ON A POSET OF TREES II

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Abstract. In this paper we study problems where one has to prove that certain graph parameter attains its maximum at the star and its minimum at the path among the trees on a fixed number of vertices. We give many applications of the so-called generalized tree shift which seems to be a powerful tool to attack the problems of the above mentioned kind. We show that the generalized tree shift increases the largest eigenvalue of the adjacency matrix and Laplacian matrix, decreases the coefficients of the characteristic polynomials of these matrices in absolute value. We will prove similar theorems for the independence polynomial and the edge cover polynomial. The generalized tree shift induces a partially ordered set on trees having fixed number of vertices. The smallest element of this poset is the path, largest element is the star. Hence the above mentioned results imply the extremality of the path and the star for these parameters.

1. Introduction

In many extremal problems concerning trees it turns out that the maximal (minimal) value of the examined parameter is attained at the star and the minimal (maximal) value is attained at the path among trees on n vertices. For instance, the star has the greatest largest eigenvalue and the path has the smallest largest eigenvalue among the trees on n vertices. Other example is the Wiener-index which is the sum of the distances of any two vertices; here it turns out that the star has the minimal Wiener-index and path has the largest Wiener-index. In many cases it is not hard to prove the extremality of the star, but sometimes to prove the extremality of the path needs some effort. In this paper we introduce a method which is very efficient proving these kinds of results.

The heart of this method is a transformation called generalized tree shift. This transformation determines a partially ordered set on trees with fixed number of vertices. The minimal element of this poset is the path, while the maximal element is the star. In this paper we give various examples of parameters changing along this poset proving the extremality of the star and the path. Of course, we gain much more than just the extremality of the path and the star.

In [4] we proved that the generalized tree shift increases the number of closed walks of length ℓ for every $\ell \geq 0$. This yields that the star has the largest number, the path has the smallest number of closed walks of length ℓ among trees on n vertices. In [3] B. Bollobás and M. Tyomkyn proved that the same holds for the number of arbitrary walks of length ℓ. In this paper we mainly concentrate on graph parameters

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arising from graph polynomials. This means that our results will have the following shape. Assume that $P(G,x) = x^n + a_{n-1}(G)x^{n-1} + \dots a_1(G)x + a_0(G)$ is some graph polynomial (characteristic polynomial of the adjacency matrix, independence polynomial, etc.). Let T be a tree and T' be some tree obtained from T by some generalized tree shift then $|a_k(T)| \geq |a_k(T')|$ for all $1 \leq k \leq n-1$ and the largest real root of $P(T',x)$ is larger than the largest real root of $P(T,x)$. (Of course, the actual relation will depend on the graph polynomial.) We will prove results of the above type for the characteristic polynomial of the adjacency matrix, Laplacian matrix and for the independence polynomial and edge cover polynomial.

This paper is arranged as follows. In Section 2 we introduce the concept of the generalized tree shift and the induced poset of the generalized tree shift. In Section 3 we revisit the theorems concerning the spectral radius of trees and their complements. In Section 4 we give an overview how to use the generalized tree shift when one studies graph polynomials of trees. In Section 5 we prove the so-called General Lemma, which unifies many computations concerning graph polynomials of trees. In Section 6, 7, 8 and 9 we will prove many theorems on the extremal values of the coefficients and roots of the characteristic polynomial of the adjacency matrix and Laplacian matrix, the independence polynomial and the edge cover polynomial. In Section 10 we give a little discussion on related graph transformations. We end the paper with some concluding remarks.

Notations: We will follow the usual notation: G is a graph, $V(G)$ is the set of its vertices, $E(G)$ is the set of its edges, $e(G)$ denotes the number of edges, $N(x)$ is the set of the neighbors of x, $|N(v_i)| = \deg(v_i) = d_i$ denote the degree of the vertex v_i. We will also use the notation $N[v]$ for the closed neighbor $N(v) \cup \{v\}$. The complement of the graph G will be denoted by $\overline{G}$.

For $S \subset V(G)$ the graph $G - S$ denotes the subgraph of G induced by the vertices $V(G)\backslash S$. If $S = \{v\}$ then we will use the notation $G - v$ and $G - \{v\}$ as well.

If $e \in E(G)$ then $G - e$ denotes the graph with vertex set $V(G)$ and edge set $E(G)\backslash\{e\}$.

Let P_n and S_n denote the path and the star on n vertices. We also use the notation xPy for the path with endvertices x and y.

The matrix $A(G)$ will denote the adjacency matrix of the graph G, i.e., $A(G)_{ij}$ is the number of edges going between the vertices v_i and v_j. Since $A(G)$ is symmetric, its eigenvalues are real and we will denote them by $\mu_1 \geq \mu_2 \geq \dots \geq \mu_n$. We will also use the notation $\mu(G)$ for the largest eigenvalue and we will call it the spectral radius of the graph G. The characteristic polynomial of the adjacency matrix will be denoted by

$$\phi(G,x) = \det(xI - A(G)) = \prod_{i=1}^{n}(x - \mu_i).$$

We will simply call it the adjacency polynomial.

The Laplacian matrix of G is $L(G) = D(G) - A(G)$ where $D(G)$ is the diagonal matrix for which $D(G)_{ii} = d_i$, the degree of the vertex v_i. The matrix $L(G)$ is symmetric, positive semidefinite, so its eigenvalues are real and non-negative, the smallest one is 0; we will denote them by $\lambda_1 \geq \lambda_2 \geq \dots \lambda_{n-1} \geq \lambda_n = 0$. We will also use the notation $\lambda_{n-1}(G) = a(G)$ for the so-called algebraic connectivity of the graph G. We introduce the notation $\theta(G)$ for the Laplacian spectral radius $\lambda_1(G)$. The characteristic polynomial of the Laplacian matrix will be denoted by

$$L(G,x)=\det(xI-L(G))=\prod_{i=1}^{n}(x-\lambda_i).$$

We will simply call it the Laplacian polynomial.

If the polynomial $P(G,x)$ has the form

$$P(G,x)=\sum_{k=0}^{n}(-1)^{n-k}s_k(G)x^k,$$

where $s_k(G)\geq 0$, then $\widehat{P}(G,x)$ denotes the polynomial

$$\widehat{P}(G,x)=(-1)^nP(G,-x)=\sum_{k=0}^{n}s_k(G)x^k.$$

For polynomials P_1 and P_2 we will write $P_1(x)\gg P_2(x)$ if they have the same degree and the absolute value of the coefficient of x^k in $P_1(x)$ is at least as large as the absolute value of the coefficient of x^k in $P_2(x)$ for all $0\leq k\leq n$.

Let M_1 and M_2 be two graphs with u_1 and u_2 vertices of M_1 and M_2, respectively. Let $M_1:M_2$ be the graph obtained from M_1, M_2 by identifying the vertices of u_1 and u_2. So $|V(M_1:M_2)|=|V(M_1)|+|V(M_2)|-1$ and $E(M_1:M_2)=E(M_1)\cup E(M_2)$. Note that this operation depends on the vertices u_1,u_2, but we do not sign it in the notation. Sometimes to avoid the confusion we use the notation $(M_1|u_1):(M_2|u_2)$.

Additional definitions and notation will be given in the appropriate sections.

2. Generalized tree shift

In this section we introduce our main tool.

Definition 2.1. Let T be a tree and x and y be vertices such that all the interior points of the path xPy (if they exist) have degree 2 in T. The generalized tree shift (GTS) of T is the tree T' obtained from T as follows: let z be the neighbor of y lying on the path xPy, let us erase all the edges between y and $N(y)\backslash\{z\}$ and add the edges between x and $N(y)\backslash\{z\}$. See Figure 1.

In what follows we call x the beneficiary and y the candidate (for being a leaf) of the generalized tree shift. Observe that we can interchange the role of the beneficiary and the candidate, the resulting trees will be isomorphic. Hence the resulting tree T' only depends on the tree T and the path xPy.

Note that if x or y is a leaf in T then $T'\cong T$, otherwise the number of leaves in T' is the number of leaves in T plus one. In this latter case we call the generalized tree shift proper.

Remark 2.2. Note that x and y need not have degree 2.

