Applications of Estrada Indices and Energy to a family of compound graphs

Enide Andrade∗

CIDMA-Center for Research and Development in Mathematics and Applications
Departamento de Matemática, Universidade de Aveiro, 3810-193, Aveiro, Portugal.

Pamela Pizarro, María Robbiano, B. San Martín and Katherine Tapia
Departamento de Matemáticas, Facultad de Ciencias. Universidad Católica del Norte.
Av. Angamos 0610 Antofagasta, Chile.

Abstract

To track the gradual change of the adjacency matrix of a simple graph $G$ into the signless Laplacian matrix, V. Nikiforov in [36] suggested the study of the convex linear combination $A_\alpha$ ($\alpha$-adjacency matrix),

$$A_\alpha (G) = \alpha D (G) + (1 - \alpha) A (G),$$

for $\alpha \in [0,1]$, where $A(G)$ and $D(G)$ are the adjacency and the diagonal vertex degrees matrices of $G$, respectively. Taking this definition as an idea the next matrix was considered for $a, b \in \mathbb{R}$. The matrix $A_{a,b}$ defined by

$$A_{a,b} (G) = a D (G) + b A (G),$$

extends the previous $\alpha$-adjacency matrix. This matrix is designated the $(a,b)$-adjacency matrix of $G$. Both adjacency matrices are examples of universal matrices already studied by W. Haemers. In this paper, we study the $(a,b)$-adjacency spectra for a family of compound graphs formed by disjoint balanced trees whose roots are identified to the vertices of a given graph.

∗Corresponding author

Email addresses: enide@ua.pt (Enide Andrade),
pizarro01@ucn.cl,mrobbiano@ucn.cl,sanmarti@ucn.cl,ktapia@ucn.cl (Pamela Pizarro, María Robbiano, B. San Martín and Katherine Tapia)
In consequence, new families of cospectral (adjacency, Laplacian and signless Laplacian) graphs, new hypoenergetic graphs (graphs whose energy is less than its vertex number) and new explicit formulae for Estrada, signless Laplacian Estrada and Laplacian Estrada indices of graphs were obtained. Moreover, sharp upper bounds of the above indices for caterpillars, in terms of length of the path and of the maximum number of its pendant vertices, are given.

Keywords:
\(\alpha\)-adjacency matrix, universal matrix, compound graph, Estrada index, signless Laplacian Estrada index, Laplacian Estrada index, hypoenergetic graph, isospectral graph.

2000 MSC: 05C50, 05C05, 15A18

1. Introduction

In this work we deal with undirected simple graphs herein called graphs. Before we present some motivation to our problem it is introduced some usual notation in graph theory. Given a graph \(\mathcal{G}\), we write \(V(\mathcal{G})\) and \(E(\mathcal{G})\) for the sets of vertices and edges of \(\mathcal{G}\), respectively. An edge with end vertices \(v_i\) and \(v_j\) is denoted by \(v_i v_j\) and we say that the vertices \(v_i\) and \(v_j\) are adjacent or neighbors. Sometimes, after a labeling of the vertices of \(\mathcal{G}\), a vertex \(v_i\) is simply identified by its label \(i\) and an edge \(v_i v_j\) can be simply written as \(ij\). The cardinality of the set of neighbors of \(v_i\), \(N_G(v_i)\), is \(d(v_i)\) or simply \(d_i\), and it is the degree of \(v_i\). The following matricial notation will be used. The all zeros matrix and the identity matrix of appropriated orders are denoted by 0 and \(I\), respectively. If the order is specified, one writes \(I_\ell\) for the identity matrix of order \(\ell\). The all one matrix of order \(n\) is denoted by \(J_n\). Moreover, if \(M\) is a square matrix we use \(|M|\) or \(\det(M)\) to denote the determinant of \(M\) and \(M^T\) for its transpose. We will denote the adjacency matrix and the diagonal matrix of vertex degrees of a graph \(\mathcal{G}\) by \(A(\mathcal{G})\) and \(D(\mathcal{G})\), respectively. The Laplacian matrix and the signless Laplacian matrix of \(\mathcal{G}\) are given by

\[
L(\mathcal{G}) = D(\mathcal{G}) - A(\mathcal{G})
\]

and

\[
Q(\mathcal{G}) = D(\mathcal{G}) + A(\mathcal{G}),
\]

respectively.
Since the matrices $A(G)$, $L(G)$ and $Q(G)$ are real and symmetric, it follows that all of them have real spectrum. Moreover, their spectra are independent of the labeling of the vertices of $G$, as two distinct labeling of the vertices of $G$ yields similar matrices to $A(G)$, $L(G)$ and $Q(G)$, respectively. Some results related with the adjacency matrix and its spectra can be found for instance in [3, 4, 10, 11, 13]. Results related with properties of the Laplacian matrix are well known, see [25, 33, 34, 35] and the references therein. Also, applications of the Laplacian spectrum to Chemistry can be found in [41].

Another interesting result is that the spectra of $L(G)$ and $Q(G)$ coincide if and only if $G$ is a bipartite graph, see [12, 24, 25].

The spectrum of the adjacency matrix of a graph $G$ is called the spectrum of $G$ and it is denoted by $\sigma(G)$. The eigenvalues of $A(G)$ are the eigenvalues of the graph $G$. Throughout the paper, $\lambda_1 \geq \cdots \geq \lambda_n$, $q_1 \geq \cdots \geq q_n$ and $\mu_1 \geq \cdots \geq \mu_n$ will denote the adjacency, the signless Laplacian, and the Laplacian eigenvalues of a graph $G$.

