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Spectral ordering and 2-switch transformations

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Abstract

We address the problem of ordering trees with the same degree sequence by their spectral radii. To achieve that, we consider 2-switch transformations which preserve the degree sequence and establish when the index decreases. Our main contribution is to determine a total ordering of a particular family by their indices according to a given parameter related to sizes in the tree.

1 Introduction

Giving a graphical degree sequence, a general, natural, and well-studied problem is to determine, with respect to a given parameter, the extremal members in the family of graphs satisfying this degree sequence.

The main purpose of this note is to address the problem of finding extremal members in families of graphs having the same degree sequence, with respect to the *spectral radius (or index)*, which is the largest eigenvalue of the adjacency matrix. We remark that this problem has been studied in great generality in the celebrated paper by T. Biyikoğlu and J. Leydold [5], where the authors show that, in the maximum element, the degree sequence is non-increasing with respect to an ordering of the vertices induced by breadth-first search that is consistent with the eigenvector associated with the index. In [1], the authors determined the tree having maximum spectral radius among all caterpillar with a fixed degree sequence.

As a way to illustrate how this class of problems may be approached, we study how the spectral radius varies, upon transformations that preserve the degree, in the family $\mathfrak{F}(n)$ of trees given in Figure 1. The technique we use is a powerful algorithmic tool that allows one to compare the indices of two trees without computing them. Our main result is a total ordering in this family and, as a consequence, we obtain the extremal members.

We believe that this result is remarkable, since it is quite unusual to obtain a total order by any graph parameter. Spectral parameters have been used to classify many families, however it is rare that a total order is obtained. As examples, we refer to the papers [2, 3, 6, 9, 12, 13, 14], where the ordering of graphs by the index is studied.

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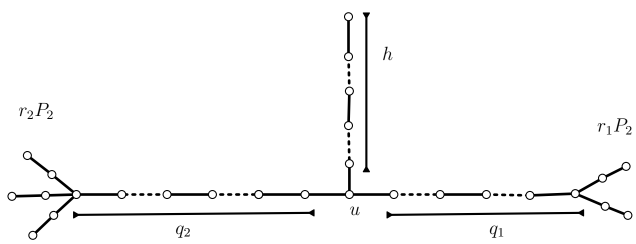

Figure 1: The family of trees $\mathfrak{F}(n)$.

The remaining of the paper is as follows. In order to explain that the family we study is not arbitrary, we devote the rest of this introduction to justify our choice. In Section 2, we define the family $\mathfrak{F}(n)$ and the transformations we perform. Moreover, we explain our powerful technique to obtain the order, that is based on an algorithmic tool, allowing to compare indices of trees without computing them. In Section 3 we obtain necessary analytical properties of some recurrence relations that appear in our comparison method. In Section 4 we show how the spectral radius varies upon the transformations. In Section 5, we use the results to obtain a total ordering in $\mathfrak{F}(n)$.

1.1 Motivation for choosing the family

We start by introducing some notation from [11] which is specially useful to represent the trees in the family $\mathfrak{F}(n)$. In that paper, it was proven that the number of Laplacian eigenvalues less than the average degree $2 - \frac{2}{n}$ of a tree having n vertices is at least $\lceil \frac{n}{2} \rceil$. We remark that pendant paths of length 2 play an important role there and serve as a motivation for our choice.

Let T be a tree with n vertices, and let u be a vertex of degree at least ℓ of T having $\ell \geq 1$ pendant paths attached at u. We denote the *sum* of pendant paths attached at u by $P(u) = P_{q_1} \oplus \cdots \oplus P_{q_\ell}$, as illustrated in Figure 2. The number of edges in each path is denoted by $\sharp P_q = q$. A subgraph obtained by a vertex u attached to $r \geq 1$ paths of

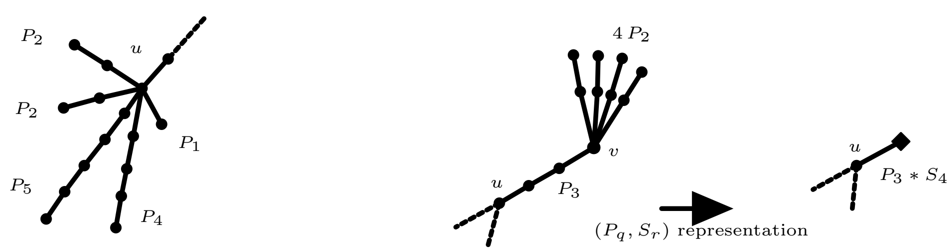

Figure 2: Vertex u with $P(u) = P_1 \oplus 2P_2 \oplus P_4 \oplus P_5$ (left) and (P_q, S_r) representation of a generalized pendant path (right).

length 2 is called a *sun with r rays* and denoted by S_r. To simplify the representation, we use the concatenation symbol and write $P_q * S_r$. To further simplify the graphic part of the representation, we will use a black square ■ to represent a pendant sun S_r attached to a vertex, and a single edge to represent the entire path P_q, omitting the r pendant P_2's and the q vertices. We will refer to this as the (P_q, S_r) *representation* of this generalized pendant path $P_q * S_r$, as shown in Figure 2 (right). We can consider $q = 0$ for paths P_q of length 0, as well as $r = 0$ for no pendant S_r. However, we do *not* allow both $r = q = 0$ simultaneously. We say a vertex u is a starlike vertex if it has degree ≥ 3 and has at least two generalized pendant paths attached to it. Using this notation, we can write any tree T having a single starlike vertex u as $T = u + P_{q_1} * S_{r_1} \oplus \cdots \oplus P_{q_\ell} * S_{r_\ell}$ where $\ell \geq 1$.

In particular, any member of $\mathfrak{F}(n)$, as in the Figure 1, has a single starlike vertex u and is represented as

$$T = u + P_h * S_0 \oplus P_{q_1} * S_{r_1} \oplus P_{q_2} * S_{r_2},$$

for $h, q_1, q_2 \geq 2$.

Our choice of the family is related to the fact that we would like to study the spectral radius ordering on trees having a single starlike vertex. We notice that the general family of trees $\mathfrak{H}$ with just one starlike vertex in this notation is given by,

$$\mathfrak{H} := \{T \,|\, T = u + P_h * S_{r_0} \oplus P_{q_1} * S_{r_1} \oplus P_{q_2} * S_{r_2},\ q_0, q_1, q_2 \geq 0, r_0, r_1, r_2 \geq 0\}.$$

In this generality, our tool becomes too involved and, hence, in order to simplify the computations and to obtain symmetry, we have chosen to study a special case of this family $\mathfrak{H}$, where we replace S_{r_0} by S_0 (no pendant P_2's on the path P_h).

We observe that the results of this note may be seen as a generalization of the total ordering of starlike trees obtained in [13], which are tree with a single vertex of degree ≥ 3. In the above notation starlike trees are written as $u + P_1 * S_0 \oplus \cdots \oplus P_m * S_0$, for $m \geq 3$.

