathcal{CS}(G)$$

Since F_2 has n complementary eigenvalues and $\varrho(F_2) \neq \varrho(F_1) \neq \varrho(G)$, we conclude that $|\mathcal{CS}(G)| \geq n+2$. This can't be, since $|\mathcal{CS}(G)| = n+1$. Thus $r = 1$.

Conclusion: G contains only one connected induced subgraph with $n-1$ vertices which is elementary, and so G must also be elementary. □

The fact that we don't know if there is a direct relation between the number of vertices of G and the cardinality of its complementary spectrum is an open problem and of great interest. It is worth to highlight that, not existing such relation, we can have two graphs with a distinct number of vertices, but with the same number of complementary eigenvalues, which didn't occur at all with the eigenvalues of the adjacency, laplacian nor of the signless laplacian matrices.

Using Lemma 4.3, we can also obtain the following result:

Lemma 4.4. *Let G be a conneted graph with at least 2 vertices. Then, the second greatest complementary eigenvalue of G is obtained by taking the maximum of the indexes of all* *connected induced subgraphs of G with one less vertex and that are not isomorphic to one another, that is,*

$$\max \{\lambda(G-v); v \in V(G) \ \textit{e v is not a cut vertex of } G\}.$$

The adopted nomenclature will be $\varrho(G)$ for the greatest complementary eigenvalue of the graph G, $\varrho_2(G)$ for the second greatest and so on.

4.3 Determining the complementary spectrum

Now we show a practical example as to how calculate the first four complementary eigenvalues of a graph G with the objetive of better illustrating the procedure we just detailed. Let G be the graph defined below:

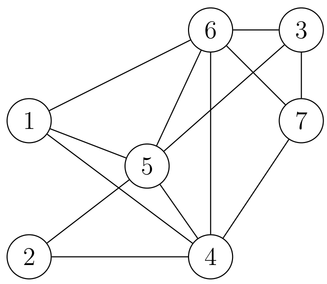


Figure 4.3: Connected graph with 7 vertices.

The first step is to associate the adjacency matrix to the graph and then calculate the index of G. We have $spect(G) = \{3.98316, 1, 0.19947, -1.46865, -1.71397, -2\}$. Thus $ind(G) = \varrho(G) = 3.98316$.

The computation for $\varrho_2(G)$ is done by utilization of the result of 4.4. This means we will take out all vertices v that are not cut vertices and calculate the index of $G - v$. We enumerate the vertices of G so that the reader can accompany the procedure, and denote by $G - i$ the graph obtained from G by taking out the vertex i.

In this way, we generate the following table and compare the greatest index that will come up from the connected induced subgraphs.

i	$ind(G-i)$
1	3.46793
2	**3.77846**
3	3.59261
4	3.01433
5	3.01433
6	2.90321
7	3.59261

Table 4.1: Computation of ϱ_2.

So we have that $\varrho_2(G) = ind(G-2) = 3.77846$. Note that all the distinct indexes found on Table 4.1 are complementary eigenvalues of G, but we want to order this eigenvalues.

Now we shall determine $\varrho_3(G)$ and, firstly, we will determine the candidates to being $\varrho_3(G)$. One of the candidates is 3.59261, that is the index of the induced subgraphs $G-3$ and $G-7$. We know, by the interlacing Theorem [26], that the index of a graph G is greater than the index of any induced subgraph of G. This means we don't have to consider the induced subgraphs of graphs that already have an index lower than 3.59261, which would be the case for graphs $G-1$, $G-4$, $G-5$ and $G-6$.

The other candidate to be $\varrho_3(G)$ is the index of an connected induced subgraph of $G-2$, since that certainly is a number lower than 3.77846 and that may also be greater than 3.59261, assuming, as such, the position of third greatest complementary eigenvalue of G. So let's look at the induced subgraphs of graph $G-2$.

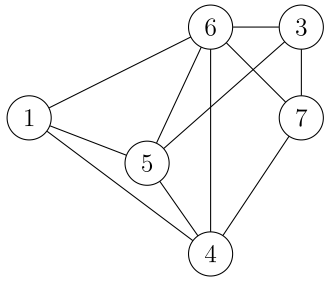


Figure 4.4: Graph $G-2$ obtained from G by taking out the vertex 2.

The procedure is the same: we take out each of the vertices that are not cut vertices from $G-2$ and verify which one have the greatest index.

i	$ind((G-2)-i)$
1	3.23607
3	3.32340
4	2.93543
5	2.93543
6	2.48119
7	3.32340

Table 4.2: Computation of ϱ_3.

Hence we conclude that $\varrho_3(G) = 3.59261$, being that the indexes of the induced subgraphs of $G-2$ do not surpass this value.

An aspect that the reader may have the interest to know why it's not considered is the following: graphs with a different number of vertices being cospectral with respect to the complementary spectrum. The cardinality of $\mathcal{CS}(G)$, as have already been said, is not a parameter pre-determined by the number of vertices of G. Hence, graphs with a different number of vertices could have the same set of complementary eigenvalues. Although, we don't consider this relevant aspect by the simple fact that the cospectrality problem in graphs is connected directly to the number of vertices that the graph has.