Notation: In the following we call the vertices of the path xPy $1,2,\dots,k$ if the path consists of k vertices such way that x will be 1 and y will be k. The set $A\subset V(T)$ consists of the vertices which can be reached with a path from k only through 1, and similarly the set $B\subset V(T)$ consists of those vertices which can be reached with a path from 1 only through k. For the sake of simplicity let A and B denote the corresponding sets in T'. The set of neighbors of 1 in A is called A_0, and similarly B_0

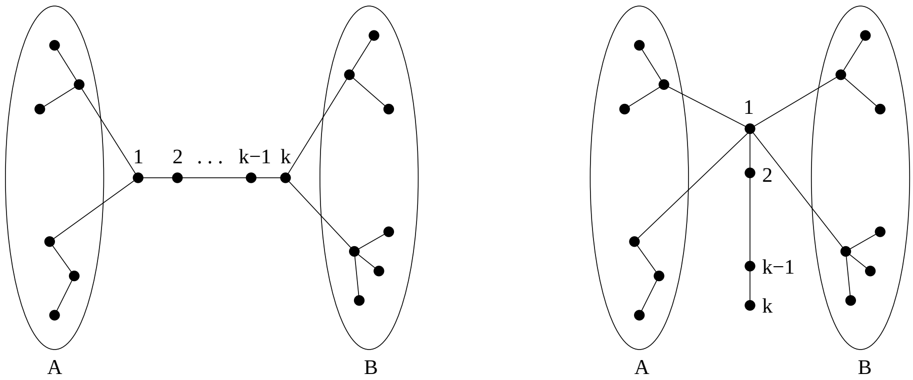

FIGURE 1. The generalized tree shift.

is the set of neighbors of 1 in $B \subset V(T')$ and set of neighbors of k in $B \subset V(T)$. Let H_1 be the tree induced by the vertices of $A \cup \{1\}$ in T, similarly let H_2 denote the tree induced by the vertices of $B \cup \{k\}$ in T. Note that H_1 and H_2 are both subtrees of T'.

Definition 2.3. Let us say that $T' > T$ if T' can be obtained from T by some proper generalized tree shift.

Remark 2.4. The relation $>$ induces a poset on the trees on n vertices, since the number of leaves of T' is greater than the number of leaves of T, more precisely the two numbers differ by one. Hence the relation $>$ is indeed extendable. See Figure 2.

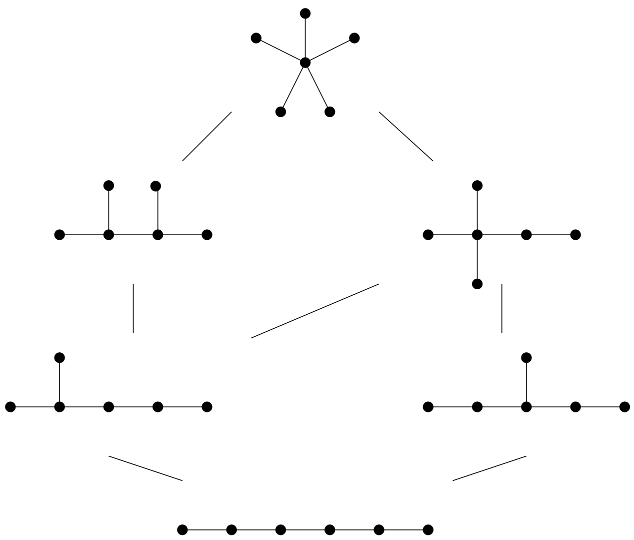

FIGURE 2. The poset of trees on 6 vertices.

One can always apply a proper generalized tree shift to any tree which has at least two vertices that are not leaves. This shows that the only maximal element of the induced poset is the star. The following theorem shows that the only minimal element of the induced poset, i.e., the smallest element is the path.

Theorem 2.5. [4] *Every tree different from the path is the image of some proper generalized tree shift, i.e., the only minimal element of the poset is the path.*

3. Spectral radius

The following theorem was proved in [4] where it was a corollary of a theorem on closed walks of trees. Since the proof of this latter result was rather long we wish to give a concise proof.

Theorem 3.1. *The generalized tree shift increases the spectral radius of the tree.*

Proof. Let u and v be the beneficiary and the candidate of the generalized tree shift, respectively. First of all, recall that if we change the role of the beneficiary and the candidate then the resulting tree will not change up to isomorphism.

Let $\underline{x}$ be the non-negative eigenvector of unit length corresponding to the largest eigenvalue of the tree T, such a vector exists by the Perron-Frobenius theorem. By the previous paragraph we can assume that $x_u \geq x_v$.

Furthermore, let $A(T)$ and $A(T')$ be the adjacency matrices of the tree T and T'. Then

$$\mu(T) = \underline{x}^T A(T)\underline{x} = \underline{x}^T A(T')\underline{x} - 2(x_u - x_v) \sum_{w \in B_0} x_w \leq \underline{x}^T A(T')\underline{x} \leq$$

$$\leq \max_{||y||=1} \underline{y}^T A(T')\underline{y} = \mu(T').$$

Hence $\mu(T) \leq \mu(T')$.

□

Corollary 3.2. *The path minimizes, the star maximizes the spectral radius of the adjacency matrix among the trees on n vertices.*

Remark 3.3. Corollary 3.2 was known, it was proved by L. Lovász and J. Pelikán [18]. In fact, they proved their theorem by the aid of some graph transformation which is a special case of the generalized tree shift.

We mention that Nikiforov's inequality [21]

$$\mu(G) \leq \sqrt{2e(G)\left(1 - \frac{1}{\omega(G)}\right)}$$

also implies that the star has maximal spectral radius for trees since we have $e(G) = n-1$ and $\omega(G) = 2$ and the greatest eigenvalue of the star is exactly $\sqrt{n-1}$. (It was Nosal who proved that for triangle-free graphs $\mu(G) \leq \sqrt{e(G)}$ holds, later Nikiforov [22] proved that in Nosal's inequality equality holds if and only if the graph is complete bipartite with some isolated vertices.)

Theorem 3.4. *The generalized tree shift increases the spectral radius of the complement of a tree.*

Proof. Let u and v be the beneficiary and the candidate of the generalized tree shift, respectively. Let $\underline{x}$ be the non-negative eigenvector of unit length corresponding to the largest eigenvalue of the graph $\overline{T}$. As before, we can assume that $x_v \geq x_u$.

Furthermore, let $A(\overline{T})$ and $A(\overline{T'})$ be the adjacency matrix of the $\overline{T}$ and $\overline{T'}$. Then

$$\mu(\overline{T}) = \underline{x}^T A(\overline{T'})\underline{x} - 2(x_v - x_u) \sum_{w \in B_0} x_w \leq \underline{x}^T A(\overline{T'})\underline{x} \leq$$

$$\leq \max_{||y||=1} \underline{y}^T A(\overline{T'})\underline{y} = \mu(\overline{T'}).$$

Hence $\mu(\overline{T}) \leq \mu(\overline{T'})$. □

Corollary 3.5. *If T is a tree on n vertices, P_n and S_n are the path and the star on n vertices and $\mu(G)$ is the spectral radius of a graph then*

$$\mu(\overline{P_n}) \leq \mu(\overline{T}) \leq \mu(\overline{S_n}).$$

4. Graph polynomials and the generalized tree shift

In this section we give a general overview how to use the generalized tree shift in the situations when we would like to prove that certain graph polynomial has the largest coefficients for the star and smallest coefficients for the path among the trees on n vertices, or we would like to prove that the largest real root of the polynomial is maximal for the star and minimal for the path.

Assume that given a graph polynomial $f(G,x)$. We will see that in many cases we have an identity of the following kind:

$$f(T',x) - f(T,x) = c_1 h(P_k,x) h(H_1,x) h(H_2,x),$$

where $h(G,x) = c_2 f(G,x) + c_3 g(G|v,x)$ and c_1, c_2, c_3 are rational functions of x and $g(G|v,x)$ is some graph polynomial depending on G and some special vertex v. (Recall that H_1 and H_2 are the subtrees of T and T' induced by the vertex set $A \cup \{1\}$ and $B \cup \{k\}$, respectively.) Generally, the graph polynomial $g(G|v,x)$ is very strongly related to $f(G,x)$, in many cases it will be $f(H,x)$ for some subgraph H of G. This means that the difference $f(T',x) - f(T,x)$ factorizes to polynomials of trees which are subtrees of both T and T'. Then we use some monotonicity property of the studied parameter to deduce that the generalized tree shift increases (decreases) this parameter. Clearly, it yields the desired result for the extremality of the star and the path. We have to emphasize that the monotonicity of the parameter is indeed crucial in many applications. In most of the cases it will be more tedious to settle the suitable monotonicity property than to prove the proper identity for $f(T',x) - f(T,x)$.