If $G$ is connected, $A(G)$, $L(G)$ and $Q(G)$ are irreducible. Our motivation comes from [36], where the author studies hybrids of $A(G)$ and $D(G)$ similarly to the definition of signless Laplacian matrix put forward by Cvetković [8]. The research related with this matrix shows that it is an interesting matrix and, although $Q(G)$ is simply the sum of $A(G)$ and $D(G)$, the study of $Q(G)$ put forward some similarities and differences between the two matrices. In order to understand to what extent each of the summands $A(G)$ and $D(G)$ determine the properties of $Q(G)$ the author in [36] introduced the convex linear combinations of the previous two matrices defined by

$$A_\alpha(G) = \alpha D(G) + (1 - \alpha) A(G), \quad (1)$$

for $\alpha \in [0,1]$. Clearly $A(G) = A_0(G)$, $Q(G) = 2A_{\frac{1}{2}}(G)$ and $D(G) = A_1(G)$, and the author in [36] estimates that the matrices $A_\alpha(G)$ can support a unified theory of $A(G)$ and $Q(G)$. In this context, these matrices can be seen in a new perspective and some problems can arise. In [29] the universal adjacency matrices of a graph with $n$ vertices are defined as:

$$U = U_G(\alpha, \beta, \gamma, \delta) = \alpha A(G) + \beta I_n + \gamma J_n + \delta D(G),$$

where $\alpha, \beta, \gamma, \delta \in \mathbb{R}$ and $\alpha \neq 0$. Moreover, in [15] the generalized adjacency matrix of a graph $G$ with $n$ vertices were defined as:

$$A(\alpha, \beta, \gamma) = \alpha A(G) + \beta I_n + \gamma J_n,$$
where $\alpha, \beta, \gamma \in \mathbb{R}$ and $\alpha \neq 0$ and it corresponds to the case $\delta = 0$ in the definition of universal adjacency matrix in [29]. Therefore, it is worth to recall (and also recalled in [36]) that this family of matrices is a small subset of the generalized adjacency matrices defined in [15], and the universal adjacency matrices defined in [29]. However, results that can fail in a more general class of matrices can be proven from the definition of $A_\alpha (G)$, although the definition of these matrices is more restricted than the others.

New results concerning $A_\alpha$ matrices of Bethe trees and generalized Bethe trees can be found in [37]. Moreover, in [37], for a tree with maximal degree, an upper bound for its spectral radius was found implying previous bounds determined by Godsil, Lovász, and Stevanović. Some bounds for the spectral radius of $A_\alpha$ for general graphs were also deduced.

Attending to the definition of $A_\alpha (G)$ and as $\alpha \in [0, 1]$, we consider an immediate extension for the $A_\alpha$ matrices that is the following linear combination.

For $a, b \in \mathbb{R}$, 
\[ A_{a,b} (G) = aD (G) + bA (G). \] (2)

**Remark 1.** The following simple facts follow directly from the definition of $A_{a,b}$.

1. $A_{a,b} (G) = U (G)(a, 0, 0, b);$  
2. $A_{0,1} (G) = A (G);$  
3. $A_{1,1} (G) = Q (G);$  
4. $A_{1,-1} (G) = L (G);$  
5. For $\alpha \in [0, 1]$ , $A_{\alpha,1-\alpha} (G) = A_\alpha (G).$

Then, the matrix under consideration is a linear combination of the adjacency matrix and the diagonal matrix of vertex degrees, which covers the usual adjacency, Laplacian and signless Laplacian spectra at once. We introduce here the following specific definition.

**Definition 2.** Let $G_1$ and $G_2$ be two graphs with disjoint vertex sets, where $|V(G_1)| = n_1$ and $|V(G_2)| = n_2$. Let $u \in V(G_1)$ and $v \in V(G_2)$. The graph $G_1 \circ G_2$ is obtained by identifying the vertices $u$ and $v$. The graph $G = G_1 \circ G_2$ is known as the *coalescence* of $G_1$ and $G_2$ with respect to $u$ and $v$. Clearly, $G_1 \circ G_2$ has $n_1 + n_2 - 1$ vertices.
Let $\mathcal{H}_r$ be a connected graph with $r$ vertices and let $\mathcal{T} = \{\mathcal{B}_i\}_{i=1}^r$ be a family of generalized Bethe trees. In [39], the authors gave a complete characterization of the spectrum of the weighted Laplacian matrix of the graphs $\mathcal{H}_r(\mathcal{T})$ obtained by the coalescence of the root vertex of $\mathcal{B}_i \in \mathcal{T}$ and the vertex $v_i \in V(\mathcal{H}_r)$, for $i = 1, \ldots, r$.

In what follows we list the results of the paper that characterize the $(a, b)$-adjacency spectra of the described graphs, present new families of cospectral (adjacency, Laplacian and signless Laplacian) graphs and new hypoenergetic graphs (graphs whose energy is less than its vertex number). The results are Theorem 3, Theorem 5 and Theorem 7.

**Theorem 3.** Let $\mathcal{H}_r$ be a connected graph with $r$ vertices. Let $\mathcal{T} = \{S_i\}_{i=1}^r$ be a family of stars with $(a, b)$-eigenvalues $\{\alpha_i\}_{i=1}^r$. For $i = 1, \ldots, r$, suppose that $S_i$ has $k+1$ vertices, with $k \geq 1$. Then $\mathcal{H}_r(\mathcal{T})$ has the following $(a, b)$-eigenvalues:

1. $\alpha_i$ with multiplicity $r(k-1)$;
2. For $i = 1, 2, \ldots, r$ the remaining eigenvalues are:

$$
\frac{\alpha_i + a(k + 1) + \sqrt{a^2(k - 1)^2 + 2k a \alpha_i + 4b^2 - 2a \alpha_i + \alpha_i^2}}{2},
$$

$$
\frac{\alpha_i + a(k + 1) - \sqrt{a^2(k - 1)^2 + 2k a \alpha_i + 4b^2 - 2a \alpha_i + \alpha_i^2}}{2}.
$$

In a natural way the next definition can be stated.