If we think in a way to determine the graphs from their complementary eigenvalues, we would use the known lexicographic order given by $G = (n, \varrho, \varrho_2, \varrho_3, \ldots, \varrho_k)$, where ϱ_i is the i^{th} complementary eigenvalue of G. This means that the graph G will be determined, firstly, by the number of its vertices, which leaves our analysis restricted only to sets of graphs with the same number of vertices.

Knowing the importance of the contribution of Godsil and Schwenk to the construction of cospectral graphs, a natural question is if those constructions would hold for the complementary spectrum. The answer is negative, which gives us even more evidence that the complementary spectrum is a relevant aspect to determine graphs. Beyond that, another important fact is that for trees until 14 vertices, there are no cospectral trees, and it is only necessary to compute until the third greatest complementary eigenvalue.

5 DETERMINIG GRAPHS BY THE COMPLEMENTARY SPECTRUM

In this chapter, we exhibit graphs and families of graphs that are determined by their complementary spectrum.

In this section, we present our paper [40] that has already been accepted for publication in *Discussiones Mathematicas Graph Theory*. We present an adapted version wiith the objective of not repeating concepts that have already been mentioned.

5.1 Introduction

The main purpose of this note is to underscore and to understand a recent new proposal for representing a graph using complementary eigenvalues. Instead of changing the matrix associated with G, the suggestion is to modify the concept of eigenvalue. In order to explain the new proposal and its consequences, we will recall here a few facts.

Definition 5.1. *Let A be a real matrix of order n. A real number λ is called a complementary eigenvalue of A if there exists a nonzero vector $x \in \mathbb{R}^n$ satisfying the complementarity system*

$$0 \leq x \perp (Ax - \lambda x) \geq 0$$

where $\perp$ stands for orthogonality and $x \geq 0$ means that every entry of vector x is nonnegative.

Fernandes et al. [21], studied the complementary eigenvalues of matrices associated to graphs (Laplacian, adjacency, etc) and we say that the *complementary spectrum of a graph G* is the set of complementary eigenvalues of its adjacency matrix.

Seeger [42] proposes to represent a graph by its complementary spectrum. As an example, the smallest pair of two nonisomorphic A-cospectral graphs of Figure 5.1 have different complementary spectra.

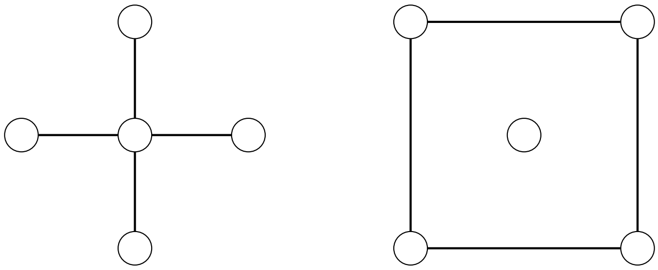


Figure 5.1: Nonisomorphic graphs with the same spectrum, but distinct complementary spectrum.

Indeed, the spectrum of both graphs is the multiset $\{-2, 0, 0, 0, 2\}$, whereas the complementary spectrum of the graph on the left is $\{0, 1, \sqrt{2}, \sqrt{3}, 2\}$ and the Complementary spectrum of the graph on right is $\{0, 1, \sqrt{2}, 2\}$. (See Section 5.3 how to compute the complementary spectrum of graphs).

In this paper, we shall reason that this new spectral way of representing a graph may do a better job in distinguishing them. For this, we formalize the proper definitions. Two graphs are said to be *complementary cospectral* if they have the same complementary spectrum.

Definition 5.2. *We say that a connected graph G is determined by its complementary spectrum – DCS for short – if any cospectral graph H is either isomorphic to G or the number of vertices of H and G are distinct.*

Throughout the paper, while reviewing some well known facts about spectra of graphs, we pose research questions that seem to be relevant in light of this new look on the spectra of graphs. In particular, we address the question of whether there exist pairs of non isomorphic graphs with the same complementary spectrum. We advance this by saying that we have found no examples of non isomorphic graphs with the same complementary spectrum.

The remainder of the paper is organized as follows. In the next Section 5.2 we review and discuss the issue of distinguishing graphs by their spectra. In Section 5.3 we show how to compute the complementary spectrum of a graph G - an interesting interplay between algebraic and combinatorial problems. We also explain Seeger's proposal for determining graphs from their complementary spectra. In Section 5.4 we show that some graphs are DCS. The path, the cycle, the complete and the star are DCS. We also show that all graph with less than 8 vertices are DCS. In section 5.5 we find several classes of graphs $\mathcal{G}$ whose elements have unique complementary spectrum in $\mathcal{G}$. Finally, in Section 5.6, we discuss the advantages and disadvantages of the proposal representation of the graphs. Particularly, we address the question of the cardinality of the complementary spectrum of a graph.