2 A family and our tool

In this section we define the family which we will determine a spectral radius ordering when performing a degree preserving operation, as well as an algorithmic tool that we believe it is powerful for this class of problems.

2.1 Our Family

By definition, the family $\mathfrak{F}(n)$ contains all trees depicted in Figure 1 fulfilling the following constraints.

1) $q_1, q_2, h \geq 2$;

2) $r_1, r_2 \geq 2$ and $r_1 < r_2$;

Notice that, in this case, the number of vertices is $n = |T| = 1 + h + q_1 + q_2 + 2(r_1 + r_2) \geq 7 + 2(r_1 + r_2) \geq 17$.

We are interested in ordering by the index (spectral radius) the trees with a fixed degree sequence, in $\mathfrak{F}(n)$. As a particular case, we obtain the extreme members of the family, that is, the trees in $\mathfrak{F}(n)$ having largest and minimum spectral radius. The degree sequence of $T \in \mathfrak{F}(n)$ is given by

$$d := [r_1 + 1, r_2 + 1, 3, 2^{n-(r_1+r_2)-4}, 1^{r_1+r_2+1}].$$

In order to keep the degree sequence we fix $r_2 > r_1 \geq 2$. In this way each element in $\mathfrak{F}(n)$, with n vertices and degree sequence d is uniquely determined by the 3-tuple $[h, q_1, q_2]$ that is,

$$\mathfrak{F}(n) := \{T = [h, q_1, q_2] \mid h + q_1 + q_2 = n - 1 - 2(r_1 + r_2)\}.$$

Now we consider two types of transformations on $T = [h, q_1, q_2] \in \mathfrak{F}(n)$. Later, in Section 4, we determine how to order, by their spectral radii, the trees obtained by these operations. These transformations are within the realm of *2-switch transformations*. For a graph $G = (V, E)$ having four distinct vertices $a, b, c, d \in V$ such that $ab, cd \in E$ and $ac, bd \notin E$, the removal of the edges ab and cd from G and the addition of ac and bd to G is referred to as a *2-switch* in G. This is a well studied classical operation (see, for example [4, 7]). It is straightforward to check that 2-switch operations preserve the degree sequence.

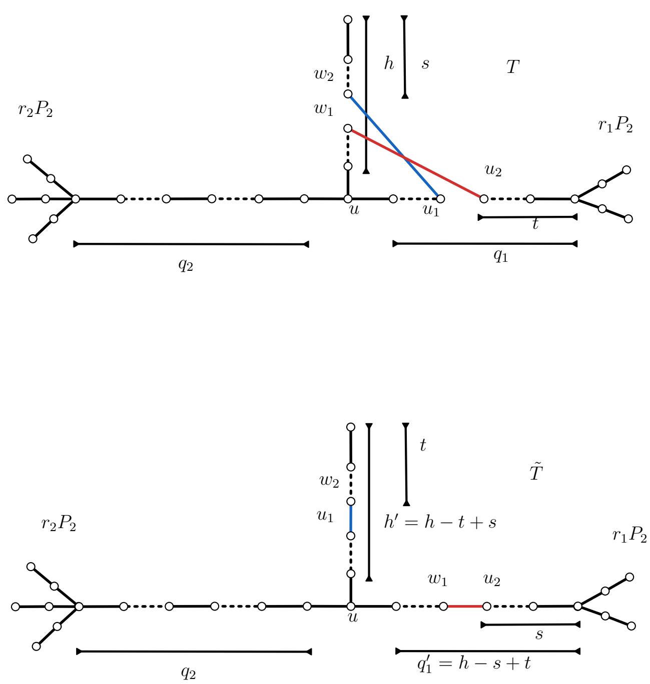

Figure 3: The 2-switch of type I.

Type I. We switch the vertices between the central path and the right (or the left) branch of T obtaining a new tree T(see Figure 3). More precisely, we have a new member of $\mathfrak{F}(n)$, where the parameters are changed by $q_1' = h - s + t$ (the closest to $r_1 P_2$) and $h' = q_1 - t + s$ (the new central path after some relabeling). Let us call that a (s, t)-2-switch of type I (see Figure 3). In order to do the 2-switch, we disconnect the edges $[u_1, u_2]$ and $[w_1, w_2]$ and reconnect $[u_1, w_2]$ and $[w_1, u_2]$.

Type II. We switch the vertices between the right and the left branches of T obtaining a new tree T'; Notice that this transformation is indeed a 2-switch preserving the degree sequence ($d := [r_1+1, r_2+1, 3, 2^{n-(r_1+r_2)-4}, 1^{r_1+r_2+1}]$). More precisely, we have a new member of $\mathfrak{F}(n)$, where the parameters are changed by $q_1' = q_2 + t - s$ (the closest to $r_1 P_2$) and $q_2' = q_1 - t + s$ (the closest to $r_1 P_2$). Let us call that a (s,t)-2-switch of type II. In order to do the 2-switch, we disconnect the edges $[u_1, u_2]$ and $[v_1, v_2]$ and reconnect $[u_1, v_2]$ and $[v_1, u_2]$.

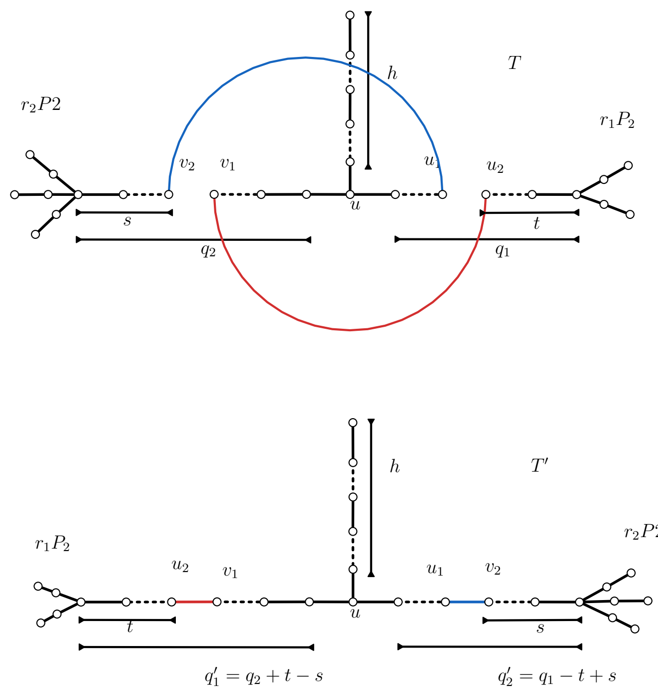

Figure 4: The 2-switch of type II.

We can always assume that $\lambda = \rho(T) > \sqrt{r_2+2}$ for all T in $\mathfrak{F}(n)$ because the sun S_{r_2+1}, whose spectral radius is $\sqrt{r_2+2}$, is a proper subgraph of T, since $q_2 \geq 2$. But in fact, we need a larger lower bound for $\lambda = \rho(T)$ for our results.

