

Research Article

## Signed bicyclic graphs with minimal index

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**Abstract:** The index  $\lambda_1(\Gamma)$  of a signed graph  $\Gamma=(G,\sigma)$  is just the largest eigenvalue of its adjacency matrix. For any  $n\geqslant 4$  we identify the signed graphs achieving the minimum index in the class of signed bicyclic graphs with n vertices. Apart from the n=4 case, such graphs are obtained by considering a starlike tree with four branches of suitable length (i.e. four distinct paths joined at their end vertex u) with two additional negative independent edges pairwise joining the four vertices adjacent to u. As a byproduct, all signed bicyclic graphs containing a theta-graph and whose index is less than 2 are detected.

Keywords: Signed Graph, Bicyclic Graph, Index, Extremal Graph Theory

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#### 1. Introduction

A signed graph  $\Gamma = (G, \sigma)$  is a pair  $(G, \sigma)$ , where  $G = (V_G, E_G)$  is a simple graph and  $\sigma \colon E_G \longrightarrow \{+1, -1\}$  is the sign function (or the signature) defined on the edge set of G. The unsigned graph G is called the underlying graph of  $\Gamma$ . The order and the size of  $\Gamma$  are the order and the size of its underlying graph. The sign of a cycle C in  $\Gamma$  is given by  $\operatorname{sign}(C) = \prod_{e \in C} \sigma(e)$ . If all edges in  $\Gamma$  are positive, then  $\Gamma$  is denoted by (G, +). A cycle is called positive (resp., negative) if  $\operatorname{sign}(C)$  is 1 (resp., -1). A signed graph is balanced if no negative cycles exist; otherwise it is unbalanced. The negation  $-\Gamma$  is obtained by reversing the sign of every edge of  $\Gamma$ .

Most of the concepts defined for unsigned graphs are directly extended to signed graphs. For example, a signed graph is said to be k-cyclic if the underlying graph

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is k-cyclic. This means that G is connected and  $|E_G| = |V_G| + k - 1$ . We use the adjectives unicyclic and bicyclic as synonyms of 1-cyclic and 2-cyclic respectively. The adjacency matrix  $A_{\Gamma}$  of  $\Gamma = (G, \sigma)$  is obtained from the standard adjacency matrix  $A_G$  by replacing 1 by -1 whenever the corresponding edge is negative. By the spectrum of  $\Gamma$ , we mean the spectrum of  $A_{\Gamma}$ . Since  $A_{\Gamma}$  is symmetric, its eigenvalues  $\lambda_1(\Gamma) \geqslant \lambda_2(\Gamma) \geqslant \cdots \geqslant \lambda_n(\Gamma)$  are real. Moreover, since the trace of  $A_{\Gamma}$  is equal to zero, we have  $\lambda_1(\Gamma)\lambda_n(\Gamma) \leqslant 0$ , with equality if and only if  $\Gamma$  is empty (without edges). The index of  $\Gamma$  is simply the largest eigenvalues  $\lambda_1(\Gamma)$ , whereas the  $spectral\ radius$  is the largest absolute value of its eigenvalues.

The 'spectral' sub-branch of extremal graph theory essentially consists in identifying those objects which are extremal with respect to a fixed spectral parameter within a given class of graphs. In the last few years, some extremal problems have been solved in the context of signed graphs. For instance, in [17] Koledin and Stanić studied connected signed graphs of fixed order, size and number of negative edges that maximize the index. In the wake of that paper, signed graphs maximizing the index in suitable subsets of complete signed graphs have been studied in [2, 13]. Let  $\mathfrak{U}_n$  (resp.,  $\mathfrak{B}_n$ ) denote the class of unbalanced unicyclic (resp., bicyclic) signed graphs of order n. Akbari et al. [1] determined signed graphs with extremal index in the class  $\mathfrak{U}_n$ . Some of the same authors studied in [19] signed graphs achieving the maximum index among all graphs in  $\mathfrak{U}_n$  of fixed girth. The first five largest indices among graphs in  $\mathfrak{B}_n$  with  $n \geq 36$  are detected by He et al. [14]. Signed graphs in  $\mathfrak{U}_n$  and  $\mathfrak{B}_n$ with extremal spectral radius were identified in [4]. Extremal graphs in  $\mathfrak{U}_n$  and  $\mathfrak{B}_n$ with respect to the least Laplacian eigenvalue were studied in [7] and [3], respectively. The first author and Stanić detected in [10] the signed graphs achieving the extremal spectral radii and the extremal indices in the set  $\mathcal{U}_n$  of all unbalanced connected signed graphs with  $n \ge 3$  vertices. Finally, the procedure in [10] to determine unbalanced graphs with largest index has been improved in [9], where it has been employed to find out the first few signed graphs ordered by the index in the class of connected signed graphs, or connected unbalanced signed graphs, or complete signed graphs. This paper is devoted to prove that the signed graphs achieving the minimal index in  $\mathfrak{B}_n$  for  $n \geq 5$  are precisely those obtained by taking a starlike tree with four branches of suitable length, such graphs are obtained by considering four distinct paths joined at their end vertex u with two additional negative independent edges pairwise joining

As made precise in Corollary 3.5, it follows that the same graphs also minimize the index in the class of all bicyclic graphs of given order.

the four vertices adjacent to u (see Fig. 1). The length of each branch depends on

the congruence class of n modulo 4 (see Theorem 2.1).

The remainder of the paper is structured as follows. The main result, Theorem 2.1, is contained in Section 2 with some directions that help to guide one along the intermediate steps of the theorem's proof. Apart from fixing notation and terminology, Section 3 contains some basic tools of spectral graph theory and some bounds for the index of the possible index-minimizers. Results in Section 4 are all part of the proof of Theorem 2.1. For its completion, we employ a signless Laplacian variant of the celebrated Jacobs-Trevisan algorithm, originally defined to locate adjacency eigenvalues

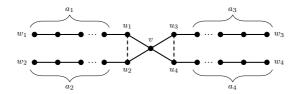


Figure 1. The signed graph  $\Gamma_{a_1,a_2,a_3,a_4}$ . Here and in the forthcoming figures, negative edges are depicted by dashed lines.

of trees. In fact, as made clear in Section 3, the indices of the signed graphs which seemingly are candidates to be index-minimizers (essentially, the graphs  $\Gamma_{a_1,a_2,a_3,a_4}$  and  $\Gamma^p_{a_1,a_2,a_3,a_4}$  respectively depicted in Fig. 1 and Fig. 4), are related with the algebraic connectivity, i.e. the second smallest (signless) Laplacian eigenvalue, of several H-shape trees. Since the arguments to perform the algorithm are quite technical, they are postponed to Section 5.

## 2. Description of the main result

We now state the main result of this paper. The notion of switching equivalence is recalled in Section 3. For the definition of the signed graph  $\Gamma_{a_1,a_2,a_3,a_4}$ , see Fig. 1. Clearly, the order of  $\Gamma_{a_1,a_2,a_3,a_4}$  is  $5 + \sum_{i=1}^4 a_i$ . In particular, for r > 0, the signed graph

$$\Phi_{r,2} := \Gamma_{r,r-1,r-1,r-1} \tag{1}$$

has 4r + 2 vertices.

**Theorem 2.1.** Let  $\tilde{\Gamma}_n$  be a signed graph achieving the minimum index in the set  $\mathfrak{B}_n$  of signed bicyclic graphs. Then:

- i)  $\tilde{\Gamma}_4$  is a diamond with two unbalanced triangles;
- ii)  $\tilde{\Gamma}_n$  with n > 4 is a switching equivalent to the signed graph

$$\Phi_{\{n\}} = \begin{cases}
\Phi_{1,2} := \Gamma_{1,0,0,0} & \text{for } n = 6 \\
\widetilde{\Phi}_{r,2} := \Gamma_{r,r,r-1,r-2} & \text{for } n = 4r + 2 \text{ and } r \geqslant 2, \\
\Phi_{r,3} := \Gamma_{r,r,r-1,r-1} & \text{for } n = 4r + 3 \text{ and } r \geqslant 1, \\
\Phi_{r,4} := \Gamma_{r,r,r-1} & \text{for } n = 4r + 4 \text{ and } r \geqslant 1, \\
\Phi_{r,5} := \Gamma_{r,r,r,r} & \text{for } n = 4r + 5 \text{ and } r \geqslant 0.
\end{cases} \tag{2}$$

The proof of Theorem 2.1 is long and requires many intermediate steps. In fact, it will only be completed in Section 5. Because of its intricacy, we give here a plan for the proof, describing how it is executed.

The case n = 4 is easy; therefore, we assume  $n \ge 5$ . Let  $P_k$  denote the (unsigned) path of order k. A first key result is given by the inequalities

$$\lambda_1(\Phi_{\{n\}}) < \lambda_1(P_{\nu_n+2}) = 2\cos\frac{\pi}{\nu_n+3} < 2, \quad \text{where } \nu_n := \left\lfloor \frac{n}{2} \right\rfloor \text{ (see Proposition 3.9)},$$

having two important consequences:

- 1. the diameter of  $\tilde{\Gamma}_n$  cannot exceed  $\nu_n$  (see Corollary 3.10);
- 2. the signed graph  $\tilde{\Gamma}_n$  lies in the subset  $\mathfrak{B}_n^*$  of bicyclic signed graphs of order n whose index is less than 2.

As better explained in Section 4, we regard  $\mathfrak{B}_n^*$  as the union of the three disjoint subsets  $\mathfrak{d}_n$ ,  $\mathfrak{i}_n$  and  $\mathfrak{th}_n$ . Signed graphs in  $\mathfrak{d}_n$  contain a dumbbell (two disjoint cycles joined by a non-trivial path); those in  $\mathfrak{i}_n$  contain an  $\infty$ -graph (two cycles with just one vertex in common); those in  $\mathfrak{th}_n$  contain a theta-graph (the union of three edge-disjoint paths of length  $\geq 2$  between two vertices).

We shall prove that  $\lambda_1(\Phi_{\{n\}}) < \lambda_1(\Theta)$  for each  $\Theta \in \mathfrak{th}_n$  (see Theorem 4.7). Since  $\Phi_{\{n\}}$  belongs to  $\mathfrak{i}_n$ , it follows that  $\tilde{\Gamma}_n$  must be searched in  $\mathfrak{d}_n \sqcup \mathfrak{i}_n$ . The detection of index-minimizers in  $\mathfrak{d}_n \sqcup \mathfrak{i}_n$  is performed in Section 4.1.

After noticing that all elements in  $\mathfrak{d}_n \sqcup \mathfrak{i}_n$  have girth 3 and circumference  $s \leq 5$ , by separately analyzing the cases s = 5, s = 4 and s = 3 (which are  $Case\ 1$ , 2 and 3 respectively in Section 4.1), we discover that a signed graph in  $\bigsqcup_{n\geq 5} (\mathfrak{d}_n \sqcup \mathfrak{i}_n)$  is switching equivalent to one of the items listed below:

- 1. a graph of type  $\Gamma^p_{a_1,a_2,a_3,a_4}$  (see Fig. 4);
- 2. one of the graphs  $\Gamma_i$  ( $1 \le i \le 16$ ) depicted in Fig. 5;
- 3. a graph of type  $\Lambda_{h,k;\ell}^p$  (see Fig. 6);
- 4. a graph of type  $X_{a_1,a_2,a_3,a_4}^p$  (see Fig. 7).

It turns out that index-minimizers are of type 1. In fact,

- a direct analysis is sufficient to show that no graph of type 2 is an indexminimizer (the several  $\lambda_1(\Gamma_i)'s$  are listed in the Appendix);
- the only graphs of type 3 whose diameter is sufficiently small to be indexminimizers are  $\Lambda^1_{0,0;0}$  of order 6,  $\Lambda^1_{1,1;0}$  of order 8, and  $\Lambda^1_{2,2;0}$  of order 10, but one easily checks that  $\lambda_1(\Phi_{\{6\}}) < \lambda_1(\Lambda^1_{0,0;0}), \ \lambda_1(\Phi_{\{8\}}) < \lambda_1(\Lambda^1_{1,1;0}),$  and  $\lambda_1(\Phi_{\{10\}}) < \lambda_1(\Lambda^1_{2,2;0});$
- no graphs of type 4 are index-minimizers by Proposition 4.5.

The proof ends by considering the only graphs of type 1 of order n whose diameter does not exceed  $\nu_n$ . If n is odd, there is just  $\Phi_{\{n\}}$ , and there is nothing else to prove. If n = 4r + 2 (resp., n = 4r + 4) index-minimizers are in the set  $\mathcal{G}_{4r+2} = \{\widetilde{\Phi}_{r,2}, \Phi_{r,2}, \Gamma^2_{r-1,r-1,r-1}, \Gamma^2_{r,r,r-2,r-2}\}$  (resp.,  $\mathcal{G}_{4r+4} = \{\Phi_{r,4}, \Gamma_{r+1,r,r-1,r-1}, \Gamma^2_{r,r,r-1,r-1}\}$ ).

Finally, in order to establish that only  $\widetilde{\Phi}_{r,2}$  (resp.  $\Phi_{r,4}$ ) minimizes the index in  $\mathcal{G}_{4r+2}$  (resp.,  $\mathcal{G}_{4r+4}$ ) we compare the algebraic connectivities of some H-shaped graphs related to graphs in  $\mathcal{G}_{4r+2} \cup \mathcal{G}_{4r+4}$  according to the formula (12). This comparison is performed in Section 5 by using the algorithm presented in Figure 12.

## 3. Basic tools and preliminaries

Let  $\Gamma = (G, \sigma)$  be a signed graph. As usual, we denote by  $\phi_A(G, \lambda) = \det(\lambda I_n - A_G)$  and  $\phi_A(\Gamma, \lambda) = \det(\lambda I_n - A_\Gamma)$  the characteristic polynomial of  $A_G$  and  $A_\Gamma$ , respectively. In Section 4, we shall also consider the characteristic polynomial  $\phi_Q(G, \lambda)$  of the signless Laplacian matrix  $Q_G = D_G + A_G$ , where  $D_G$  is the vertex degree matrix of G.