5.2 Distinguishing graphs by their spectra

When is a graph G M-DS? This means that G has a unique M-spectrum over all the graphs having the same number of vertices of G. As van Dam and Haemers [44] point out, it is very hard to prove that a graph G is M-DS, for any matrix M. In fact it seems easier to find families of graphs that have M-cospectral mates.

The milestone work of Schwenk [41] shows that almost all trees have an A-spectral mate, meaning that hardly any tree can be characterized by its A-spectrum. This result has been extended to Laplacian, signless Laplacian and distance matrix by McKay in [35]. In 1982, Godsil and Mckay [24] introduced an operation, now called the GM-switching, that has been used to construct families of cospectral graphs with respect to the adjacency and other matrices associated to a graph.

These developments seem to go against the conjecture that almost all graphs are DS. This conjecture has been forged by van Dam and Haemers in the papers [44, 45, 27]. The conjecture means, if true, that among all non-isomorphic graphs on at most n vertices, the fraction that is DS goes to 1 when n goes to infinity. We observe that since the number of trees compared to the number of all graphs is negligible, the fact that almost all trees have a cospectral mate does not interfere with the general conjecture. This conjecture appears to be formulated for any matrix M associated to graphs (Laplacian, Adjacency, signless Laplacian, etc). However, it is our understanding that the conjecture is far from being settled. We noticed that there even exist a few arguments against the validity of the conjecture [27].

Before the conjecture was firmly stated, there was a debate whether any particular matrix would distinguish more graphs than other matrices. More precisely, it was discussed whether the portion of DS graphs among all graphs on at most n vertices is larger for a particular matrix M associated to a graph. In 2009, Cvetković and Simić, in the beautiful series of papers [14, 15, 16], introduced many properties of the signless Laplacian matrix for graphs and, in particular, advocate that the signless Laplacian matrix would distinguish more graphs. From the table

n	4	5	6	7	8	9	10	11
r_n	0	0.059	0.064	0.105	0.139	0.186	0.213	0.211
s_n	0	0	0.026	0.125	0.143	0.155	0.118	0.090
q_n	0.182	0.118	0.103	0.098	0.097	0.069	0.053	0.038

where r_n, s_n and q_n are the *spectral uncertainty* associated with the adjacency, Laplacian and signless Laplacian, respectively, that is the portion of graphs on n vertices that have a cospectral mate among graphs on n vertices. Quoting the authors: "We see that numbers q_n are smaller than the numbers r_n and s_n for $n \geq 7$. In addition, the sequence q_n is decreasing for $n \leq 11$ while the sequence r_n is increasing for $n \leq 10$. This is a strong basis for believing that studying graphs by Q-spectra is more efficient than studying them by their (adjacency) spectra."

Even though it is no longer clear that the Q matrix distinguishes more graphs than other matrices, it is a fact that these computational results were used for a long time by many authors to justify the use of this matrix. It is worth mentioning a somewhat unexpected result by Carvalho et al. [10] which shows the existence of exponentially many Q-cospectral threshold graphs.

Nevertheless, the series of papers by Cvetković and Simić presented the Q-theory for graphs. The signless Laplacian matrix is now considered an important matrix that determines many structural properties of graphs. The following question still remains.

Problem 5.1. *Is there a matrix M associated to graphs such that the M-spectra distinguish more graphs than other matrices?*

5.3 Computing the complementary spectrum of a graph

Let G be a connected graph with n vertices. The largest eigenvalue of the adjacency matrix $A(G)$ of G, denoted by $\lambda(A(G))$, is called the *spectral radius* or the *index* of G. The most important information about computing the complementary spectrum is the following result [21].

Theorem 5.1. *Let G be a connected graph with n vertices. The complementary spectrum $\mathcal{CS}(G)$ of G is the set composed by the spectral radius of all induced connected subgraphs of G.*

We observe that the complementary spectrum has only nonnegative and no repeated values. Moreover, because the complementary spectrum of a disconnected graph is the union of the complementary spectrum of its components, we may consider, without loss of generality, only connected graphs.

We refer to [42] for several important properties of the complementary spectrum $\mathcal{CS}(G)$ of G, but recall here a few facts that are relevant to this paper. Let us denote by $\varrho = \varrho(G)$ the largest complementary eigenvalue and by $\varrho_2 = \varrho_2(G)$ its second largest complementary eigenvalue.

Fact 1: 0 is the smallest complementary eigenvalue of any graph G.

Fact 2: $\varrho = \lambda(A(G))$ is the spectral radius of $A(G)$.

Fact 3: $\varrho_2 = \max\{\lambda(G - v); v \in V(G) \text{ and } v \text{ is not a cut vertex of } G\}$.

Theorem 5.1 is an interplay between a combinatorial problem – the determination of connected induced subgraphs – an algebraic problem – the computation of spectral radii of principal submatrices of the adjacency matrix – and an optimization problem – the computation of complementary eigenvalues.