Let $T_j := [\underbrace{2, 2, ..., 2}_{r_2 \text{ times}}, j]$ be the starlike tree composed by r_2 legs of P_2 and a path of length j, with $j \geq 3$ as Figure 5 illustrates.

Theorem 2.1. *Let $T \in \mathfrak{F}(n)$. If $j \geq 3$, then*

$$\rho(T) > \rho(T_j).$$

This result may be proven by our comparison method that will be explained next, but there is a simpler proof, for which we need the following definitions and known result of Lemma 2.2.

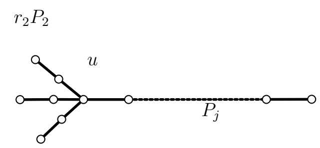

Figure 5: The graph T_j.

An internal path in a graph G, denoted by $v_1v_2, \dots v_{r-1}v_r$, is a path beginning at v_1 and ending at v_r, where v_1 and v_r both have degree bigger than two, while all other vertices have degree two. The vertices v_1 and v_r are not necessarily distinct. We denote by C_n, the cycle on n vertices and by W_n the tree with n vertices where two vertices have degree three and the distance between them is $n-5$. The following result appears in the work by Hoffman and Smith [8].

Lemma 2.2. *Let G be a graph with n vertices, $G \neq C_n, W_n$. Let G' be the graph with $n+1$ vertices obtained from G by inserting a new vertex of degree two in an edge e. Then*

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

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

Proof. (Theorem 2.1) Let $T = [h, q_1, q_2] \in \mathfrak{F}(n)$ and $3 \leq j$.

Let H_1' be the tree obtained by adding an edge in the internal path starting from u to the vertex r_1P_2. We notice that $T \neq W_n$, as it has a vertex u of degree $r_2 + 1 > 3$, and hence, by Lemma 2.2, $\rho(H_1') < \rho(T)$. We now remove the pendant vertex of the path P_h in T, obtaining a tree H_1, a proper subtree of H_1'. If follows that $\rho(H_1) < \rho(T)$. We apply this process successively h times, obtaining a tree H_h composed by the starlikes r_2P_2 and r_1P_2 linked in their centers by a path of length $q_2 + h + q_1 + 1$ such that $\rho(H_h) < \rho(T)$.

Now, if $3 \leq j \leq q_2 + h + q_1 + 1$, we see that T_j is a proper subtree of H_h and therefore, $\rho(T_j) < \rho(H_h) < \rho(T)$.

For $j > q_2 + h + q_1 + 1$, we keep adding edges in the internal path starting at r_2P_2 and ending at r_1P_2 until the length of the path is at least j, obtaining a tree H_j. This operation, according the Lemma 2.2, decreases the spectral radius. As T_j is a proper subtree of H_j, it follows that $\rho(T_j) < \rho(H_j) < \rho(T)$.

□

2.2 Our tool

We would like to recall the algorithm **Diagonalize(T, α)**. For a tree T and a real number α this algorithm outputs a sequence $(d_v)_{v \in V(T)}$.

Algorithm Diagonalize(T, α)

1. List the vertices of T in postorder as $v_1, \dots, v_n$.

2. For each $i = 1, \dots, n$ set $d_{v_i} \leftarrow \alpha$.

3. For each $i = 1, \ldots, n$:

4. If v_i has a child v_j such that $d_{v_j} = 0$,
then
set $d_{v_i} \leftarrow -\frac{1}{2}$ and $d_{v_j} \leftarrow 2$.
Further, if v_i has a parent v_p, remove the edge $v_p v_i$ from T.

5. Otherwise, set $d_{v_i} \leftarrow d_{v_i} - \sum d_{v_j}^{-1}$, summing over all children v_j of v_i.

The above algorithm of Jacobs and Trevisan [10] can be used to estimate eigenvalues of a given tree. It finds a diagonal matrix D that is congruent to the matrix $A(T) + \alpha I$, where $A(T)$ is the adjacency matrix of T and α is a real number. Its nice feature is that it can be easily executed manually directly on the drawing of a tree. The authors proved that the following result holds.

Theorem 2.3. *For a tree T, let $(d_v)_{v\in V(T)}$ be the values produced by* **Diagonalize**$(T, -\alpha)$. *Then the diagonal matrix $D = \text{diag}(d_v)_{v\in V(T)}$ is congruent to $A(T) + \alpha I$, hence the number of (positive | negative | zero) entries in $(d_v)_{v\in V(T)}$ is equal to the number of eigenvalues of $A(T)$ that are (greater than α | smaller than α | equal to α).*

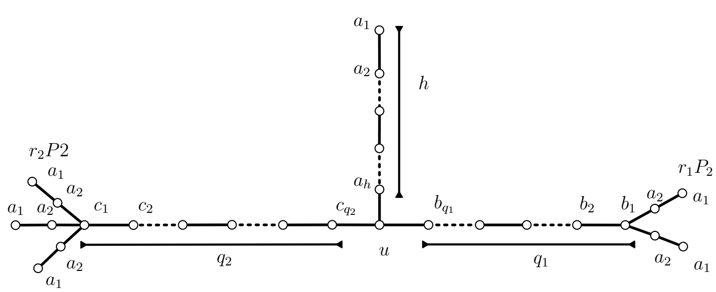

Figure 6: The algorithm Diagonalize(T, $-\lambda$) applied to a generic member of trees $\mathfrak{F}(n)$.

Let $(d_v)_{v\in V}$ be the sequence obtained by executing **Diagonalize** $(T, -\lambda)$, when $T \in \mathfrak{F}(n)$ (see Figure 6) and u is the root of the tree. Since we are going to use this algorithm in different trees, it is useful to adopt a new notation, recording the tree we are using and the vertex where we are applying, which is

$$f_T(v) := d_v, \ \forall v \in V(T).$$

Taking $\lambda = \rho(T)$, the vertices labeled with the values of the numeric sequences generated by the application of the algorithm **Diagonalize** $(T, -\lambda)$ appear in Figure 6.

By the application of the algorithm, we know that $a_j, b_j, c_j < 0$ for all indices appearing in the picture and

$$f_T(u) = -\lambda - \frac{1}{a_h} - \frac{1}{b_{q_1}} - \frac{1}{c_{q_2}} = 0, \tag{2.1}$$

otherwise, if some previous vertex produces zero then, the step (4) of the algorithm will produce a positive value which is not possible because λ is the index of T.

Furthermore, we have

$$a_1 = -\lambda, \qquad b_1 = -\lambda - \frac{r_1}{a_2}, \text{ and } c_1 = -\lambda - \frac{r_2}{a_2}.$$

From these vertices towards the root u we obtain three sequences a_j, b_j and c_j, obeying the same relation, that is, $a_{j+1} = -\lambda - \frac{1}{a_j}$, $\quad b_{j+1} = -\lambda - \frac{1}{b_j}$ and $c_{j+1} = -\lambda - \frac{1}{c_j}$.

Now suppose that we have a new tree $\tilde{T}$ with new parameters $[h', q_1', q_2']$ (same number of vertices and with the same r_1 and r_2). We now execute **Diagonalize**$(\tilde{T}, -\lambda)$.

