AUSTRALASIAN JOURNAL OF COMBINATORICS
Volume **84(1)** (2022), Pages 220–237

Complementarity eigenvalues and graph determination

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Abstract

Determination of connected graphs is a fundamental theme of spectral graph theory. In this work, the task of separating a pair of connected graphs is done with the help of the spectral code function. The verb "to separate" is used here as a synonym of the verb to discriminate or to distinguish. By definition, the spectral code of a connected graph G is an eventually zero sequence $\Gamma(G) := (\varrho_1(G), \varrho_2(G), \varrho_3(G), \dots)$ whose kth term is the k-largest complementarity eigenvalue of the graph. The spectral code of a graph is a convenient vector representation of the so-called complementarity spectrum of the graph. The spectral code separation technique runs as follows: while comparing two connected graphs, say G and H, we start by considering ϱ_1, which is nothing but the spectral radius function; in case of equality $\varrho_1(G) = \varrho_1(H)$, the second largest complementarity eigenvalue function ϱ_2 enters into action; in case of a new equality, we pass to ϱ_3, and so on. Complementarity eigenvalues perform more efficiently the separation role usually played by classical eigenvalues.

* Partially supported by FONDECYT (Chile) through grant 11220268.

ISSN: 2202-3518

1 Introduction

All graphs considered in this work are finite, undirected, unlabeled, loopless and without multiple edges. The attention is further restricted to graphs that are connected. We denote by $\mathcal{C}$ the set of connected graphs of arbitrary order. As discovered by Collatz and Sinogowitz [3] in the fifties, two distinct connected graphs may have the same characteristic polynomial. This means that the eigenvalues of a graph may not provide enough information to identify the graph itself, i.e., the classical spectrum could be unable to separate or distinguish a pair of connected graphs. This phenomenon is nowadays called cospectrality or spectral indetermination. A word of clarification is in order: labeled graphs that are isomorphic are considered simply as the same graph. We are using unlabeled graphs in order to avoid the nuisance of graph isomorphism. For handling the difficult problem of identifying a graph by means of a collection of spectral parameters, we shift the attention from classical eigenvalues to complementarity eigenvalues. Although the idea of using complementarity eigenvalues as tools for identifying and enumerating connected graphs was already suggested in Seeger [13] and further explored in Pinheiro et al. [10], this area of research is still at the embryonic stage. The transition from classical eigenvalues to complementarity eigenvalues is a major change in the way of perceiving the concept of spectral information contained in a graph.

For the reader's convenience, we recall that a scalar $\lambda \in \mathbb{R}$ is a complementarity eigenvalue of a graph G if it is a complementarity eigenvalue (or Pareto eigenvalue) of the associated adjacency matrix, i.e., if there exists a nonzero vector $x \in \mathbb{R}^n$ satisfying the complementarity system

$$x \geq 0\,,\ A_G x - \lambda x \geq 0\,,\ \langle x, A_G x - \lambda x\rangle = 0\,, \tag{1}$$

where n is the order of G, $\langle \cdot, \cdot \rangle$ is the inner product of $\mathbb{R}^n$, and $x \geq 0$ means that x is componentwise nonnegative. The complementarity spectrum or set of complementarity eigenvalues of G is denoted by $\Pi(G)$. See Seeger [12] for the theory of complementarity spectra of general matrices, and Fernandes et al. [5] for the first published paper on complementarity spectra of graphs. The adjacency matrix of G depends on the way of labeling the vertices, but the set $\Pi(G)$ does not. Indeed, the complementarity spectrum of a matrix is invariant under permutation similarity transformations. As shown in [5], the complementarity spectrum of a connected graph G admits the representation

$$\Pi(G) = \{\varrho(F) : F \in \mathcal{S}(G)\}, \tag{2}$$

where $\varrho(F)$ is the spectral radius of F and $\mathcal{S}(G)$ is the set of connected induced subgraphs of G. Hence, $\Pi(G)$ can be computed by evaluating the spectral radius of each connected induced subgraph of G or, alternatively, by solving the complementarity system (1) with the help of any existing algorithm.

Classical spectra and complementarity spectra differ in many ways. To start with, there is no such a thing as a characteristic polynomial whose zeros are the complementarity eigenvalues of the graph. Secondly, complementarity eigenvalues are not counted with associated multiplicities: the complementarity spectrum of a graph is a set and not a multiset as is the case of the classical spectrum. Perhaps the most striking difference between classical spectra and complementarity spectra concerns cardinality: the number of eigenvalues of a connected graph of order n is at most n, whereas the number of complementarity eigenvalues is at least n and usually much larger than n. As shown in [5], the maximum number of complementarity eigenvalues of a connected graph of order n increases faster than any polynomial in the variable n. The recent paper of Seeger and Sossa [14] provides updated information on cardinality of complementarity spectra of various classes of connected graphs. The complementarity spectrum of any connected graph belongs to $\mathfrak{F}(\mathbb{R})$, the set of nonempty finite subsets of $\mathbb{R}$. The reader should be aware that $c(G) := \mathrm{card}[\Pi(G)]$ may change significatively if G is replaced by another graph of the same order. By way of example, Figure 1 displays a graph of order 14 with as many as 5085 complementarity eigenvalues. Such a graph is to be compared with a star of order 14, which has only 14 complementarity eigenvalues.

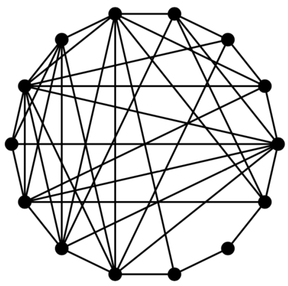

Figure 1: Graph of order 14 with 5085 complementarity eigenvalues

Our numerical experience with low order connected graphs suggests that the complementarity spectral map $\Pi : \mathcal{C} \to \mathfrak{F}(\mathbb{R})$ is a promising separation tool. The verb "to separate" is used here as a synonym of the verb to discriminate or to distinguish. In the parlance of classical set theory, an abstract function f separates the points of a set X (in short, f separates X) if the values $f(x_1)$ and $f(x_2)$ are different when the points $x_1, x_2 \in X$ are different. This amounts to saying that f is an injection on X. The purpose of this work is to explore whether Π serves to separate the members of $\mathcal{C}$ or, at least, to separate the members of some large subset of $\mathcal{C}$.