**Definition 4.** Let $a, b \in \mathbb{R}$. The graphs $\mathcal{H}_r$ and $\mathcal{J}_r$ are two $(a, b)$-isospectral graphs if the spectrum of the $(a, b)$-adjacency matrices coincide.

The next theorem follows directly from Theorem 3.

**Theorem 5.** Let $\mathcal{H}_r$ and $\mathcal{J}_r$ be two $(a, b)$-isospectral graphs with $r$ vertices. Let $\mathcal{T} = \{S_i\}_{i=1}^r$ be a family of stars. For $i = 1, \ldots, r$, suppose that $S_i$ has $k + 1$ vertices, with $k \geq 1$. Then the graphs $\mathcal{H}_r(\mathcal{T})$ and $\mathcal{J}_r(\mathcal{T})$ are also $(a, b)$-isospectral graphs.

The energy of a graph $\mathcal{G}$, $\epsilon(\mathcal{G})$, is the sum of the absolute values of the eigenvalues of $\mathcal{G}$. The motivation for the introduction of this graph invariant
comes from Chemistry where results on the energy were obtained already in 1940’s (in a more-or-less implicit way) (see for instance, [7, 26, 30]) but it was I. Gutman who in the 1970’s consider the previous description as a definition noticing that all the results until then related with the chemical concept total $\pi$ electron energy (see [27, 32] for more detailed reading) pertain to the previous quantity. In the chemical literature it has been noticed that for the vast majority of molecular graphs (connected graphs in which there are no vertices of degree greater than three) the energy exceeds the number of vertices. In 1973 England and Ruedenberg published a paper [16] where they posed the following question-Why does the graph energy exceeds the number of vertices? Therefore it made sense to construct the next definition.

**Definition 6.** [27, 32] A graph $G$ with $n$ vertices is called **hypoenergetic** if the sum of the absolute values of its eigenvalues is less than $n$.

For a survey on hypoenergetic graphs the readers should refer to [27]. In this paper by using Theorem 3 we prove the following.

**Theorem 7.** Let $\mathcal{H}_n$ be an hypoenergetic graph with eigenvalues $\{\lambda_i\}_{i=1}^n$. Let $\mathcal{T} = \{E_i\}_{i=1}^n$ be a family of stars. For $i = 1, \ldots, n$, suppose that $E_i = S_{k+1}$ with $k \geq 4$. Then $\mathcal{H}_n(\mathcal{T})$ is hypoenergetic.

Ernesto Estrada in [22] introduced a molecular descriptor known as Estrada Index. This concept, associated to the eigenvalues of a graph $G$, is presented below.

**Definition 8.** [22] The Estrada Index of a graph $G$ with $n$ vertices is defined as

$$EE(G) = \sum_{\lambda \in \sigma(G)} \exp \lambda.$$ 

This graph invariant is used in many areas. Concerning weighted graphs, Estrada Index can be used in molecular structures, [17, 18, 22]. For graphs without weights the reader should refer to [19, 20] where the authors present a measure of centrality and bipartivity of certain networks such as the metabolism, social communities, individual proteins and trophic interactions in food networks. A relation between the Estrada Index and an atomic branch can be seen in [21].

For a graph $G$ with $n$ vertices, the Laplacian Estrada Index and the signless Laplacian Estrada Index were defined in a natural way as the following:
Definition 9. [2, 31, 42, 43] For a graph $G$ with $n$ vertices the Laplacian Estrada Index and the signless Laplacian Estrada Index are respectively:

1. $\text{LEE}(G) = \sum_{i=1}^{n} \exp \mu_i$
2. $\text{SLEE}(G) = \sum_{i=1}^{n} \exp q_i$.

We list here the main results related to the above indices, that are Theorem 10, Corollaries 11 and 12 and Theorems 13 and 14.

Theorem 10. Let $\mathcal{H}_n$ be a graph whose eigenvalues are $\{\lambda_i\}_{i=1}^{n}$. Let $\mathcal{T} = \{E_i\}_{i=1}^{n}$ be a family of stars, such that, $E_i = S_{k+1}$, for $i = 1, \ldots, n$. Then

$$EE(\mathcal{H}_n(\mathcal{T})) = n(k-1) + \sum_{i=1}^{n} 2 \exp \frac{\lambda_i}{2} \cosh \frac{\sqrt{\lambda_i^2 + 4k}}{2}$$