The first result we mention is very well-known and involves the spectrum of the (unsigned) path  $P_n$  with n vertices.

**Proposition 3.1.** [12, p. 73] The characteristic polynomial  $\phi(P_n, \lambda)$  is equal to  $U_n(\lambda/2)$ , where  $U_n(x)$  is the *n*-th Chebyshev polynomial of the second kind defined through the following identity

$$U_n(\cos \omega) \sin \omega = \sin((n+1)\omega).$$

Therefore, the eigenvalues of  $A_{P_n}$  are

$$\lambda_k(P_n) = 2\cos\frac{k\pi}{n+1}$$
 for  $1 \leqslant k \leqslant n$ .

For a signed graph  $\Gamma = (G, \sigma)$  and a function  $\theta \colon V_G \longrightarrow \{+1, -1\}$ , we can build a new signed graph  $\Gamma^{\theta} = (G, \sigma^{\theta})$ , where  $\sigma^{\theta}(e) = \theta(v_i)\sigma(e)\theta(v_j)$  for each edge  $e = v_i v_j \in E_G$ . The signed graphs  $\Gamma$  and  $\Gamma^{\theta}$  are said to be *switching equivalent*; they share the same spectrum and the same set of positive cycles. In fact,  $A_{\Gamma^{\theta}} = D^{-1}A_{\Gamma}D$ , where D is the diagonal matrix diag  $(\theta(v_1), \theta(v_2), \dots, \theta(v_n))$ . It can also be proved [21, Proposition 3.2] that two signed graphs sharing the same underlying graph are switching equivalent if and only if  $\Gamma$  is switching equivalent to (G, +). In particular, any signed forest  $(F, \sigma)$  is balanced, the matrices  $A_{(F, \sigma)}$  and  $A_F$  are similar and we denote their shared eigenvalues by  $\lambda_1(F) \geqslant \dots \geqslant \lambda_{|V_F|}(F)$ .

For the same reason, all balanced (resp., unbalanced) cycles of fixed order are spectrally indistinguishable. With a slight abuse of notation we denote by  $C_n^b$  (resp.,  $C_n^u$ ) any balanced (resp., unbalanced) cycle of order  $n \ge 3$ .

We say that  $\Lambda = (H, \tau)$  is an induced subgraph of  $\Gamma = (G, \sigma)$ , and write  $\Lambda \subseteq \Gamma$ , if H is an induced subgraph of G and  $\tau = \sigma|_{H}$ . Furthermore, we write  $\Lambda \subset \Gamma$  and say that  $\Gamma$  properly contains  $\Lambda$  if  $\Lambda \subseteq \Gamma$  and  $H \neq G$ .

Let  $\Gamma - v$  denote the signed graph obtained from  $\Gamma$  by deleting the vertex v. The following result is known as the *Interlacing Theorem for Signed Graphs*, which is a consequence of the Cauchy Interlacing Theorem holding, in its general form, for principal submatrices of any Hermitian matrix (see [12, Theorem 0.10]).

**Theorem 3.2.** Let  $\Gamma = (G, \sigma)$  be a signed graph of order  $n \ge 2$ , and let v be one of its vertices. The eigenvalues of  $A_{\Gamma}$  and those of  $A_{\Gamma-v}$  interlace as follows:

$$\lambda_1(\Gamma) \geqslant \lambda_1(\Gamma - v) \geqslant \lambda_2(\Gamma) \geqslant \lambda_2(\Gamma - v) \geqslant \cdots \geqslant \lambda_{n-1}(\Gamma - v) \geqslant \lambda_n(\Gamma).$$

By using Theorem 3.2 the suitable number of times, we get the following corollary.

Corollary 3.3. If  $\Lambda \subseteq \Gamma$  and  $\Lambda'$  is switching equivalent to  $\Lambda$ , then  $\lambda_1(\Lambda') = \lambda_1(\Lambda) \leq \lambda_1(\Gamma)$ .

The two parts of the following result respectively come from [1, Theorem 2.5] and [20, Lemma 2.1].

**Theorem 3.4.** The index of a signed graph  $\Gamma = (G, \sigma)$  never exceeds  $\lambda_1(G, +)$ . Moreover, if  $\Gamma$  is connected, then  $\lambda_1(\Gamma) = \lambda_1(G, +)$  if and only if  $\Gamma$  is balanced.

Theorem 3.4 has the following immediate consequence.

**Corollary 3.5.** Let  $n \geq 4$ . A signed graph  $\tilde{\Gamma}_n$  minimizes the index among the signed bicyclic graphs of order n if and only if it is unbalanced and minimizes the index in  $\mathfrak{B}_n$ .

The next theorem encapsulates a Schwenk-like formula which will be repeatedly used along the paper.

**Theorem 3.6.** [6, Theorem 3.1] Let  $\Gamma$  be a signed graph and u be an arbitrary vertex of  $\Gamma$ . Then the following holds:

$$\phi(\Gamma, \lambda) = \lambda \, \phi(\Gamma - u, \lambda) - \sum_{u \sim v} \phi(\Gamma - u - v, \lambda) - 2 \sum_{C \in \mathcal{C}_u} \operatorname{sign}(C) \cdot \phi(\Gamma \setminus V(C), \lambda), \tag{3}$$

where  $u \sim v$  means that u and v are adjacent and  $C_u$  is the set of cycles passing through u.

We now prove some bounds for the index of the graphs defined in (1) and (2).

**Lemma 3.7.** For  $t \in \{1, 2\}$ , the following inequalities hold:

$$2\cos\frac{\pi}{2r+t+2} < \lambda_1(\Phi_{r,2t}) \leqslant \lambda_1(\Phi_{r,2t+1}),\tag{4}$$

and

$$2\cos\frac{\pi}{2r+3} < \lambda_1(\widetilde{\Phi}_{r,2}) \leqslant \lambda_1(\Phi_{r,3}). \tag{5}$$

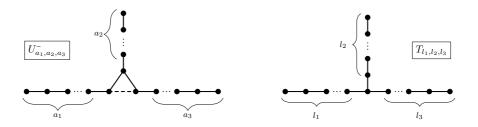


Figure 2. The signed graph  $U_{a_1,a_2,a_3}^-$  and the T-shape graph  $T_{l_1,l_2,l_3}$ 

Proof. Since  $\Phi_{r,2t} \subseteq \Phi_{r,2t+1}$  and  $\widetilde{\Phi}_{r,2} \subseteq \Phi_{r,3}$ , the second inequalities of both (4) and (5) come from interlacing. Let now  $u_2$  be the vertex of  $\Phi_{r,2t}$  as in Fig. 1. The signed graph  $\Phi_{r,2t} - u_2$  has two connected components. One is  $P_{r+t-2}$ . The other one is the signed unicyclic graph  $U_{r+1,r+t-2,r-1}^-$  (see Fig. 2), whose index is strictly larger than  $\lambda_1(P_{2r+t+1})$  (see [1, Theorem 3.4]). Thus, by interlacing,

$$2\cos\frac{\pi}{2r+t+2} < \lambda_1(U_{r+1,r+t-2,r-1}^-) \leqslant \lambda_1(\Phi_{r,2t}) \leqslant \lambda_1(\Phi_{r,2t+1}).$$

The argument to prove the first inequality of (5) is analogous.

**Lemma 3.8.** For  $t \in \{1, 2\}$ ,  $\lambda_2(\Phi_{r, 2t+1}) = \lambda_1(P_{2r+2}) = 2\cos(\pi/(2r+3))$ .

*Proof.* Let v the only vertex of  $\Phi_{r,2t+1}$  of degree 4. We first deal with the case t=2 which is easier. Since  $\Phi_{r,5} - v = 2P_{2r+2}$ , by Proposition 3.1 and Theorem 3.2 we arrive at

$$2\cos\frac{\pi}{2r+3} = \lambda_1(2P_{2r+2}) \geqslant \lambda_2(\Phi_{r,5}) \geqslant \lambda_2(2P_{2r+2}) = 2\cos\frac{\pi}{2r+3},$$

proving the statement for t=2.

Let now t=1. Note that  $\Phi_{r,3}-v=P_{2r+2}\sqcup P_{2r}$ . Therefore, by interlacing and (4),  $\lambda_1(\Phi_{r,3})>\lambda_1(P_{2r+2})\geqslant \lambda_2(\Phi_{r,3})$ . The proof will be over once we show that  $\lambda_1(P_{2r+2})$  is an eigenvalue of  $\Phi_{r,3}$ .

If we use the Schwenk-like formula of Theorem 3.6 starting from the central vertex v of  $\Phi_{r,3}$ , we obtain

$$\phi(\Phi_{r,3};\lambda) = \phi(2r+2) \left(\lambda \phi(2r) - 2\phi(r)\phi(r-1) + 2\phi(r-1)^2\right) + -2\phi(2r)\phi(r) \left(\phi(r+1) - \phi(r)\right), \quad (6)$$

where we set  $\phi(k) = \phi(P_k; \lambda)$ . From (6) it is immediately seen that

$$\phi(\Phi_{r,3}; \lambda_1(P_{2r+2})) = 0 \iff \phi(P_{r+1}; \lambda_1(P_{2r+2})) = \phi(P_r; \lambda_1(P_{2r+2})).$$

The latter equality actually holds and comes from Proposition 3.1. In fact,  $\lambda_1(P_{2r+2}) = 2\cos\alpha$  for  $\alpha = \frac{\pi}{2r+3}$ , and

$$\phi\left(P_{r+1}; 2\cos\alpha\right) = \frac{\sin((r+2)\alpha)}{\sin\alpha} = \frac{\sin((r+1)\alpha)}{\sin\alpha} = \phi\left(P_r; 2\cos\alpha\right),$$

since 
$$\sin((r+2)\alpha) = \sin(\pi - (r+1)\alpha) = \sin((r+1)\alpha)$$
.

**Proposition 3.9.** The indices of the signed graphs  $\Phi_{r,\epsilon}$  and  $\widetilde{\Phi}_{r,2}$  in (2) and (1) satisfy the following inequalities:

$$2\cos\frac{\pi}{2r+3} < \lambda_1(\Phi) < 2\cos\frac{\pi}{2r+4} \quad \text{for } \Phi \in \{\widetilde{\Phi}_{r,2}, \Phi_{r,2}, \Phi_{r,3}\},\tag{7}$$

and

$$2\cos\frac{\pi}{2r+4} < \lambda_1(\Phi_{r,\epsilon}) < 2\cos\frac{\pi}{2r+5} \quad \text{for } \epsilon \in \{4,5\}.$$
 (8)

*Proof.* The lower bounds of (7) and (8) immediately come from Lemma 3.7. To prove the upper bounds, let  $\beta = \pi/(2r+4)$  and  $\gamma = \pi/(2r+5)$ .

With the aid of Proposition 3.1, (6) and the software Wolfram|Alpha, the evaluation of  $\phi(\Phi_{r,3},\lambda)$  at  $\lambda_1(P_{2r+3}) = 2\cos\beta$  gives

$$\phi\left(\Phi_{r,3}; 2\cos\beta\right) = \frac{32}{\sin^3\beta} \cdot \sin^7\frac{\beta}{2} \cdot \cos\frac{\beta}{2} \cdot \left(2\cos\beta + 1\right)^2 \tag{9}$$

which is clearly a positive number. Since, by Lemma 3.8,  $\lambda_2(\Phi_{r,3}) < 2\cos\beta$ , the positivity of (9) and interlacing imply  $\max\{\lambda_1(\widetilde{\Phi}_{r,2}),\lambda_1(\Phi_{r,2})\} \leq \lambda_1(\Phi_{r,3}) < 2\cos\beta$ . Thus, (7) is proved.

The argument to prove the upper bound of (8) is similar. If we use the Schwenk-like formula (3) obtained by considering the central vertex v of  $\phi(\Phi_{r,5}; \lambda)$  we arrive at

$$\phi(\Phi_{r,5};\lambda) = \phi(2r+2) \left(\lambda \phi(2r+2) + 4\phi(r)(\phi(r) - \phi(r+1))\right), \tag{10}$$

where, once again, we set  $\phi(k) := \phi(P_k; \lambda)$ .

With the aid of Proposition 3.1, (10) and the software Wolfram Alpha, the evaluation of  $\phi(\Phi_{r,5}, \lambda)$  at  $\lambda_1(P_{2r+4}) = 2\cos\gamma$  gives

$$\phi(\Phi_{r,5}; 2\cos\gamma) = 64\sin^6\frac{\gamma}{2}\cos^2\frac{\gamma}{2} > 0,$$

proving, together with Lemma 3.8, that the largest root of  $\phi(\Phi_{r,5}, \lambda)$  – and a fortiori of  $\phi(\Phi_{r,4}, \lambda)$  – is smaller than  $2\cos\gamma$ . Hence, the upper bound of (8) follows.

Table 1 in the Appendix involves the candidates to minimize the index in the several  $\mathfrak{B}_n$ 's for  $5 \leq n \leq 9$ . As many entries of Table 2, the values for the index from the second column of Table 1 on are approximated. Obviously, they are consistent with the bounds (7) and (8).

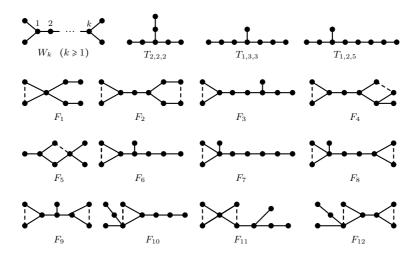


Figure 3. Some forbidden graphs

Corollary 3.10. The diameter of a signed graph minimizing the index in  $\mathfrak{B}_n$  does not exceed  $\nu_n := \lfloor \frac{n}{2} \rfloor$ .

