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On the Laplacian coefficients of acyclic graphs

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Abstract

Let G be a graph of order n and let $\Lambda(G,\lambda) = \sum_{k=0}^{n}(-1)^k c_k \lambda^{n-k}$ be the characteristic polynomial of its Laplacian matrix. Zhou and Gutman recently proved that among all trees of order n, the kth coefficient c_k is largest when the tree is a path, and is smallest for stars. A new proof and a strengthening of this result is provided. A relation to the Wiener index is discussed.

1 Introduction

Let G be a graph of order $n = |G|$ and let $L(G) = D(G) - A(G)$ be its Laplacian matrix. The *Laplacian polynomial* of G is the characteristic polynomial of its Laplacian matrix, $\Lambda(G,\lambda) = \det(\lambda I_n - L(G))$. Let $c_k = c_k(G)$ $(0 \le k \le n)$ be the absolute values of the coefficients of $\Lambda(G,\lambda)$, so that

$$\Lambda(G,\lambda) = \sum_{k=0}^{n}(-1)^k c_k \lambda^{n-k}.$$

It is easy to see that $c_0 = 1$, $c_1 = 2\|G\|$, $c_n = 0$, and $c_{n-1} = n\tau(G)$, where $\tau(G)$ denotes the number of spanning trees of G. We refer to [5] and [6, 7] for a detailed introduction to graph Laplacians.

For a graph G, let $m_k(G)$ be the number of matchings of G containing precisely k edges (shortly *k-matchings*), and let $S(G)$ denote the *subdivision*

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of G. Zhou and Gutman [10] proved that for every acyclic graph T of order n,

$$c_k(T) = m_k(S(T)), \qquad 0 \le k \le n. \tag{1}$$

Using this correspondence, Zhou and Gutman [10] proved a conjecture from [3] that the extreme values of Laplacian coefficients among all n-vertex trees are attained on one side by the path P_n of length $n-1$, and on the other side by the star $S_n = K_{1,n-1}$ of order n. In other words,

$$c_k(S_n) \le c_k(T) \le c_k(P_n), \qquad 0 \le k \le n \tag{2}$$

holds for all trees T of order n.

In this note we present a different proof of (2) and obtain a strengthening of Zhou and Gutman's result. We prove that all Laplacian coefficients are monotone under two operations called π and σ. It is shown that by using π consecutively, every tree can be transformed into a path, and successive application of the operation σ transforms any tree into the star. This in particular implies (2).

It is well-known that the Laplacian coefficient c_{n-2} of an n-vertex tree T is equal to the sum of all distances between unordered pairs of vertices (see, e.g. [9]), also known as the *Wiener index* $W(T)$ of T:

$$c_{n-2}(T) = W(T) = \sum_{\{u,v\}} \operatorname{dist}(u,v).$$

In the last section we discuss some questions suggested by this correspondence.

2 The transformation π

Let u_0 be a vertex of a tree T. Suppose that $P = u_0u_1 \dots u_p$ $(p \ge 1)$ is a path in T whose internal vertices $u_1, \dots, u_{p-1}$ all have degree 2 in T and where u_p is a *leaf* (i.e., a vertex of degree 1 in T). Then we say that P is a *pendant path* of *length* p attached at u_0.

Suppose that $\deg_T(u_0) \ge 3$ and that $P = u_0u_1 \dots u_p$ and $Q = u_0v_1 \dots v_q$ are distinct pendant paths attached at u_0. Then we form a tree $T' = \pi(T, u_0, P, Q)$ by removing the paths P and Q and replacing them with a longer path $R = u_0u_1 \dots u_pv_1v_2 \dots v_q$. We say that T' is a *π-transform* of T.

Proposition 2.1 *Every tree which is not a path contains a vertex of degree at least three at which (at least) two pendant paths are attached. In* *particular, every tree can be transformed into a path by a sequence of π-transformations.*

Proof. Let T be a tree which has at least one vertex of degree 3 or more. To prove that T contains a vertex of degree at least 3 with two pendant paths, consider a path S in T which contains the maximum number of vertices of degree different from 2. Then S joins two leaves x and y. Let u be a vertex on S of degree ≥ 3 which is closest to x. Let Q be a path joining u with some leaf of T such that $Q \cap S = \{u\}$. If Q would not be a pendant path, this would contradict the maximality of S. So, Q and the segment of S from u to x are two pendant paths attached at u.

The second part of the proposition is easily proved by induction on the number of leaves of the tree since every π-transformation eliminates one leaf.