How will we obtain the above identity for $f(T',x) - f(T,x)$? There is a very straightforward way of doing that. We only need to compute a recursion formula for $M_1 : M_2$ (this graph was defined in the introduction among the notations).

Observe that $T = (H_1 : P_k) : H_2$, where we identify $1 \in V(H_1)$ and $1 \in V(P_k)$ and then we identify $k \in V(P_k)$ and $k \in V(H_2)$. While for the image of T at the generalized tree shift applied to the tree T and P_k, we have $T' = (H_1 : H_2) : P_k$, where we identify $1 \in V(H_1)$ and $1 \in V(H_2)$ and then we identify $1 \in V(H_1 : H_2)$ and $1 \in V(P_k)$. So if we have some recursion formula for $M_1 : M_2$ then we can express

$$f(T,x) = h_1(f(P_k,x), g(P_k|1,x), f(H_1,x), g(H_1|1,x), f(H_2,x), g(H_2|k,x))$$

and

$$f(T',x) = h_2(f(P_k,x), g(P_k|1,x), f(H_1,x), g(H_1|1,x), f(H_2,x), g(H_2|k,x)).$$

Although this strategy would be very straightforward, the amount of computation we need to perform heavily depends on the polynomial $f(G,x)$ and sometimes it is indeed a huge work. To avoid this, we will prove a theorem which directly computes $f(T,x) - f(T',x)$ from the recursion formula of $f(M_1 : M_2)$.

5. General lemma

Theorem 5.1. *(General lemma.) Assume that the graph polynomials f and g satisfy the following recursion formula.*

$$f(M_1 : M_2, x) = c_1 f(M_1,x) f(M_2,x) + c_2 f(M_1,x) g(M_2|u_2,x) +$$

$$+c_2 g(M_1|u_1,x) f(M_2,x) + c_3 g(M_1|u_1,x) g(M_2|u_2,x),$$

where c_1, c_2, c_3 are rational functions of x. Let K_2 and P_3 be the paths on two and three vertices, respectively. Assume that $c_2 f(K_2) + c_3 g(K_2|1) \neq 0$. Then

$$f(T) - f(T') = c_4(c_2 f(P_k) + c_3 g(P_k|1))(c_2 f(H_1) + c_3 g(H_1|1))(c_2 f(H_2) + c_3 g(H_2|k)),$$

where

$$c_4 = \frac{g(P_3|1) - g(P_3|2)}{(c_2 f(K_2) + c_3 g(K_2|1))^2}.$$

Proof. Since $T = (((H_1|1) : (P_k|1))|k) : (H_2|k)$ we have

$$f(T) = c_1 f(H_1 : P_k) f(H_2) + c_2 f(H_1 : P_k) g(H_2|k) =$$
$$+c_2 g(H_1 : P_k|k) f(H_2) + c_3 g(H_1 : P_k|k) g(H_2|k).$$

Similarly, $T' = (((H_1|1) : (P_k|1))|1) : (H_2|1)$ so

$$f(T') = c_1 f(H_1 : P_k) f(H_2) + c_2 f(H_1 : P_k) g(H_2|1) +$$
$$+c_2 g(H_1 : P_k|1) f(H_2) + c_3 g(H_1 : P_k|1) g(H_2|1).$$

Note that $g(H_2|1) = g(H_2|k)$, since 1 and k denote the same vertex, only their names are different in the different trees. Hence

$$f(T) - f(T') = (c_2 f(H_2) + c_3 g(H_2|k))(g(H_1 : P_k|k) - g(H_1 : P_k|1)).$$

Now let us consider

$$\frac{f(T) - f(T')}{(c_2 f(H_1) + c_3 g(H_1|1))(c_2 f(H_2) + c_3 g(H_2|k))} = \frac{g(H_1 : P_k|k) - g(H_1 : P_k|1)}{c_2 f(H_1) + c_3 g(H_1|1)}.$$

The left hand side is symmetric in H_1 and H_2 so if we switch them we obtain that

$$\frac{g(H_1 : P_k|k) - g(H_1 : P_k|1)}{c_2 f(H_1) + c_3 g(H_1|1)} = \frac{g(H_2 : P_k|k) - g(H_2 : P_k|1)}{c_2 f(H_2) + c_3 g(H_2|1)}.$$

Since H_1 and H_2 can be chosen arbitrarily, this expression is the same for every graph H_1. In particular, we can apply it to K_2:

$$\frac{g(H_1 : P_k|k) - g(H_1 : P_k|1)}{c_2 f(H_1) + c_3 g(H_1|1)} = \frac{g(K_2 : P_k|k) - g(K_2 : P_k|1)}{c_2 f(K_2) + c_3 g(K_2|1)}.$$

In fact, applying the above computation for $H_1 = H_2 = K_2$ we obtain that

$$\frac{f(P_{k+2}) - f(Q_{k+2})}{(c_2 f(K_2) + c_3 g(K_2|1))^2} = \frac{g(K_2 : P_k|k) - g(K_2 : P_k|1)}{c_2 f(K_2) + c_3 g(K_2|1)},$$

where Q_{k+2} is the tree that we obtain from P_{k+1} by attaching a pendent edge to the second vertex. This will be the GTS-transform of P_{k+2} if we apply it to $H_1 = H_2 = K_2$ and the path P_k. Note that $Q_{k+2} = P_3 : P_k$, where we identified the middle vertex of P_3 and the endvertex of P_k. On the other hand, $P_{k+2} = P_3 : P_k$, where we identified the endvertices of P_3 and P_k. Hence

$$f(Q_{k+2}) = c_1 f(P_3) f(P_k) + c_2 g(P_3|2) f(P_k) + c_2 f(P_3) g(P_k|1) + c_3 g(P_3|2) g(P_k|1).$$

Similarly,

$$f(P_{k+2}) = c_1 f(P_3) f(P_k) + c_2 g(P_3|1) f(P_k) + c_2 f(P_3) g(P_k|1) + c_3 g(P_3|1) g(P_k|1).$$

Hence

$$f(P_{k+2}) - f(Q_{k+2}) = (g(P_3|1) - g(P_3|2))(c_2 f(P_k) + c_3 f(P_k|1)).$$

Putting all together we obtain that

$$f(T) - f(T') = c_4(c_2 f(P_k) + c_3 g(P_k|1))(c_2 f(H_1) + c_3 g(H_1|1))(c_2 f(H_2) + c_3 g(H_2|k)),$$

where

$$c_4 = \frac{g(P_3|1) - g(P_3|2)}{(c_2 f(K_2) + c_3 g(K_2|1))^2}.$$

□

Remark 5.2. Throughout this paper we will refer to Theorem 5.1 as General Lemma.

6. The adjacency polynomial

In this section we are concerned with the characteristic polynomial of the adjacency matrix. We have already seen that the GTS increases the spectral radius of the adjacency matrix. The main result of this section is that it decreases the coefficients in absolute value.

Theorem 6.1. *The generalized tree shift decreases the coefficients of the characteristic polynomial in absolute value, i.e., if the tree T' is obtained from the tree T by some generalized tree shift then*

$$\phi(T,x) \gg \phi(T',x).$$

(Recall that $\phi(T,x) \gg \phi(T',x)$ means that each coefficient of $\phi(T,x)$ in absolute value is at least as large as the corresponding coefficient of $\phi(T',x)$ in absolute value.)

Lemma 6.2. [18] *For arbitrary forest T we have*

$$\phi(T,x) = \sum_{k=0}^{n} (-1)^k m_k(T) x^{n-2k},$$

where $m_k(T)$ denotes the number of ways one can choose k independent edges of the forest T.

Remark 6.3. So we need to prove that $m_k(T) \geq m_k(T')$ for every $1 \leq k \leq n$. One can do it by purely combinatorial tools, but in order to show our strategy in work we have chosen an algebraic way.