*Proof.* Let  $\tilde{\Gamma}_n$  be a signed graph minimizing the index in  $\mathfrak{B}_n$ . If diam  $\tilde{\Gamma}_n = k - 1$ , then  $\tilde{\Gamma}_n$  contains a signed path of order k and, by Corollary 3.3,  $2\cos\frac{\pi}{k+1} = \lambda_1(P_k) \le \lambda_1(\tilde{\Gamma}_n)$ . The statement now follows by looking at the upper bounds of (7) and (8).  $\square$ 

The importance of Corollary 3.10 is transitory. In fact,  $\nu_n$  is the diameter of the several  $\Phi_{r,\epsilon}$ 's and  $\widetilde{\Phi}_{r,2}$ 's . Therefore, Theorem 2.1, whose proof requires Corollary 3.10, will ensure that the diameter of index-minimizers in  $\mathfrak{B}_n$  is precisely equal to  $\nu_n$ .

Throughout the rest of the paper we say that a signed graph  $\Lambda$  is forbidden if and only if  $\lambda_1(\Lambda) \geq 2$ . The reason for this naming is readily explained. Let  $\tilde{\Gamma}_n$  be a signed graph minimizing the index in  $\mathfrak{B}_n$  for  $n \geq 4$ . From Proposition 3.9 and the fact that there are signed diamonds of order 4 whose index is less than 2, we immediately deduce that  $\lambda_1(\tilde{\Gamma}_n) < 2$ . Therefore, Corollary 3.3 implies that every forbidden signed graph cannot be contained in  $\tilde{\Gamma}_n$ . In particular, since  $\lambda_1(C_n^b) = 2$ , all graphs containing an induced balanced cycle are forbidden. Fig. 3 depicts a certain number of minimal forbidden signed graphs: in fact, their index is 2 and all their proper induced subgraphs have index in the interval [0,2). Graphs on the top row of Fig. 3, together with the cycles  $C_n$ , are known as Smith graphs.

We end this section by giving a rationale for the comparisons of algebraic connectivities performed in Section 5. Let G be an (unsigned) connected graph G with n vertices. We denote by  $\mathcal{L}(G)$  its line graph, and by  $0 \leq \mu_1(G) \leq \mu_2(G) \leq \cdots \leq \mu_n(G)$  the eigenvalues of  $Q_G$ . When G is a tree, the signless Laplacian eigenvalues are also

the eigenvalues of  $L_G = D_G - A_G$ . Therefore, for every tree T,  $\mu_1(T) = 0$  and  $\mu_2(T) \neq 0$  is known as the algebraic connectivity of T.

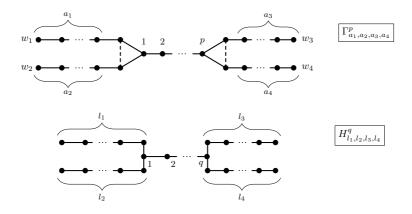


Figure 4. The signed graph  $\Gamma^p_{a_1,a_2,a_3,a_4}$  and the H-shape tree  $H^q_{l_1,l_2,l_3,l_4}$ 

**Proposition 3.11.** The following equalities hold:

$$\mu_2(T_{l_1,l_2,l_3}) = 2 - \lambda_1(U_{l_1-1,l_2-1,l_3-1}^-), \tag{11}$$

and

$$\mu_2(H_{l_1,l_2,l_3,l_4}^q) = 2 - \lambda_1(\Gamma_{l_1-1,l_2-1,l_3-1,l_4-1}^{q-1}), \tag{12}$$

where  $T_{l_1,l_2,l_3}$  is the T-shape graph depicted in Fig. 2, whereas  $\Gamma^p_{a_1,a_2,a_3,a_4}$  and the H-shape tree  $H^q_{l_1,l_2,l_3,l_4}$  are depicted in Fig. 4.

*Proof.* It is immediately seen that  $\mathcal{L}(T_{l_1,l_2,l_3})$  and  $\mathcal{L}(H^q_{l_1,l_2,l_3,l_4})$  are the underlying graphs of  $U:=U^-_{l_1-1,l_2-1,l_3-1}$  and  $\Gamma=\Gamma^{q-1}_{l_1-1,l_2-1,l_3-1,l_4-1}$  respectively. The signed graphs -U and  $-\Gamma$  are both balanced; therefore, they are spectral undis-

The signed graphs -U and  $-\Gamma$  are both balanced; therefore, they are spectral undistinguishable from their underlying graphs. Moreover, if n is the order of both U and  $\Gamma$ , then  $\lambda_1(U) = \lambda_n(-U)$  and  $\lambda_1(\Gamma) = \lambda_n(-\Gamma)$ .

The equalities (11) and (12) now come from the well-known identity  $\phi_A(\mathcal{L}(T), \lambda) = (\lambda + 2)^{-1}\phi_Q(T, \lambda + 2)$  holding for every tree T (see, for instance [11, Eq. 2]).

# 4. Chasing index-minimizers

The diamond, i.e. the graph made by two triangles sharing an edge, is the only bicyclic graph of order 4. By a direct calculation, the index of any diamond with two unbalanced triangles is  $(\sqrt{17}-1)/2 < 2$ . Other types of diamonds contain at

least one induced balanced triangle; hence, they are forbidden. This proves Part i) of Theorem 2.1.

From now on we assume  $n \geq 5$ . Note that there exists a unique pair  $(r, \epsilon) \in \mathbb{N}_0 \times \{2, 3, 4, 5\}$  such that  $n = 4r + \epsilon$ . The proof consists in showing that if the signed bicyclic graph  $\Gamma$  belongs to  $\mathfrak{B}_n$  and it is not switching equivalent to  $\Phi_{\{n\}}$  defined in (2), then  $\lambda_1(\Gamma) > \lambda_1(\Phi_{\{n\}})$ . By Proposition 3.9, we can take into consideration only graphs in the set  $\mathfrak{B}_n^*$  of bicyclic signed graphs of order n whose index is less than 2. As already observed in Section 3, a signed graph in  $\mathfrak{B}_n^*$  does not contain any balanced cycle.

We recall that the *base* of a bicyclic graph  $\Gamma = (G, \sigma)$ , denoted by  $\hat{\Gamma} = (\hat{G}, \sigma|_{\hat{G}})$ , is the (unique) minimal bicyclic signed subgraph of  $\Gamma$ .

It is easy to verify that  $\hat{\Gamma}$  is the unique bicyclic subgraph of  $\Gamma$  without pendant vertices (i.e. vertices of degree is 1), and  $\Gamma$  can be obtained from  $\hat{\Gamma}$  by attaching signed trees to some vertices of  $\hat{\Gamma}$ .

The underlying graph  $\hat{G}$  of  $\hat{\Gamma}$  can be either a dumbbell, an  $\infty$ -graph, or a theta-graph. In other words,  $\mathfrak{B}_n^* = \mathfrak{d}_n \sqcup \mathfrak{t}_n \sqcup \mathfrak{th}_n$ , where

$$\mathfrak{d}_n := \{ \Gamma \in \mathfrak{B}_n^* \mid \hat{G} \text{ is a dumbbell} \}, \qquad \mathfrak{i}_n := \{ \Gamma \in \mathfrak{B}_n^* \mid \hat{G} \text{ is an } \infty \text{-graph} \},$$

and

$$\mathfrak{th}_n := \{ \Gamma = (G, \sigma) \in \mathfrak{B}_n^* \mid \hat{G} \text{ is a theta-graph} \}.$$

The cases  $\Gamma \in \mathfrak{d}_n \sqcup \mathfrak{i}_n$  and  $\Gamma \in \mathfrak{th}_n$  will be dealt in two separate subsections.

## 4.1. Index-minimizers in $\mathfrak{d}_n \sqcup \mathfrak{i}_n$

Graphs in  $\mathfrak{d}_n \sqcup \mathfrak{i}_n$  just contain two cycles, which are both unbalanced. Let  $C_r^u$  and  $C_s^u$  (with  $r \leq s$ ) be the two signed cycles contained in a signed graph  $\Gamma \in \mathfrak{d}_{4r+\epsilon} \sqcup \mathfrak{i}_{4r+\epsilon}$ . Once we set

$$\mathcal{D}(\Gamma) = \min\{d(v, w) \mid v \in C_r^u, w \in C_s^u\},\$$

it is clear that a graph  $\Gamma \in \mathfrak{d}_n \sqcup \mathfrak{i}_n$  belongs to  $\mathfrak{i}_n$  if and only if  $\mathcal{D}(\Gamma) = 0$ .

**Lemma 4.1.** Let  $\Gamma = (G, \sigma) \in \mathfrak{d}_n \sqcup \mathfrak{i}_n$ . The two cycles of  $\Gamma$  have order r = 3 and  $s \leq 5$ .

*Proof.* Assume by contradiction that  $r \ge 4$ . In this case G would contain a double snake  $W_k$  (see Fig. 3) for a suitable  $k \ge 1$ , yet, double snakes are all forbidden. Therefore, r = 3. Now,  $s \le 5$ , otherwise  $\Gamma$  would contain an induced subgraph switching equivalent to either  $T_{2,2,2}$  or the graph  $F_1$  of Fig. 3; yet,  $T_{2,2,2}$  and  $F_1$  are both forbidden.

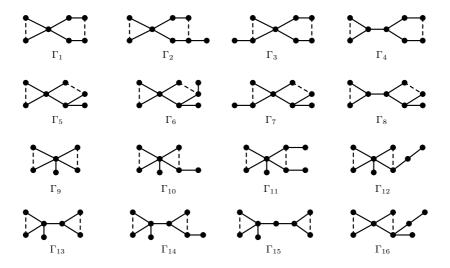


Figure 5. Some graphs in  $i_6$ ,  $i_7$ ,  $i_8$ ,  $o_7$  and  $o_8$ 

Our investigation on graphs in  $\mathfrak{d}_n \sqcup \mathfrak{i}_n$  will proceed from the biggest possible circumference (which is 5, by Lemma 4.1) to the smallest one (which is 3).

#### Case 1. s = 5.

Let  $C_3^u$  and  $C_5^u$  be the two unbalanced cycles of a signed graph  $\Gamma = (G, \sigma)$  in  $\mathfrak{d}_n \sqcup \mathfrak{i}_n$ . Note that  $\mathcal{D}(\Gamma) \leqslant 1$ , otherwise  $\Gamma$  would contain a graph switching equivalent to one of the following forbidden graphs in Fig. 3: the graph  $F_2$  if  $\mathcal{D}(\Gamma) = 2$ ; the graph  $F_3$  if  $\mathcal{D}(\Gamma) = 3$ ;  $T_{1,2,5}$  if  $\mathcal{D}(\Gamma) > 3$ .

A direct analysis shows that  $\Gamma$  is switching equivalent to one of the graphs  $\Gamma_i$  ( $1 \le i \le 4$ ) depicted in Fig. 3. In fact, by adding to them an additional pendant vertex in every possible way, if the resulting signed graphs is not in  $\{\Gamma_2, \Gamma_3, \Gamma_4\}$ , then it is forbidden.

#### Case 2. s = 4.

Let  $C_3^u$  and  $C_4^u$  be the two unbalanced cycles of a signed graph  $\Gamma = (G, \sigma)$  in  $\mathfrak{d}_n \sqcup \mathfrak{i}_n$ , and let  $v \in C_3^u$  and  $w \in C_4^u$  be the vertices such that  $d(v, w) = \mathcal{D}(\Gamma)$ . Clearly, v and w are the ending vertices of the (possibly trivial) path in  $\hat{\Gamma}$  connecting the two cycles. We denote by w' and w'' the vertices in  $C_4^u$  adjacent to w, and by  $d_G(u)$  the degree of a vertex u in G.

## **Subcase 2.1.** $d_G(w')d_G(w'') > 4$ .

As above,  $\mathcal{D}(\Gamma) \leq 1$ , otherwise  $\Gamma$  would contain a graph switching equivalent to one of the following forbidden graphs in Fig. 2: the graph  $F_4$  if  $\mathcal{D}(\Gamma) = 2$ ; the graph  $F_3$  if  $\mathcal{D}(\Gamma) = 3$ ;  $T_{1,2,5}$  if  $\mathcal{D}(\Gamma) > 3$ . The non-forbidden signed graphs are switching equivalent to the graphs  $\Gamma_i$  ( $5 \leq i \leq 8$ ) depicted in Fig. 5.

**Subcase 2.2.**  $d_G(w')d_G(w'') = 4$ .

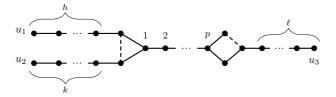


Figure 6. The signed graph  $\Lambda_{h,k:\ell}^p$ 

Since the double snakes  $W_k$ 's and  $F_5$  are forbidden, the graph  $\Gamma$  is switching equivalent to a signed graph of type  $\Lambda_{h,k;\ell}^p$ , where  $p = \mathcal{D}(\Gamma) + 1$ ,  $0 \le h \le k$ ,  $\ell \ge 0$ , with pendant vertices  $u_1, u_2$  and  $u_3$  (see Fig. 6). Since we are looking for possible index-minimizers, by Corollary 3.10 neither of the three distances  $d(u_1, u_2)$ ,  $d(u_1, u_3)$  and  $d(u_2, u_3)$  should exceed  $\nu_n = \lfloor \frac{n}{2} \rfloor$ . This leads to the following algebraic constraints:

$$h + k \le \nu_n - 1$$
,  $h + p + \ell \le \nu_n - 2$ , and  $k + p + \ell \le \nu_n - 2$ , (13)

where  $\ell = n - h - k - p - 5$ .