We will see further in this note that the cardinality of the set $\mathcal{CS}(G)$ plays an important role. Only as an observation, we point out that two graphs with the same number of vertices may have a different number of complementary eigenvalues. As an example the cycle C_4 on 4 vertices has $\mathcal{CS}(C_4) = \{0, 1, \sqrt{2}, 2\}$, while the graph H composed by a triangle with a pendent vertex has $\mathcal{CS}(H) = \{0, 1, \sqrt{2}, 2, \lambda(H)\}$, where $\lambda(H) \approx 2.17009$. Additionally, there may exist nonisomorphic subgraphs of G having the same index, hence the following holds [21].

Corollary 5.1. *Let G be a connected graph with n vertices and $\mathfrak{b}(G)$ be the number of induced nonisomorphic connected subgraphs of G. Then*

$$|\mathcal{CS}(G)| \leq \mathfrak{b}(G) \quad \text{and} \quad n \leq \mathfrak{b}(G) \leq 2^n - 1.$$

The lower bound of Theorem 5.1 is nicely settled by Seeger [42] as follows. For a given n, we say that the complete graph K_n, the star S_n, the path P_n and the cycle C_n, all with n vertices, are *elementary graphs.*

Theorem 5.2. *Let G be a connected graph with n vertices. Then*

$$n \leq |\mathcal{CS}(G)|.$$

Equality holds if and only if G is an elementary graph.

5.4 Graphs determined by the complementary spectrum

The number of complementary eigenvalues of a graph G is not determined by the number of vertices of G, instead it depends on the number of different spectral radii of the induced subgraphs of G. Hence, an interesting strategy to characterize graphs or classes of graphs by this spectral property is to study the cardinality of the complementary spectrum. For example, if we show that a graph G with n vertices is the only graph among all graphs on n vertices that has k complementary eigenvalues, we will have shown that this graph is DCS.

Let K_n, C_n, P_n and S_n be, respectively, the complete graph, the cycle, the path and the star on n vertices. Following Seeger, we will call them elementary graphs.

Theorem 5.3. *Elementary graphs are DCS.*

Proof. Let $\mathcal{S}(G)$ denote the set of all induced connected subgraphs of G and $\mathcal{CS}(G)$ denote the set of complementary spectrum of G. We know that

$$\mathcal{S}(K_n) = \{K_1, K_2, \ldots, K_{n-1}, K_n\}$$
$$\mathcal{S}(C_n) = \{P_1, P_2, \ldots, P_{n-1}, C_n\}$$
$$\mathcal{S}(P_n) = \{P_1, P_2, \ldots, P_{n-1}, P_n\}$$
$$\mathcal{S}(S_n) = \{S_1, S_2, \ldots, S_{n-1}, S_n\}.$$

So, we have

$$\mathcal{CS}(K_n) = \{0, 1, 2, \ldots, n-1\}$$
$$\mathcal{CS}(C_n) = \{\omega_1, \omega_2, \ldots, \omega_{n-1}, 2\}$$
$$\mathcal{CS}(P_n) = \{\omega_1, \omega_2, \ldots, \omega_{n-1}, \omega_n\}$$
$$\mathcal{CS}(S_n) = \{0, 1, \sqrt{2}, \ldots, \sqrt{n-1}\},$$

where $\omega_i = 2\cos\left(\dfrac{\pi}{i+1}\right)$. As we know the set of all induced subgraphs of the elementary graphs, we also know that their complementary spectra are different from each other. Actually, except for C_5 and S_5, we just need to compute the spectral radius of the elementary graphs to see this. And for C_5 and S_5, we just need to compute the second largest complementary eigenvalue to see that $\varrho_2(C_5) \neq \varrho_2(S_5)$, in spite of $\varrho(C_5) = \varrho(S_5)$.

Moreover, by Theorem 5.2, these are the only graphs G having $|\mathcal{CS}(G)| = n$, hence their complementary spectrum is different from any other graph with n vertices. This proves the result. □

Notice that we know all the induced connected subgraphs of K_n, C_n, P_n and S_n. Hence, we not only determine these graphs by their complementary spectrum, but we can also compute the whole complementary spectra of the elementary graphs K_n, C_n, P_n and S_n.

5.4.1 Ordering of Graphs

In this subsection, we give further details of the spectral representation of graphs proposed by Seeger [42].

As a motivation, consider the set $\mathcal{C}_6$ of all graphs with $n \leq 6$ vertices. Denote by $|G|$ the number of vertices of G. Define in $\mathcal{C}_6$ the following order

$$H \preceq G \leftrightarrow (|H|, \varrho(H), \varrho_2(H)) \preceq_{\text{lex}} (|G|, \varrho(G), \varrho_2(G)), \tag{5.1}$$

where $\preceq_{\text{lex}}$ is the lexicographic order in $\mathbf{R}^3$.

Seeger has shown, by computing numerically the complementary spectrum, that this lexicographic rule is a total ordering in $\mathcal{C}_6$, that is, all graphs with $n \leq 6$ vertices can be distinguished either by the largest or the second largest complementary eigenvalue. According to our definition, this means that all graphs up to 6 vertices are DCS.