Lemma 6.4. *With the notation introduced in the introduction, for the trees T and T' we have*

$$\phi(T,x) - \phi(T',x) = \phi(P_{k-2},x)(\phi(H_1,x) - x\phi(H_1 - \{1\},x))(\phi(H_2,x) - x\phi(H_2 - \{1\},x)).$$

To prove this lemma we need the following formula for the characteristic polynomial of $M_1 : M_2$.

Lemma 6.5. *For the graph $M_1 : M_2$ we have*

$$\phi(M_1 : M_2, x) = \phi(M_1,x)\phi(M_2 - u_2,x) + \phi(M_1 - u_1,x)\phi(M_2,x) - x\phi(M_1 - u_1,x)\phi(M_2 - u_2,x).$$

Proof. This was first proved by A. J. Schwenk in [23]. It can be found in [9] too: this is Corollary 3.3 in Chapter 4. Another proof can be given by copying the argument of Lemma 7.7. □

Proof of Lemma 6.4. By the previous lemma we can apply the General Lemma for $f(G,x) = \phi(G,x)$, $g(G|v,x) = \phi(G - v,x)$ and $c_1 = 0, c_2 = 1, c_3 = -x$.

We have $\phi(K_2,x) - x\phi(K_1,x) = (x^2 - 1) - x^2 = -1$ and

$$\phi(P_3 - \{1\},x) - \phi(P_3 - \{2\},x) = (x^2 - 1) - x^2 = -1.$$

Finally,

$$x\phi(P_{k-1},x) - \phi(P_k,x) = \phi(P_{k-2},x).$$

Hence

$$\phi(T,x)-\phi(T',x)=\phi(P_{k-2},x)(\phi(H_1,x)-x\phi(H_1-\{1\},x))(\phi(H_2,x)-x\phi(H_2-\{1\},x)).$$

□

From this one can easily deduce Theorem 6.1 as follows.

Proof of Theorem 6.1. Note that from Lemma 6.2 we have

$$(-i)^n\phi(ix)=\sum_{r=0}^{\lfloor n/2\rfloor} m_r(G)x^{n-2r},$$

where i is the square root of -1. Hence

$$\sum_{r=0}^{n}(m_r(T)-m_r(T'))x^{n-2r}=(-i)^n(\phi(T,ix)-\phi(T',ix))=$$

$$=(-i)^{k-2}\phi(P_{k-2},ix)((-i)^{a+1}\phi(H_1,ix)-(-i)^{a+1}(ix)\phi(H_1-\{1\},ix))\cdot$$
$$\cdot((-i)^{b+1}\phi(H_2,ix)-(-i)^{b+1}(ix)\phi(H_2-\{1\},ix)),$$

where $|V(H_1)|=a+1$, $|V(H_2)|=b+1$ and $|V(T)|=|V(T')|=n=a+b+k$. Note that $x\phi(H_j-\{1\},x)$ is the characteristic polynomial of the forest H_j^* which can be obtained from H_j by deleting the edges incident to the vertex 1 (but we do not delete the vertex). Hence

$$\sum_{r=0}^{n}(m_r(T)-m_r(T'))x^{n-2r}=$$

$$=\left(\sum_{r=0}^{n}m_r(P_{k-2})x^{n-2r}\right)\left(\sum_{r=0}^{n}(m_r(H_1)-m_r(H_1^*))x^{n-2r}\right)\left(\sum_{r=0}^{n}(m_r(H_2)-m_r(H_2^*))x^{n-2r}\right).$$

Since $m_r(H_j)\geq m_r(H_j^*)$, each coefficient of the right hand side is non-negative. Hence $m_r(T)\geq m_r(T')$. □

Remark 6.6. Theorem 3.1 can be deduced from Lemma 6.4 as well.

7. The Laplacian characteristic polynomial

Recall that we denote the Laplacian matrix of G by $L(G)$ and $L(G,x)=\det(xI-L(G))$ denotes the characteristic polynomial of the Laplacian matrix of G.

Let $L(G|u)$ be the matrix obtained from $L(G)$ be deleting the row and the column corresponding to the vertex u (warning: this is not $L(G-u)$ because of the diagonal elements). Furthermore, let $L(G|u,x)$ denote the characteristic polynomial of $L(G|u)$.

We will subsequently use the following two classical facts, for details see [10].

Statement 7.1. *The eigenvalues of* $L(G)$ *are non-negative real numbers, at least one of them is* 0*. Hence we can order them as* $\lambda_1\geq\lambda_2\geq\cdots\geq\lambda_n=0$.

Corollary 7.2. *The Laplacian polynomial can be written as*

$$L(G,x)=x^n-a_{n-1}x^{n-1}+a_{n-2}x^{n-2}-\cdots+(-1)^{n-1}a_1x,$$

where $a_1,a_2,\ldots,a_{n-1}$ *are non-negative integers.*

Recall that we use the notation $\lambda_{n-1}(G) = a(G)$ for the so-called algebraic connectivity of the graph G and the notation $\theta(G)$ for the Laplacian spectral radius $\lambda_1(G)$.

The main result of this section is the following.

Theorem 7.3. *The generalized tree shift decreases the coefficients of the Laplacian polynomial in absolute value, i.e., if T' is obtained from T by a generalized tree shift then*

$$L(T,x) \gg L(T',x)$$

or in other words $a_k(T) \geq a_k(T')$ for $k = 1, \dots, n-1$. Furthermore, $\theta(T') \geq \theta(T)$ and $a(T') \geq a(T)$.

Corollary 7.4. *Let $L(G,x) = \sum_{k=1}^{n} (-1)^{n-k} a_k(G) x^k$. Then*

$$a_k(P_n) \geq a_k(T) \geq a_k(S_n).$$

for any tree T on n vertices and $k = 1, \dots, n-1$. Furthermore,

$$\theta(P_n) \leq \theta(T) \leq \theta(S_n),$$

and

$$a(P_n) \leq a(T) \leq a(S_n).$$

Remark 7.5. All parts of Corollary 7.4 are known. The first statement concerning the coefficients of the Laplacian polynomial was conjectured in [14] and was proved by B. Zhou and I. Gutman [2] by the aid of a surprising connection between the Laplacian polynomial and the adjacency polynomial of trees. A different proof was given by B. Mohar [20] using graph transformations. The same approach was used by D. Stevanović and A. Ilić [24] when they studied the extremal values of Laplacian coefficients of unicyclic graphs.

The maximality of the star concerning the Laplacian spectral radius is trivial since $\theta(S_n) = n$, because $\overline{S_n}$ is not connected and this is the maximal value for a graph on n vertices. The minimality of the path is proved in [15].

The first statement concerning the algebraic connectivity (the minimality of the path) was proved by R. Grone and R. Merris [11], the second statement was proved by R. Merris [19]. J.-M. Guo [12] gave new proofs for both parts by using graph transformations.

Again we will prove a product formula for $L(T,x) - L(T',x)$.

Lemma 7.6. *With our usual notation we have*

$$L(T,x) - L(T',x) = \frac{1}{x} L(P_{k-1},x)(L(H_1,x) - xL(H_1|1,x))(L(H_2,x) - xL(H_2|k,x)).$$

Lemma 7.7. *As usual, let $M_1 : M_2$ denote the graph obtained from M_1, M_2 by identifying the vertices of u_1 and u_2. Then*

$$L(M_1 : M_2, x) = L(M_1,x)L(M_2|u_2,x) + L(M_2,x)L(M_1|u_1,x) -$$
$$-xL(M_1|u_1,x)L(M_2|u_2,x).$$

Proof. Let $|V(M_1)| = n_1$ and $|V(M_2)| = n_2$. Furthermore, let d_1 and d_2 be the degree of u_1 and u_2 in M_1 and M_2, respectively.

Let the rows and columns of $A = L(M_1 : M_2)$ be ordered in such a way that the first n_1 rows and columns correspond to the vertices of M_1, while the last n_2 rows and columns correspond to the vertices of M_2. Hence, the n_1th row and column correspond to the vertex $u_1 = u_2$.

The key observation is that if we consider the expansion of $\det(xI - A)$, none of the non-zero terms contain $a_{i,n_1}, a_{n_1,j}$ together where $i < n_1 < j$. Indeed, a non-zero product should contain $n_1 - 1$ non-zero elements from the first $n_1 - 1$ columns and together with $a_{i,n_1}, a_{n_1,j}$, this would be $n_1 + 1$ elements from the first n_1 rows.