For even integers n = 2q, Conditions (13) are equivalent to

$$3 \leqslant q \leqslant 5, \quad q - 3 \leqslant h \leqslant k, \quad h + k < q. \tag{14}$$

If instead n = 2q + 1, Conditions (13) are only satisfied for n = 7, h = 1 and k = 1, but in this case  $\ell$  would be negative.

There are only three graphs of type  $\Lambda^p_{h,k;\ell}$  satisfying (14). Namely:  $\Lambda^1_{0,0;0}$  of order 6,  $\Lambda^1_{1,1;0}$  of order 8, and  $\Lambda^1_{2,2;0}$  of order 10.

#### Case 3. s = 3.

Let  $\Gamma$  be a graph in  $\mathfrak{d}_n \sqcup \mathfrak{i}_n$  containing two unbalanced triangles, and let  $P_{\Gamma}$  be the path connecting the two triangles in the base  $\hat{\Gamma}$ . Clearly, the order of  $P_{\Gamma}$  is  $\mathcal{D}(\Gamma) + 1$ .

**Subcase 3.1.** There are some vertices in  $V(\Gamma) \setminus V(\hat{\Gamma})$  adjacent to  $P_{\Gamma}$ . Since the graphs  $T_{1,3,3}$ ,  $F_6$ ,  $F_7$ , and  $F_8$  in Fig. 3 are forbidden, we have  $\mathcal{D}(\Gamma) \leq 2$ . The non-forbidden signed graphs are switching equivalent to the graphs  $\Gamma_i$  ( $9 \leq i \leq 15$ ) depicted in Fig. 5 (note that the graph  $F_9$  in Fig. 3 is forbidden).

**Subcase 3.2.** There are no vertices in  $V(\Gamma) \setminus V(\tilde{\Gamma})$  adjacent to  $P_{\Gamma}$ . Since the double snakes  $W_k$ 's, together with  $T_{1,2,5}$ ,  $T_{1,3,3}$  and the graphs  $F_{10}$ ,  $F_{11}$  and  $F_{12}$  in Fig. 3 are forbidden, apart from graph  $\Gamma_{16}$  of Fig. 5, signed graphs of this type in  $\mathfrak{d}_n \sqcup \mathfrak{i}_n$  are switching equivalent to an element in the set  $\mathcal{S}'_n \cup \mathcal{S}''_n$ , where

$$\mathcal{S}'_n = \{ \Gamma^p_{a_1, a_2, a_3, a_4} \in \mathfrak{d}_n \sqcup \mathfrak{i}_n \mid p \geqslant 1, \ a_1 \geqslant a_2 \geqslant 0, \quad \text{and} \quad a_1 \geqslant a_3 \geqslant a_4 \geqslant 0 \}$$

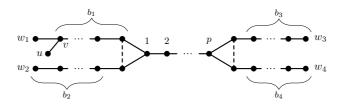


Figure 7. The signed graph  $X_{b_1,b_2,b_3,b_4}^p$ 

and

$$S_n'' = \{X_{b_1,b_2,b_3,b_4}^p \in \mathfrak{d}_n \sqcup \mathfrak{i}_n \mid p \geqslant 1, \ b_1 \geqslant 0, \ b_2 \geqslant 0 \quad \text{and} \quad b_3 \geqslant b_4 \geqslant 0\}.$$

Elements in  $\mathcal{S}'_n$  and in  $\mathcal{S}''_n$  are respectively depicted in Figg. 4 and 7. Clearly,  $\Gamma^1_{a_1,a_2,a_3,a_4}$  is precisely the graph  $\Gamma_{a_1,a_2,a_3,a_4}$  of Fig. 1. We first seek for indexminimizers in  $\mathcal{S}'_n$ . Note that every positive integer n can be uniquely written in the form

$$n = 2\nu_n + \omega$$
, where  $\nu_n = \left\lfloor \frac{n}{2} \right\rfloor$  and  $\omega = \frac{1}{2} (1 + (-1)^n)$ .

Clearly,  $\omega \in \{0,1\}$  depends on the parity of n.

**Lemma 4.2.** If the diameter of  $\Gamma_{a_1,a_2,a_3,a_4}^p \in \mathcal{S}'_n$  does not exceed  $\nu_n$ , then

$$a_1 + a_3 = \nu_n - p - 1$$
 and  $a_2 + a_4 = \nu_n + \omega - 3$  with  $1 \le p \le 2 - \omega$ . (15)

*Proof.* Since  $d(w_1, w_3) \leq \nu_n$  and  $n = 2\nu_n + \omega = \sum_{i=1}^4 a_i + p + 4$ , we can write

$$d(w_1, w_3) = a_1 + a_3 + p + 1 = \nu_n - k$$
 and  $a_2 + a_4 = \nu_n + \omega + k - 3$  (16)

for some  $k \ge 0$ . With Equations (16) at hand, the inequality  $a_1 + a_3 \ge a_2 + a_4$  implies  $2k + \omega \le 2 - p \le 1$ , which is only possible for k = 0. Hence,  $p \le 2 - \omega$ , and Equations (16) specialize to (15).

By Corollary 3.10 and Lemma 4.2, we immediately realize that if  $\Gamma_{a_1,a_2,a_3,a_4}^p$  minimizes the index in  $S'_{2\nu_n+\omega}$ , then  $(\omega,p)\in\{(0,1),(0,2),(1,1)\}.$ 

**Subcase 3.2.1.**  $(\omega, p) = (0, 1)$ .

Equations (15) now read

$$a_1 + a_3 = \nu_n - 2 = (a_2 + a_4) + 1,$$
 (17)

implying that  $a_1 \ge (\nu_n - 2)/2$  and  $a_2 \ge (\nu_n - 3)/2$ . These two inequalities, together with  $\nu_n \ge d(w_1, w_2) = a_1 + a_2 + 1$ , give

$$\nu_n - 2 \le a_1 + a_2 \le \nu_n - 1.$$

By plugging  $a_1 \ge a_2$  and  $a_3 \ge a_4$  into (17) one at a time, we also obtain  $a_{i+1} \le a_i \le a_{i+1} + 1$ . for  $i \in \{1, 3\}$ . With these constraints at hand, it is now straightforward to check that  $\Phi_{r,2}$  (for  $r \ge 1$ ) and  $\widetilde{\Phi}_{r,2}$  (for r > 1) are the only possible index-minimizers in  $S'_{4r+2} \cap \mathfrak{i}_{4r+2}$ . On the other hand,  $\Phi_{r,4}$  and  $\Gamma_{r+1,r,r-1,r-1}$  are the only possible index-minimizers in  $S'_{4r+4} \cap \mathfrak{i}_{4r+4}$ .

**Subcase 3.2.2.**  $(\omega, p) = (0, 2)$ .

Equations (15) become  $a_1 + a_3 = \nu_n - 3 = a_2 + a_4$  which, together with  $a_1 \ge a_2$  and  $a_3 \ge a_4$  gives  $a_1 = a_2$  and  $a_3 = a_4$ . From  $d(w_1, w_2) = 2a_1 + 1 \le \nu_n$  and  $a_1 = \nu_n - a_3 - 3$  we arrive at

$$\frac{\nu_n - 5}{2} \leqslant a_3 = a_4 \leqslant a_1 = a_2 \leqslant \frac{\nu_n - 1}{2}.$$
 (18)

It is straightforward to check that the only signed graphs in  $\mathcal{S}'_{4r+2} \cap \mathfrak{d}_{4r+2}$  satisfying (18) are  $\Gamma^2_{r,r,r-2,r-2}$  and  $\Gamma^2_{r-1,r-1,r-1}$ . In  $\mathcal{S}'_{4r+4} \cap \mathfrak{d}_{4r+4}$ , instead, constraints (18) are only satisfied by  $\Gamma^2_{r,r,r-1,r-1}$ .

**Subcase 3.2.3.**  $(\omega, p) = (1, 1)$ .

The argument is similar to the previous subcase. Equations (15) become  $a_1 + a_3 = \nu_n - 2 = a_2 + a_4$  which, together with  $a_1 \ge a_2$  and  $a_3 \ge a_4$  gives  $a_1 = a_2$  and  $a_3 = a_4$ . From  $d(w_1, w_2) = 2a_1 + 1 \le \nu_n$  and  $a_1 = \nu_n - a_3 - 2$  we arrive at

$$\frac{\nu_n - 3}{2} \leqslant a_3 = a_4 \leqslant a_1 = a_2 \leqslant \frac{\nu_n - 1}{2}.$$
 (19)

For n=4r+3, the sum  $a_1+a_3=\nu_n-2$  is odd; therefore,  $a_1\neq a_3$ . Moreover,  $(\nu_n-3)/2=r-1$  and  $(\nu_n-1)/2=r$ . The only signed graph in  $\mathcal{S}'_{4r+3}$  satisfying (19) is  $\Phi_{r,3}=\Gamma_{r,r,r-1,r-1}$ . For n=4r+5, instead,  $(\nu_n-2)/2=r$ , whereas the numbers  $(\nu_n-3)/2$  and  $(\nu_n-1)/2$  are not integers. Hence, the only integral 4-tuple  $(a_1,a_2,a_3,a_4)$  satisfying (19) is (r,r,r,r). In other words, the only index-minimizer in  $\mathcal{S}'_{4r+5}$  is  $\Phi_{r,5}$ .

**Proposition 4.3.** For each  $n \ge 5$  the set  $S'_n$  contains just one signed graph minimizing the index. Such graph is  $\Phi_{\{n\}}$  defined in (2).

*Proof.* Subcase 3.2.3 analyzed above makes the statement trivial when n is odd. Let n be an even integer larger than 4. For n = 6, a direct check shows that  $\lambda_1(\Phi_{1,2}) < \lambda_1(\Gamma_{0,0,0,0}^2)$ . For  $n \ge 8$  we use Proposition 3.11 and the several comparison of algebraic

connectivities performed in Section 5. More precisely, for n = 4r + 2 and r > 1, Propositions 5.6-5.8 will ensure that  $\widetilde{\Phi}_{r,2}$  has the smallest index in the set

$$\{\widetilde{\Phi}_{r,2},\Phi_{r,2},\Gamma^2_{r-1,r-1,r-1,r-1},\Gamma^2_{r,r,r-2,r-2}\}.$$

Similarly, for n = 4r + 4 and  $r \ge 1$ , Propositions 5.9 and 5.10 will suffice to prove that  $\Phi_{r,4}$  minimizes the index in the set

$$\{\Phi_{r,4}, \Gamma_{r+1,r,r-1,r-1}, \Gamma^2_{r,r,r-1,r-1}\}.$$

The next step consists in showing that no graph in  $\mathcal{S}''_n$  minimizes the index in  $\mathfrak{d}_n \sqcup \mathfrak{i}_n$ . Note that  $\mathcal{S}''_n$  is nonempty for  $n \geq 7$ . Let  $\Gamma$  be a signed graph. For every eigenvalue  $\lambda$  of  $A_{\Gamma}$ , we denote by  $\mathbf{y}_v$  the component of the  $\lambda$ -eigenvector  $\mathbf{y}$  correspondent to a fixed vertex  $v \in V(\Gamma)$ .

**Lemma 4.4.** Let w be a pendant vertex of the index-minimizer  $\tilde{\Gamma}'_n$  in  $\mathcal{S}'_n$  for  $n \geq 7$ , and let  $\mathbf{x}$  be a  $\lambda_1(\tilde{\Gamma}'_n)$ -eigenvector. Then,  $\mathbf{x}_w$  is nonzero.

*Proof.* Let v,  $\lambda$  and  $\mathbf{x}$  be a vertex of a signed graph  $\Gamma$ , an eigenvalue of  $A_{\Gamma}$  and a  $\lambda$ -eigenvector respectively. It is well known that if  $\mathbf{x}_v = 0$ , then  $\lambda$  is also an eigenvalue of  $A_{\Gamma-v}$  (see, for instance, [16]). From the eigenvalue equations, we also see that if  $\Gamma$  is in  $S'_n$  and w is a pendant vertex such that  $\mathbf{x}_w = 0$ , then  $\lambda$  is also an eigenvalue of the graph obtained by cutting the vertices of the path connecting w to the base. This fact will be repeatedly used along all the cases. For terminology, we shall always refer to Fig. 1.

Case 1.  $n = 4r + 2 \ (r \ge 2)$ .

For  $1 \leq i \leq 4$ , the graphs  $\widetilde{\Phi}_{r,2}(i)$ 's obtained by removing from  $\widetilde{\Phi}_{r,2} = \Gamma_{r,r,r-1,r-2}$  the path connecting  $w_i$  to  $u_i$  are all induced subgraph of  $U_{r,r}^-$ , whose index is  $\lambda_1(P_{2r+2})$  (see [1, Theorem 3.4]). Yet, by interlacing and [1, Theorem 3.4]

$$\lambda_1(\widetilde{\Phi}_{r,2}) \geqslant \lambda_1(\widetilde{\Phi}_{r,2} - w_1) = \lambda_1(U_{r+1,r-1,r-2}^-) > \lambda_1(P_{2r+2}).$$

Hence,  $\lambda_1(\widetilde{\Phi}_{r,2}) > \lambda_1(\widetilde{\Phi}_{r,2}(i))$  and  $\mathbf{x}_{w_i} \neq 0$  for  $1 \leqslant i \leqslant 4$ .

Case 2.  $n = 4r + 3 \ (r \ge 1)$ .