Since the tree $\tilde{T}$ has the same properties of T, when $\rho(T) > \rho(\tilde{T})$, we obtain similar sequences and a similar formula at the root $\tilde{u}$ of the tree $\tilde{T}$. More precisely, the execution of **Diagonalize**$(\tilde{T}, -\lambda)$ produces the same sequences, a_j, b_j, c_j and

$$f_{\tilde{T}}(\tilde{u}) = -\lambda - \frac{1}{a_{h'}} - \frac{1}{b_{q_1'}} - \frac{1}{c_{q_2'}} \tag{2.2}$$

From Theorem 2.3 it follows that $\rho(T) > \rho(\tilde{T})$ if and only if $-\lambda - \frac{1}{a_{h'}} - \frac{1}{b_{q_1'}} - \frac{1}{c_{q_2'}} < 0$ and all $a_j, b_j, c_j < 0$.

We will see that in order to determine the sign of Equation (2.2), we need to deal in great detail with the recurrences appearing when the algorithm **Diagonalize**$(\tilde{T}, -\lambda)$ is implemented. For that we will determine some analytical properties of the recurrences a_j, b_j and c_j.

3 Analytical properties of recurrence sequences

As we observed in the previous section, the only information needed is the sign of the numeric sequences generated. All the recurrence relations are of the same kind, differing only by the initial value. More precisely, they are of the form

$$z_{j+1} = \varphi(z_j) \quad \text{where} \quad \varphi(t) = -\lambda - \frac{1}{t} \tag{3.1}$$

for $t \neq 0$ and $\lambda = \rho(T) > \rho(T_j) > 2$. Hence it depends only on the analytical behavior of the function $\varphi(t)$.

In [3] this sequence was extensively studied and its behavior can be summarized by the following result whose proof is a combination of the results found in [3].

Theorem 3.1. *Let z_j be the recurrence in formula* (3.1)*, then*

(a) $\varphi(t) = t$ *has two roots* $\theta = \frac{-\lambda - \sqrt{\lambda^2 - 4}}{2} < -1$ *and* θ^{-1}*, which are also fixed points of* $\varphi(t) = t$*;*

(b) $\theta(\lambda)$ *is decreasing as a function of* λ*;*

(c) $z_j = \theta + \frac{\theta^{-1} - \theta}{\beta(\theta^2)^j + 1}$*, where the constant* $\beta \in \mathbb{R}$ *is obtained when computing the given value* z_1*;*

(d) The sequence a_j obtained from z_j by taking $a_1 = -\lambda$ is given by $a_j = \theta - \frac{\sqrt{\lambda^2-4}}{(\theta^2)^j-1} < 0$, for any $j \geq 1$. In particular, a_j is increasing and $\lim_{j\to\infty} a_j = \theta$.

We also need to understand the sequences b_j and c_j obtained from z_j by considering $b_1 = -\lambda - \frac{r_1}{a_2}$ and $c_1 = -\lambda - \frac{r_2}{a_2}$, $2 \leq r_1 < r_2$, respectively.

We are going to study both at the same time by considering a parametric sequence

$$z_{j+1}(r) = \varphi(z_j(r)) \tag{3.2}$$

with $z_1(r) := -\lambda - \frac{r}{a_2}$ for some $r \geq 2$.

The main facts can be summarized in the following result.

Theorem 3.2. *Let z_j be the recurrence in formula (3.2), then*

(a) $z_j(r) = \theta + \frac{\theta^{-1}-\theta}{\beta(\theta^2)^j+1}$, where the constant $\beta := \beta(r) \in \mathbb{R}$ is given by

$$\beta := \frac{r - a_2\theta}{a_2\theta - r\theta^2};$$

(b) $\beta(r)$ is a continuous function of r in $(2, \infty) \setminus r_*$, where $r_* := \frac{a_2}{\theta}$. Moreover $\beta(r)$ has a single root in $r^* = a_2\theta$ and $\beta(r) > 0$, for $r \in (r_*, r^*)$

(c) The sequence $z_j(r) < 0$, for $j \geq 1$, is decreasing and $\lim_{j\to\infty} z_j = \theta$.

Proof. **(a)** Using Theorem 3.1 (c) and the fact that $-\lambda = \theta + \theta^{-1}$ and $\theta - \theta^{-1} = -\sqrt{\lambda^2 - 4}$ we obtain

$$z_1 = -\lambda - \frac{r}{a_2} = \theta + \theta^{-1} - \frac{r}{a_2} \text{ and } z_1 = \theta + \frac{\theta^{-1} - \theta}{\beta(\theta^2)^1 + 1},$$

producing

$$\beta := \beta(r) = \frac{\theta^{-1}\frac{r}{a_2} - 1}{1 - \theta\frac{r}{a_2}} = \frac{r\theta^{-1} - a_2}{a_2 - r\theta} = \frac{r - a_2\theta}{a_2\theta - r\theta^2}.$$

(b) We notice that $\beta(r)$ is a rational function, hence continuous, apart from the roots of the denominator. Thus, the discontinuity occurs at $r_* := \frac{a_2}{\theta}$. Also, $\beta(r)$ has only one possible root in $r^* = a_2\theta$.

Additionally, $\lim_{r\to r_*^+} \beta(r) = +\infty$. To see that we just take $r := r_* + \delta$ for $\delta > 0$, then

$$\beta(r_* + \delta) = \frac{r_* + \delta - a_2\theta}{a_2\theta - (r_* + \delta)\theta^2} = \frac{\delta + (r_* - a_2\theta)}{(a_2\theta - r_*\theta^2) - \delta\theta^2} = \frac{\delta + (r_* - a_2\theta)}{-\delta\theta^2} \overset{\delta\to 0^+}{\to} +\infty$$

because $r_* - a_2\theta = \frac{a_2}{\theta} - a_2\theta = a_2(\frac{1-\theta^2}{\theta}) < 0$.

As $r^* - r_* = a_2(\theta - \theta^{-1}) = a_2(-\sqrt{\lambda^2 - 4}) > 0$, we see that $r_* < r^*$. Also, differentiating with respect to r we conclude that $\beta(r)$ is decreasing and take the value zero only for $r^* := a_2\theta > r_*$. Thus we conclude that $\beta(r) > 0$ for $r \in (r_*, r^*)$. Figure 7 illustrates a typical

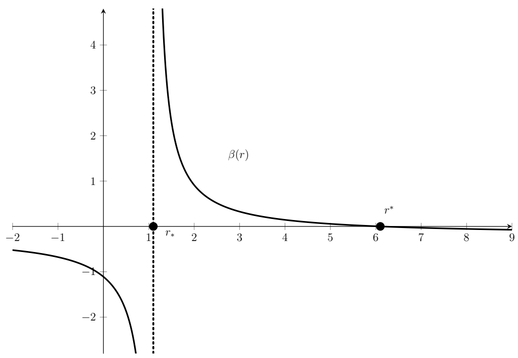

Figure 7: The behavior of $\beta(r)$.

behavior of the function $\beta(r)$.