Corollary 11. Let $\mathcal{H}_n$ be a graph with $n$ vertices and $\{q_i\}_{i=1}^{n}$ be its signless Laplacian eigenvalues. Let $\mathcal{T} = \{E_i\}_{i=1}^{n}$ be a family of stars, such that, $E_i = S_{k+1}$, for $i = 1, \ldots, n$. Then,

$$\text{SLEE}(\mathcal{H}_n(\mathcal{T})) = \exp(1)n(k-1) + \sum_{i=1}^{n} 2 \exp \frac{q_i + k + 1}{2} \times \Psi_1,$$

where

$$\Psi_1 = \cosh \frac{\sqrt{(q_i - 1)^2 + k^2 + 2k(1+q_i)}}{2}.$$

Corollary 12. Let $\mathcal{H}_n$ be a graph with $n$ vertices and $\{\mu_i\}_{i=1}^{n}$ be its Laplacian eigenvalues. Let $\mathcal{T} = \{E_i\}_{i=1}^{n}$ be a family of stars, such that, $E_i = S_{k+1}$, for $i = 1, \ldots, n$. Then

$$\text{LEE}(\mathcal{H}_n(\mathcal{T})) = \exp(1)n(k-1) + \sum_{i=1}^{n} 2 \exp \frac{\mu_i + k + 1}{2} \cosh \frac{\sqrt{(\mu_i - 1)^2 + k^2 + 2k(1+\mu_i)}}{2}.$$

Applications of these results are listed below.
Theorem 13. Let $G$ be a graph of order $n \geq 4$ with the minimum vertex degree one and the maximum vertex degree at least two.

Let $H$ be the subgraph of $G$ induced by the set

$$\{v \in V(G) : d(v) \geq 2\}. \quad (3)$$

Looking at the pendant vertices, let us consider all the stars coalescence to $H$ with respect to their central vertex and the vertices of $H$, and choose some with maximum number of pendant vertices, say $k$. If $H$ has $r$ vertices, then

$$EE(G) \leq r(k - 1) + \sum_{i=1}^{r} 2 \exp \frac{\lambda_i}{2} \cosh \frac{\sqrt{\lambda_i^2 + 4k}}{2},$$

where $\lambda_i := \lambda_i(H)$, is the $i$-th eigenvalue of $H$. In particular, if the maximum above is $k = 1$, it is obtained

$$EE(G) \leq \sum_{i=1}^{r} 2 \exp \frac{\lambda_i}{2} \cosh \frac{\sqrt{\lambda_i^2 + 4}}{2}.$$

Theorem 14. Let $G$ be a graph of order $n \geq 4$ with the minimum vertex degree one and the maximum vertex degree at least two. Let $H$ be the subgraph of $G$ induced by the set in (3). Moreover, let $v_0 \in V(H)$ be a vertex with maximum number, called $k$, of pendant neighbors. Let $\{\mu_i\}_{i=1}^{r}$ (resp. $\{q_i\}_{i=1}^{r}$) be the Laplacian (resp. signless Laplacian) eigenvalues of $H$. Then

$$LEE(G) \leq \exp(1)r(k - 1) + \sum_{i=1}^{r} 2 \exp \frac{\mu_i + k + 1}{2} \cosh \frac{(\mu_i - 1)^2 + k^2 + 2k(1 + \mu_i)}{2},$$

$$SLEE(G) \leq \exp(1)r(k - 1) + \sum_{i=1}^{r} 2 \exp \frac{q_i + k + 1}{2} \cosh \frac{(q_i - 1)^2 + k^2 + 2k(1 + q_i)}{2}.$$

In both cases equality holds if and only if $G = H(\mathcal{T})$, where $\mathcal{T} = \{E_i\}_{i=1}^{n}$ is a family of stars, such that, $E_i = S_{k+1}$, for $i = 1, \ldots, n$. In particular, for $k = 1$, it is obtained

$$LEE(G) \leq \sum_{i=1}^{r} 2 \exp \frac{\mu_i + 2}{2} \cosh \frac{\sqrt{\mu_i^2 + 4}}{2},$$
and
\[ SLEE(G) \leq \sum_{i=1}^{r} 2 \exp \frac{q_i + 2}{2} \cosh \frac{\sqrt{q_i^2 + 4}}{2}, \]
respectively.

Some more concepts used throughout the paper can be found, for instance in [10]. The paper is organized as follows. The first section introduces some general notation that will be used in the paper. Here, some motivation is referred and the main results are exhibited. At Section 2 the \((a, b)\)-adjacency matrix for a graph using a connected graph \(H_r(T)\) with \(r\) vertices and a family \(T = \{\mathcal{B}_i\}_{i=1}^{r}\) of \(r\) stars coalescing with respect to the root vertex of \(\mathcal{B}_i\) and the vertex \(v_i \in V(H_r(T))\) is exhibited. At Section 3, the characteristic polynomial of the \((a, b)\)-adjacency matrix is obtained. At Section 4 its eigenvalues are characterized and the proofs of the theorems 3, 7, 10, and corollaries 11, 12 are given. At Section 5 the proofs of the theorems 13 and 14 are presented. Moreover, we apply to a path with a certain number of vertices the obtained formulas for Estrada and Laplacian Estrada Indices and sharp upper bounds of the above indices for caterpillars in terms of length of the path and of the maximum number of its pendant vertices are presented.

2. Balanced Trees

In this section we assume that \(G\) is a graph with a root vertex. We say that a vertex \(v \in V(G)\) is at level \(j + 1\) if its distance to the root vertex is \(j\). An edge is at level \(j\) if it is connecting a vertex at level \(j\) to other one at level \(j + 1\). A generalized Bethe tree is a rooted tree where vertices at the same level have the same degree. A star graph is a generalized Bethe tree with two levels. In [40], the authors gave a complete characterization of the spectra of the Laplacian and adjacency matrices of these weighted trees. Some further developments can be found for instance in [5, 6, 23, 38]. Unlike the previous results already obtained on this type of graphs, a more general context of families of distinct weighted Bethe graphs (constructed using weighted generalized Bethe trees) was considered in [1].