Definition 1. *Let $\mathcal{G}$ be a class of connected graphs. We say that $\mathcal{G}$ is separable if the restriction of Π to $\mathcal{G}$ is an injection; i.e., if two graphs in $\mathcal{G}$ have the same complementarity spectrum, then they are the same graph.*

For the sake of precision, the concept of separability introduced in Definition 1 should be called Π-separability. However, we prefer to omit the reference to Π and use an alleviated terminology. Classical spectra will no longer show up in the discussion. A word of caution is in order: the class under examination may have infinitely many members, so we could be comparing in fact the complementarity spectra of connected graphs that are not necessarily of the same order. A class of connected graphs is called finite if it has finitely many members and homogeneous if all its members have the same order. We are mainly interested in the classes

$$\begin{aligned} \mathbb{C}_n &:= \text{ connected graphs of order } n, \\ \mathbb{T}_n &:= \text{ trees of order } n, \end{aligned}$$

but we shall consider also some more specialized examples. A first question that comes to mind is whether the class of connected graphs is separable, i.e., whether the map Π is able to separate the universal class $\mathcal{C}$. In spite of massive numerical experimentation, we have not yet found a pair of distinct connected graphs with the same complementarity spectrum. Of course, failure in finding a counterexample is not a proof that $\mathcal{C}$ is separable. This issue is difficult and probably a long time will pass before we get a formal proof of the separability of $\mathcal{C}$ or before we find a counterexample. In this work we would like to present at least some partial advances in this research area.

The organization of the paper is as follows. Section 2 introduces the concept of spectral code of a connected graph and the associated concept of separability index of a class of connected graphs. The spectral code is a representation of the complementarity spectrum as a sequence formed with the complementarity eigenvalues arranged in decreasing order. The separability index of a class, say $\mathcal{G}$, is the minimal number of successive complementarity eigenvalues (starting from the largest one) that are needed to separate $\mathcal{G}$. Computing separability indices is a major concern of this work.

Section 3 deals with the separability indices of classes of connected graphs of low or moderate order. For such classes, it is possible to compute the separability index as a result of exhaustive numerical experimentation. In this section, we also comment on separation of pairs of cospectral graphs.

Section 4 gives the exact separability index for many important classes of connected graphs. The classes under consideration are homogeneous, or finite nonhomogeneous, or infinite.

2 Spectral code of a graph

The notation that we use in this work is for the most part standard. For instance, the symbols K_n, P_n, S_n, and C_n indicate respectively the complete graph, the path, the star, and the cycle on n vertices. The cycle C_n is defined starting from $n = 3$. As said before, the function Π takes values in $\mathfrak{F}(\mathbb{R})$. It is not always easy to work with a function whose values are finite sets of various cardinalities. Instead of the set-valued function Π, we can use an equivalent function $\Gamma : \mathcal{C} \to \ell(\mathbb{R})$ with values on the vector space of real sequences with finitely many nonzero terms. By an obvious reason, a sequence of that sort is called an eventually zero sequence. By definition,

Γ assigns to a connected graph G an eventually zero sequence

$$\Gamma(G) := (\varrho_1(G), \varrho_2(G), \varrho_3(G), \dots)$$

called the spectral code of G. Here, $\varrho_k(G)$ stands for the kth largest complementarity eigenvalue of G, with the convention $\varrho_k(G) = 0$ for all $k \geq c(G)$. For instance, for a complete graph of order 8 and a star of order 6, we get

$$\begin{aligned} \Gamma(K_8) &= (7, 6, 5, 4, 3, 2, 1, 0, 0, \dots), \\ \Gamma(S_6) &= (\sqrt{5}, 2, \sqrt{3}, \sqrt{2}, 1, 0, 0, \dots), \end{aligned}$$

respectively. Three additional examples are given in Table 1 to help familiarize the reader with the general look of a spectral code.

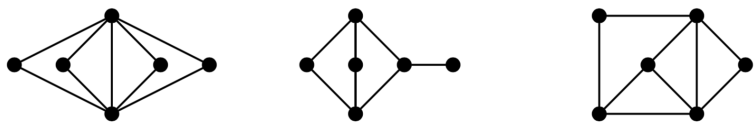

Figure 2: Graphs with 8, 10, and 15 complementarity eigenvalues, respectively

In general, a complementarity eigenvalue is either an integer or an irrational. This is clear from the representation formula (2) and the fact that the spectral radius of any graph is either an integer or an irrational. The first two graphs mentioned in Table 1 are somewhat special, because it is rather unusual to get a radical representation for each complementarity eigenvalue. By a radical representation we mean an expression involving only integers and square roots. In our numerical experiments, complementarity eigenvalues are always computed with double-precision arithmetic,x but we display them with 6 decimal places only. The third graph mentioned in Table 1 is also special, but for a different reason. That graph has the maximum number of complementarity eigenvalues among all graphs on 6 vertices. In principle, we could change the spectral code of G by the finite vector

$$\gamma(G) := (\varrho_1(G), \varrho_2(G), \varrho_3(G), \dots, 1, 0) \tag{3}$$

obtained by dropping all the zeros after the first one. However, working with (3) is not always a convenient strategy, mainly because the number of components of this vector may change from one graph to another, even if we focus on graphs of a prescribed order. The number of components of (3) is equal to $c(G)$. The concept of separability can be reworded in terms of the spectral code function: a class $\mathcal{G}$ of connected graphs is separable if and only if the restriction of Γ to $\mathcal{G}$ is an injection, i.e., if two graphs in $\mathcal{G}$ have the same spectral code, then they are the same. The spectral code is a sort of password that is intended to identify the graph, the kth letter of the password being the kth largest complementarity eigenvalue of the graph. It would be disturbing of course if two or more graphs share the same spectral code. For this reason, it is helpful to know in advance if the graphs under consideration

Table 1: Complementarity eigenvalues arranged in decreasing order, cf. graphs in Figure 2