Similarly, none of the non-zero terms contain $a_{i,n_1}, a_{n_1,j}$ together where $i > n_1 > j$.

So we can divide the non-zero terms of $\det(xI - A)$ into three classes. The first class contains those terms in which $x - a_{n_1,n_1} = x - d_1 - d_2$ appears. Their sum is clearly

$$(x - d_1 - d_2)L(M_1|u_1, x)L(M_2|u_2, x).$$

The second class are those non-zero terms which contain an element $-a_{i,n_1}$ where $i < n_1$. These terms should contain $-a_{n_1,j}$ for some $j < n_1$. These terms contribute the sum $\det(B_1)L(M_2|u_2, x)$ where B_1 is the matrix obtained from $xI - L(M_1)$ by replacing $x - a_{n_1,n_1}$ with 0. Then

$$\det(B_1) = L(M_1, x) - (x - d_1)L(M_1|u_1, x).$$

Finally, the third class are those non-zero terms which contain an element $-a_{i,n_1}$, where $i > n_1$. These terms should contain $-a_{n_1,j}$ for some $j > n_1$. These terms contribute the sum $\det(B_2)L(M_1|u_1, x)$ where B_2 is the matrix obtained from $xI - L(M_2)$ by replacing $x - a_{n_1,n_1}$ with 0. Then

$$\det(B_2) = L(M_2, x) - (x - d_2)L(M_2|u_2, x).$$

Putting all these together we get

$$L(M_1 : M_2, x) = (x - d_1 - d_2)L(M_1|u_1, x)L(M_2|u_2, x)+$$

$$+(L(M_1, x)-(x-d_1)L(M_1|u_1, x))L(M_2|u_2, x)+(L(M_2, x)-(x-d_2)L(M_2|u_2, x))L(M_1|u_1, x)$$

$$= L(M_1, x)L(M_2|u_2, x) + L(M_2, x)L(M_1|u_1, x) - xL(M_1|u_1, x)L(M_2|u_2, x).$$

□

Proof of Lemma 7.6. By Lemma 7.7 we can apply the General Lemma with $f(G, x) = L(G, x)$, $g(G|v, x) = L(G|v, x)$ and $c_2 = 1, c_3 = -x$. In this case,

$$L(K_2, x) - xL(K_2|1, x) = x(x - 2) - x(x - 1) = -x$$

and

$$L(P_3|1, x) - L(P_3|2, x) = ((x - 2)(x - 1) - 1) - (x - 1)^2 = -x.$$

Furthermore, expanding the matrix of $L(P_k, x)$ according to the first row, we have

$$L(P_k, x) = (x - 1)L(P_{k-1}|1, x) - L(P_{k-2}|1, x).$$

Hence

$$L(P_k, x) - xL(P_{k-1}, x) = -L(P_{k-1}|1, x) - L(P_{k-2}, x) = -L(P_{k-1}, x).$$

Putting all together we get that

$$L(T, x) - L(T', x) = \frac{1}{x}L(P_{k-1}, x)(L(H_1, x) - xL(H_1|1, x))(L(H_2, x) - xL(H_2|k, x)).$$

□

Now we are ready to prove Theorem 7.3. For the sake of convenience we repeat the corresponding part of the theorem which we prove.

Theorem 7.3 (First part.)

$$L(T,x) \gg L(T',x).$$

Proof. Let $|V(A)| = a$, $|V(B)| = b$, then $|V(T)| = |V(T')| = a+b+k$. Because of the alternating sign of the coefficients we have to prove that each coefficient of

$$(-1)^{a+b+k}(L(T,-x) - L(T',-x))$$

is non-negative. Let $\widehat{L}(G,x) = (-1)^{|V(G)|}L(G,-x)$ and $\widehat{L}(G|v,x) = (-1)^{|V(G)|-1}L(G,-x)$, then $\widehat{L}(G,x)$ and $\widehat{L}(G|v,x)$ have only non-negative coefficients.

By Lemma 7.6 we have

$$\widehat{L}(T,x) - \widehat{L}(T',x) = (-1)^{a+b+k}(L(T,-x) - L(T',-x)) =$$

$$= (-1)^{a+b+k}\frac{L(P_{k-1},-x)}{-x}(L(H_1,-x) + xL(H_1|1,-x))(L(H_2,-x) + xL(H_2|1,-x)) =$$

$$= \frac{(-1)^{k-1}L(P_{k-1},-x)}{x}((-1)^{a+1}L(H_1,-x) - x(-1)^{a}L(H_1|1,-x))\cdot$$

$$\cdot((-1)^{b+1}L(H_2,-x) - x(-1)^{b}L(H_2|1,-x)) =$$

$$= \frac{1}{x}\widehat{L}(P_{k-1},x)(\widehat{L}(H_1,x) - x\widehat{L}(H_1|1,x))(\widehat{L}(H_2,x) - x\widehat{L}(H_2|1,x)).$$

We know that all coefficients of $\widehat{L}(P_{k-1},x)$ are non-negative. We show that the coefficients of the polynomials $\widehat{L}(H_1,x) - x\widehat{L}(H_1|1,x)$ and $\widehat{L}(H_2,x) - x\widehat{L}(H_2|1,x)$ are also non-negative. Clearly, it is enough to show it for the former one.

For any matrix B we have

$$f(B,x) = \det(xI - B) = \sum_{r=0}^{n}(-1)^{n-r}\left(\sum_{|S|=r}\det(B_S)\right)x^r,$$

where the matrix B_S is obtained from by deleting the rows and columns corresponding to the elements of the set S. In other words,

$$\widehat{f}(B,x) = (-1)^n\det(-xI - B) = \det(xI + B) = \sum_{r=0}^{n}\left(\sum_{|S|=r}\det(B_S)\right)x^r.$$

Hence

$$\widehat{L}(H_1,x) - x\widehat{L}(H_1|1,x)) = \sum_{r=0}^{n}\left(\sum_{|S|=r,1\notin S}^{n}\det(L(H_1)_S)\right)x^r.$$

Since $L(H_1)$ is a positive semidefinite matrix, all subdeterminants of it are non-negative. This proves that the coefficients are indeed non-negative. □

Remark 7.8. In [4] it was shown that the generalized tree shift decreases the Wiener-index of a tree. (The Wiener-index of a graph is the sum $\sum_{x,y} d(x,y)$, where $d(x,y)$ is the distance of the vertices x and y.) One can consider Theorem 7.3 as a generalization of this fact since the signless coefficient of x^2 in the Laplacian polynomial is just the Wiener-index (see [25]).

Theorem 7.3 (Second part.)

$$a(T') \geq a(T).$$

We will need some preparation. We will use the following fundamental lemmas.

Lemma 7.9. *(Interlacing lemma) Let G be a graph and e an edge of it. Let $\lambda_1 \geq \lambda_2 \geq \dots \lambda_{n-1} \geq \lambda_n = 0$ be the roots of $L(G,x)$ and let $\tau_1 \geq \tau_2 \geq \dots \tau_{n-1} \geq \tau_n = 0$ be the roots of $L(G-e,x)$. Then*

$$\lambda_1 \geq \tau_1 \geq \lambda_2 \geq \tau_2 \geq \dots \geq \lambda_{n-1} \geq \tau_{n-1}.$$

Corollary 7.10. *Let T_1 be a tree and T_2 be its subtree. Then $a(T_1) \leq a(T_2)$.*

Proof. It is enough to prove the statement for $T_1 - v = T_2$ where the degree of the vertex v is one. Let e be the pendant edge whose one of the end vertex is v. Then we can get T_2 by deleting the edge e and then the isolated vertex v. First we get that $\lambda_{n-2}(T_2 \cup \{v\}) \geq \lambda_{n-1}(T_1) \geq \lambda_{n-1}(T_2 \cup \{v\})$ by the interlacing lemma. After deleting the isolated vertex v we exactly delete the $\lambda_{n-1}(T_2 \cup \{v\}) = 0$ from the Laplacian spectra and we get that

$$a(T_2) = \lambda_{n-2}(T_2) = \lambda_{n-2}(T_2 \cup \{v\}) \geq \lambda_{n-1}(T_1) = a(T_1).$$

□

For the sake of simplicity, we introduce the polynomials

$$h(G,x) = (-1)^{n-1}\frac{1}{x}L(G,x) \quad \text{and} \quad r(G,x) = (-1)^{n-1}L(G|u,x),$$

where G is a graph on n vertices. It will be convenient to use the notation $a(p(x))$ for the smallest positive root of the polynomial $p(x)$.