Suppose that \(T = \{\mathcal{B}_i\}_{i=1}^{r}\) is a family of stars. Using results from [1] and [39], explicit eigenvalues for the \((a, b)\)-adjacency matrices are obtained in the next section. Therefore, in order to write the \((a, b)\)-adjacency matrix of this graph we need to introduce some notation and the labeling of its vertices. Let \(H_r\) be a connected graph with vertices \(v_1, v_2, \ldots, v_r\) and \(d_1, \ldots, d_r\), the
corresponding degrees, respectively. Let \( A(H_r) = (\varepsilon_{i,j}) \) be its adjacency matrix. Consider \( \{h_i\}_{i=1}^r \) a sequence of positive integers and the following notation for the family of stars \( \mathcal{T} = \{S_{h_i+1}\}_{i=1}^r \). The following labeling of the vertices of \( H_r(\mathcal{T}) \) (taking into account the labeling of the vertices of \( H_r(\mathcal{T}) \)) is established:

1. For \( i = 1, \ldots, r \), let \( v_{1,i}, \ldots, v_{h_i,i} \) be the labels for the vertices of degree 1 that are adjacent to \( v_i \) in \( H_r(\mathcal{T}) \).
2. Finally, the vertex \( v_i \) in \( V(H_r) \) is labeled as \( v_{h_i+1,i} \).

Therefore, the \((a,b)\)-adjacency matrix of \( H_r(\mathcal{T}) \) takes the form:

\[
A_{a,b}(H_r(\mathcal{T})) = \begin{bmatrix}
A_{a,b}(B_1) + ad_1T_1 & \varepsilon_{1,2}bF_{1,2} & \cdots & \varepsilon_{1,r}bF_{1,r} \\
\varepsilon_{1,2}bF_{1,2}^T & A_{a,b}(B_2) + ad_2T_2 & \cdots & \varepsilon_{2,r}bF_{2,r} \\
\vdots & \vdots & \ddots & \vdots \\
\varepsilon_{1,r}bF_{1,r}^T & \varepsilon_{2,r}bF_{2,r}^T & \cdots & A_{a,b}(B_r) + ad_rT_r
\end{bmatrix}
\]

(4)

where \( T_i \) is the null matrix except for the entry \((h_i + 1, h_i + 1)\) that is equal to 1 and \( A_{a,b}(B_i) \) is the \((a,b)\)-adjacency matrix of \( B_i \) in \( H_r(\mathcal{T}) \). The next theorem plays an important role in this study and its proof can be found in [39].

In what follows denote by \( \tilde{B} \) the submatrix obtained from a matrix \( B \) deleting its last row and column. Let \( F_{i,j} = (\varphi_{rs}) \) be the matrix of order \( n_i \times n_j \) whose entries are zero except for the entry \( \varphi_{n_i,n_j} \) that is equal to 1.

**Theorem 15.** [39] Let \( \{n_i\}_{i=1}^r \) be a sequence of positive integers and \( B_i \) be a square matrix of order \( n_i \) with \( i = 1, 2, \ldots, r \). Let \( \{\mu_{ij}\}_{i,j} \) be a family of \( r \) \((r-1)\) arbitrary scalars and \( \{F_{i,j}\}_{i,j} \) be a family of \( r \) \((r-1)\) matrices, where \( F_{i,j} \) is of order \( n_i \times n_j \) such that the entries \( F_{i,j} \) are all zero except for the entry \( n_i, n_j \), that is equal to 1. Let

\[
M = \begin{bmatrix}
\lambda I - B_1 & -\mu_{1,2}F_{1,2} & \cdots & -\mu_{1,r-1}F_{1,r-1} & -\mu_{1,r}F_{1,r} \\
-\mu_{2,1}F_{2,1}^T & \lambda - B_2 & \cdots & \cdots & \cdots \\
-\mu_{3,1}F_{3,1}^T & -\mu_{3,2}F_{2,2}^T & \cdots & \cdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & B_{r-1} \\
-\mu_{r,1}F_{r,1}^T & -\mu_{r,2}F_{r,2}^T & \cdots & -\mu_{r,r-1}F_{r,r-1} & \lambda - B_r
\end{bmatrix}
\]
Therefore, $\det M$ is the following

$$
\begin{vmatrix}
|\lambda I - B_1| & -\mu_{1,2} |\lambda I - \tilde{B}_2| & \cdots & -\mu_{1,r-1} |\lambda I - \tilde{B}_{r-1}| & -\mu_{1,r} |\lambda I - \tilde{B}_r| \\
-\mu_{2,1} |\lambda I - \tilde{B}_1| & |\lambda I - B_2| & \cdots & \cdots & -\mu_{2,r} |\lambda I - \tilde{B}_r| \\
-\mu_{3,1} |\lambda I - \tilde{B}_1| & -\mu_{3,2} |\lambda I - \tilde{B}_2| & \cdots & \cdots & \cdots \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
-\mu_{r,1} |\lambda I - \tilde{B}_1| & -\mu_{r,2} |\lambda I - \tilde{B}_2| & \cdots & -\mu_{r,r-1} |\lambda I - \tilde{B}_{r-1}| & |\lambda I - B_r| \\
\end{vmatrix}
$$

### 3. Characteristic polynomial of the $(a, b)$-adjacency matrix

In this section we determine the characteristic polynomial of the matrix in (4). The next result follows easily from [4, Lemma 2.3.1].