	1st graph in Fig 2		2nd graph in Fig 2		3rd graph in Fig 2
	exact	numerical	exact	numerical	
ϱ_1	$(1/2)(1+\sqrt{33})$	3.372281	$[(1/2)(7+\sqrt{33})]^{1/2}$	2.524338	3.169195
ϱ_2	3	3.000000	$\sqrt{6}$	2.449490	2.935432
ϱ_3	$(1/2)(1+\sqrt{17})$	2.561553	$[(1/2)(5+\sqrt{17})]^{1/2}$	2.135779	2.855773
ϱ_4	2	2.000000	2	2.000000	2.685544
ϱ_5	$\sqrt{3}$	1.732051	$[2+\sqrt{2}]^{1/2}$	1.847759	2.561553
ϱ_6	$\sqrt{2}$	1.414214	$\sqrt{3}$	1.732051	2.481194
ϱ_7	1	1.000000	$(1/2)(1+\sqrt{5})$	1.618034	2.302776
ϱ_8	0	0.000000	$\sqrt{2}$	1.414214	2.170086
ϱ_9	0	0.000000	1	1.000000	2.135779
ϱ_{10}	0	0.000000	0	0.000000	2.000000
ϱ_{11}	0	0.000000	0	0.000000	1.732051
ϱ_{12}	0	0.000000	0	0.000000	1.618034
ϱ_{13}	0	0.000000	0	0.000000	1.414214
ϱ_{14}	0	0.000000	0	0.000000	1.000000
ϱ_{15}	0	0.000000	0	0.000000	0.000000

belong or not to a separable class. If yes, then we can trust the spectral code as discriminating tool; otherwise the spectral code does not fulfill properly its assigned task. Should we use the spectral code in full extent or just the most relevant part of it? If we truncate the spectral code of G after the tth entry, then we get the finite dimensional vector

$$\Gamma_t(G) := (\varrho_1(G), \varrho_2(G), \ldots, \varrho_t(G)).$$

Using the function Γ_t instead of Γ is like using the first t letters of a password instead of the entire password. This is of course a metaphorical way of speaking. The first two terms in a spectral code are by far the most important ones. Fortunately, these terms are easy to compute because they are given by the explicit formulas

$$\varrho_1(G) = \varrho(G)\,, \tag{4}$$

$$\varrho_2(G) = \max_{\substack{F \in \mathcal{S}(G) \\ |F| = |G|-1}} \varrho(F)\,. \tag{5}$$

Recall that $\varrho(G)$ is the spectral radius of G and $\mathcal{S}(G)$ is the set of connected induced subgraphs of G. Parenthetically, any graph in the feasible set of (5) is called a child of G. An eldest child of G is a child that achieves the maximal value (5). In our numerical experiments, we use (4) and (5) if we need to compute only the first two complementarity eigenvalues of a graph, but we rely on Theorem 4.1 in Seeger [12] if we need to compute the entire complementarity spectrum. The theorem just mentioned tells us how to compute the complementarity spectrum of an arbitrary matrix, say A, by examining some special eigenvalues in each principal submatrix of A. The details can be consulted in [12]. The representation formula (2) is quite useful when it comes to addressing theoretical issues concerning highly structured graphs of large order.

2.1 The concept of separability index

Truncated spectral codes can be used to measure the degree of separability of a class $\mathcal{G}$ of connected graphs. It is implicitly understood that $\mathcal{G}$ has at least two members, otherwise the separation or discrimination problem has no sense. We define the separability index of $\mathcal{G}$ as the minimum number of complementarity eigenvalues needed for separating $\mathcal{G}$, i.e.,

$$\mathfrak{s}(\mathcal{G}) := \inf\{t \geq 1 : \Gamma_t \text{ separates } \mathcal{G}\}.$$

We use the convention $\mathfrak{s}(\mathcal{G}) = \infty$ if no truncated spectral code is able to separate $\mathcal{G}$, but we do not know yet if such a situation could arise in practice. A sufficient condition for a class to be separable is to have a finite separability index. Note that:

- $\mathfrak{s}(\mathcal{G}) = 1$ means that the spectral radius alone suffices to separate $\mathcal{G}$. This happens if $\mathcal{G}$ is for instance the infinite class of complete graphs.
- $\mathfrak{s}(\mathcal{G}) = 2$ means that the spectral radius is not sharp enough to separate $\mathcal{G}$, but the spectral radius together with the second largest complementarity eigenvalue function do the separation job. By way of example, the infinite class of complete bipartite graphs belongs to this category.
- $\mathfrak{s}(\mathcal{G}) = 3$ means that also the 3rd largest complementarity eigenvalue function is needed for separating $\mathcal{G}$, but we can dispense from the 4th largest complementarity eigenvalue function. An example of this case is the finite nonhomogeneous class of connected graphs with 8 edges.

The smaller the value of $\mathfrak{s}(\mathcal{G})$, the easier it is to separate $\mathcal{G}$. The separability index is monotonic in the sense that $\mathcal{G}_1 \subseteq \mathcal{G}_2$ implies $\mathfrak{s}(\mathcal{G}_1) \leq \mathfrak{s}(\mathcal{G}_2)$. However, it is not because $\mathcal{G}$ has many members that $\mathfrak{s}(\mathcal{G})$ should be large. The term $\mathfrak{s}(\mathcal{G})$ depends more on the structure of the members of $\mathcal{G}$ than in their number.

3 Experimental results on separability indices

In what follows, the symbol

$$\mathbb{C}(n_1, n_2) := \cup_{n=n_1}^{n_2} \mathbb{C}_n \tag{6}$$

stands for the class of connected graphs of order between n_1 and n_2, both extremes inclusive. In particular, $\mathbb{C}(1, n)$ is the set of connected graphs of order up to n. Note that, for each $n \geq 2$, the class $\mathbb{C}(1, n)$ is finite but not homogeneous. A matter of exhaustive numerical testing shows that

$$\begin{cases} \Gamma_3 \text{ separates the 143 members of } \mathbb{C}(1,6), \text{ but } \Gamma_2 \text{ does not,} \\ \Gamma_4 \text{ separates the 996 members of } \mathbb{C}(1,7), \text{ but } \Gamma_3 \text{ does not,} \\ \Gamma_9 \text{ separates the 12113 members of } \mathbb{C}(1,8), \text{ but } \Gamma_8 \text{ does not,} \\ \Gamma_{16} \text{ separates the 273193 members of } \mathbb{C}(1,9), \text{ but } \Gamma_{15} \text{ does not.} \end{cases} \tag{7}$$

As mentioned in (7), the connected graphs of order up to 9 can be separated with Γ_{16}, but not with Γ_{15}, cf. Figure 3. Checking this statement took around 22 hours in a computer OS High Sierra, processor 3.4 GHz Intel Core i5 and memory 8GB. The codes were implemented with Matlab R2017a.