Let  $\lambda$  be the index of  $\Phi_{r,3} = \Gamma_{r,r,r-1,r-1}$ , and let  $\mathbf{x}$  be a  $\lambda$ -eigenvector. By symmetry,  $\mathbf{x}_{w_1} = \mathbf{x}_{w_2}$ ,  $\mathbf{x}_{u_1} = \mathbf{x}_{u_2}$  and  $\mathbf{x}_{u_3} = \mathbf{x}_{u_4}$ . Suppose that  $\mathbf{x}_{w_1} = 0$ . The eigenvalue equations show that  $\mathbf{x}_{w_2} = \mathbf{x}_{u_1} = \mathbf{x}_{u_2} = \mathbf{x}_v = 0$  and  $\mathbf{x}_{u_3} = -\mathbf{x}_{u_4}$ . This should be possible only if all components of  $\mathbf{x}$  were null, and this cannot occur. The cases  $\mathbf{x}_{w_i} = 0$  for i > 1 are treated similarly.

Case 3.  $n = 4r + 4 \ (r \ge 1)$ .

For  $1 \leq i \leq 4$ , let  $\Phi_{r,4}(i)$  be the graph obtained by removing from  $\Phi_{r,4} = \Gamma_{r,r,r,r-1}$  the path connecting  $w_i$  to  $u_i$ . The graphs  $\Phi_{r,4}(i)$  for i < 4 are all induced subgraph

of  $U_{r,r,r}^-$ , whose index is  $\lambda_1(P_{2r+2})$  (see [1, Theorem 3.4]), whereas  $\Phi_{r,4}(4) = U_{r+1,r,r}^-$ . Yet, by Proposition 3.9,  $\lambda_1(\Phi_{r,4}) > \lambda_1(P_{2r+2})$ . This implies that  $\lambda_1(\Phi_{r,4}) > \lambda_1(\Phi_{r,4}(i))$  for i < 4; therefore  $\mathbf{x}_{w_i} \neq 0$  for i < 4. Now, suppose by contradiction that  $\mathbf{x}_{w_4} = 0$ . This would imply  $\lambda_1(\Phi_{r,4}) = \lambda_1(U_{r+1,r,r}^-)$  which, by (11) and (12), is equivalent to  $\mu_2(H_{r+1,r+1,r+1,r}^2) = \mu_2(T_{r+2,r+1,r+1})$  against Corollary 5.5.

Case 4.  $n = 4r + 5 \ (r \ge 1)$ .

Let  $\lambda$  be the index of  $\Phi_{r,5} = \Gamma_{r,r,r,r}$ , and let  $\mathbf{x}$  be a  $\lambda$ -eigenvector. By symmetry, if  $\mathbf{x}_{w_j} = 0$  for some  $j \in \{1, 2, 3, 4\}$  then  $\mathbf{x}_{w_i} = 0$  for all  $i \in \{1, 2, 3, 4\}$ . Through the eigenvalue equation we shall infer that all components of  $\mathbf{x}$  were null, and this is not possible. Hence, the statement is proved.

**Proposition 4.5.** Let  $n \ge 7$ . For each signed graph  $\Gamma''$  in  $\mathcal{S}''_n$  there exists a graph  $\tilde{\Gamma}'$  in  $\mathcal{S}'_n$  such that  $\lambda_1(\tilde{\Gamma}') < \lambda_1(\Gamma'')$ .

Proof. Let  $\Gamma'' := X_{b_1,b_2,b_3,b_4}^p$  a graph in  $\mathcal{S}''_n$ . We consider the graph  $\Gamma' = \Gamma^p_{b+1,b_2,b_3,b_4}$  in  $\mathcal{S}'_n$  obtained by replacing the positive edge uv with the positive edge  $uw_1$  (see Fig. 7). We set  $\lambda = \lambda_1(\Gamma')$  and consider a  $\lambda$ -eigenvector  $\mathbf{x}$  of  $A_{\Gamma'}$  with  $\mathbf{x}_u \geqslant 0$ . From the eigenvalue equations we deduce

$$\mathbf{x}_{w_1} = \lambda \mathbf{x}_u; \text{ and } \mathbf{x}_v = \left(\lambda - \frac{1}{\lambda}\right) \mathbf{x}_{w_1}.$$

By definition, either  $\Phi_{1,2}$  or the graph  $U_{2,1,0}^-$  defined in [1] are induced subgraph of  $\Gamma'$ . Therefore, by interlacing,  $\lambda > (\sqrt{5} + 1)/2$ . This implies that  $\mathbf{x}_v \leq \mathbf{x}_{w_1}$ . By [1, Lemma 2.8] it follows that  $\lambda_1(\Gamma') \leq \lambda_1(\Gamma'')$ , where the inequality is surely strict if  $\mathbf{x}_u$  is nonzero. Now, if  $\Gamma'$  is an index-minimizer in  $\mathcal{S}'_n$ , then the statement comes from Lemma 4.4. Otherwise, there exists a  $\tilde{\Gamma}'_n$  in  $\mathcal{S}'_n$  such that  $\lambda_1(\tilde{\Gamma}'_n) < \lambda_1(\Gamma') \leq \lambda_1(\Gamma'')$ , as claimed.

**Proposition 4.6.** For each  $n \ge 5$ , every index-minimizer in the set  $\mathfrak{d}_n \sqcup \mathfrak{i}_n$  is switching equivalent to  $\Phi_{\{n\}}$ .

Proof. The case analysis performed in this subsection detected all potential indexminimizers. Let  $n_i$  be the order of the signed graph  $\Gamma_i$  in Fig. 5. Note that  $n_i \leq$ 8. From Table 2 in the Appendix we learn that  $\lambda_1(\Phi_{\{n_i\}}) < \lambda_1(\Gamma_i)$  for  $1 \leq i \leq$ 16,  $\lambda_1(\Phi_{\{6\}}) < \min\{\lambda_1(\Lambda_{0,0;0}^1, \lambda_1(\Gamma_{0,0,0,0}^2)\}$  and  $\lambda_1(\Phi_{\{8\}}) < \lambda_1(\Lambda_{1,1;0}^1)$ . Moreover,  $\lambda_1(\Phi_{\{10\}}) < \lambda_1(\Lambda_{2,2;0}^1) = 1.93295$ . The statement now comes from Propositions 4.3 and 4.5.

#### 4.2. A closer look to $\mathfrak{th}_n$

The entire subsection can be regarded as a proof of the following result.

**Theorem 4.7.** The inequality  $\lambda_1(\Phi_{\{n\}}) < \lambda_1(\Theta)$  holds for each  $n \ge 5$  and for each  $\Theta \in \mathfrak{th}_n$ .

It is immediately seen that Theorem 4.7 and Proposition 4.6, together with the introductory remarks at the beginning of Section 4, prove Theorem 2.1. Even when not explicitly stated, we always assume  $n \ge 5$ .

**Lemma 4.8.** Every  $\Theta \in \mathfrak{th}_n$  has two unbalanced cycles sharing precisely one edge.

*Proof.* Suppose that the base  $\hat{\Lambda}$  of a signed graph  $\Lambda$  of order n is a theta-graph. If  $\hat{\Lambda}$  does not contain two unbalanced cycles sharing precisely one edge, then  $\hat{\Lambda}$  (and  $\Lambda$  as well) contains as induced subgraph at least one balanced cycle. Thus,  $\lambda_1(\Lambda) \geq 2$ ; hence,  $\Lambda \not\in \mathfrak{th}_n$ .

For  $3 \leqslant r \leqslant s$ , let  $\Theta(C_r, C_s)$  denote the set of signed graphs whose base has two unbalanced cycles of order r and s sharing precisely one edge, and let  $\mathfrak{th} = \bigcup_{n \geqslant 4} \mathfrak{th}_n$ . We could rephrase Lemma 4.8 by saying that  $\mathfrak{th} \subset \bigcup_{3 \leqslant r \leqslant s} \Theta(C_r, C_s)$ .

**Lemma 4.9.** If  $\mathfrak{th} \cap \Theta(C_r, C_s)$  is nonempty, then  $r \leq 4$ . Moreover, if  $\mathfrak{th} \cap \Theta(C_4, C_s)$  is nonempty, then  $s \leq 6$ .

*Proof.* Let  $5 \leq r \leq s$ . The underlying graph of every  $\Theta \in \Theta(C_r, C_s)$  contains the double snake  $W_1$  (see Fig. 3) which is forbidden. For  $s \geq 7$ , a graph  $\Theta \in \Theta(C_4, C_s)$  contains a subgraph switching equivalent to the forbidden graph  $F_{13}$  in Fig. 10.

Up to switching equivalence, there are just eight signed graphs in  $\mathfrak{th} \cap \bigcup_{4 \leq r \leq s \leq 6} \Theta(C_r, C_s)$ . Referring to the notation of Fig. 8, we find

$$\Theta_{i} \in \begin{cases}
\Theta(C_{4}, C_{6}) & \text{if } i = 1; \\
\Theta(C_{4}, C_{5}) & \text{if } 2 \leqslant i \leqslant 4; \\
\Theta(C_{4}, C_{4}) & \text{if } 5 \leqslant i \leqslant 8.
\end{cases}$$

In fact, every signed graph obtained by adding an additional pendant vertex to an item in  $\mathcal{T}_{(1)} = \{\Theta_i \mid 1 \leqslant i \leqslant 8\}$ , if not in  $\mathcal{T}_{(1)}$ , has either  $T_{1,3,3}$ ,  $T_{2,2,2}$ , a double snake, or a forbidden graph in  $\{F_i \mid 13 \leqslant i \leqslant 16\}$  (see Fig. 10) among their induced subgraphs.

We now take into account the signed graphs in th containing triangles.

**Lemma 4.10.** For each  $s \ge 3$ ,  $p \ge q \ge 0$  and  $p \ne 0$ , let  $Z_{s;p}$  be the signed graph in Fig. 9, and let  $\Delta_{p,q}$  and  $\Delta'_{p,q}$  be the graphs in Fig. 11. Then,

- (i)  $\phi_A(Z_{s:p}, 2) = 4$ ;
- (ii)  $\phi_A(\Delta_{p,q}, 2) = 4;$
- (iii)  $\phi_A(\Delta'_{p,q}, 2) = 4 pq$ .

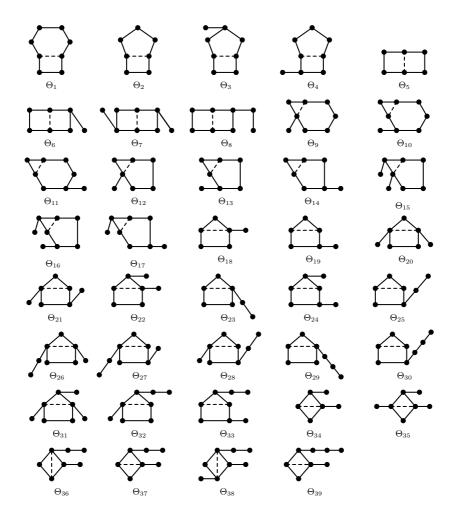


Figure 8. Some graphs in  $\mathfrak{th}_n$  for  $6 \leqslant n \leqslant 8$ .



Figure 9. The signed graphs  $Z_{s;p}$  and  $Z_{s;p}^{\prime}$ .

*Proof.* Let  $\Theta$  be a signed graph of type  $Z_{s;p}$ ,  $\Delta_{p,q}$ , or  $\Delta'_{p,q}$ , and let w denote the vertex depicted in Figg. 9 and 11. The Schwenk decomposition (3) with respect to the vertex w (see Fig. 9) gives:

$$\phi(Z_{s;p}) = \lambda \phi(C_s^u) \phi(P_{p-1}) - 2\phi(P_{s-1})\phi(P_{p-1}) - \phi(P_{p-2})\phi(C_s^u) + 2\phi(P_{p-1})\phi(P_{s-2}) - 2\phi(P_{p-1}), \quad (20)$$

$$\phi(\Delta_{p,q}) = \phi(P_p) \left(\lambda \phi(T_{1,1,q}) - 2\phi(P_{q+2}) - \phi(P_q)(\lambda^2 - 4\lambda + 2)\right) - \phi(P_{p-1})\phi(T_{1,1,q}), \quad (21)$$

and

$$\phi(\Delta'_{p,q}) = \lambda \phi(P_{p+q+3}) - \phi(P_p) \left( \phi(P_{q+2}) - 2\phi(P_{q+1}) + 2\phi(P_q) \right) - \phi(P_q) \left( \phi(P_{p+2}) - 2\phi(P_{p+1}) \right) - \phi(P_{p+1}) \phi(P_{q+1}), \quad (22)$$

where  $\phi(\Gamma)$  stands for  $\phi_A(\Gamma, \lambda)$ ,  $T_{1,1,0} := P_3$  and the pair  $(\phi(P_0), \phi(P_{-1}))$  must be read as (1,0). By plugging in 20-22  $\phi_A(C_s^u, 2) = \phi(T_{1,1,q}, 2) = 4$  and  $\phi_A(P_h, 2) = h + 1$ , we easily arrive at the three equations in the statement.

**Proposition 4.11.** For each  $s \ge 3$ ,  $p \ge q \ge 0$  and  $p \ne 0$ , the graphs  $Z_{s;p}$  and  $\Delta_{p,q}$  belong to  $\mathfrak{th}$ , whereas the only graphs of type  $\Delta'_{p,q}$  in  $\mathfrak{th}$  are  $\Delta'_{p,0}$ ,  $\Delta'_{1,1}$  and  $\Delta'_{2,1}$ .

*Proof.* Let  $\Theta$  be a signed graph of type  $Z_{s;p}$ ,  $\Delta_{p,q}$  or  $\Delta'_{p,q}$ , and let w denote the vertex depicted in Figg. 9 and 11. We observe that in all cases  $\lambda_1(\Theta - w) < 2$ . Since, by interlacing,  $\lambda_2(\Theta) < 2$ , the condition  $\lambda_1(\Theta) < 2$  is equivalent to  $\phi_A(\Theta, 2) > 0$ . The statement now follows from Lemma 4.10.

It is worthwhile to notice that  $\Delta'_{(p,0)} = Z_{3;p}$ .