For graphs with 7 vertices, we report the following experiment. For the first step, we computed the index of all 853 graphs on 7 vertices. Notice that when the spectral radii of these graphs are different, it means that these graphs are determined by their complementary spectrum once that the largest complementary eigenvalue of them are all different.

In case two graphs G and H have $\varrho(G) = \varrho(H)$, we compute the second largest complementary eigenvalue. We removed all non-cut vertices of these graphs obtaining all possible connected induced subgraphs (with 6 vertices), after that we compute the spectral radii of all these connected induced subgraphs and chose the largest one. In this second step we looked for the graphs with the same ϱ_2 and, for this set, it was necessary to compute ϱ_3.

In the third step we determined the candidate subgraphs to be ϱ_3 for these graphs, based on the interlacing of eigenvalues. We then computed the ϱ_3 and, for those where ϱ_3 was the same, we computed ϱ_4 in the same way we did for ϱ_3. Finally, this was the final step. There is no pair of graphs that has the same ϱ, ϱ_2, ϱ_3 and ϱ_4.

This means that the order given by equation 5.1 is not enough to distinguish all graphs with 7 vertices. However, we only need to compute the first four largest complementary eigenvalues to determine all graphs on 7 vertices. In any event, we can state the following result.

Theorem 5.4. *All graphs with $n \leq 7$ vertices are DCS.*

This may suggest that this complementary spectrum approach may be an alternative spectral technique that defines a greater portion of graphs.

To finish this section, we give the complete ordering formulation given by Seeger. For the set $\mathcal{C}$ of all connected graphs, define the function

$$G \in \mathcal{C} \longrightarrow \Psi_q(G) = (|G|, \varrho(G), \varrho_2(G), \ldots, \varrho_q(G)),$$

where $\varrho_k(G) = 0$ if $k > |\mathcal{CS}(G)|$. Define the order

$$H \preceq_q G \Leftrightarrow \Psi_q(H) \preceq \Psi_q(G), \tag{5.2}$$

a natural problem is to determine whether there exists q such that this defines a total ordering in $\mathcal{C}$.

Problem 5.2. *Let $\mathcal{C}$ be the set of all connected graphs. Does there exist q such that (5.2) defines a total order in $\mathcal{C}$?*

A positive answer to this question is equivalent to say that all graphs are DCS.

5.5 Classes with unique complementary spectrum

Consider a class of graphs $\mathcal{G}$ in which each element $G \in \mathcal{G}$ has a unique complementary spectrum. More precisely, if for $H, G \in \mathcal{G}$ we have $\varrho(H) = \varrho(G) \iff H$

and G are isomorphic. We say in this case that the graphs of $\mathcal{G}$ are determined by their complementary spectrum in $\mathcal{G}$. For short we say that $\mathcal{G}$ is DCS. Notice that the graphs of these classes are DCS just inside the class they belong to, which may be a first step to show they are DCS.

It is well known that the largest complementary eigenvalue of a graph G is the spectral radius of G. If a class $\mathcal{G}$ is such that each element $G \in \mathcal{G}$ has a unique spectral radius, then by the above definition, we say that $\mathcal{G}$ is DCS.

In this section we find a few classes $\mathcal{G}$ which are DCS.

5.5.1 Complete bipartite graphs

We say that a graph G on n vertices is complete bipartite if the set of vertices of G can be partitioned into two disjoint sets of cardinality r and s such that none of the vertices in each set are adjacent and every vertex in one bipartition is adjacent to every vertex in the other bipartition. We will denote this graph by $K_{r,s}$. It is well known that

$$\varrho(K_{r,s}) = \sqrt{rs}. \tag{5.3}$$

If we fix the number of vertices, we have $r + s = n$, in order to prove the uniqueness of the spectral radius, we shall take two different partitions of n, say $n = p+q = r+s$, and show that if $K_{p,q}$ and $K_{r,s}$ have the same spectral radius then they are isomorphic.

Notice that $rs = rn - r^2$ and $pq = np - p^2$. Suppose $pq = rs$, so that $K_{p,q}$ and $K_{r,s}$ have the same spectral radius. Then $(r-p)n = (r-p)(r+p)$. If $p = r$, then $q = s$ and $K_{p,q}$ and $K_{r,s}$ are isomorphic. If $p \neq r$, then $n = p+r$. But $n = p+q$, so $q = r$ and, consequently, $p = s$. We conclude once again that $K_{p,q}$ and $K_{r,s}$ are isomorphic.

This means that the class of the complete bipartite graphs is DCS.

In this class of graphs, we can actually compute the spectral radius of the graphs. We notice there are methods of ordering a whole class of graphs by their spectral radius, without computing them. This will also allows one to conclude that this class is DCS without really knowing what the spectral radius is.

5.5.2 Lollipops

A lollipop with n vertices, denoted by $H_{n,k}$, is a graph obtained by pending in a vertex of the cycle C_k, a terminal vertex of the path P_{n-k}, where $3 \leq k \leq n$. In order to prove that the class of lollipop graphs is DCS, we need the following concept.