**Lemma 16.** Let $S_{n+1}$ be a star with $n$ pendant vertices. Its $(a, b)$-characteristic polynomial is given by

$$q(\lambda) = (\lambda^2 - \lambda a (n + 1) + n (a^2 - b^2)) (\lambda - a)^{(n-1)}.$$ 

Let $(A_{a,b})_i$ and $(\tilde{A}_{a,b})_i$ be the matrices $A_{a,b}(B_i)$ and $\tilde{A}_{a,b}(B_i)$, respectively. Moreover, consider the sequence of $\{\lambda_i^{a,b}\}_{i=1}^r$ as the sequence of the $(a, b)$-eigenvalues of $\mathcal{H}_r$.

**Theorem 17.** Let $\mathcal{H}_r$ be a connected graph with $r$ vertices. Let $\mathcal{T} = \{B_i\}_{i=1}^r$ be a family of graphs isomorphic to $S_{k+1}$ stars. Let $\{\lambda_i^{a,b}\}_{i=1}^r$ be the sequence of the $(a, b)$-eigenvalues of $\mathcal{H}_r$. Then, the characteristic polynomial of $A_{a,b}(\mathcal{H}_r(\mathcal{T}))$ is

$$|\lambda I - A_{a,b}(\mathcal{H}_r(\mathcal{T}))| = (\lambda - a)^{(r-1)} \prod_{i=1}^r \left( \lambda^2 - \lambda \left( \lambda_i^{a,b} + (k + 1) a \right) + k (a^2 - b^2) + a \lambda_i^{a,b} \right).$$

**Proof.**

Applying Theorem 15 to the matrix $\lambda I - A_{a,b}(\mathcal{H}_r(\mathcal{T}))$, we obtain

$$p(\lambda) := |\lambda I - A_{a,b}(\mathcal{H}_r(\mathcal{T}))| =$$
where have
where the last equality follows from Lemma 16. Therefore, replacing in (6), we
is obtained, the characteristic polynomial
property for determinants we have,
By simplicity the matrices
Note that in this case the matrices \( F_{i,j} \) are of orders \((k+1) \times (k+1)\).
Thus, as deleting the last row and column of \( \lambda I - (A_{a,b}) \), the matrix \((\lambda - a) I_k\)
is obtained, the characteristic polynomial \( p(\lambda) \) takes the form
\[
\begin{array}{cccc}
|\lambda I_{k+1} - (A_{a,b})| & -\varepsilon_{1,2} b |\lambda I - (\hat{A}_{a,b})_2| & \ldots & -\varepsilon_{1,r} b |\lambda I - (\hat{A}_{a,b})_r| \\
-\varepsilon_{1,2} b |\lambda I - (\hat{A}_{a,b})_1| & |\lambda I - (A_{a,b})_2| & \ldots & -\varepsilon_{2,r} b |\lambda I - (\hat{A}_{a,b})_r| \\
\vdots & \vdots & \ddots & \vdots \\
-\varepsilon_{1,r} b |\lambda I - (\hat{A}_{a,b})_1| & -\varepsilon_{1,2} b |\lambda I - (\hat{A}_{a,b})_2| & \ldots & |\lambda I - (A_{a,b})_r| \\
\end{array}
\]
\((5)\)

By simplicity the matrices \( A_{a,b} (B_i) \) are denoted by \((A_{a,b})\). All the matrices \( T_i \)
(each one of order \(k+1\)) will be simply denoted by \( T \). Therefore, by the multilinear
property for determinants we have,
\[
p(\lambda) = |(\lambda - a) I_k|^r
\]
\[
\begin{array}{cccc}
|\lambda I_{k+1} - (A_{a,b}) - ad_i T| & -\varepsilon_{1,2} b |(\lambda - a) I_k| & \ldots & -\varepsilon_{1,r} b |(\lambda - a) I_k| \\
-\varepsilon_{1,2} b |(\lambda - a) I_k| & |\lambda I_{k+1} - (A_{a,b}) - ad_2 T| & \ldots & -\varepsilon_{2,r} b |(\lambda - a) I_k| \\
\vdots & \vdots & \ddots & \vdots \\
-\varepsilon_{1,r} b & -\varepsilon_{1,2} b & \ldots & |\lambda I_{k+1} - (A_{a,b}) - ad_r T| \\
\end{array}
\]
\((6)\)

Now, note that for \( i \in I \)
\[
|\lambda I_{k+1} - (A_{a,b}) - ad_i T| = |\lambda I_{k+1} - (A_{a,b})| - ad_i |\lambda I_k - (\hat{A}_{a,b})| \\
= |\lambda I_{k+1} - (A_{a,b})| - ad_i (\lambda - a)^k \\
= (\lambda^2 - \lambda a (k+1) + k (a^2 - b^2)) (\lambda - a)^{k-1} - ad_i (\lambda - a)^k,
\]
where the last equality follows from Lemma 16. Therefore, replacing in (6), we
have
\[
p(\lambda) = |(\lambda - a) I_k|^r
\]
\[
\begin{array}{cccc}
\theta_1 & -\varepsilon_{1,2} b & \ldots & -\varepsilon_{1,r} b \\
-\varepsilon_{1,2} b & \theta_2 & \ldots & -\varepsilon_{2,r} b \\
\vdots & \vdots & \ddots & \vdots \\
-\varepsilon_{1,r} b & -\varepsilon_{2,r} b & \ldots & \theta_r \\
\end{array}
\]
where \( \theta_i = \frac{\lambda^2 - \lambda a (k+1) + k (a^2 - b^2) - ad_i (\lambda - a)}{(\lambda - a)}, i = 1, \ldots, r \). Thus \( p(\lambda) \) is equal to