**Proposition 4.12.** For every  $s \ge 3$  and  $p \ge 1$ , the index of the signed graphs  $Z'_{s;p}$  in Fig. 9 is 2.

*Proof.* Let v be the vertex of  $Z'_{s;p}$  as in Fig. 9. We set  $Z_{s;0} := C^u_s$ . By interlacing and Proposition 4.11,  $\lambda_2(Z'_{s;p}) \le \lambda_1(Z_{s;p-1}) < 2$ . The statement will be proved once we show that  $\phi_A(Z'_{s;p}, 2) = 0$ . The Schwenk decomposition (3) with respect to the vertex v (see Fig. 9) gives:

$$\phi(Z'_{s;p}) = \begin{cases} \phi(Z_{s;p-1})(\lambda^3 - 2\lambda) - \lambda^2 \phi(Z_{s;p-2}) & \text{if } p \geqslant 2, \\ \phi(C_s^u)(\lambda^3 - 2\lambda) - 2\lambda^2 \left(\phi(P_{s-1}) - \phi(P_{s-2}) + 2\right) & \text{if } p = 1, \end{cases}$$

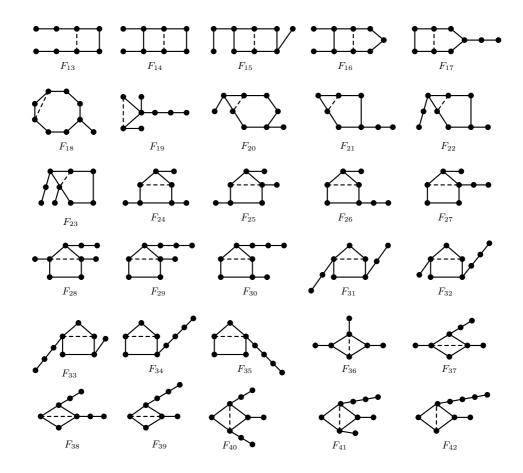


Figure 10. Further forbidden graphs.

where we have adopted the same convention as in the proof of Lemma 4.10 to denote characteristic polynomials. Recalling from Lemma 4.10 that  $\phi_A(Z_{s;p-1},2) = \phi_A(C_s^u,2) = 4$  for all  $p \ge 1$ , and knowing that  $\phi(P_h,2) = h+1$ , we see that 2 is indeed a root of the polynomial  $\phi(Z'_{s;p})$ .

For  $s \geq 3$ , we now describe the set  $\mathcal{U}_s := \Theta(C_3, C_s) \cap \mathfrak{th}$ .

**Lemma 4.13.** For  $s \ge 7$ , every  $\Theta \in \mathcal{U}_s$  is switching equivalent to  $Z_{s,p}$  for some  $p \ge 1$ .

*Proof.* Let  $s \ge 7$ . If there exists a  $\Theta \in \mathcal{U}_s$  which is not switching equivalent to any  $Z_{s;p}$ , then it contains a subgraph switching equivalent to either a graph of type  $Z'_{s;q}$  or a forbidden graph in the set  $\{T_{1,3,3}, F_6, F_{18}, F_{19}\}$ . Hence,  $\lambda_1(\Theta) \ge 2$ .

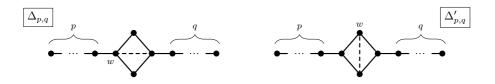


Figure 11. The signed graphs  $\Delta_{p,q}$  and  $\Delta'_{p,q}$ .

Up to switching equivalence, it turns out that

(i) 
$$U_6 = \{\Theta_i \mid 9 \le i \le 11\} \cup \{Z_{6;p} \mid p \ge 1\}$$
 (see Figg. 8 and 9);

(ii) 
$$U_5 = \{\Theta_i \mid 12 \le i \le 14\} \cup \{Z_{5,p} \mid p \ge 1\};$$

(iii) 
$$U_4 = \{\Theta_i \mid 15 \le i \le 33\} \cup \{Z_{4:p} \mid p \ge 1\};$$

(iv) 
$$\mathcal{U}_3 = \{\Theta_i \mid 34 \le i \le 39\} \cup \{Z_{3:p} \mid p \ge 1\} \cup \{\Delta_{p,q} \mid p \ge q \ge 0\} \cup \{\Delta'_{1,1}, \Delta'_{2,1}\}.$$

In fact, up to switching equivalence, every signed graph obtained by adding an additional pendant vertex to an item in  $\mathcal{T}_{(2)} = \{\Theta_i \mid 9 \leqslant i \leqslant 33\}$ , if not in  $\mathcal{T}_{(2)}$ , contains a double snake, a graph of type  $Z'_{s;q}$ , or a forbidden graph in  $\{T_{2,2,2}, F_1, F_6, F_{13}, F_i \mid 19 \leqslant i \leqslant 35\}$  (see Figg. 3 and 10). Similarly, every signed graph obtained by adding an additional pendant vertex to an item in  $\mathcal{T}_{(3)} = \{\Theta_i \mid 9 \leqslant i \leqslant 35\}$ , if not in  $\mathcal{T}_{(3)}$ , contains a double snake, a graph of type  $Z'_{3;q}$ , or a forbidden graph in  $\{F_i, \Delta'_{p,q} \mid 36 \leqslant i \leqslant 42, pq = 4\}$ .

The next proposition is the last result we need to prove Theorem 4.7.

**Proposition 4.14.** Let n be the order of  $\Theta \in \{\Delta'_{1,1}, \Delta'_{2,0}, Z_{s;p}, \Delta_{p,q} \mid p \geqslant q \geqslant 0, p \neq 0\}$ . If diam  $\Theta \leqslant \nu_n = \lfloor n/2 \rfloor$ , then

- (i)  $\Theta \in \{Z_{4;1}, \Delta_{1,0}\}$  for n = 5;
- (ii)  $\Theta \in \{Z_{5,1}, Z_{4,2}, \Delta_{1,1}, \Delta_{2,0}\}$  for n = 6;
- (iii)  $\Theta \in \{Z_{n-1;1}, Z_{n-2;2}\}$  for even n > 6;
- (iv)  $\Theta \in \{Z_{n-1:1}\}$  for odd n > 5.

*Proof.* We immediately see that  $\Delta'_{1,1}$  and  $\Delta'_{2,0}$  have order 6 and diameter  $4 > \nu_6 = 3$ . Now, let  $Z_{s;p}$  be a signed graph of order  $n = 4r + \epsilon$  with  $2 \le \epsilon \le 5$ . It is not hard to check that

diam 
$$Z_{s;p} = p + \left\lceil \frac{s}{2} \right\rceil - 1 = \begin{cases} p+k-1 \text{ for even } s = 2k\\ p+k \text{ for odd } s = 2k+1. \end{cases}$$

By studying separately the four cases

- 1) s even and  $\epsilon \in \{2,3\}$ , 2) s even and  $\epsilon \in \{4,5\}$ ,
- 3) s odd and  $\epsilon \in \{2,3\}$ , 4) s odd and  $\epsilon \in \{4,5\}$ ,

we discover that the conditions

$$s + p = n = 4r + \epsilon$$
 and  $p + \left\lceil \frac{s}{2} \right\rceil - 1 \leqslant \left\lfloor \frac{n}{2} \right\rfloor = \left\lfloor 2r + \frac{\epsilon}{2} \right\rfloor$ 

are both satisfied only if (s, p) = (n - 1, 1) and (s, p) = (n - 2, 2) when n is even, and only if (s, p) = (n - 1, 1) when n is odd. Analogously, since diam  $\Delta_{p,q} = p + q + 1$ , by distinguishing the cases  $\epsilon \in \{2, 3\}$  and  $\epsilon \in \{4, 5\}$ , we check without difficulty that the conditions

$$|V_{\Delta_{p,q}}| = p + q + 4 = n = 4r + \epsilon$$
 and  $p + q + 1 \le \left|\frac{n}{2}\right| = \left|2r + \frac{\epsilon}{2}\right|$ 

are only satisfied for 
$$\epsilon = 1$$
,  $r = 0$  and  $(p, q) = (1, 0)$ , and  $\epsilon = 3$ ,  $r = 1$  and  $p + q = 2$ , i.e.  $(p, q) = (1, 1)$  or  $(p, q) = (2, 0)$ .

We are now ready to finish the proof of Theorem 4.7. Summarizing the results gathered so far, we have proved that, up to switching equivalence,

$$\bigcup_{n \ge 5} \mathfrak{th}_n = \{\Theta_i, | 1 \le i \le 39\} \cup \{\Delta'_{1,1}, \Delta'_{2,1}, Z_{s;p}, \Delta_{p,q}, s \ge 3, p \ge q \ge 0, p \ne 0\}. \tag{23}$$

If we add to (23) the diamond  $\Delta_{0,0}$  with four vertices and two unbalanced triangles we obtain the switching equivalence representatives of all signed bicyclic graphs whose base is a theta-graph and whose index is smaller than 2.

Denoted by  $n_i$  the order of  $\Theta_i$  for  $1 \le i \le 39$  in Fig. 8, from Table 4 in the Appendix we learn that  $\lambda_1(\Phi_{(n_i)}) < \lambda_1(\Theta_i)$  for  $1 \le i \le 39$ . Now, by Corollary 3.10 and Proposition 4.6 we only need to check the inequalities  $\lambda_1(\Phi_{\{s+p\}}) < \lambda_1(Z_{s;p})$  and  $\lambda_1(\Phi_{\{p+q+4\}}) < \lambda_1(\Delta_{p,q})$  for the graphs listed in Proposition 4.14(i)-(iii). On Table 4 we read that  $\lambda_1(\Phi_{\{6\}}) < \min\{\lambda_1(\Delta_{1,1}), \lambda_1(\Delta_{2,0})\}$ . For the remaining signed graphs we distinguish three cases.

#### Case 1. n = 4r + 2.

For r = 1, a direct computation shows that  $\lambda_1(Z_{5;1}) = 1.75660$  and  $\lambda_1(Z_{4;2}) = 1.81361$  are both larger than  $\lambda_1(\Phi_{1,2}) = 1.67828$ . For  $r \ge 2$ , we consider the vertex w in Fig. 9. By interlacing and Proposition 3.9, we arrive at

$$\lambda_1(Z_{4r+1;1}) \geqslant \lambda_1(Z_{4r+1;1} - w) = \lambda_1(C_{4r+1}^u) = 2\cos\frac{\pi}{4r+1} > 2\cos\frac{\pi}{2r+4} > \lambda(\Phi_{\{4r+2\}}),$$

and

$$\lambda_1(Z_{4r;2}) \geqslant \lambda_1(Z_{4r;2} - w) = \lambda_1(C_{4r}^u) = 2\cos\frac{\pi}{4r} \geqslant 2\cos\frac{\pi}{2r+4} > \lambda(\Phi_{\{4r+2\}}).$$

Case 2. n = 4r + 4.

Again by interlacing and Proposition 3.9, we see that

$$\lambda_1(Z_{4r+3;1}) \geqslant \lambda_1(Z_{4r+3;1} - w) =$$

$$\lambda_1(C_{4r+3}^u) = 2\cos\frac{\pi}{4r+3} \geqslant 2\cos\frac{\pi}{2r+5} > \lambda(\Phi_{\{4r+4\}}), \quad \text{for all } r \geqslant 1.$$

Moreover,

$$\lambda_1(Z_{4r+2;2}) \geqslant \lambda_1(Z_{4r+2;2} - w) =$$

$$\lambda_1(C_{4r+2}^u) = 2\cos\frac{\pi}{4r+2} \geqslant 2\cos\frac{\pi}{2r+5} > \lambda(\Phi_{\{4r+4\}}), \quad \text{for all } r \geqslant 2.$$

Finally, for r = 1,  $\lambda_1(Z_{6,2}) = 1.87228 > 1.76893 = \lambda(\Phi_{\{8\}})$ .

Case 3. n = 4r + 2t + 1 with  $t \in \{1, 2\}$ .

Arguing as above,

$$\lambda_1(Z_{4r+2t;1}) \geqslant \lambda_1(Z_{4r+2t;1} - w) = \lambda_1(C_{4r+2t}^u) = 2\cos\frac{\pi}{4r+2t} \geqslant 2\cos\frac{\pi}{2r+3+t} > \lambda(\Phi_{\{4r+2t+1\}}).$$

# 5. A comparison of algebraic connectivities

In this section we compare the algebraic connectivity of some pairs of graphs of type  $T_{l_1,l_2,l_3}$  or  $H^q_{l_1,l_2,l_3,l_4}$  (see Figg. 2 and 4). The main tools for doing that is the algorithm presented in Figure 12, which may be used to determine the number of Q-eigenvalues of a given tree in any interval. It is a Q-variant of the Jacobs-Trevisan algorithm [15] originally devised for the adjacency matrix. Recently, such Q-variant has been successfully employed to compare Q-indices of quipus [5]. The algorithm is based on the diagonalization of the matrix  $Q(T) + \alpha I$ , where  $\alpha$  is a given real number. In fact, it produces a diagonal matrix D congruent to  $Q(T) + \alpha I$ . Consequently, the following result holds.

**Theorem 5.1.** [5, Theorem 3.1] Let T be a tree and consider  $Diagonalize(T, -\alpha)$ . Let  $(d_v)_{v \in V(T)}$  be the sequence it produces. Then, the diagonal matrix  $D = \operatorname{diag}(d_v)_{v \in V(T)}$  is congruent to  $Q(T) - \alpha I$ . So the number of (positive | negative | zero) entries in  $(d_v)_{v \in V(T)}$  is equal to the number of eigenvalues of Q(T) that are (greater than  $\alpha$  | smaller than  $\alpha$  | equal to  $\alpha$ ).