An internal path in a graph G, denoted by $v_1 v_2 \ldots v_{r-1} v_r$, is a path beginning at v_1 and ending at v_r, where v_1 and v_r both have degree bigger than two, while all other vertices have degree two. The vertices v_1 and v_r are not necessarily distinct. We denote by W_n the tree with n vertices where two vertices have degree three and the distance between them is $n-5$. In the following we denote by λ the spectral radius of the graph we are considering. The following result, according to Belardo [7], appears in the work by Hoffman and Smith [29].

Lemma 5.1. *Let G be a graph with n vertices, $G \neq C_n, W_n$. Let G' be the graph with $n+1$ vertices obtained from G by inserting a new vertex of degree two in an edge e. Then*

i) if e lies on an internal path then $\lambda(G') < \lambda(G)$;

ii) if e does not lie on an internal path then $\lambda(G') > \lambda(G)$.

Theorem 5.5. *Given n, if we take $3 \leq k \leq n-1$, then $\lambda(H_{n,k+1}) < \lambda(H_{n,k})$.*

Proof. Consider the graph $H_{n,k}$. By Lemma 5.1, If we add a vertex in an edge of C_k, we have $\lambda(H_{n+1,k+1}) < \lambda(H_{n,k})$. If we delete the end vertex of the path P_{n-k} in $H_{n+1,k+1}$, we obtain $\lambda(H_{n,k+1}) < \lambda(H_{n+1,k+1})$, because $H_{n,k+1}$ is a proper subgraph of $H_{n+1,k+1}$. This proves the result. □

From this result we conclude that lollipops with n vertices are determined by their spectral radius. Hence they the class is DCS.

5.5.3 Starlike trees

A starlike tree is a tree having a unique vertex of degree greater than 2. In [37], the authors prove that, for a fixed n, all starlike trees with n vertices have distinct spectral radius. In the next paragraph, we explain the result in a more precise way.

A starlike tree with n vertices may be represented as a partition of $n-1$, say $T = [m_1, m_2, \ldots, m_k]$, where $, m_i \geq 1, n-1 = m_1 + m_2 + \cdots + m_k$, $k \geq 3$ and the paths P_{m_i} are attached to common vertex v. Moreover, without loss of generality we assume that $1 \leq m_1 \leq m_2 \leq \cdots \leq m_k$. In the paper [37], it is proven that the lexicographic order of the k-tuple $[m_1, m_2, \ldots, m_k]$ gives a total ordering of the spectral radii of the starlike trees with n vertices.

This shows that the class of starlike trees is DCS.

5.5.4 Trees - computational results

A tree T is a connected graph without cycles. With respect to the complementary spectrum of a tree, we have performed some experiments and the following results arise.

Considering all trees up to 14 vertices, we observe that there are no cospectral pairs if we consider the complementary spectrum. The experiment consists in fixing n and computing the spectral radii of all trees on n vertices. For trees with the same spectral radius, we further compute the second largest complementary eigenvalue taking all non-cut vertices and compute the spectral radii of all possible induced subgraphs.

For n up to 6 vertices, no tree has the same spectral radius. For $n \leq 10$ there are no pairs of cospectral trees with respect to the complementary spectrum. More than that, they are determined just by ϱ and ϱ_2. We summarize the results in Table 5.1 and notice that we need only ϱ, ϱ_2 and ϱ_3 to distinguish all trees up to 14 vertices. In Seeger notation, it means that $\Psi_3(G) = (|G|, \varrho(G), \varrho_2(G), \varrho_3(G))$ is a total order in the class of trees up to 14 vertices.

n	Trees	Cospectral Trees	ϱ equal	same ϱ, ϱ_2	same ϱ, ϱ_2, ϱ_3
7	11	0	2 graphs 1 pair	0	0
8	23	2 graphs 1 pair	4 graphs 2 pairs	0	0
9	47	10 graphs 5 pairs	18 graphs 7 pairs 1 quartet	0	0
10	106	8 graphs 4 pairs	24 graphs 9 pairs 2 triples	0	0
11	235	60 graphs 27 pairs 2 triples	106 graphs 31 pairs, 9 triples, 3 quartets and 1 quintet	2 graphs 1 pair	0
12	551	119 graphs 49 pairs 7 triples	197 graphs 57 pairs, 48 triples, 2 quartets and 5 quintets	8 graphs 4 pairs	0
13	1301	192 sets	662 graphs	29 graphs 10 pairs 3 triples	0
14	3159	390 sets	1245 graphs	51 graphs 24 pairs 1 triple	0

Table 5.1: Experiment

5.6 Final Remarks

In this note, following the ideas of [21] and [42], we have shown how to use complementary eigenvalues of the adjacency matrix to represent the spectrum of a graph. We have defined the notion of a connected graph being *defined by the complementary spectrum* - *DCS* - when it has a unique complementary spectrum among all graphs with the same order. We show that the elementary graphs (the path, the cycle, the star and the complete graph) are DCS. We show, by computing the complementary spectra, that all graphs with less than 8 vertices are DCS. Additionally, we have not found two non isomorphic connected graphs with the same complementary spectrum.