(c) We recall that $r^* = a_2\theta$, moreover, from Theorem 3.1 (d), we know that $\lim_{j\to\infty} a_j = \theta$ hence

$$r^* = \lim_{j\to\infty} a_2 a_j. \tag{3.3}$$

By Theorem 2.1, we know that $\rho(T_j) < \rho(T)$, where T_j is the tree of Figure 5. Now, we apply **Diagonalize**$(T_j, -\lambda)$ with the root at S_{r_2}, for $\lambda = \rho(T)$. By our comparison method, we see that

$$f_{T_j}(u) = -\lambda - \frac{1}{a_j} - \frac{r_2}{a_2} < 0$$

or, equivalently, $a_{j+1} < \frac{r_2}{a_2}$, and since $a_2 < 0$, we get $r_2 < a_2 a_{j+1}$.
Taking the limit on both sides and using Equation (3.3), we obtain

$$r_2 \le \lim_{j\to\infty} a_2 a_{j+1} = \lim_{j\to\infty} a_2 a_j = r^*.$$

We also observe that $r_* < r_1$, because $r_* = \frac{a_2}{\theta} = 2\,\frac{\lambda^2-1}{\lambda\left(\lambda+\sqrt{\lambda^2-4}\right)} < 2 \le r_1$.

Since $z_j = \theta + \frac{\theta^{-1}-\theta}{\beta(r)(\theta^2)^j+1}$, for $\theta^{-1} - \theta = \sqrt{\lambda^2-4} > 0$ and $\theta < 0$, we see that z_j is always negative and decreasing, as long as $\beta(r) > 0$. Now, because $r_* < r_1 < r_2 \le r^*$, we see from item (b), that $\beta(r) > 0$. Moreover z_j tends to θ as $j \to \infty$. □

4 Ordering the 2-switches of $\mathfrak{F}(n)$

We show in this section how the spectral radius varies in each case for all the possible 2-switching positions in the appropriate interval. We notice that $\mathfrak{F}(n)$ is preserved by both types of (s,t)-2-switch, only changing $[h, q_1, q_2]$ (see Figure 6). For 2-switches of Type I, h decreases to 2, while q_1 increases to $q_1 + h - 2$ and q_2 is constant. For 2-switches of Type II, h is constant, q_1 decreases to 2, while q_2 increases to $q_2 + q_1 - 2$.

4.1 Warmup: Ordering 2-switches of Type I

Given a 2-switch of Type I such that $T = [h, q_1, q_2] \to \tilde{T} = [h', q_1', q_2']$ (see Figure 3), we observe that the actual result of the operation in the tree is an increment (decrement) of the length h with a decrement (increment) of the length q_1, while q_2 remains unchanged.

In order to study the behavior of the spectral radius of members of this family, it is enough to study the 2-switch $T = [h, q_1, q_2] \to \tilde{T} = [h' = h-1, q_1' = q_1 + 1, q_2' = q_2]$, since this will cover all possible positions.

We will prove that $\rho(T) > \rho(\tilde{T})$ using our comparison method, hence we need to prove that if $-\lambda - \frac{1}{a_h} - \frac{1}{b_{q_1}} - \frac{1}{c_{q_2}} = 0$ then $-\lambda - \frac{1}{a_{h'}} - \frac{1}{b_{q_1'}} - \frac{1}{c_{q_2}} = -\lambda - \frac{1}{a_{h-1}} - \frac{1}{b_{q_1+1}} - \frac{1}{c_{q_2}} < 0$. Notice that, from the first equation, we obtain $-\lambda - \frac{1}{c_{q_2}} = \frac{1}{a_h} + \frac{1}{b_{q_1}}$ and substituting in the second one it is equivalent to $\frac{1}{a_h} + \frac{1}{b_{q_1}} - \frac{1}{a_{h-1}} - \frac{1}{b_{q_1+1}} < 0$, which in turn is equivalent to

$$(a_h - a_{h+1}) + (b_{q_1+2} - b_{q_1+1}) < 0. \tag{4.1}$$

From Theorem 3.1, the sequence a_j is increasing thus $a_h - a_{h+1} < 0$. From Theorem 3.2, the sequence b_j is decreasing thus $b_{q_1+2} - b_{q_1+1} < 0$.

We remark that the transformation $T = [h, q_1, q_2] \to \tilde{T} = [h' = h-1, q_1' = q_1, q_2' = q_2+1]$ is also of Type-I, and we can show that the index decreases as well by using a similar argument. This proves the following theorem.

Theorem 4.1. *Let $T = [h, q_1, q_2]$ be a tree in $\mathfrak{F}(n)$ and $\tilde{T} = [h', q_1', q_2']$ be the graph obtained by a 2-switch in Figure 3. If $h' = h-1, q_1' = q_1 + 1$ and $q_2' = q_2$ or if $h' = h-1, q_1' = q_1$ and $q_2' = q_2 + 1$ then $\rho(T) > \rho(\tilde{T})$.*

We remark that this result may be obtained also by using Lemma 2.2 due to Hoffman & Smith [8]. We add an edge on the internal path from u to $r_1 P_2$ (or from u to $r_2 P_2$) and then erase the pendant vertex from P_h, so that the spectral radius decreases even more, keeping both with the same number of vertices.

Our method, after we obtained that the sequence b_j is decreasing, is simple enough to provide the alternative proof. On the contrary, we are not aware of any alternative known method to prove Theorem 4.2, that deals with 2-switching of Type II. Additionally, or perhaps because of that, the application of our method requires to overcome quite a few technical difficulties.

4.2 Ordering 2-switches of Type II

We observe that a 2-switch of type II can be seen as a displacement of the central path of length h from the position closest to $r_1\,P_2$ to the closest to $r_2\,P_2$ (or vice versa). Indeed, if we take $s = q_2$ then $q_1' = q_2 + t - s = t$ and $q_2' = q_1 - t + q_2 = q_1 + q_2 - t$, for $1 \leq t \leq q_1 - 1$. For instance, taking $t = 1$ we can apply the 2-switch sequentially.

Since every configuration $[h, q_1, q_2]$ can be obtained by successive changes by 1, we only need to consider the case where $T = [h, q_1, q_2] \to \tilde{T} = [h, q_1' = q_1 - 1, q_2' = q_2 + 1]$. We will prove that this operation decreases the spectral radius

By using our method of Section 2, given a 2-switch of Type II we need to prove that if $-\lambda - \frac{1}{a_h} - \frac{1}{b_{q_1}} - \frac{1}{c_{q_2}} = 0$ then $-\lambda - \frac{1}{a_h} - \frac{1}{b_{q_1-1}} - \frac{1}{c_{q_2+1}} < 0$.