The slight advantage of these polynomials is that they are non-negative at 0, more precisely $r(G,0)$ is the number of spanning trees while $h(G,0)$ is n times the number of spanning trees. So for a tree T we have $h(T,0) = n$ and $r(T,0) = 1$.

Now we are ready to prove the second part of Theorem 7.3.

Proof. Let us rewrite the formula of Lemma 7.6 in terms of polynomials h and r. For the sake of brevity, let $h(H_i,x) = h_i(x)$ and $r(H_i,x) = r_i(x)$. Since $V(H_1) = a+1,\ V(H_2) = b+1,\ V(P_k) = k$ we have

$$(-1)^{a+b+k}x(h(T,x) - h(T',x)) =$$

$$(-1)^{k-1}h(P_{k-1},x)((-1)^a x h_1(x) - x(-1)^a r_1(x))((-1)^b x h_2(x) - x(-1)^b r_2(x)).$$

Hence

$$h(T',x) = h(T,x) + x h(P_{k-1},x)(h_1(x) - r_1(x))(h_2(x) - r_2(x)).$$

Since all of these polynomials are positive in 0 we have

$$a(T') \geq \min(a(T), a(P_{k-1}), a(h_1 - r_1), a(h_2 - r_2)).$$

We only need to show that

$$\min(a(T), a(P_{k-1}), a(h_1 - r_1), a(h_2 - r_2)) = a(T).$$

Clearly, $a(P_{k-1}) \geq a(T)$ because P_{k-1} is a subtree of T, so we can apply Corollary 7.10. Next we show that $a(h_1 - r_1) \geq a(T)$. In fact, it will turn out that $a(h_1 - r_1) \geq a(h_1)$; but then we are done since H_1 is a subtree of T so $a(h_1) \geq a(T)$.

Now we prove that $a(h_1 - r_1) \geq a(h_1)$. The roots of the polynomial h_1 are the roots of $L(H_1,x)$ without 0: $\lambda_1 \geq \dots \geq \lambda_a > 0$. The roots of the polynomial r_1 are the roots of $L(H_1|1,x)$: $\lambda_1' \geq \dots \geq \lambda_a' > 0$. By the interlacing theorem for symmetric matrices, we have

$$\lambda_1 \geq \lambda_1' \geq \lambda_2 \geq \lambda_2' \geq \dots \geq \lambda_a \geq \lambda_a' > 0.$$

Assume for a moment that these roots are all different. Since $h_1 - r_1$ is positive in 0, namely $h_1(0) - r_1(0) = (a+1) - 1 = a$ we get that $h_1 - r_1$ is positive in the interval $[\lambda_j', \lambda_j]$ if $a - j$ is odd and negative if $a - j$ is even, because the sign of h_1 and r_1 are different at these intervals. So there must be a root of $h_1 - r_1$ in the interval $(\lambda_j, \lambda_{j-1}')$ for $j = 1, \dots, a-1$. But $h_1 - r_1$ is a polynomial of degree $a-1$, so we have found all of its roots. Hence there cannot be any root in the interval $[0, \lambda_a]$. Clearly, this argument with a slight modification still holds if some roots coincide: one can consider the intervals of length 0 as infinitely small intervals. Hence $a(h_1 - r_1) \geq a(h_1)$ and similarly $a(h_2 - r_2) \geq a(h_2)$. Hence $a(T') \geq a(T)$.

□

Theorem 7.3 (Third part.)

$$\theta(T') \geq \theta(T).$$

Disclaimer: the proof of this part is very similar to the proof of the previous part.

Here we need another corollary of Lemma 7.9.

Corollary 7.11. *Let G_2 be a subgraph of G_1 then $\theta(G_2) \leq \theta(G_1)$.*

Proof. First we delete all edges belonging to $E(G_1) \setminus E(G_2)$. This way we obtain that $\theta(G_1) \geq \theta(G_2')$ where $G_2' = (V(G_1), E(G_2))$. Then we delete the isolated vertices consisting of $V(G_1) \setminus V(G_2)$, this way we deleted some 0's from the Laplacian spectrum of G_2'. Clearly, this does not affect $\theta(G_2') = \theta(G_2)$. Hence $\theta(G_1) \geq \theta(G_2)$. □

Now we are ready to prove the third part of Theorem 7.3.

Proof. We will show that

$$L(T,x) - L(T',x) = \frac{1}{x} L(P_{k-1},x)(L(H_1,x) - xL(H_1|1,x))(L(H_2,x) - xL(H_2|k,x)) \geq 0$$

for $x \geq \theta(T')$ implying that $\theta(T') \geq \theta(T)$.

It is enough to show that $L(H_1,x) - xL(H_1|1,x) \leq 0$ for $x \geq \theta(H_1)$. Then by symmetry, we have $L(H_2,x) - xL(H_2|k,x) \leq 0$ for $x \geq \theta(H_2)$. Thus $L(T,x) - L(T',x) \geq 0$ for $x \geq \max(\theta(P_k), \theta(H_1), \theta(H_2))$. Since P_k, H_1, H_2 are all subgraphs of T' we have $\theta(T') \geq \max(\theta(P_k), \theta(H_1), \theta(H_2))$ by Corollary 7.11. Hence $L(T,x) - L(T',x) \geq 0$ for $x \geq \theta(T')$.

Now let us prove that $L(H_1,x) - xL(H_1|1,x) \leq 0$ for $x \geq \theta(H_1)$. First of all, let us observe that $L(H_1,x) - xL(H_1|1,x)$ is a polynomial of degree a with main coefficient $-d_1$, where $|V(H_1)| = a+1$ and d_1 is the degree of the vertex 1. Let the roots of the polynomial $L(H_1,x)$ be $\lambda_1 \geq \dots \geq \lambda_a = \lambda_{a+1} = 0$. The roots of the polynomial $L(H_1|1,x)$ are $\lambda_1' \geq \dots \geq \lambda_a' \geq 0$. By the interlacing theorem for symmetric matrices, we have

$$\lambda_1 \geq \lambda_1' \geq \lambda_2 \geq \lambda_2' \geq \dots \geq \lambda_a \geq \lambda_a' > 0.$$

Assume for a moment that these roots are all different. Then $L(H_1,x) - xL(H_1|1,x)$ is positive in the interval $[\lambda_j', \lambda_j]$ if j is odd and negative if j is even since both terms have the same sign. Hence there must be a root in the interval $(\lambda_{j+1}, \lambda_j')$ for

$j = 1, \dots, a-1$ and 0 is also a root of the polynomial $L(H_1, x) - xL(H_1|1, x)$. This way we find all roots of this polynomial, thus $L(H_1, x) - xL(H_1|1, x) \leq 0$ if $x > \lambda'_1$, in particular if $x > \lambda_1$. Clearly, this argument also works if some λ_i, λ'_i coincide since the interlacing property still holds. □

8. The independence polynomial

In this section we study the independence polynomial.

Definition 8.1. The *independence polynomial* of the graph G is defined as

$$I(G, x) = \sum_{k=0}^{n} (-1)^k i_k(G) x^k,$$

where $i_k(G)$ denotes the number of independent sets of size k and $\beta(G)$ denotes the smallest real root of $I(G, x)$.

Remark 8.2. Some authors call the polynomial $I(G, -x)$ the independence polynomial; since the transformation between the two forms is trivial, it will not cause any confusion to work with this definition.

The graph parameter $\beta(G)$ is examined in various papers. D. Fisher and A. Solow proved that $\beta(G)$ is the smallest root in absolute value [8]. The fundamental result on $\beta(G)$ due to D. Fisher and J. Ryan [7] is the following: if G_1 is a subgraph of G_2 then $\beta(G_1) \geq \beta(G_2)$. We will prove a bit stronger monotonicity property which will be more suitable for our purposes. This stronger property will imply the above mentioned result of D. Fisher and J. Ryan. We mention that their result already implies that for nonempty graph G the value $\beta(G)$ indeed exists and in fact, it is at most 1; the one-node graph is a subgraph of every graph and 1 is the (smallest real) root of $I(K_1, x) = 1 - x$.