As we have seen, the complementary spectrum of a graph G is the set composed by the spectral radii of all connected induced subgraphs of G. This result may be seen as a nice relationship between the algebraic problem of computing the complementary eigenvalues of the adjacency matrix and the combinatorial problem of determining the connected induced subgraphs of G. On the other hand, it also may be seen as an evidence of the difficulty of the problem. Which is harder? Computing the complementary eigenvalues of an adjacency matrix or to find all connected induced subgraphs?

The difficulty of these problems is related to the cardinality $|\mathcal{CS}(G)|$ of the complementary spectrum of a graph G. Moreover, we notice that $|\mathcal{CS}(G)|$ can be related to the isomorphism problem in the following way. If $|\mathcal{CS}(G)|$ were bounded by a polynomial in n, the order of G, then the complementary spectrum could be computed in polynomial time. In this case, if all graphs were DCS, the conclusion would be that the isomorphism problem is polynomial. Clearly, this line of reasoning is very speculative and perhaps the only merit is to show that proving that a graph G is DCS, or computing the complementary spectrum of G or merely bounding its cardinality are very hard problems. Indeed, as we see next, the cardinality $|\mathcal{CS}(G)|$ is not bounded by a polynomial.

Let $\mathcal{G}_n$ be the set of all connected graphs of order n. Corollary 5.1 shows that for $G \in \mathcal{G}_n, |\mathcal{CS}(G)| \leq 2^n - 1$. Can we find a better than exponential upper bound? In [21], the authors determined that $|\mathcal{CS}(G)|$ grows faster than any polynomial in n. More precisely, they showed that, for fixed n, there is a starlike tree T with n vertices whose

$$|\mathcal{CS}(T)| \sim \frac{\exp \pi\sqrt{2\sqrt{n}/3}}{4\sqrt{3n}}.$$

This means that $|\mathcal{CS}(G)|$ can not be bounded by a polynomial in n. It is still unknown whether there is an upper bound whose growth is smaller than an exponential. We finish this note by posing the following question.

Problem 5.3. *Is there a function of n bounding the cardinality $|\mathcal{CS}(G)|$ for all $G \in \mathcal{G}_n$ whose growth is smaller than exponential?*

6 FINAL REMARKS

Initially, let's resume some questioning made in the Introduction and verify if we can conjecture some answers.

1. Are there indicatives that a matrix determines a greater number of graphs than other?

2. Does changing the matrix associated to the graph is, or seem to be, a solution to the problem of cospectrality?

3. Is there another parameter that we can associate to a graph and that ends up uniquely describing it?

The first and second questions may be treated together. Indeed, if we have evidence that a kind of matrix is better to determine graphs by their spectrum, then this kind of matrix is closer to give us a solution to the problem of cospectrality. Conversely, if there's a matrix that seems to solve the problem of cospectrality, it obviously must determine more graphs by their spectrum than other matrices. That being said, it seems the more we study constructions of cospectral graphs and how they work, the more we discover an infinitude of graphs that are not DS with respect to any of matrix M. In a nut shell, there seems that no matrix will solve the problem of cospectrality

Do we have graphs determined by their complementary spectrum? The answer for this question is directly related to the final question we asked before. And we can cite the elementary graphs that are determined by the complementary spectrum. Although the elementary graphs are a relatively small class, to say that a graph with n vertices is determined by the spectrum, that is, that no other graph with n vertices has the same set of eigenvalues as its, has a great relevance in the literature.

In fact we show now that the graph $K_n - \{e\}$ is determined by the complementary spectrum. Consider the graph $K_n - \{e\}$, we know it is the only graph with n

vertices and $\frac{n(n-1)}{2} - 1$ edges. Therefore,

$$\lambda_1(G) < \lambda_1(K_n - \{e\}) < \lambda_1(K_n)$$

for all G with n vertices. This result is guaranteed since K_n has one more edge than $K_n - \{e\}$, and G is a graph with less edges than $K_n - \{e\}$.

There are some families of graphs we can say are determined by their complementary spectrum at least inside their own family. For example, consider the collection of all starlike graphs. We know that there are no two starlike graphs with the same complementary spectrum, but we still cannot say they are determined by their complementary spectrum, since there may exist a graph that is not starlike and that has the same complementary spectrum as a starlike graph. This is also the case for the complete bipartite graphs, the double brooms and the lollipops.

Almost all trees have a cospectral pair with respect to all the types of matrices we worked with here, those being the adjacency, laplacian and signless laplacian matrices. However, if we consider the complementary spectrum, we know there are no pairs of cospectral trees up until $n = 14$ vertices. Another experiment with positive results was made for unicyclic graphs. For $n = 8$ and $n = 9$, and considering the universe of unicyclic graphs, these graphs are all DCS.