12
\[
(\lambda - a)^k \begin{vmatrix}
\frac{\lambda^2 - \lambda a(k+1) + k(a^2 - b^2)}{(\lambda - a)} & -\varepsilon_1 b & \ldots & -\varepsilon_r b \\
-\varepsilon_1 b & \frac{\lambda^2 - \lambda a(k+1) + k(a^2 - b^2)}{(\lambda - a)} & -\varepsilon_2 b & \ldots & -\varepsilon_r b \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
-\varepsilon_1 b & -\varepsilon_2 b & \ldots & \frac{\lambda^2 - \lambda a(k+1) + k(a^2 - b^2)}{(\lambda - a)} & -\varepsilon_r b
\end{vmatrix} = (\lambda - a)^r \prod_{i=1}^{k-1} \left( \frac{\lambda^2 - \lambda a(k+1) + k(a^2 - b^2)}{(\lambda - a)} \right).
\]

Since
\[
\lambda^2 - \lambda a(k + 1) + k(a^2 - b^2) - (\lambda - a) \lambda_i^{a,b}(H_r)
\]
is equal to
\[
\lambda^2 - \lambda \left( \lambda_i^{a,b}(H_r) + (k + 1) a \right) + k(a^2 - b^2) + a\lambda_i^{a,b}(H_r),
\]
the result follows.

4. Characterization of the eigenvalues of \(H_r(\mathcal{T})\)

In this section we characterize the \((a,b)\)-eigenvalues of the previously described graphs, \(H_r(\mathcal{T})\). In fact, it is possible to obtain in an explicit way the eigenvalues, Laplacian eigenvalues and signless Laplacian eigenvalues in function of those from the original graph. By a direct computation the Theorem 3 can be obtained.

**Proof.** of Theorem 3. This result is a consequence of Theorem 17 and it is a direct computation of the roots of polynomial in the statement.
Proof. of Theorem 7. Notice that $H_n(T)$ has $n(k+1)$ vertices. Recall that if $(a,b) = (0,1)$ then $A_{a,b}(G) = A(G)$, the adjacency matrix of $G$. By Theorem 3, the non zero eigenvalues of $H_n(T)$ become, for $i = 1, \ldots, n$,
\[
\begin{cases}
\lambda_i + \sqrt{\lambda_i^2 + 4k}, \\
\lambda_i - \sqrt{\lambda_i^2 + 4k}
\end{cases}
\]

Then we get
\[
\epsilon(H_n(T)) = \sum_{i=1}^{n} \sqrt{\lambda_i^2 + 4k}
\leq \sum_{i=1}^{n} (|\lambda_i| + 2\sqrt{k})
< (n + 2\sqrt{kn})
= n \left(1 + 2\sqrt{k}\right) \leq (n+1)k
\]
as
\[
2\sqrt{k} \leq k \iff 4k \leq k^2 \iff k \geq 4.
\]
Thus, the result, follows.

Recalling the Definitions 8 and 9 the following results are shown.

Proof. of Theorem 10. In order to obtain the explicit form of the eigenvalues of $A(H_r(T))$, $(a,b) = (0,1)$ is used in Theorem 3. Then, the formula in Theorem 10 is directly obtained from the expression for $EE(H_r(T))$. Finally, the result follows from the definition of $\cosh(x) \left( = \frac{e^x + e^{-x}}{2}\right)$.

Proof. of Corollary 11. In order to obtain the explicit form of the eigenvalues of $Q(H_r(T))$, $(a,b) = (1,1)$ is used in Theorem 3. Then, the formula in Corollary 11 is directly obtained from the expression for $SLEE(H_r(T))$.

Proof. of Corollary 12. In order to obtain the explicit form of the $L(H_n(T))$ we use $(a,b) = (1,-1)$ at Theorem 3. Then, the formula in Corollary 12 is directly obtained from the expression for $LEE(H_n(T))$. 

14
5. An Application

In what follows we apply previous results to a graph \( G \) (with order \( n \geq 4 \)) with the minimum vertex degree one and the maximum vertex degree at least two. The idea is, after performing an operation of coalescence of one vertex of \( K_2 \), a certain number of times (if necessary) with respect to the vertices of an induced subgraph of \( G \) obtained by the set of vertices of \( G \) that have degree greater or equal than 2, to reach to a graph in the form \( H_r (T) \) where \( T \) is a family of stars and apply the results of previous section. Our aim is to give upper bounds for the Estrada Indices of \( G \) in terms of the number of pendant vertices and of the eigenvalues of the induced subgraph by the set of its non pendant vertices.

Proof. of Theorem 13. Consider the function \( \varphi \) defined by:

\[
\varphi : V (H) \longrightarrow N \cup \{0\}, \quad \varphi (v) = \left| \{w \in N_G (v) : d(w) = 1\} \right|
\]

As \( G \) has at least one pendant vertex there exists \( v \in V (H) \) such that \( \varphi (v) \geq 1 \). Let \( \bar{v} \in V (H) \) such that \( k = \varphi (\bar{v}) \geq \varphi (v) \), for all \( v \in V (H) \). We perform in \( G \) the following operation:

Each vertex \( v \in V (H) \setminus \{\bar{v}\} \) is identified by coalescence, more than once if it is necessary, to a vertex of \( K_2 \), in order to obtain \( k \) pendant vertices, neighbors to \( v \). With this operation, it is obtained a new graph \( H_r (T) \) where \( T \) is a family of \( r \) stars all of them isomorphic to \( S_{k+1} \).