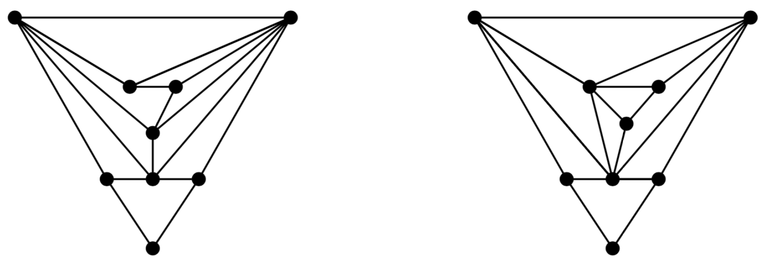

Figure 3: Graphs of order 9 sharing the 15 largest complementarity eigenvalues, but not the 16th largest

Tables 2 and 3 include part of the information provided in (7), and also display the separability index of some particular classes, among which are $\mathbb{C}_n$, $\mathbb{T}_n$, and

$$\begin{aligned} \mathbb{ST}_n &:= \text{ starlike trees of order } n, \\ \mathbb{U}_n &:= \text{ unicyclic graphs of order } n, \\ \mathbb{R}_n &:= \text{ regular connected graphs of order } n, \\ \mathbb{BP}_n &:= \text{ bipartite connected graphs of order } n. \end{aligned}$$

By passing to union as in (6), we form the class $\mathbb{T}(n_1, n_2) := \cup_{n=n_1}^{n_2} \mathbb{T}_n$. The same mechanism is used to form $\mathbb{ST}(n_1, n_2)$, $\mathbb{U}(n_1, n_2)$, and so on. Since a starlike tree has at least 4 vertices, the class $\mathbb{ST}(n_1, n_2)$ is defined only if $n_1 \geq 4$. Consistently, $\mathbb{ST}(4, n)$ corresponds to the class of starlike trees on at most n vertices. The classes $\mathbb{U}(3, n)$, $\mathbb{R}(1, n)$, and $\mathbb{BP}(2, n)$ are defined in a similar way.

Table 2: Separability index of some particular classes of connected graphs

n	$\mathbb{C}_n$	$\mathbb{C}(1,n)$	$\mathbb{U}_n$	$\mathbb{U}(3,n)$	$\mathbb{R}_n$	$\mathbb{R}(1,n)$	$\mathbb{BP}_n$	$\mathbb{BP}(2,n)$
4	1	2	1	2	1	2	1	1
5	2	2	1	2	1	2	1	2
6	2	3	1	2	2	2	2	3
7	4	4	1	2	2	2	3	3
8	9	9	2	2	3	3	3	3
9	16	16	3	3	3	3	3	4

Due to a prohibitive computational cost, Table 2 runs for values of n up to 9 only. Computing the separability index of $\mathbb{C}(1, 10)$ would require computation of the complementary spectrum of 11 989 764 connected graphs in all, among them the 11 716 571 connected graphs of order 10. In the considered experimental range, the separability indices $\mathfrak{s}(\mathbb{C}_n)$, $\mathfrak{s}(\mathbb{U}_n)$, $\mathfrak{s}(\mathbb{R}_n)$, and $\mathfrak{s}(\mathbb{BP}_n)$, are nondecreasing as a function of n. This observation is somehow consistent with intuition, but we do not have a formal proof of such a monotonicity behavior for larger values of n.

Table 3: Separability index of some particular classes of trees

n	$\mathbb{T}_n$	$\mathbb{T}(1,n)$	$\mathbb{ST}_n$	$\mathbb{ST}(4,n)$
4	1	1	1	1
5	1	2	1	1
6	1	2	1	1
7	2	2	1	2
8	2	3	1	2
9	2	3	1	2
10	2	3	1	2
11	3	3	1	2
12	3	4	1	2
13	3	4	1	2
14	3	6	1	2
15	4	7	1	2

Table 3 runs for values of n up to 15. The column $\mathbb{T}_n$, for n until 14, is filled with information provided in Pinheiro et al. [10, Table 1]. The case $n = 15$ is added now. Note that $\mathbb{T}_{15}$ is the class of smaller order trees for which 3 complementarity eigenvalues are not enough to accomplish separation. The column $\mathbb{ST}_n$ is filled with ones, because distinct starlike trees of the same order have different spectral radii, cf. Oliveira et al. [9]. However, the spectral radius alone is not able to separate starlike trees of different order; see the last column of Table 3.

Connected graphs can be partitioned according to the number of vertices, but also according to the number of edges. We could consider for instance the problem of computing the separability index of the class $\mathbb{C}^m$ of connected graphs with m edges. The class $\mathbb{C}^m$ is finite but not homogeneous. Table 4 displays the separability index of $\mathbb{C}^m$ for values of m up to 9.

Table 4: Spectral separability index of $\mathbb{C}^m$

m	1	2	3	4	5	6	7	8	9
$\mathfrak{s}(\mathbb{C}^m)$	1	1	1	2	2	2	2	3	3

Connected graphs can be partitioned according to even more sophisticated criteria, for instance, a combination of order and cyclomatic number. By definition, the cyclomatic number of a connected graph G is the nonnegative integer $e(G) - |G| + 1$, where $e(G)$ is the number of edges. A k-cyclic graph is a connected graph whose cyclomatic number is equal to k. Table 5 displays the separability index of the class $\mathbb{C}_n^k$ of k-cyclic graphs of order n. Note that $\mathbb{C}_n^0 = \mathbb{T}_n$ and $\mathbb{C}_n^1 = \mathbb{U}_n$. The case $\mathbb{C}_n^2$ corresponds to the class of bicyclic graphs of order n, and so on. The parameter k ranges from 0 to $k_n := (n-1)(n-2)/2$.