Theorem 4.2. *Let $T = [h, q_1, q_2]$ be a tree obtained by a 2-switch in Figure 4. If $r_2 > r_1 \geq 2$, $q_1' = q_1 - 1$ and $q_2' = q_2 + 1$ then $\rho(T) > \rho(T')$.*

Proof. Given a 2-switch of Type II, we need to prove that if $-\lambda - \frac{1}{a_h} - \frac{1}{b_{q_1}} - \frac{1}{c_{q_2}} = 0$ then $-\lambda - \frac{1}{a_h} - \frac{1}{b_{q_1-1}} - \frac{1}{c_{q_2+1}} < 0$. We define

$$\mathcal{I} := -\frac{1}{a_h} + \left(-\lambda - \frac{1}{b_{q_1-1}}\right) - \frac{1}{c_{q_2+1}} = -\frac{1}{a_h} + b_{q_1} - \frac{1}{c_{q_2+1}}.. \tag{4.2}$$

Now, equation $-\frac{1}{a_h} - \frac{1}{b_{q_1}} + \left(-\lambda - \frac{1}{c_{q_2}}\right) = 0$ may be read as $c_{q_2+1} = \frac{1}{a_h} + \frac{1}{b_{q_1}}$. Substituting that in (4.2) we obtain

$$\mathcal{I} = -\frac{1}{a_h} + b_{q_1} - \frac{1}{\frac{1}{a_h} + \frac{1}{b_{q_1}}}. \tag{4.3}$$

Using the fact that $a_h < 0$ and $b_{q_1} < 0$ conclude that $\mathcal{I} < 0$ if and only if

$$a_h(b_{q_1}^2 - 1) < b_{q_1}. \tag{4.4}$$

We already know that $a_h < \theta < b_{q_1}$ but we do not know the sign of $b_{q_1}^2 - 1$. We claim that $b_{q_1}^2 - 1 > 0$. To see that, we recall that b_j is decreasing and b_1 is given by $b_1 := -\lambda - \frac{r_1}{-\lambda + \frac{1}{\lambda}} = \phi(\lambda, r_1)$ where the auxiliary function $\phi : A \to \mathbb{R}$ is given by

$$\phi(t, r) := -t - \frac{r}{-t + \frac{1}{t}},$$

defined on the set $A = \{(t, r) \,|\, t \geq 2,\, r \geq 2\} \subset \mathbb{R}^2$.

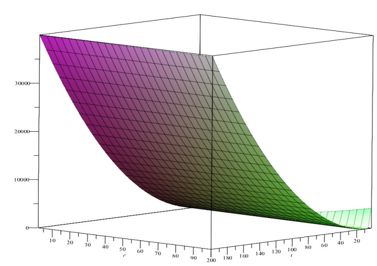

Figure 8: The graph of $\phi(t, r)^2 - 1$ plotted in A.

It is easy to see that $\phi(t, r)^2 - 1 > 0$ for $(t, r) \in A$, see Figure 8. In other words, $b_1^2 - 1 > 0$ and $b_1 < -1$ because it is negative. For any $T \in \mathfrak{F}(n)$ we conclude that $\theta < b_{q_1} < -1 = b_1$, for any $T \in \mathfrak{F}(n)$. In particular $b_{q_1}^2 - 1 > 0$.

From these facts, we can rewrite equation (4.4) in the equivalent form

$$a_h < \frac{b_{q_1}}{b_{q_1}^2 - 1}. \tag{4.5}$$

In order to conclude our proof, it is sufficient to prove that $\theta < \frac{b_{q_1}}{b_{q_1}^2-1}$ because $a_h < \theta$ for all h. At this point, it is useful to introduce a second auxiliary function

$$\psi(t) := \frac{t}{t^2-1}, t < 0.$$

This function is obviously decreasing in the interval $(-\infty, -1)$. As the correspondence $j \to b_j$ is also decreasing, we conclude that the correspondence $j \to \psi(b_j)$ is increasing and, as a consequence, $\frac{b_1}{b_1^2-1} < \frac{b_{q_1}}{b_{q_1}^2-1}$.

We claim that $\frac{b_1}{b_1^2-1} > \theta$ or equivalently

$$\frac{\left(-\lambda - \frac{r_1}{-\lambda+\frac{1}{\lambda}}\right)}{\left(-\lambda - \frac{r_1}{-\lambda+\frac{1}{\lambda}}\right)^2 - 1} > \frac{-\lambda - \sqrt{\lambda^2-4}}{2}, \tag{4.6}$$

for $\lambda = \rho(T)$.

The inequality (4.6) is equivalent to $g(x,r) > 0$ for $x \geq \rho(T) \geq \sqrt{r_2+2} \geq \sqrt{r_1+3}$ and $r = r_1 \geq 2$, where $g : B \to \mathbb{R}$ is given by

$$g(x,r) = \frac{\left(-x - \frac{r}{-x+\frac{1}{x}}\right)}{\left(-x - \frac{r}{-x+\frac{1}{x}}\right)^2 - 1} + \frac{x+\sqrt{x^2-4}}{2},$$

defined on $B = \{(x,r) \,|\, x \geq \sqrt{r+3},\ r \geq 2\} \subset \mathbb{R}^2$.

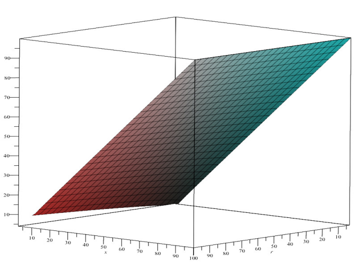

Figure 9: The graph of g on B.

As we can see in Figure 9, the function is always positive in this set concluding our proof. □

5 Spectral radius ordering in $\mathfrak{F}(n)$

In this section we provide a total ordering by the spectral radius in the family $\mathfrak{F}(n)$. In order to recall our notation, we notice that $r_1 > r_2 \geq 2$ and the number n of vertices is fixed, hence each element in $\mathfrak{F}(n)$ is uniquely determined by the 3-uple $[h, q_1, q_2]$, that is,

$$\mathfrak{F}(n) := \{T = [h, q_1, q_2] \mid h + q_1 + q_2 = n - 1 - 2(r_1 + r_2),\ h, q_1, q_2 \geq 2\}.$$

The degree sequence of an element $T \in \mathfrak{F}(n)$ is given by $d := [r_1+1, r_2+1, 3, 2^{n-(r_1+r_2)-2}, 1^{r_1+r_2+1}]$, for a fixed pair $r_1 > r_2 \geq 2$. We recall the well known result from [7] (also [4]):

Theorem 5.1. *If G and H have the same degree sequence, then there exists a 2-switch sequence transforming G into H.*

As a consequence, given an element in $\mathfrak{F}(n)$, it maybe transformed into any other by a sequence of 2-switch transformations.

The remarkable fact is that, as we will see next, we can reach any element from another using only two types of 2-switches. Additionally, the sequence of 2-switches is closed in the family, that is, any intermediate member is also a member. Given $T = [h, q_1, q_2] \in \mathfrak{F}(n)$ we define the following operations.