Note that \( G \) is an induced subgraph of \( H_r (T) \). Therefore, the Interlacing Theorem, [10] and the increasing of the exponential function implies that

\[
EE (G) \leq EE (H_r (T))
\]

and

\[
EE (H_r (T)) = r (k - 1) + \sum_{i=1}^{r} 2 \exp \left( \frac{\lambda_i (H)}{2} \cosh \frac{\sqrt{\lambda_i (H)^2 + 4k}}{2} \right)
\]

Analogously, the next upper bounds are obtained for \( LEE(G) \) and \( SLEE(G) \).

Proof. of Theorem 14. The same argument proceeds for both cases, in consequence, we consider only the Laplacian case. Let \( G^+ \) be the graph obtained from \( G \) by adding isolated vertices and \( G^{++} \) be the graph obtained
from \( G^+ \) by adding edges between those last isolated vertices and the vertices of the set \( H \), the subgraph of \( G \) induced by the set in (3). It is clear that

\[
LEE(G^+) \geq LEE(G)
\]

and by a similar argument used in [28]

\[
LEE(G^{++}) \geq LEE(G^+)
\]

with equality if and only if \( G^{++} = G^+ \).

The result follows directly from the fact that, in the above arguments, adding pendant vertices to an arbitrary graph its Laplacian Estrada Index strictly increases.

In the paper [14] it was proven that the Estrada Index of the star and the path with \( n \) vertices are the maximum and minimum Estrada Index, respectively for all trees with \( n \) vertices. In consequence, its values, \( 2 \cosh \sqrt{n - 1} \) and \( \sum_{j=1}^{n} \exp(2 \cos \left( \frac{\pi j}{n+1} \right)) \), are upper and lower bounds, respectively, for the Estrada Index of the caterpillar graph with \( n \) vertices. Taking these results from [14] as motivation, in this section explicit formulae for the Estrada Index of some caterpillars, whose values can now be directly compared with the values of \( EE(S_n) \) and \( EE(P_n) \), are obtained. Moreover, the next example yields upper bounds for the Estrada and Laplacian Estrada indices of a caterpillar graph.

**Example 18.** Let \( P_r \) be a path with \( r \) vertices. Let \( \mathcal{T} = \{S_{b_i+1}\}_{i=1}^{r} \) be a family of stars such that, for each \( i = 1, \ldots, r \), \( S_{b_i+1} \) stands for a star with \( b_i + 1 \) vertices where \( b_i \geq 0 \). Let \( k = \max_{1 \leq i \leq r} b_i \). The graph \( P_r(\mathcal{T}) \) is called the caterpillar graph \( C = C(b_1, \ldots, b_r) \). Since the eigenvalues and Laplacian eigenvalues of \( P_r \) are of the form \( 2 \cos \left( \frac{j\pi}{r+1} \right), (j = 1, \ldots, r) \) and \( 2 - 2 \cos \left( \frac{j\pi}{r} \right), (j = 0, \ldots, r - 1) \), respectively (see, for instance [4]), with previous results the following upper bounds are directly obtained:

\[
EE(C) \leq EE(C(k, \ldots, k)) = r(k - 1) + \sum_{j=1}^{r} 2 \exp \cos \left( \frac{\pi j}{r+1} \right) \cosh \sqrt{\cos^2 \left( \frac{\pi j}{r+1} \right) + k} \\
\leq EE(S_{r(k+1)}) = 2 \cosh \sqrt{rk + r - 1}.
\]
and

\[ LEE(C) \leq LEE(C(k, \ldots, k)) \]
\[ = er(k - 1) + \sum_{j=0}^{r-1} 2\Psi_1 \exp \frac{3 - 2 \cos \left( \frac{\pi j}{r} \right) + k}{2}, \]

with

\[ \Psi_1 = \cosh \sqrt{\frac{(1 - 2 \cos \left( \frac{\pi j}{r} \right))^2 + k^2 + 2k(3 - 2 \cos \left( \frac{\pi j}{r} \right))}{2}}, \]

where the last inequality is an equality if and only if \( b_i = k \), for all \( i = 1, \ldots, r \).

In particular, for \( k = 1 \) we obtain

\[ EE(C(1,1,\ldots,1)) = \sum_{j=1}^{r} 2 \exp \cos \left( \frac{\pi j}{r + 1} \right) \cosh \sqrt{\cos^2 \left( \frac{\pi j}{r + 1} \right) + 1} \]
\[ \geq EE(P_{2r}) \]
\[ = \sum_{j=1}^{2r} \exp \left( 2 \cos \left( \frac{\pi j}{2r + 1} \right) \right), \]

and

\[ LEE(C(1, \ldots, 1)) = \sum_{j=0}^{r-1} 2\Psi_2 \exp \frac{3 - 2 \cos \left( \frac{\pi j}{r} \right) + 1}{2} \]

where

\[ \Psi_2 = \cosh \sqrt{\frac{(1 - 2 \cos \left( \frac{\pi j}{r} \right))^2 + 7 - 4 \cos \left( \frac{\pi j}{r} \right)}{2}}. \]

Acknowledgments. E. Andrade was supported in part by the Portuguese Foundation for Science and Technology (FCT-Fundaç~ao para a Ciência e a Tecnologia), through CIDMA - Center for Research and Development in Mathematics and Applications, within project UID/MAT/04106/2013. M. Robbiano was
partially supported by project Proyecto VRIDT UCN16115. P. Pizarro was supported by grant CONICYT-PCHA/Doctorado Nacional/2017-21170312. K. Tapia was supported by grant CONICYT-PCHA/Doctorado Nacional/2016-21160357. The author thank the anonymous referees for their contribution which led to an improvement of the paper.