Table 5 shows that, at least in the considered experimental range, $\mathfrak{s}(\mathbb{C}_n^k)$ is nondecreasing as a function of n. Observe however that $\mathfrak{s}(\mathbb{C}_n^k)$ is rather chaotic as a

Table 5: Spectral separability index of $\mathbb{C}_n^k$

	n=4	n=5	n=6	n=7	n=8	n= 9
k=0	1	1	1	2	2	2
k=1	1	1	1	1	2	3
k=2	1	1	2	2	3	4
k=3	1	1	2	2	3	4
k=4	-	1	2	4	7	10
k=5	-	1	1	3	5	9
k=6	-	-	1	4	7	10
k=7	-	-	1	4	7	12
k=8	-	-	1	3	9	15
k=9	-	-	1	2	8	16
k=10	-	-	1	2	7	15
k=11	-	-	-	1	7	13
k=12	-	-	-	1	6	12

function of k. For instance, the column $n = 8$ gives us no clue about the value of $\mathfrak{s}(\mathbb{C}_8^{13})$. In general, we can only assert that $\mathfrak{s}(\mathbb{C}_n^k)$ goes down to 1 as k approaches k_n. We should be aware that, for a fixed k, the term $\mathfrak{s}(\mathbb{C}_n^k)$ could be highly sensitive with respect to n. Consider for instance the row $k = 8$. Note that $\mathfrak{s}(\mathbb{C}_n^8)$ jumps abruptly when n passes from 7 to 8. Another big jump occurs when n passes from 8 to 9. Presumably, $\mathfrak{s}(\mathbb{C}_n^8)$ will continue increasing at a fast rate as n goes to infinity.

3.1 Cospectral graphs that can be separated with the spectral code

Two graphs with the same characteristic polynomial are said to be cospectral. Pairs of cospectral connected graphs are not hard to find. As explained in Schwenk [11], cospectrality among trees is the rule rather than the exception. Many authors have developed general techniques for constructing cospectral pairs, cf. [6, 7, 8]. What is quite surprising is that cospectrality may occur abundantly even in a narrow class of graphs. For instance, Mowshowitz [8] shows how to construct infinitely many pairs of cospectral double-brooms. Figure 4 displays one of these pairs.

Figure 4: Example of a Mowshowitz's pair of cospectral double-brooms

Preliminary numerical experiments of ours show that complementarity eigenvalues are more efficient as tools for separating connected graphs than classical eigenvalues. Some partial theoretical results corroborate this impression. Let us examine for instance the family of Mowshowitz's pairs of cospectral double-brooms. Metaphorically speaking, a double-broom is a broomstick with bristles on both extremes. At a more formal level, a double broom is a tree obtained by coalescing stars at the end-vertices of a path. More precisely, a double-broom graph $\mathrm{DB}_m(r,s)$ with parameters $m \geq 2$ and $r, s \geq 0$ is a tree obtained by attaching r leaves to one endvertex of a path P_m and s leaves to the other endvertex of the path. When $\min\{r,s\} \leq 1$, the double-broom $\mathrm{DB}_m(r,s)$ degenerates into a broom (with bristles only on one side of the broomstick), which further degenerates into a path if $\max\{r,s\} \leq 1$.

Proposition 1. *For each positive integer k, the double-brooms*

$$A_k := \mathrm{DB}_2\,(3+k, 3+2k) \quad \textit{and} \quad B_k := \mathrm{DB}_3\,(1+k, 4+2k)$$

are cospectral, but they have a different second largest complementarity eigenvalue.

Proof. The cases $k=0$ and $k=1$ can be checked by hand, cf. Table 6, so we work with $k \geq 2$. Note that $|A_k| = |B_k| = 8+3k$. The double-brooms A_k and B_k have the same characteristic polynomial, cf. [8, Theorem 10]. By applying the variational formula (5), we get $\varrho_2(A_k) = \varrho(\tilde{A}_k)$ and $\varrho_2(B_k) = \varrho(\tilde{B}_k)$, where $\tilde{A}_k := \mathrm{DB}_2\,(2+k, 3+2k)$ and $\tilde{B}_k := \mathrm{DB}_3\,(k, 4+2k)$ are the eldest children of A_k and B_k, respectively. We must prove that the spectral radii of $\tilde{A}_k$ and $\tilde{B}_k$ are different. As mentioned in Del Vecchio et al. [4], for all integers $m, r, s \geq 2$, the characteristic polynomial of $\mathrm{DB}_m\,(r,s)$ is given by

$$\varphi(\lambda, \mathrm{DB}_m\,(r,s)) = \lambda^{r+s-2}\left[\lambda^2\varphi(\lambda, P_m) - (r+s)\lambda\varphi(\lambda, P_{m-1}) + rs\,\varphi(\lambda, P_{m-2})\right]$$

with the convention $\varphi(\lambda, P_{m-2}) = 1$ if $m=2$. In particular,

$$\begin{aligned}
\varphi(\lambda, \mathrm{DB}_2\,(r,s)) &= \lambda^{r+s-2}\left[\lambda^4 - (r+s+1)\lambda^2 + rs\right], \\
\varphi(\lambda, \mathrm{DB}_3\,(r,s)) &= \lambda^{r+s-1}\left[\lambda^4 - (r+s+2)\lambda^2 + (r+s+rs)\right].
\end{aligned}$$

The largest roots of these polynomials are

$$\begin{aligned}
\varrho(\mathrm{DB}_2\,(r,s)) &= (1/2)^{1/2}\left[r+s+1+\sqrt{(r+s+1)^2 - 4rs}\right]^{1/2} \\
\varrho(\mathrm{DB}_3\,(r,s)) &= (1/2)^{1/2}\left[r+s+2+\sqrt{(r+s+2)^2 - 4(r+s+rs)}\right]^{1/2},
\end{aligned}$$

respectively. Hence,

$$\begin{aligned}
\varrho(\tilde{A}_k) &= (1/2)^{1/2}\left[6+3k+\sqrt{k^2+8k+12}\right]^{1/2}, \\
\varrho(\tilde{B}_k) &= (1/2)^{1/2}\left[6+3k+\sqrt{k^2+8k+20}\right]^{1/2},
\end{aligned}$$

from where we see that $\varrho(\tilde{A}_k)$ is smaller than $\varrho(\tilde{B}_k)$. $\square$

Remark 1. We could multiply the number of separation results in the same vein as Proposition 1. As shown in Table 2, Γ_{16} suffices to separate all members of $\mathbb{C}_9$, be they cospectral or not. However, much more than 16 complementarity eigenvalues are needed for separating cospectral connected graphs of order 10. In fact, a matter of exhaustive numerical testing shows that Γ_{29} separates all cospectral connected graphs of order 10, but Γ_{28} does not, cf. Figure 5.