- $\alpha : \mathfrak{F}(n) \to \mathfrak{F}(n)$, given by $\alpha([h, q_1, q_2]) = [h-1, q_1+1, q_2]$, for $h \geq 3$;
- $\beta : \mathfrak{F}(n) \to \mathfrak{F}(n)$, given by $\beta([h, q_1, q_2]) = [h, q_1-1, q_2+1]$, for $q_1 \geq 3$.
- $\gamma : \mathfrak{F}(n) \to \mathfrak{F}(n)$, given by $\beta([h, q_1, q_2]) = [h-1, q_1, q_2+1]$, for $h \geq 3$.

We remark that the transformations make sense for $h, q_1, q_2 \geq 1$, and the results from Section 4 do apply. However, we observe that the original $T = [h, q_1, q_2]$ and the transformed tree $T' = [h', q'_1, q'_2]$ must have parameters $h, h', q_1, q'_1, q_2, q'_2 \geq 2$, otherwise they will not be 2-switches, because the degree sequence changes.

Theorem 5.2. *Let α, β and γ be the transformations defined in $\mathfrak{F}(n)$. Let $T^* = [h_0, 2, 2]$, where $h_0 := n - 5 - 2(r_1 + r_2) \geq 2$. The following facts are true*

(a) α, β and γ are 2-switch transformations;

(b) α, β and γ are index decreasing transformations;

(c) Any $T \in \mathfrak{F}(n)$ can be obtained from T^* by a sequence of α and β transformations;

(d) Any $T \in \mathfrak{F}(n)$ can be obtained from T^* by a sequence of α and γ transformations.

Proof. From our definition of Section 2, we see that α and γ are Type-I 2-switches, while β is a Type-II 2-switch and our results of Theorem 4.1 and Theorem 4.2 apply, hence they decrease the index. This proves (a) and (b).
(c) To see that, consider the tree $T^* = [h_0, 2, 2]$. As $T^* = u + P_{h_0} * S_0 \oplus P_2 * S_{r_1} \oplus P_2 * S_{r_2}$, and $h_0 = n - 5 - 2(r_1 + r_2) \geq 2$, because $n \geq 7 + 2(r_1 + r_2)$, we see that $T^* \in \mathfrak{F}(n)$. Let $T = [h', q'_1, q'_2]$ be any tree in $\mathfrak{F}(n)$ ($h', q'_1, q'_2 \geq 2$). Then we have the following
$\alpha([h_0, 2, 2]) = [h_0 - 1, 2 + 1, 2]$, $\alpha([h_0 - 1, 2 + 1, 2]) = [h_0 - 2, 2 + 2, 2]$, and so on, until we obtain $h_0 - k = h'$, that is $\alpha^k([h_0, 2, 2]) = [h', 2 + (h_0 - h'), 2]$.
Now we apply β transformation j times obtaining $\beta^j \alpha^k([h_0, 2, 2]) = [h', 2+(h_0-h')-j, 2+j]$.
At this point we claim that, making $2+(n-5-2(r_1+r_2)-h')-j = q'_1$ we get $2+j = q'_2$. Indeed, $2+(n-5-2(r_1+r_2)-h')-j = q'_1$ means that $j = 2+(n-5-2(r_1+r_2)-h'-q'_1)-q'_2+q'_2 = q'_2 - 2 + (n - (1 + h' + q'_1 + q'_2 + 2(r_1 + r_2))) = q'_2 - 2$. Hence $2 + j = q'_2$. Thus we conclude that there exist $k, j \in \mathbb{N}$ such that $\beta^j \alpha^k(T^*) = T$ for any $T \in \mathfrak{F}(n)$.

(d) A similar reasoning as in (c) shows that $T^* \in \mathfrak{F}(n)$. We now apply $k' = q_1' - 2$ times the transformation α, arriving at $[h_0 - k', q_1', 2]$. Reasoning as above we show that there is an integer j' so that $h_0 - k' - j' = h'$ and $q_2' = 2 + j'$. Hence applying now j' times the transformation γ, shows that $\gamma^{j'}\alpha^{k'}(T^*) = T$. □

We observe that $T^* = [h_0, 2, 2]$ has the configuration with largest possible h_0. From Theorem 5.2 (b) and (c) (or from (b) and (d)), it follows that T^* is the extremal element of $\mathfrak{F}(n)$: it has the maximum spectral radius.

The next result is quite remarkable in the sense that it provides a complete ordering of $\mathfrak{F}(n)$ using only α and γ transformations, allowing us to find also the element of minimum index.

Theorem 5.3. *Consider the family $\mathfrak{F}(n)$, where $2 \le r_1 < r_2$, $h_0 = n - 5 - 2(r_1 + r_2) \ge 2$, $T^* = [h_0, 2, 2] \in \mathfrak{F}(n)$ and $T_* = [2, 2, h_0] \in \mathfrak{F}(n)$. The following claims are true.*

(a) The elements of the ordered sequence

$$\mathcal{A} := \{T^*, \alpha(T^*), \cdots, \alpha^{h_0-2}(T^*), \gamma(T^*), \alpha(\gamma(T^*)), \cdots, \alpha^{h_0-3}(\gamma(T^*)), \cdots, \gamma^{h_0-2}(T^*) = T_*\}$$

compose the set $\mathfrak{F}(n)$;

(b) The sequence $\mathcal{A}$ is ordered by the inverse lexicographic order:
$[x, y, z] \succ [x', y', z']$ iff $z' > z$ or $z' = z$ but $y' > y$.

(c) If $[x, y, z] \succ [x', y', z']$ then $\rho([x, y, z]) > \rho([x', y', z'])$;

(d) The maximum (resp. minimum) index in $\mathfrak{F}(n)$ is $\rho(T^*)$ (resp. $\rho(T_*)$).

Before we prove Theorem 5.3 we need a technical lemma.

Lemma 5.4. *If $T^* = [h_0, 2, 2] \in \mathfrak{F}(n)$, then $\rho(\alpha^{h_0-j-2}(\gamma^j(T^*)) > \rho(\gamma^{j+1}(T^*))$, for $j = 0, 1, 2, ..., h_0 - 2$, that is,*

$$\rho([2, h_0 - j, 2]) > \rho([h_0 - (j + 1), 2, 2 + (j + 1)]).$$

Proof. We will consider the first case $j = 0$. The rest of the cases are identical. Thus, we must prove that

$$\rho([2, h_0, 2]) > \rho([h_0 - 1, 2, 3]).$$

Taking $\lambda = \rho([2, h_0, 2])$ and applying `Diagonalize`$([2, h_0, 2], -\lambda)$, we have

$$-\lambda - \frac{1}{a_2} - \frac{1}{b_{h_0}} - \frac{1}{c_2} = 0.$$

From this, we obtain $c_3 = \frac{1}{\frac{1}{a_2} + \frac{1}{b_{h_0}}}$.