The main result of this section is the following.

Theorem 8.3. *Let T be a tree and T' is a tree obtained from T by a generalized tree shift. Then $I(T', x) \gg I(T, x)$ or in other words, $i_k(T') \geq i_k(T)$ for all $k \geq 1$. Furthermore, $\beta(T') \leq \beta(T)$.*

The first statement of the theorem is quite straightforward. The second statement needs some preparation, more precisely the preparation of the suitable monotonicity property.

Fact 1. [16] The polynomial $I(G, x)$ satisfies the recursion

$$I(G, x) = I(G - v, x) - xI(G - N[v], x),$$

where v is an arbitrary vertex of the graph G.

Fact 2. [16] The polynomial $I(G, x)$ satisfies the recursion

$$I(G, x) = I(G - e, x) - x^2 I(G - N[u] - N[v], x),$$

where $e = uv$ is an arbitrary edge of the graph G.

The following definition –together with the statements following it– will be the main tool to prove the second statement of Theorem 8.3.

Definition 8.4. Let $G_1 \succ G_2$ if $I(G_2, x) \geq I(G_1, x)$ on the interval $[0, \beta(G_1)]$.

Statement 8.5. *The relation $\succ$ is transitive on the set of graphs and if $G_1 \succ G_2$ then $\beta(G_1) \leq \beta(G_2)$.*

Proof. Let $G_1 \succ G_2$. Since $I(G_1, 0) = 1$ we have $I(G_1, x) > 0$ on the interval $[0, \beta(G_1))$. Thus $I(G_2, x) \geq I(G_1, x) > 0$ on the interval $[0, \beta(G_1))$ giving that $\beta(G_2) \geq \beta(G_1)$. If $G_1 \succ G_2 \succ G_3$ then $\beta(G_1) \leq \beta(G_2) \leq \beta(G_3)$ and $I(G_3, x) \geq I(G_2, x) \geq I(G_1, x)$ on the interval $[0, \min(\beta(G_1), \beta(G_2))) = [0, \beta(G_1))$ thus $G_1 \succ G_3$. □

Statement 8.6. *If G_2 is an induced subgraph of G_1 then $G_1 \succ G_2$.*

Proof. We prove by induction on the number of vertices of G_1. For sake of simplicity, let us use the notation $G_1 = G$. By the transitivity of the relation $\succ$ it is enough to prove that $G \succ G - v$. The statement is true if $|V(G)| = 2$.

Since $G - N[v]$ is an induced subgraph of $G - v$, by the induction hypothesis we have

$$I(G - v, x) \succ I(G - N[v], x).$$

This means that

$$I(G - N[v], x) \geq I(G - v, x)$$

on the interval $[0, \beta(G - v)]$. Thus $I(G - N[v], x) \geq 0$ on the interval $[0, \beta(G - v)]$. Hence by Fact 1 we have

$$I(G, x) = I(G - v, x) - xI(G - N[v], x) \leq I(G - v, x)$$

on the interval $[0, \beta(G - v)]$. This implies that $\beta(G) \leq \beta(G - v)$; indeed, $I(G, 0) = 1$ and $I(G, \beta(G - v)) \leq 0$ so $I(G, x)$ has a root in the interval $[0, \beta(G - v)]$. Hence $I(G, x) \leq I(G - v, x)$ on the interval $[0, \beta(G)]$, i.e., $G \succ G - v$. □

Statement 8.7. *If G_2 is a subgraph of G_1 then $G_1 \succ G_2$.*

Proof. Let us apply the notation $G_1 = G$.

Clearly, it is enough to prove that $G \succ G - e$ where $e = (u, v) \in E(G)$. Let us use the recursion formula of Fact 2 to G:

$$I(G, x) = I(G - e, x) - x^2 I(G - N[u] - N[v], x).$$

By Statement 8.6 we have $G \succ G - N[u] - N[v]$ and so $I(G - N[u] - N[v], x) \geq I(G, x) \geq 0$ on the interval $[0, \beta(G)]$. Hence $I(G - e, x) \geq I(G, x)$ on this interval, i.e., $G \succ G - e$. □

Now we start to settle the suitable product formula for $I(T, x) - I(T', x)$.

Lemma 8.8. *We have*

$$I(M_1 : M_2, x) = I(M_1 - u_1, x)I(M_2 - u_2, x) - xI(M_1 - N[u_1], x)I(M_2 - N[u_2]).$$

Equivalently,

$$I(M_1 : M_2) = I(M_1)I(M_2) + xI(M_1)I(M_2 - N[u_2]) + xI(M_1 - N[u_1])I(M_2) + \\ +(x^2 - x)I(M_1 - N[u_1])I(M_2 - N[u_2]).$$

Proof. In the first formula we simply separated those terms which contain the vertex $u_1 = u_2$ (second term) from those not containing $u_1 = u_2$ (first term).

The second formula simply follows from the first one by using the identity

$$I(M_j - u_j, x) = I(M_j, x) + xI(M_j - N[u_j], x)$$

for $j = 1, 2$. □

Lemma 8.9. *Let T be tree and T' is obtained from T by a generalized tree shift. Then with the usual notation we have*

$$I(T,x)-I(T',x)=xI(P_{k-3},x)(I(A,x)-I(A-A_0,x))(I(B,x)-I(B-B_0,x)),$$

where we define $I(P_0,x)=I(P_{-1},x)=1$.

Proof. By the previous lemma we can use the General Lemma applied to $f(G,x)=I(G,x)$ and $g(G|v,x)=I(G-N[v],x)$ and $c_2=x$, $c_3=x^2-x$.

Then

$$I(P_3-N[1],x)-I(P_3-N[2],x)=(1-x)-1=-x$$

and

$$xI(K_2,x)+(x^2-x)I(K_2-N[1],x)=x(1-2x)+(x^2-x)1=-x^2.$$

Furthermore,

$$xI(P_k,x)+(x^2-x)I(P_{k-2},x)=x(I(P_{k-1},x)-xI(P_{k-2},x))+(x^2-x)I(P_{k-2},x)=$$
$$=x(I(P_{k-1},x)-I(P_{k-2},x))=-x^2I(P_{k-3},x).$$

Finally,

$$x(I(H_1-1,x)+xI(H_1-N[1],x))+(x^2-x)I(H_1-N[1],x)=$$
$$=x(I(H_1-1,x)-I(H_1-N[1],x)=x(I(A,x)-I(A-A_0,x)).$$

Similar statement holds for $xI(H_2,x)+(x^2-x)I(H_2-N[1],x)$. Putting all together we get that

$$I(T,x)-I(T',x)=xI(P_{k-3},x)(I(A,x)-I(A-A_0,x))(I(B,x)-I(B-B_0,x)).$$

□

Now we are ready to prove Theorem 8.3.

Theorem 8.3. *Let T be a tree and T' is a tree obtained from T by a generalized tree shift. Then $I(T',x)\gg I(T,x)$ or in other words $i_k(T')\geq i_k(T)$ for all $k\geq 1$. Furthermore, $T'\succ T$ and so $\beta(T')\leq\beta(T)$.*

Proof. By Lemma 8.9 we have

$$I(T',-x)-I(T,-x)=xI(P_{k-3},-x)(I(A,-x)-I(A-A_0,-x))(I(B,-x)-I(B-B_0,-x)).$$

Since on the left hand side we multiply polynomials of positive coefficients, we have $I(T',x)\gg I(T,x)$.

Now we prove the second statement. Since $A-A_0$ is a subgraph of A we have

$$I(A,x)-I(A-A_0,x)\leq 0$$

on the interval $[0,\beta(A)]$. Similarly,

$$I(B,x)-I(B-B_0,x)\leq 0$$

on the interval $[0,\beta(B)]$. Finally $I(P_{k-3},x)\geq 0$ on the interval $[0,\beta(T')]$ since $T'\succ P_{k-3}$ because P_{k-3} is a subgraph of T'. It is also true that $\beta(A),\beta(B)\geq\beta(T')$ because of the same reason. Hence

$$I(T,x)-I(T',x)=xI(P_{k-3},x)(I(A,x)-I(A-A_0,x))(I(B,x)-I(B-B_0,x))\geq 0$$

on the interval $[0,\beta(T')]$, i.e., we have $T'\succ T$ (and so $\beta(T')\leq\beta(T)$).