Table 6: Γ_2 separates each Mowshowitz's pair A_k, B_k of cospectral double-brooms

k	A_k	B_k	$\varrho(A_k)$, $\varrho(B_k)$	ϱ_2 A_k	ϱ_2 B_k
0	$DB_2(3,3)$	$DB_3(1,4)$	2.302776	2.175328	2.288246
1	$DB_2(4,5)$	$DB_3(2,6)$	2.689994	2.606010	2.681899
2	$DB_2(5,7)$	$DB_3(3,8)$	3.031927	2.971267	3.026925
3	$DB_2(6,9)$	$DB_3(4,10)$	3.340999	3.294556	3.337672
4	$DB_2(7,11)$	$DB_3(5,12)$	3.624921	3.587894	3.622583
5	$DB_2(8,13)$	$DB_3(6,14)$	3.888844	3.858430	3.887129
6	$DB_2(9,15)$	$DB_3(7,16)$	4.136396	4.110837	4.135096

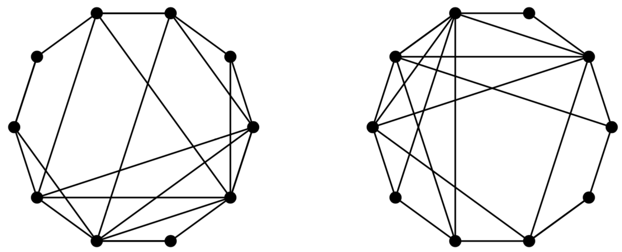

Figure 5: Γ_{28} is unable to separate these cospectral graphs

4 Theoretical results on separability indices

There are many classes of connected graphs that can be separated with the help of the spectral radius alone. Such classes have a separability index equal to 1. Propositionr 2 mentions some illuminating examples, but we shall not indulge in this case. After all, classes with separability index equal to 1 fall into the realm of classical graph spectral theory.

Recall that a lollipop graph is obtained as a graph coalescence of a path and a complete graph. While participating in a graph coalescence, a path is rooted at an endvertex and a complete graph is rooted at any vertex. Paths and complete graphs are particular instances of a lollipop graph: in a sense, they can be viewed as degenerate lollipop graphs. A wheel graph is a graph join of K_1 and a cycle, whereas a ladder graph is a Cartesian product of P_2 and another path of arbitrary order. A triangular (respectively, quadrilateral) book is a connected graph formed with two or more copies of C_3 (respectively, C_4) sharing a common edge. Metaphorically speaking, each cycle is a page of the book and the common edge is the spine or base of the book.

Proposition 2. *The class of starlike trees of order n is an example i of homogeneous class with separability index equal to* 1. *Examples of infinite classes with separability index equal to* 1 *include: the class of paths, the class of complete graphs, the class of stars, the class of wheels, the class of ladders, the class of lollipops, the class of triangular books, and the class of quadrilateral books.*

Proof. A path graph is determined by the number of vertices, which in turn is determined by the spectral radius. The same remark applies to a complete graph, a star, a wheel, and a ladder. Let us examine the case of a lollipop graph. For integers $m \geq 1$ and $q \geq 3$, let $L(m, q)$ be the lollipop graph obtained by coalescing a path P_{m+1} and a complete graph K_q. Such a connected graph has $n = m+q$ vertices. The parameter q corresponds to the clique number of the graph. It is shown in Cioabă and Gregory [2, Lemma 2.4] that

$$q - 1 + \frac{1}{q(q-1)} \, < \, \varrho(L(m, q)) \, < \, q - 1 + \frac{1}{(q-1)^2} \, .$$

From these inequalities, we see that the spectral radius determines the clique number. Once the parameter q has been identified, it is possible to deduce the parameter m because $\varrho(L(\cdot, q))$ is an increasing function. Summarizing, the spectral radius determines (m, q) and this pair of parameters describes the lollipop graph itself. The case of $\mathbb{ST}_n$ is because distinct members of this class have different spectral radii, cf. Oliveira et al. [9]. Let $\mathrm{TB}(p)$ be the triangular book with p pages and $\mathrm{QB}(q)$ be the quadrilateral book with q pages. The spectral radii $\varrho(\mathrm{TB}(p)) = (1/2)(1 + \sqrt{1 + 8p}\,)$ and $\varrho(\mathrm{QB}(q)) = 1 + \sqrt{q}$ are increasing as a function of p and q, respectively. Hence, the spectral radius of a triangular (respectively, quadrilateral) book determines the number of pages and, a posteriori, the triangular (respectively, quadrilateral) book itself. □

Let $\mathbb{CB}$ be the class of complete bipartite graphs. This class is infinite because we are not bounding the number of vertices.

Proposition 3. *$\mathbb{CB}$ has separability index equal to* 2.

Proof. Let $K_{p,q}$ be the complete bipartite graph with parameters p and q. Without loss of generality, we may assume that $1 \leq p \leq q$. Clearly, $\varrho(K_{p,q}) = \sqrt{pq}$ and $\varrho_2(K_{p,q}) = \sqrt{p(q-1)}$. Since $K_{2,6}$ and $K_{3,4}$ have the same spectral radius, we know that $\mathfrak{s}(\mathbb{CB}) \geq 2$. Let $K_{p,q}$ and $K_{r,s}$ be complete bipartite graphs with $1 \leq p \leq q$ and $1 \leq r \leq s$. Suppose that $\Gamma_2(K_{p,q}) = \Gamma_2(K_{r,s})$. In such a case, $pq = rs$ and $p(q-1) = r(s-1)$. This yields $(p, q) = (r, s)$. □

It is worthwhile noticing that the spectral radius function $\varrho : \mathcal{C} \to \mathbb{R}$ is constant on various subsets of $\mathcal{C}$. In such a situation, it is the second largest complementarity eigenvalue function ϱ_2 that plays the leading role in the task of discriminating connected graphs. By way of example, ϱ is constant on the class of sunlet graphs. Recall that a sunlet graph is obtained by attaching a pendant vertex to each vertex of a cycle. If the cycle under consideration is of order r, then the associated sunlet is a connected graph of order $2r$. The next result is advanced as a conjecture.