Analogously, applying `Diagonalize`$([h_0 - 1, 2, 3], -\lambda)$, we have

$$-\lambda - \frac{1}{a_{h_0-1}} - \frac{1}{b_2} - \frac{1}{c_3} =: \mathcal{I}.$$

We need to show that $\mathcal{I} < 0$. Writing $\mathcal{I} = a_{h_0} - \frac{1}{b_2} - \frac{1}{\frac{1}{a_2}+\frac{1}{b_{h_0}}}$, we conclude that $\mathcal{I} < 0$ if the function

$$g(\lambda, r_1, h_0) := a_{h_0} - \frac{1}{b_2} - \frac{1}{\frac{1}{a_2} + \frac{1}{b_{h_0}}}$$

is always negative for $r_1 \geq 2$, $h_0 \geq 2$ and $\lambda \geq \sqrt{r_1+3}$.

At a first glance, we cannot plot a graph as we did before because we have three variables. However, if we consider the variation of the variable h_0 we observe that the correspondence $h_0 \to g(\lambda, r_1, h_0)$ is monotonously increasing because

$$\frac{d}{dh_0} g(\lambda, r_1, h_0) = \frac{da_{h_0}}{dh_0} - \frac{1}{\left(\frac{1}{a_2} + \frac{1}{b_{h_0}}\right)^2} \frac{1}{b_{h_0}^2} \frac{db_{h_0}}{dh_0} > 0,$$

since $\frac{da_{h_0}}{dh_0} > 0$ and $\frac{db_{h_0}}{dh_0} < 0$.

Hence we just need to show that the limit function

$$f(\lambda, r_1) := \lim_{h_0 \to \infty} g(\lambda, r_1, h_0) = \theta - \frac{1}{b_2} - \frac{1}{\frac{1}{a_2} + \frac{1}{\theta}}$$

is always negative for $C := \{(\lambda, r1) \,|\, r_1 \geq 2,\ \lambda \geq \sqrt{r_1+3}\}$, as shown on Figure 10, concluding our proof. □

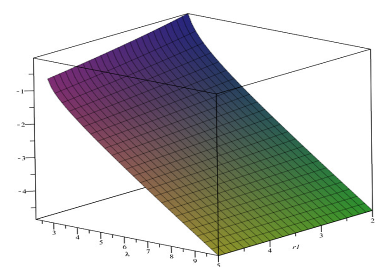

Figure 10: The graph of f on C.

Proof. **(of Theorem 5.3)**
To see (a) we first see that both transformations α and γ decrease the index. By Theorem 5.2 (d), we can reach any configuration from T^*, showing that every configuration appears in the sequence $\mathcal{A}$.
For (b), we notice that the inverse lexicographic order:
$[x, y, z] \succ [x', y', z']$ if and only if $z' > z$ or $z' = z$ but $y' > y$, is naturally produced in $\mathcal{A}$. For instance comparing $[x, y, z]$ with $[x', y', z'] = \alpha([x, y, z]) = [x-1, y+1, z]$ we obtain $z' = z$ but $y' > y$. The only possible difficulty is to compare, for example, $[x, y, z] = \alpha^{h_0-2}(T^*) = [2, h_0-2, 2]$ with $[x', y', z'] = \gamma(T^*) = [h_0-1, 2, 3]$, in this case we have $z' > z$.
For (c) we can use the same reasoning, if the next element is obtained from the previous one by α the index decreases by Theorem 4.1. Again, it remains to analyse the case $[x, y, z] =$

$\alpha^{h_0-2}(T^*) = [2, h_0 - 2, 2]$ and $[x', y', z'] = \gamma(T^*) = [h_0 - 1, 2, 3]$. In this case the index decrease by Lemma 5.4.
The item (d) is a direct consequence of the previous items. □

Example 5.5. We consider $\mathfrak{F}(23)$, with $r_1 = 2$, $r_2 = 3$ and $h_0 = n - 5 - 2(r_1 + r_2) = 8$. In this case $T^* = [h_0, 2, 2] = [8, 2, 2]$ and $T_* = [2, 2, h_0] = [2, 2, 8]$. We will use the same procedure described in the proof of Theorem 5.3 to build a table where we show the spectral radius of each intermediary tree:

Transf. / $\mathcal{A}$	Tree	Index
T^*	[8, 2, 2]	2.31431268823172996316982502630
$\alpha(T^*)$	[7, 3, 2]	2.30752321205156788164155922354
$\alpha^2(T^*)$	[6, 4, 2]	2.30509257122848263666229555974
$\alpha^3(T^*)$	[5, 5, 2]	2.30414417603593895847264293478
$\alpha^4(T^*)$	[4, 6, 2]	2.30348720654135784657134525755
$\alpha^5(T^*)$	[3, 7, 2]	2.30226165044440472718571097461
$\alpha^6(T^*)$	[2, 8, 2]	2.29881642949995094980856594643
$\gamma(T^*)$	[7, 2, 3]	2.28520768467980257500859073365
$\alpha(\gamma(T^*))$	[6, 3, 3]	2.28076523286917478390041282633
$\alpha^2(\gamma(T^*))$	[5, 4, 3]	2.27913084342903308996825366690
$\alpha^3(\gamma(T^*))$	[4, 5, 3]	2.27834791245706879712729095155
$\alpha^4(\gamma(T^*))$	[3, 6, 3]	2.27748824925244285093685838480
$\alpha^5(\gamma(T^*))$	[2, 7, 3]	2.27554403106324050144208754160
$\gamma^2(T^*)$	[6, 2, 4]	2.27010998510725135104117051475
$\alpha(\gamma^2(T^*))$	[5, 3, 4]	2.26762484634172519636930335282
$\alpha^2(\gamma^2(T^*))$	[4, 4, 4]	2.26667762008239070931668388638
$\alpha^3(\gamma^2(T^*))$	[3, 5, 4]	2.26605728367174815669677409819
$\alpha^4(\gamma^2(T^*))$	[2, 6, 4]	2.26506821261118740374393886088
$\gamma^3(T^*)$	[5, 2, 5]	2.26290253458453744084697620016
$\alpha(\gamma^3(T^*))$	[4, 3, 5]	2.26171078345443097808224085587
$\alpha^2(\gamma^3(T^*))$	[3, 4, 5]	2.26119844487818869745804831320
$\alpha^3(\gamma^3(T^*))$	[2, 5, 5]	2.26069897200749878293447592468
$\gamma^4(T^*)$	[4, 2, 6]	2.25980268994372236598891968054
$\alpha(\gamma^4(T^*))$	[3, 3, 6]	2.25927957177517211016191460326
$\alpha^2(\gamma^4(T^*))$	[2, 4, 6]	2.25898741243972985580277387992
$\gamma^5(T^*)$	[3, 2, 7]	2.25857320563154910353684549335
$\alpha(\gamma^5(T^*))$	[2, 3, 7]	2.25834278165321357168906331906
$\gamma^6(T^*) = T_*$	[2, 2, 8]	2.25810972712429442797185863240

As expected, the index ordering in $\mathfrak{F}(23)$ is total.

Remark 5.6. Theorem 5.3 has a powerful application, not only we can obtain the extremal indices in $\mathfrak{F}(n)$, but given any $[x, y, z] \in \mathfrak{F}(n)$ and a 2-switch F, such that $F([x, y, z]) = [x', y', z']$ we can immediately say if F increases or decreases the index by using the order relation in Theorem 5.3 (c).

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