Figure 12. The algorithm  $Diagonalize(T, -\alpha)$ .

```
Input: tree T, scalar \alpha Output: diagonal matrix D congruent to A(T) + \alpha I Algorithm Diagonalize(T,\alpha) initialize d(v) := \deg(v) + \alpha, for all vertices v order vertices bottom up for k=1 to n if v_k is a leaf then continue else if d(c) \neq 0 for all children c of v_k then d(v_k) := d(v_k) - \sum \frac{1}{d(c)}, summing over all children of v_k else select one child v_j of v_k for which d(v_j) = 0 d(v_k) := -\frac{1}{2} d(v_j) := 2 if v_k has a parent v_l, remove the edge v_k v_l. end loop
```

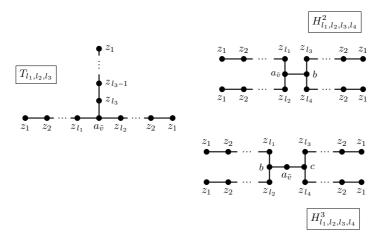


Figure 13. Valued T-shape and H-shape trees after running the algorithm

Note that the algorithm requires the choice in T of a root  $\tilde{v}$ , which is the last vertex to be processed. For each  $v \neq \tilde{v}$ , the final output  $d_v$  is given by the value d(v) computed on line 6 of the algorithm if  $d(v) \neq 0$ . The types of trees on which the algorithm will be implemented are depicted in Fig. 13.

**Lemma 5.2.** Let T be one of the trees in Fig. 13, and let l be the maximum among the labels of the  $z_i$ 's involved. Once we execute  $Diagonalize(T, -\alpha)$  with  $0 < \alpha < 1$ , and  $z_h > 0$  for a fixed  $h \le l - 1$ , then  $z_{h+1} < z_h$ .

*Proof.* By choosing as root the vertex  $\tilde{v}$  with output  $a_{\tilde{v}}$ , we arrive at the following recursive relations

$$\begin{cases} z_1 = 1 - \alpha \\ z_{i+1} = 2 - \alpha - \frac{1}{z_i}, & i = 1, \dots, l - 1. \end{cases}$$

If  $z_i > 0$ , the inequality  $z_{i+1} < z_i$  is equivalent to  $z_i^2 - (2 - \alpha)z_i + 1 > 0$ , which actually holds. In fact,  $\Delta = (2 - \alpha)^2 - 4$  is negative.

The following lemma is known to the experts and it is a consequence of [18, Theorem 3.1].

**Lemma 5.3.** Let T and T' be two trees. If  $T \subseteq T'$ , then  $\mu_2(T) \geqslant \mu_2(T')$ .

**Proposition 5.4.** For each  $r \ge 1$ ,  $\mu_2(T_{r+2,r+1,r+1}) > \mu_2(H_{r+1,r+1,r+1,1}^2)$ .

*Proof.* Let  $T := T_{r+2,r+1,r+1}$ ,  $T' = H_{r+1,r+1,r+1,1}^2$  and  $T'' = T_{3,2,2}$ . Since  $T'' \subseteq T \subset T'$ , by Lemma 5.3 or, equivalently, by Proposition 3.11 and interlacing,

$$\mu_2(T') \leqslant \mu := \mu_2(T) \leqslant \mu_2(T'') = 0.2434.$$
 (24)

In order to show that the first inequality in (24) is strict, we are going to execute  $D:=Diagonalize(T,-\mu)$  first, and  $D'=Diagonalize(T',-\mu)$  afterwards. Our claim will be proved once we show that D' provides at least two negative outputs. In the case at hand, the graph on the left of Fig. 13 has  $(z_{l_1},z_{l_2},z_{l_3})=(z_{r+2},z_{r+1},z_{r+1})$ . Since T has only one Q-eigenvalue less than  $\mu_2(T)$ , at its completion the algorithm D produces (at least) a zero and exactly one negative output. Whilst the D is processing, the case  $z_i=0$  for some i cannot occur. In fact, the appearance of 0 among  $z_1,\ldots,z_{r+1}$  would produce two negative outputs, and  $z_{r+2}=0$  (once we know that  $z_i\neq 0$  for i< r+2) would produce no zero outputs. Hence,  $z_{r+2}<0$  and

$$a_{\tilde{v}}(T) = (3 - \mu) - \frac{2}{z_{r+1}} - \frac{1}{z_{r+2}} = 0.$$
 (25)

By plugging in (25)  $z_{r+2} = 2 - \mu - z_{r+1}^{-1}$ , it turns out that  $z_{r+1}$  is the smallest root of  $(5 - 5\mu + \mu^2)x^2 - (7 - 3\mu)x + 2$ , i.e.

$$z_{r+1} = \frac{7 - 3\mu - \sqrt{9 - 2\mu + \mu^2}}{2(5 - 5\mu + \mu^2)}.$$
 (26)

From  $z_{r+2} = z_{r+1}((2-\mu)z_{r+1}-1)^{-1} < 0$ , we deduce  $z_{r+1} < (2-\mu)^{-1}$ , therefore, when we execute D', the output correspondent to the non-root of degree 3 is

$$b = 3 - \mu - \frac{1}{z_{r+1}} - \frac{1}{z_1} < 3 - \mu + (\mu - 2) - (1 - \mu)^{-1} = -\mu/(1 - \mu) < 0,$$

and with the aid of Wolfram Alpha we discover that the output at the root of T'

$$(3-\mu) - \frac{2}{z_{r+1}} - \frac{1}{b} = (3-\mu) - \frac{2}{z_{r+1}} + \frac{(1-\mu)z_{r+1}}{(1-\mu) - (2-4\mu + \mu^2)z_{r+1}}$$

is negative as well for  $\mu \in (0, 0.25)$  when we plug (26) in it.

Corollary 5.5. For each  $r \ge 1$ ,  $\mu_2(T_{r+2,r+1,r+1}) > \mu_2(H_{r+1,r+1,r+1,r}^2)$ .

*Proof.* Since  $H_{r+1,r+1,r+1,1}^2 \subseteq H_{r+1,r+1,r+1,r}^2$ , from Lemma 5.3 and Proposition 5.4 we immediately obtain

$$\mu_2(T_{r+2,r+1,r+1}) > \mu_2(H_{r+1,r+1,r+1,1}^2) \geqslant \mu_2(H_{r+1,r+1,r+1,r}^2).$$

The next three propositions compare the algebraic connectivity of H-shape trees with 4r + 3 vertices.

**Proposition 5.6.** For each  $r \ge 2$ ,  $\mu_2(H_{r+1,r,r,r}^2) < \mu_2(H_{r+1,r+1,r,r-1}^2)$ .

*Proof.* We set  $T(r) := H_{r+1,r,r,r}^2$ ,  $T'(r) := H_{r+1,r+1,r-1,r-2}^2$ , and  $\mu := \mu_2(T(r))$ . For  $r \in \{2,3\}$  the statement comes from a direct computation.

Let  $r \ge 4$ . The proof first requires the execution of  $D:=Diagonalize(T(r), -\mu)$ . Since  $T(4) \subseteq T(r)$ , Lemma 5.3 yields  $\mu := \mu_2(T(r)) \le \mu_2(T(4)) = 0.07165 < 0.0844$ . The importance of this bound will be clear later on.

Note that D produces (at least) one zero output and just one negative final value; therefore,  $z_i > 0$  for  $0 \le i \le r$ . We also have  $z_{r+1} = (2 - \mu) - z_r^{-1} > 0$ . Otherwise  $z_r^{-1} \le 2 - \mu$ , and D would produce at least two negative outputs: one along the first H-ray (or at the root if  $z_{r+1} = 0$ ) and

$$b = 3 - \mu - 2z_r^{-1} \le (3 - \mu) - (4 - 2\mu) < 0.$$

When b is firstly processed, it cannot be zero. Otherwise the outputs at the two vertices of degree 3 would be 2 and -1/2, and no zero output would come out.

So far, we have proved that  $z_i > 0$  for  $1 \le i \le r+1$  and  $b = 3 - \mu - 2z_r^{-1} < 0$ . From  $z_{r+1} > 0$  and b < 0, we deduce

$$(2-\mu)^{-1} < z_r < 2(3-\mu)^{-1}. (27)$$

A straightforward manipulation shows that  $a(\tilde{v}) = 3 - \mu - z_r^{-1} - z_{r+1}^{-1} - b^{-1}$  is zero if and only if  $f_{\mu}(z_r) = 0$ , where

$$f_{\mu}(x) = (13 - 19\mu + 8\mu^2 - \mu^3)x^3 - (24 - 21\mu + 4\mu^2)x^2 + (13 - 5\mu)x - 2. \tag{28}$$

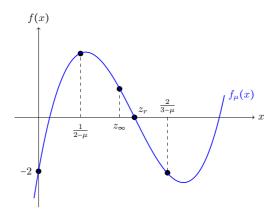


Figure 14. The function  $f_{\mu}(x)$ 

As a consequence of (7) and (12), when  $r \to \infty$ ,  $\mu$  tends to 0. Thus, by (27) and (28),  $z_r$  tends to  $z_{\infty} = (11 + \sqrt{17})/26$ , which is the only root of  $f_0(x)$  in the interval (1/2, 3/2). Condition  $\mu < 0.0844$  (holding for  $r \ge 4$ ) ensures that  $z_{\infty}$  belongs to the interval  $(1/(2 - \mu), 2/(3 - \mu))$ . Moreover,

$$f_{\mu}(z_{\infty}) = -\frac{1}{4394} \left( (95\sqrt{17} + 473)\mu^2 - 4(47\sqrt{17} + 49)\mu - (353\sqrt{17} + 555) \right)$$

is positive and belongs to the interval (0.0458, 0.052). The contour plot of the function  $f_{\mu}(x)$  is sketched in Fig. 14. It takes into account the equalities  $f_{\mu}(1/(2-\mu)) = (1-\mu)/(2-\mu)^3 > 0$  and  $f_{\mu}(2/(3-\mu)) = -4(1-\mu)/(3-\mu)^3 < 0$ . Since the number

$$f_{\mu}\left(\frac{\sqrt{5}-1}{2}\right) = -\frac{1}{2}\left(2(\sqrt{5}-2)\mu^3 + 4(11-5\sqrt{5})\mu^2 + 16(4\sqrt{5}-9)\mu - 63\sqrt{5} + 141\right)$$

is negative for  $\mu < 0.0844$ , we also infer by Fig. 14 that

$$0 < z_{\infty} < z_r < (\sqrt{5} - 1)/2. \tag{29}$$

We now consider the graph T'(r) and execute  $D':=Diagonalize(T'(r), -\mu)$ , proving that it just gives one negative output; namely b(T'). We already know that the  $z_i$ 's are all positive for  $1 \le i \le r+1$ , and

$$b(T') = 3 - \mu - z_r^{-1} - z_{r-1}^{-1} = 3 - \mu - z_r^{-1} + z_r - (2 - \mu)$$
  
=  $z_r^{-1}(z_r^2 + z_r - 1)$ .

This number is negative by (29). The output corresponding to the root is

$$a_{\tilde{v}}(T') = 3 - \mu - 2z_{r+1}^{-1} - b(T')^{-1} = \frac{\Omega(z_r)}{(z_r^2 + z_r - 1)((2 - \mu)z_r + 1)}$$

where

$$\Omega(x) = (\mu^2 - 5\mu + 4)x^3 + (\mu^2 - 3\mu + 1)x^2 - (\mu^2 - 6\mu + 6)x + 3 - \mu.$$

The proof will be over once we show that  $a_{\tilde{v}}(T') > 0$  or, equivalently,  $\Omega(z_r) < 0$ . By the Descartes's rule of signs, the polynomial  $\Omega(x)$  has two positive roots, but only one of them belongs to the interval  $((2-\mu)^{-1}, 1)$ , since

$$\Omega(1/(2-\mu)) = 2(2-\mu^3)(\mu^3 - 3\mu + 1) > 0$$
, and  $\Omega(1) = -\mu(3-\mu) < 0$ .

With the aid of Wolfram Alpha, we compute

$$\Omega(z_{\infty}) = -\frac{1}{4394} \left( 3(23\sqrt{17} - 163)\mu^2 + 2(55\sqrt{17} + 852)\mu - 777\sqrt{17} + 3023 \right)$$

which is negative for  $\mu < 0.0844$ . As claimed,  $\Omega(z_r) < 0$ . In fact,

$$z_r \in (z_{\infty}, 2(3-\mu)^{-1}) \subset (z_{\infty}, 1),$$

an interval along which  $\Omega(x)$  is always negative.

**Proposition 5.7.** For each  $r \ge 1$ ,  $\mu_2(H_{r+1,r,r,r}^2) > \mu_2(H_{r,r,r,r}^3)$ .

Proof. A direct check suffices to prove the statement for  $r \in \{2,3\}$ . Let now  $r \geqslant 4$ . We set once again  $\mu := \mu_2(H)$ , where  $H =: H^2_{r+1,r,r,r}$  and use some results obtained along the previous proof to execute  $D_{H'} := Diagonalize(H', -\mu)$ , where  $H' := H^3_{r,r,r,r}$  (see the H-shape tree on the right in Fig. 13). In fact, we already know that  $z_i > 0$  for all  $i \leqslant r+1$ , and  $b(H) := 3 - \mu - 2z_r^{-1} < 0$ . Now, the numbers b(H') and c(H') correspondent to the two vertices of degree 3 in H' are both equal to b(H). The presence of at least two negative outputs for  $D_{H'}$  prove the statement.

**Proposition 5.8.** For each  $r \ge 2$ ,  $\mu_2(H_{r+1,r+1,r,r-1}^2) > \mu_2(H_{r+1,r+1,r-1,r-1}^3)$ .

Proof. We set  $\tilde{T}(r) := H_{r,r-1,r+1}^2$  (the root we are choosing is adjacent to H-rays of different length),  $\tilde{T}'(r) := H_{r+1,r+1,r-1,r-1}^3$ , and  $\mu := \mu_2(\tilde{T}(r))$ . Since  $\mu_2(\tilde{T}(2)) = 0.18216$ , by Lemma 5.3 we know that  $\mu \leq 0.18216$  for every  $r \geq 2$ .