Conjecture 1. *The infinite class of sunlet graphs has separability index equal to* 2.

We present below an argument in favour of this conjecture. Let M_r be the sunlet whose underlying cycle has r vertices. Determining a sunlet is a matter of identifying the parameter r. The spectral radius function provides no information on this parameter, because $\varrho(M_r) = 1 + \sqrt{2}$ for all $r \geq 3$. We examine then the function

$$r \in \{3, 4, \ldots\} \mapsto g(r) := \varrho_2(M_r) = \varrho(\widetilde{M}_r),$$

where $\widetilde{M}_r$ is the unique child of M_r. Uniqueness of the child of M_r is obvious: the induced subgraph $\widetilde{M}_r$ is obtained by removing any of the r pendant vertices of M_r. Proving Conjecture 1 amounts to checking that g is injective. The adjacency matrix of $\widetilde{M}_r$ is obtained by dropping the last row and last column of

$$A_{M_r} = \begin{bmatrix} A_{C_r} & I_r \\ I_r & 0 \end{bmatrix},$$

where I_r is the identity matrix of order r and A_{C_r} is the adjacency matrix of the cycle C_r. The numerical evaluation of $g(r)$ offers no difficulty when r remains in a reasonable range. If g were strictly increasing, as is suggested by Figure 6, then Conjecture 1 would be true.

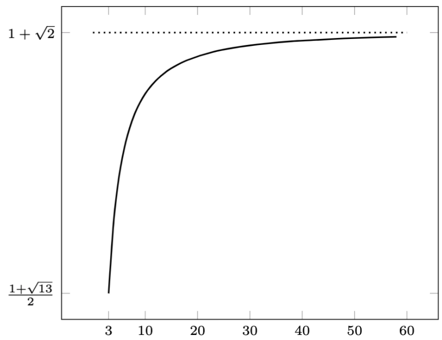

Figure 6: Behavior of $\varrho_2(M_r)$ as a function of r

Remark 2. Let $k \geq 3$ be an integer. The function ϱ is constant on the class of k-regular connected graphs. However, it is not true that the first two complementarity eigenvalues suffice to separate an arbitrary pair of k-regular connected graphs. To see this, consider the 4-regular connected graphs G and H shown in Figure 7. Since

$$(\varrho(G), \varrho_2(G)) = (\varrho(H), \varrho_2(H)) = (4.000000, 3.503224),$$

we need to call the function ϱ_3 to separate these graphs. Hence, the separability index of the class of 4-regular connected graphs is at least 3.

The proposition below concerns the separability index of a special class of trees, namely, trees of diameter 3.

Proposition 4. *Trees of diameter* 3 *form an infinite class with separability index equal to* 2.

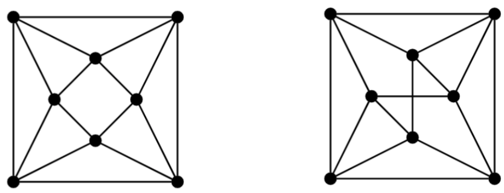

Figure 7: Pair of 4-regular graphs sharing the two largest complementarity eigenvalues

Proof. Let $\mathbb{T}^3$ be the class of trees of diameter 3. The members of $\mathbb{T}^3$ are trees of the form $T(r,s)$, where the parameters r and s are integers such that $s \geq r \geq 1$. By definition, $T(r,s)$ is constructed by attaching r pendant vertices to one endvertex of P_2 and s pendant vertices to the other endvertex of P_2. Hence, $T(r,s)$ has $r+s+2$ vertices in all. The spectral radius of $T(r,s)$ is given by

$$\varrho(T(r,s)) \;=\; \left[\frac{r+s+1+\sqrt{(r+s+1)^2-4sr}}{2}\right]^{1/2}.$$

Since $T(6,10)$ and $T(8,9)$ have the same spectral radius, it follows that $\mathfrak{s}(\mathbb{T}^3) \geq 2$. The second largest complementarity eigenvalue of $T(r,s)$ also has an explicit formula, namely,

$$\varrho_2(T(r,s)) \;=\; \varrho(T(r-1,s)) \;=\; \left[\frac{r+s+\sqrt{(r+s)^2-4s(r-1)}}{2}\right]^{1/2}.$$

Let G be a tree of diameter 3 and suppose that $a := \varrho(G)$ and $b := \varrho_2(G)$ are known. With this information at hand, it is possible to identify the parameters r and s that describe G. Indeed, we claim that the system

$$\begin{aligned} r+s+1+\sqrt{(r+s+1)^2-4rs} \;&=\; 2a^2\,, \\ r+s+\sqrt{(r+s)^2-4s(r-1)} \;&=\; 2b^2 \end{aligned}$$

has a unique solution (r,s) such that $s \geq r \geq 1$. For proving this claim, we square in

$$\begin{aligned} \sqrt{(r+s+1)^2-4rs} \;&=\; 2a^2-(r+s+1)\,, \\ \sqrt{(r+s)^2-4s(r-1)} \;&=\; 2b^2-(r+s) \end{aligned}$$

and, after simplification, we get

$$s = b^2 + \frac{b^2}{r-1-b^2}\,, \quad s = a^2 + \frac{a^2}{r-a^2}\,.$$

The above equations describe a pair of hyperbolas intersecting at a unique point in the region $s \geq r \geq 1$. The r-component of this point is equal to the smallest root of the quadratic equation

$$b^2 + \frac{b^2}{r-1-b^2} \;=\; a^2 + \frac{a^2}{r-a^2}\,.$$

The s-component is derived afterwards by substituting the obtained value of r into either of the two hyperbolas. □