An important fact to be accounted for is that of we have not found yet pairs of connected graphs with the same complementary spectrum. Though, we did find cospectral graphs with respect to the complementary spectrum that are disconnected. These pairs were not considered by us on the present research, since our main goal was to consider connected graphs. Maybe better comprehending how the construction of DCS graphs is given, even when disconnected, can be of importance on a future work.

Another important topic of our dissertation certainly was the study of matroids, which was mainly done during the period of exchange and advised by Professor Jorge Alfonsin. The result of this study, which was presented on the XXXIX National Congress of Applied and Computational Mathematics - CNMAC - shows that, as simple as it may be, there is a relation between determination of graphs and bases of matroids. Another work of interest to be done hereafter is to study more relations like this.

6.1 Matroids

A matroid [1, 39, 49] $\mathcal{M}$ is an ordered pair $(\mathcal{I}, E)$, where $E = \{1, \ldots, n\}$ and $\mathcal{I}$ is a collection of subsets of E such that:

(*i*) $\emptyset \in \mathcal{I}$;

(*ii*) $I \in \mathcal{I}, I' \subset I \Rightarrow I' \in \mathcal{I}$;

(*iii*) if $I_1, I_2 \in \mathcal{I}$ satisfy $|I_1| < |I_2|$, then there exists an element $e \in I_2 \setminus I_1$ such that $(I_1 \cup e) \in \mathcal{I}$.

The elements of $\mathcal{I}$ are called *independents of* $\mathcal{M}$. A basis of a matroid is an independent maximal set. Two matroids $\mathcal{M}_1 = (\mathcal{B}_1, E_1)$ and $\mathcal{M}_2 = (\mathcal{B}_2, E_2)$ are isomorphic if, and only if, there exists a bijection $f : E_1 \rightarrow E_2$ such that, if $B_1 \in \mathcal{B}_1$ then $f(B_1) \in \mathcal{B}_2$.

We present an application of a classical result about matroids on the determination of a family of graphs. In doing so, we will use the operation between two graphs known as *2-isomorphism*. A graph G is 2-isomorphic to a graph H if H can be transformed into a graph isomorphic to G through a sequence of operations known as *vertex indentification*, *vertex cleaving* and *twisting*.

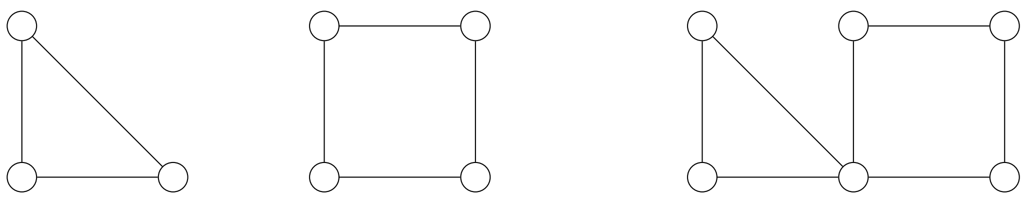


Figure 6.1: Vertex identification, vertex cleaving

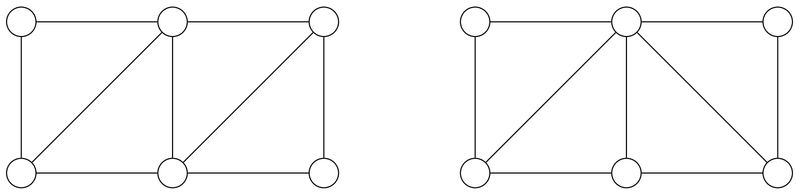


Figure 6.2: Twisting

Theorem 6.1. *[39] Let G and H be graphs with no isolated vertex. We then have that $\mathcal{M}(G)$ and $\mathcal{M}(H)$ are isomorphic if, and only if, G and H are 2-isomorphic.*

Theorem 6.2. *Let G be a k-connected graph of n vertices and m edges. For $k \geq 3$, we have that G is determined by its matroids of circuits $\mathcal{M}(G)$.*

Proof. Let G be a k-connected graph with $k \geq 3$.
Suppose that exists a graph H such that $\mathcal{M}(G)$ and $\mathcal{M}(H)$ are isomorphic. By Theorem 1, we have that G and H are 2-isomorphic. Though, to obtain (without loss of generality) G from H by use of the operations that define the 2-isomorphism, we must have both G and H being, at most, 2-connected. If they're not, the vertex identification, vertex cleaving and twisting operations would not be possible. So, since there's no possibility of obtaining the graph H 2-isomorphic to G, we have that their matroids are not isomorphic. With this, we can associate each k-connected graph with $k \geq 3$ to a list composed by the bases of their associated matroids. The matroids not being isomorphic, we would then have different bases for each matroid and, consequently, different lists associated to the graphs.

□

On future works, it will be interesting to think about more relations between matroids and graph determination. Moreover, we aim to optimize our procedure to calculate the complementary spectrum of a graph G so that it can be used more effectively to compare the complementary spectrum of graphs on the same family or with the same number of vertices.

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