The proof first requires the execution of  $\tilde{D}$ :=Diagonalize( $\tilde{T}(r)$ ,  $-\mu$ ). Since many arguments are similar to the ones used along the proof of Proposition 5.6, we shall skip some details. We know that among the final values produced by  $\tilde{D}$  at least one is zero and precisely one is negative; therefore  $z_i > 0$  for all  $i \leq r$ . Note that  $z_{r+1}$  is positive as well: if along the process  $z_{r+1} = 0$ , then the final outputs at the two vertices of degree 3 would be both negative.

Now, by Lemma 5.2, the numbers

$$b(\tilde{T}(r)) = 3 - \mu - 2z_{r+1}^{-1} = \frac{z_r}{z_r^2 + z_r - 1}$$
(30)

and  $3-\mu-z_r^{-1}-z_{r-1}^{-1}$  cannot be both zero. Thus,  $b(\tilde{T}(r))$  is the (necessarily negative) output correspondent to the non-root vertex of degree 3, whereas the output at the root is

$$a_{\tilde{v}}(\tilde{T}(r)) = 3 - \mu - z_r^{-1} - z_{r-1}^{-1} - b(\tilde{T}(r))^{-1} = 0.$$

Since  $b(\tilde{T}(r)) < 0$ , Equation (30) shows that  $z_r < (\sqrt{5} - 1)/2$ . By expressing  $a_{\tilde{v}}(\tilde{T}(r))$  only in terms of  $z_r$  and  $\mu$ , we discover that  $z_r$  is the only root of

$$g_{\mu}(x) = (4 - 5\mu + \mu^2)x^2 - (1 + 3\mu - \mu^2)x^2 - (6 - 6\mu + \mu^2)x + 3 - \mu$$

belonging to the interval (0,1). In fact, the polynomial has a negative root,  $g_{\mu}(0) > 0$  and  $g_{\mu}(1) = -\mu(3-\mu) < 0$ . We also deduce that the function  $g_{\mu}(x)$  is positive for  $x \in (0, z_r)$  and negative for  $x \in (z_r, 1)$ .

When  $r \to \infty$ ,  $z_r$  tends to  $z_{\infty} = (\sqrt{57} - 3)/8$ , which is the smallest positive root of  $g_0(x)$ . We observe that  $z_r > z_{\infty}$  since the number

$$g_{\mu}(z_{\infty}) = \frac{\mu}{128} \left( (45 - 7\sqrt{57})\mu + 27\sqrt{57} - 137 \right)$$

is positive.

We now execute  $\tilde{D}':=Diagonalize(\tilde{T}'(r), -\mu)$ . The proof will be over once we show that D' has at least two negative outputs. We already know that  $z_i > 0$  for all  $i \leq r+1$ . Let  $b(\tilde{T}'(r))$  and  $c(\tilde{T}'(r))$  denote the outputs of D' in correspondence of the two vertices of degree 3 (see Fig. 13). We have

$$b(\tilde{T}'(r)) = b(\tilde{T}(r)) = 3 - \mu - 2z_{r+1}^{-1} < 0.$$

On the contrary,

$$c(\tilde{T}'(r)) = 3 - \mu - 2z_{r-1}^{-1} = 2z_r + \mu - 1$$

is positive, since  $z_r > z_\infty > 0.568 > (1-\mu)/2$ . The last step consists in showing that  $a_{\tilde{v}}(\tilde{T}'(r)) = 2 - \mu - b(\tilde{T}'(r))^{-1} - c(\tilde{T}'(r))^{-1}$  is negative. After some calculations, it turns out that

$$a_{\tilde{v}}(\tilde{T}'(r)) = -\frac{\Upsilon_{\mu}(z_r)}{(2z_r + \mu - 1)(3 - \mu - z_r(4 - 5\mu + \mu^2))}$$

where the denominator is positive and

$$\Upsilon_{\mu}(x) = 2(2-\mu)(3-5\mu+\mu^2)x^2 - (20-34\mu+23\mu^2-8\mu^3+\mu^4)x + 8-11\mu+6\mu^2-\mu^3.$$

For  $0 < \mu < 0.18216$ ,  $\Upsilon_{\mu}(x)$  is a facing up parabola with two positive roots. Furthermore,  $\Upsilon_{\mu}(0) > 0$ ,  $\Upsilon_{\mu}(1) < 0$ , and

$$\Upsilon_{\mu}\left(\frac{\sqrt{5}-1}{2}\right) = \frac{1}{2} \cdot \left(72 - 32\sqrt{5} - 2(30\sqrt{5} - 67)\mu - (37\sqrt{5} - 77)\mu^2 + 2(5\sqrt{5} - 8)\mu^3 - (\sqrt{5} - 1)\mu^4\right) > 0$$

This implies that  $\Upsilon_{\mu}(x)$  is always positive in the interval  $(0, (\sqrt{5}-1)/2)$ . In particular, it is positive when evaluated in  $z_r$ .

The remaining two propositions compare the algebraic connectivity of H-shape trees with 4r + 5 vertices.

**Proposition 5.9.** For each  $r \ge 1$ ,  $\mu_2(H_{r+1,r+1,r+1,r}^2) > \mu_2(H_{r+2,r+1,r,r}^2)$ .

Proof. For  $r \in \{2,3\}$  the statement comes from a direct computation. Let  $r \geqslant 4$ . We set  $T(r) := H^2_{r+1,r,r+1,r+1}$  (this notation suggests that the chosen root is adjacent to H-rays of different length),  $T'(r) := H^2_{r+1,r+1,r-1,r-2}$ , and  $\mu := \mu(T(r))$ . The proof initially requires the execution of  $D := Diagonalize(T(r), -\mu)$ . Since  $T(4) \subseteq T(r)$ ,  $\mu := \mu_2(T(r)) < \mu_2(T(4)) = 0.06162 < 0.07$ . Since D produces just one negative output,  $z_i > 0$  for  $1 \leqslant i \leqslant r+1$ , and the root value  $a_{\bar{v}}(T(r))$  is zero. As a consequence of Lemma 5.2 the numbers

$$\hat{b} = 3 - \mu - 2z_{r+1}^{-1}$$
 and  $\hat{a} = 3 - \mu - z_r^{-1} - z_{r+1}^{-1}$ 

cannot be both zero. The number  $\hat{a}$  would compute the root value  $a_{\tilde{v}}(T(r))$  if it were zero  $\hat{b}$ , the first number computed by the algorithm in correspondence of the non-root of degree 3. In other words, we surely have

$$b = \hat{b} < 0$$
 and  $a_{\tilde{v}}(T(r)) = \hat{a} - b^{-1} = 0$ .

Replacing  $-z_r^{-1}$  with  $z_{r+1}-2+\mu$  in the equation  $b^{-1}=\hat{a}$ , we arrive at  $b=z_{r+1}(z_{r+1}^2+z_{r+1}-1)^{-1}$ . Knowing that b is negative, we discover that  $0 < z_{r+1} < \hat{q} := (\sqrt{5}-1)/2$ . Furthermore, by equating

$$3 - \mu - \frac{2}{z_{r+1}} = \frac{z_{r+1}}{z_{r+1}^2 + z_{r+1} - 1},$$

it turns out that  $z_{r+1}$  is the unique root of the polynomial

$$h_{\mu}(x) = (3 - \mu)x^3 - \mu x^2 - (5 - \mu)x + 2$$

in the interval  $(0,\hat{q})$ ; in fact, the Descartes' rule of signs says that  $h_{\mu}(x)$  has two positive roots, and precisely one of them is larger than  $\hat{q}$  since  $h_{\mu}(0) = 2$  and  $h_{\mu}(\hat{q}) = -(3-\sqrt{5})/2$ .

We now execute  $D':=Diagonalize(T'(r), -\mu)$ . We already realized that  $z_i > 0$  for  $i \leq r+1$ , whereas

$$z_{r+2} = 2 - \mu - z_{r+1}^{-1} < 0 \iff z_{r+1} < (2 - \mu)^{-1},$$

and the latter is precisely the case since

$$h_{\mu}\left(\frac{1}{2-\mu}\right) = 1 - \frac{9 - 9\mu + 2\mu^2}{(2-\mu)^3}$$

is negative for  $\mu \in (0,1)$ . The proof ends once we show that D' has at least a second negative output. Let us compute

$$b(T') = 3 - \mu - 2z_r^{-1} = 3 - \mu + 2(z_{r+1} - (2 - \mu)) = 2z_{r+1} - (1 - \mu).$$

This number is negative, since

$$h_{\mu}\left(\frac{1-\mu}{2}\right) = -\frac{1-12\mu - 12\mu^2 + 8\mu^3 - \mu^4}{8}$$

is negative for  $\mu < 0.07$ , implying that  $z_{r+1} < (1 - \mu)/2$ .

The *H*-shape trees involved in Propositions 5.6 and 5.9 are obtained one from another through a graph perturbation called *shifting* in [8], yet the sufficient conditions on the Fiedler vector considered in [8, Lemma 7] guaranteeing the inequality in the two statements does not hold.

**Proposition 5.10.** For each  $r \ge 1$ ,  $\mu_2(H_{r+1,r+1,r+1,r}^2) > \mu_2(H_{r+1,r+1,r,r}^3)$ .

Proof. For  $r \in \{2,3\}$  the statement comes from direct computations. Let now  $r \geq 4$ ,  $\mu := \mu_2(H_{r+1,r+1,r+1,r}^2)$  and  $T''(r) = H_{r+1,r+1,r,r}^3$  (see the *H*-shape tree on the right in Fig. 13). In order to execute the algorithm  $D'' := Diagonalize(T''(r), -\mu)$ , we acquire several data from the proof of Proposition 5.9. We know that  $z_i > 0$  for all  $i \leq r+1$ ,  $3-\mu-2z_r^{-1} < 0$  and  $3-\mu-2z_{r+1}^{-1} < 0$ . Since the latter two numbers are the output values processed by D'' for b(T''(r)) and c(T''(r)) (see Fig. 13), the algorithm D'' has (at least) two negative outputs, proving the statement.

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# Appendix: Indices of small graphs in $\mathfrak{B}_n^*$

Table 1. Indices of graphs of type (2) up to 10 vertices.

$\overline{n}$	5	6	7	8	9	10
Γ	$\Phi_{0,5}$	$\Phi_{1,2}$	$\Phi_{1,3}$	$\Phi_{1,4}$	$\Phi_{1,5}$	$\widetilde{\Phi}_{2,2}$
$\lambda_1$	$\frac{\sqrt{17}-1}{2}$	1.67828	1.69353	1.76893	1.79129	1.81784

Table 2. Indices of some 'small' graphs considered along the paper

Graph	$\lambda_1$	Graph	$\lambda_1$	Graph	$\lambda_1$	Graph	$\lambda_1$
n=5		n = 7		n = 8		n = 8 (continuation)	
$\Phi_{0,1}$	1.56155	$\Phi_{1,3}$	1.69353	$\Phi_{1,3}$	1.76893	$\Theta_{11}$	1.97446
$\Delta_{1,0}$	1.74912	$\Gamma_1$	1.90321	$\Gamma_2$	1.96607	$\Theta_{15}$	1.97121
		$\Gamma_5$	1.94242	$\Gamma_3$	1.97722	$\Theta_{16}$	1.97597
		$\Gamma_{10}$	1.95546	$\Gamma_4$	1.98010	$\Theta_{17}$	1.97722
n = 6		$\Gamma_{13}$	1.96202	$\Gamma_6$	1.97280	$\Theta_{26}$	1.96255
$\Phi_{1,2}$	1.67828	$\Theta_2$	1.87939	$\Gamma_7$	1.97926	$\Theta_{27}$	1.97086
$\Gamma_9$	1.90321	$\Theta_6$	1.90211	$\Gamma_8$	1.98166	$\Theta_{28}$	1.97280
$\Lambda^{1}_{0,0;0}$	1.81361	$\Theta_{12}$	1.92103	$\Gamma_{11}$	1.98227	$\Theta_{29}$	1.98011
$\Gamma^2_{0,0,0,0}$	$\sqrt{3}$	$\Theta_{13}$	1.93230	$\Gamma_{12}$	1.98407	$\Theta_{30}$	1.98237
$\Theta_5$	$\sqrt{3}$	$\Theta_{14}$	1.93543	$\Gamma_{14}$	1.98595	$\Theta_{31}$	1.95197
$\Theta_{18}$	1.84943	$\Theta_{20}$	1.87939	$\Gamma_{15}$	1.98708	$\Theta_{32}$	1.97825
$\Theta_{19}$	1.87112	$\Theta_{21}$	1.92022	$\Gamma_{16}$	1.98552	$\Theta_{33}$	1.98095
$\Theta_{34}$	1.89420	$\Theta_{22}$	1.93543	$\Lambda^{1}_{1,1;0}$	1.89761	$\Theta_{38}$	1.97908
$\Delta_{1,1}$	1.79129	$\Theta_{23}$	1.94011	$\Theta_1$	1.95630	$\Theta_{39}$	1.98460
$\Delta_{2,0}$	1.85133	$\Theta_{24}$	1.94551	$\Theta_3$	1.93894		
$\Delta'_{1,1}$	1.90321	$\Theta_{25}$	1.94781	$\Theta_4$	1.95069		
$\Delta'_{2,0}$	1.86620	$\Theta_{35}$	1.94341	$\Theta_7$	1.95630		
,		$\Theta_{36}$	1.95423	$\Theta_8$	1.96962		
		$\Theta_{37}$	1.95546	$\Theta_9$	1.96884		
				$\Theta_{10}$	1.97230		