□

9. Edge cover polynomial

The concept of the edge cover polynomial was introduced by S. Akbari and M. R. Oboudi [1]. The edge cover polynomial is defined as follows.

Definition 9.1. Let G be a graph on n vertices and m edges. Let $e_k(G)$ denote the number of ways one can choose k edges that cover all vertices of the graph G. We call the polynomial

$$E(G,x)=\sum_{k=1}^{m} e_k(G)x^k$$

the *edge cover polynomial* of the graph G. Clearly, if the graph G has an isolated vertex then the edge cover polynomial is 0.

Let $\xi(G)$ denote the smallest real root of the edge cover polynomial.

Unfortunately, the parameter $\xi(G)$ is not a monotone parameter of graphs, not even for trees. Surprisingly, in spite of this fact, one can use the generalized tree shift to prove that the path and the star are the extremal cases. (Although, the star is not the only tree for which $\xi(T)=0$.)

Theorem 9.2. *Let T be a tree on n vertices. Then*

$$\xi(P_n)\le \xi(T)\le \xi(S_n).$$

Furthermore, for any $1\le k\le n-1$ we have

$$e_k(S_n)\le e_k(T)\le e_k(P_n).$$

As usual, we prove a lemma connecting $E(T,x)$ and $E(T',x)$.

Lemma 9.3. *Let T be a tree and T' be the tree obtained from the tree T by a generalized tree shift. Then*

$$E(T,x)-E(T',x)=\frac{1}{x}E(P_k,x)E(H_1,x)E(H_2,x).$$

Lemma 9.4.

$$E(M_1:M_2)=E(M_1)E(M_2)+E(M_1)E(M_2-u_2)+E(M_1-u_1)E(M_2).$$

Proof. The terms of $E(M_1:M_2)$ are separated according to the vertex $u_1=u_2$ is covered in the graph M_1, M_2 or both. □

Proof of Lemma 9.3. According to the previous lemma we can apply the General Lemma to $f(G,x)=E(G,x)$ and $g(G|v,x)=E(G-v,x)$ and $c_2=1$, $c_3=0$.

Then $E(P_3-1,x)-E(P_3-2,x)=x-0=x$ and $c_2E(K_2,x)+c_3E(K_2-1,x)=x$. Hence

$$E(T,x)-E(T',x)=\frac{1}{x}E(P_k,x)E(H_1,x)E(H_2,x).$$

□

Proof of Theorem 9.2. Since all the coefficients of the edge cover polynomial are non-negative we have $\xi(T)\le 0=\xi(S_n)$. (Note that $E(S_n,x)=x^{n-1}$.)

To prove the extremality of the path, we make the observation that

$$E(P_n,x)=\sum_{k=0}^{n}\binom{n-2-k}{k}x^{n-1-k}.$$

Indeed, $E(P_n,x) = x(E(P_{n-1},x)+E(P_{n-2},x))$ and $E(P_1,x) = 0, E(P_2,x) = x$. Thus $E(P_n,x)$ is a simple transform of the Chebyshev polynomial of the second kind. This implies that

$$\xi(P_n) = -4\cos^2\frac{\pi}{n-1}$$

if $n \geq 3$. In particular, $-\xi(P_n) > -\xi(P_{n-1}) > \cdots > -\xi(P_2)$.

Let $\lambda \geq -\xi(P_n)$ and set $c(T) = (-1)^{n-1}E(T,-\lambda)$. Clearly, $c(P_n) > 0$. We show that for all trees on n vertices we have $c(T) \geq c(P_n) > 0$. We prove it by induction on the number of vertices. By the main lemma

$$c(T') - c(T) = \frac{1}{\lambda}c(P_k)c(H_1)c(H_2).$$

By the induction hypothesis all terms on the right hand side are positive; indeed, $c(H_1) > c(P_{a+1}) > 0$ because $\lambda > -\xi(P_n) > -\xi(P_{a+1})$. Thus $c(T') > c(T)$. Since the smallest element of the poset induced by the generalized tree shift is the path on n vertices, this implies that $c(T) > c(P_n)$ indeed holds. Hence $E(T,x)$ has no root in the interval $(-\infty, \xi(P_n))$.

The second claim is trivial from Lemma 9.3 and from the fact that the star is the largest, the path is the smallest element of the induced poset of the generalized tree shift.

□

Remark 9.5. Although, we have no monotonicity for $\xi(T)$ in general, the weak monotonicity for the paths was enough to prove the statement.

In [5] one can find a strengthening of Theorem 9.2.

10. The generalized tree shift and related transformations of trees

Originally, the author developed the generalized tree shift to overcome a certain weakness of the Kelmans transformation. Although, it turned out that the generalized tree shift is indeed the generalization of many transformations for trees found in the literature. In this section we survey some of them.

In [18] L. Lovász and J. Pelikán proved that the star has the largest, the path has the smallest spectral radius among trees on n vertices. Their proof for settling the minimality of the path used a certain transformation of trees. This transformation is nothing else than the generalized tree shift applied in the case when the degree of the candidate vertex is 2, so it moves one edge. We also mention that they used the same ordering for the polynomials that we used for the independence polynomial.

In [20] B. Mohar defined the operation σ and π. Both transformations are special cases of the generalized tree shift; more precisely, the inverse of π is the special case of the generalized tree shift. In the language of the generalized tree shift, the inverse of π-transformation is nothing else than the generalized tree shift when H_2 itself is a path. The σ-transformation is the generalized tree shift when H_2 is a star and $k = 2$ (so the path has no interior vertices). This transformations were also used by D. Stevanović and A. Ilić [24]. Surprisingly, H. Deng [6] used exactly the same transformations for proving the extremality of the star and the path at the Estrada index. In fact, he also solved the problem for the number of closed walks as well. They needed two transformations, one for settling the extremality of the star and one for settling the extremality of the path.

In [12] J.-M. Guo studied the algebraic connectivity of graphs, the transformation "separating an edge" is the generalized tree shift applied to adjacent vertices x, y.

(In fact, he defined it for every graph, but Theorem 2.1 of [12] shows that it was useful only when the separated edge was a cut edge.) In this paper Guo used another transformation also called "grafting an edge". This transformation is not the special case of the generalized tree shift, but surprisingly they have a nontrivial common special transformation. In the language of the generalized tree shift this special case is when the graph H_2 is a path. Then the generalized tree shift acts as if the graph H_1 had been shifted from the end of a long path to the middle of this path. Guo showed that this can be refined in such a way that the graph H_1 gets closer and closer to the center of the path, the algebraic connectivity becomes greater and greater. This suggests that maybe one can refine the poset induced by the generalized tree shift.

We mention that a more and more refined poset of trees could have a serious application. In chemistry one often measures molecules by some parameter. In this case it is useless that the star maximizes, the path minimizes this parameter since these are not the graph of molecules in general. Still a graph transformation could be useful to compare molecules in a fast way or to give a hint where to find the proper molecule.

11. Concluding remarks

In this section we collected the parameters of trees into a table which increase or decrease by applying the generalized tree shift. The common property of this parameters is that they are all monotone parameters of trees. In fact, most of them are monotone parameters of all graphs.

We hope that the many examples could convince everybody that this transformation is much more natural than it seems to be at first sight. The simple form of the General Lemma is also a clue of this naturality.

	Parameter	Change	Maximum
1	largest eigenvalue of the adjacency matrix	increasing	star
2	coefficients of the adjacency characteristic polynomial	decreasing	path
3	number of closed walks of length ℓ (ℓ fixed) [4]	increasing	star
4	number of walks of length ℓ (ℓ fixed) [3]	increasing	star
5	algebraic connectivity	increasing	star
6	largest real root of the Laplacian polynomial	increasing	star
7	coefficients of the Laplacian characteristic polynomials	decreasing	path
8	smallest real root of the independence polynomial	decreasing	path
9	coefficients of the independence polynomial	increasing	star
10	coefficients of the edge cover polynomial	decreasing	path

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