As reported in Tables 2 to 5, separability index equal to 3 is obtained for instance with the homogeneous classes

$$\begin{cases} \mathbb{C}_7^8,\ \mathbb{C}_8^2,\ \mathbb{C}_8^3,\ \mathbb{U}_9, \\ \mathbb{R}_8,\ \mathbb{R}_9,\ \mathbb{BP}_7,\ \mathbb{BP}_8,\ \mathbb{BP}_9, \\ \mathbb{T}_{11},\ \mathbb{T}_{12},\ \mathbb{T}_{13},\ \mathbb{T}_{14}, \end{cases}$$

and the finite nonhomogeneous classes

$$\begin{cases} \mathbb{C}^8,\ \mathbb{C}^9,\ \mathbb{C}(1,6),\ \mathbb{U}(3,9), \\ \mathbb{R}(1,8),\ \mathbb{R}(1,9),\ \mathbb{BP}(2,6),\ \mathbb{BP}(2,7),\ \mathbb{BP}(2,8), \\ \mathbb{T}(1,8),\ \mathbb{T}(1,9),\ \mathbb{T}(1,10),\ \mathbb{T}(1,11). \end{cases}$$

The next proposition presents two infinite classes with separability index equal to 3. The first class is denoted by $\mathbb{E}$ and it is formed with all elementary graphs. An elementary graph is understood as a graph of any order that is either a path, a cycle, a star or a complete graph. The second class is denoted by $\mathbb{SL}$ and it is formed with all Smith-like graphs. By definition, a Smith-like graph is a connected graph whose spectral radius is less than or equal to 2.

Table 7: The three largest complementarity eigenvalues of each Smith-like graph

G	$\lvert G\rvert$	$\varrho(G)$	$\varrho_2(G)$	$\varrho_3(G)$
P_1	1	0	0	0
P_2	2	1	0	0
P_n	$n \geq 3$	$2\cos(\pi/(n+1))$	$2\cos(\pi/n)$	$2\cos(\pi/(n-1))$
S_4	4	$2\cos(\pi/6)$	$2\cos(\pi/4)$	1
Y_n	$n \geq 5$	$2\cos(\pi/(2n-2))$	$2\cos(\pi/(2n-4))$	$2\cos(\pi/(2n-6))$
$S(2,2,1)$	6	$2\cos(\pi/12)$	$2\cos(\pi/8)$	$2\cos(\pi/6)$
$S(3,2,1)$	7	$2\cos(\pi/18)$	$2\cos(\pi/12)$	$2\cos(\pi/10)$
$S(4,2,1)$	8	$2\cos(\pi/30)$	$2\cos(\pi/18)$	$2\cos(\pi/12)$
$S(2,2,2)$	7	2	$2\cos(\pi/12)$	$2\cos(\pi/8)$
$S(3,3,1)$	8	2	$2\cos(\pi/18)$	$2\cos(\pi/12)$
$S(5,2,1)$	9	2	$2\cos(\pi/30)$	$2\cos(\pi/18)$
S_5	5	2	$2\cos(\pi/6)$	$2\cos(\pi/4)$
C_n	$n \geq 3$	2	$2\cos(\pi/n)$	$2\cos(\pi/(n-1))$
H_n	$n \geq 6$	2	$2\cos(\pi/(2n-4))$	$2\cos(\pi/(2n-6))$

Proposition 5. *Examples of infinite classes with separability index equal to* 3 *include* $\mathbb{E}$ *and* $\mathbb{SL}$.

Proof. Since S_5 and C_6 are such that $\varrho(S_5) = \varrho(C_6) = 2$ and $\varrho_2(S_5) = \varrho_2(C_6) = \sqrt{3}$, we know already that $\mathfrak{s}(\mathbb{E}) \geq 3$. In fact, $\{S_5, C_6\}$ is the only pair of elementary graphs that cannot be separated with the help of Γ_2. For showing that Γ_3 separates

$\mathbb{E}$, we simply observe that

$$\begin{aligned}
\Gamma_3(K_n) &= (n-1,\, n-2,\, n-3) \\
\Gamma_3(S_n) &= \left(\sqrt{n-1},\, \sqrt{n-2},\, \sqrt{n-3}\right) \\
\Gamma_3(P_n) &= (2\cos(\pi/(n+1)),\, 2\cos(\pi/n),\, 2\cos(\pi/(n-1))) \\
\Gamma_3(C_n) &= (2,\, 2\cos(\pi/n),\, 2\cos(\pi/(n-1))).
\end{aligned}$$

Note that $\varrho_3(S_5) = \sqrt{2}$ is different from $\varrho_3(C_6) = 2\cos(\pi/5)$. Consider now the class $\mathbb{SL}$. All the Smith-like graphs are listed in [1, Theorem 3.1.3]. Since S_5 and C_6 are Smith-like graphs, we know already that $\mathfrak{s}(\mathbb{SL}) \geq 3$. Besides $\{S_5, C_6\}$, there are other pairs of Smith-like graphs that cannot be separated with the help of Γ_2. The complete list of "unseparable" pairs is

$$\{S_5, C_6\},\ \{H_n, C_{2n-4}\},\ n \geq 6,$$

where H_n is the tree of order n obtained by joining with a path the central vertices of two copies of S_3. Table 7 shows $\varrho(G)$, $\varrho_2(G)$, and $\varrho_3(G)$, for each Smith-like graph G. The notation $S(n_1, n_2, n_3)$ stands for the T-shape tree with parameters $n_1 \geq n_2 \geq n_3 \geq 1$. For each $n \geq 5$, $Y_n := S(n-3, 1, 1)$ is called the snake graph of order n. Table 7 shows that $\Gamma_3(G) \neq \Gamma_3(H)$ if G and H are distinct Smith-like graphs. Note that, for all $n \geq 6$, the third largest complementarity eigenvalues

$$\begin{aligned}
\varrho_3(H_n) &= 2\cos(\pi/(2n-6)) \\
\varrho_3(C_{2n-4}) &= 2\cos(\pi/(2n-5))
\end{aligned}$$

are different. In conclusion, $\mathfrak{s}(\mathbb{SL}) = 3$. □

Acknowledgements

The authors would like to thank Vilmar Trevisan (UFRGS, Porto Alegre) for useful discussions on the subject of this work.

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(Received 18 Mar 2022; revised 16 June 2022)