□

Theorem 2.2 *Let $T' = \pi(T, u_0, P, Q)$ be a π-transform of a tree T of order $n = |T|$. For $d = 1, \ldots, k-1$, let n_d be the number of vertices in $T - P - Q$ that are at distance d from u_0 in T. Then*

$$c_k(T) \leq c_k(T') - \sum_{d=1}^{k-1} n_d \binom{n-3-d}{k-1-d} \quad \text{for} \quad 2 \leq k \leq n-2$$

and $c_k(T) = c_k(T')$ for $k \in \{0, 1, n-1, n\}$.

Proof. As mentioned before, the coefficients $c_0 = 1$ and $c_n = 0$ are constant, while c_1 and c_{n-1} "count" the number of edges and the number of spanning trees (multiplied by n), respectively, so they are the same for all trees with the same number of vertices. This shows that $c_k(T) = c_k(T')$ for $k \in \{0, 1, n-1, n\}$, and so we henceforth assume that $2 \leq k \leq n-2$.

By a theorem of Zhou and Gutman, our Eq. (1), it suffices to see that $m_k(S) \leq m_k(S') - \sum_{d=1}^{k-1} n_d \binom{n-3-d}{k-1-d}$, where $S = S(T)$ and $S' = S(T')$. We let $P = u_0 u_1 \ldots u_p$, $Q = u_0 v_1 \ldots v_q$, and $R = u_0 u_1 \ldots u_p v_1 \ldots v_q$. In the subdivision graphs we have the corresponding paths $\hat{P} = u_0 \hat{u}_1 u_1 \hat{u}_2 u_2 \ldots \hat{u}_p u_p$, $\hat{Q} = u_0 \hat{v}_1 v_1 \hat{v}_2 v_2 \ldots \hat{v}_q v_q$, and $\hat{R} = u_0 \hat{u}_1 u_1 \ldots \hat{u}_p u_p \hat{v}_1 v_1 \ldots \hat{v}_q v_q$, where the vertices with the "hats" are those subdividing the edges of T and T'.

We consider the vertex-sets and edge-sets of T and T' and then also of S and S' to be the same under the obvious correspondence. In particular, the edge $e_1 = u_0 \hat{v}_1$ of S is identified with the edge $u_p \hat{v}_1$ of S'.

Let M be a k-matching of S. If $e_1 \notin M$ or $e_2 = \hat{u}_p u_p \notin M$, then we set M' be the corresponding k-matching of S'. Every matching M' of S'

obtained in this way is said to be of *type* 1. If e_1 and e_2 are both in M, then we define the k-matching M' of S' as follows. We let M and M' agree on $E(S) \setminus E(\hat{P})$, but we replace the edges in $M \cap E(\hat{P})$ with the edge-set $\{\hat{u}_i u_i \mid u_{p-i}\hat{u}_{p-i+1} \in M\} \cup \{u_{i-1}\hat{u}_i \mid \hat{u}_{p-i+1}u_{p-i+1} \in M\}$. (We think of replacing the path $\hat{P}$ with its inverse path $u_p\hat{u}_p \dots u_1\hat{u}_1u_0$.) It is obvious that M' is a k-matching of S' also in this case. We say that M' is a matching of *type* 2. All other matchings of S' are of *type* 0.

It is easy to see that a matching of S' cannot be of types 1 and 2 at the same time. This shows that the correspondence $M \mapsto M'$ is 1-1. Therefore, $m_k(S) \leq m_k(S')$ and hence $c_k(T) \leq c_k(T')$. In order to prove stronger inequalities of the theorem, we have to find additional $\sum_{d=1}^{k-1} n_d \binom{n-3-d}{k-1-d}$ k-matchings of S' which are of type 0.

It is easy to see that for every vertex $v \in V(S')$, there is a (unique) $(n-1)$-matching M_v of S' such that the vertex v is not covered by the edges in M_v. For our purpose, we shall consider the vertex $v = v_q$. Then $M_v \cap E(\hat{R})$ contains the edge $u_p\hat{v}_1$ and edges $\{u_{i-1}\hat{u}_i \mid 1 \leq i \leq p\} \cup \{v_{j-1}\hat{v}_j \mid 2 \leq j \leq q\}$. Let u be a vertex of $T - P - Q$ that is at distance d from u_0. In S', there is a path U of length $2d$ joining u_0 with u. Every second edge on this path belongs to M_v. Let us now form an $(n-2)$-matching $M_v^u = (M_v + E(U)) \setminus \{u_0\hat{u}_1\}$, where $+$ denotes the symmetric difference of edge-sets. Finally, let $\mathcal{N}_k^u$ be the set of all k-matchings contained in M_v^u which contain the edge $u_p\hat{v}_1$ and all d edges of $M_v^u \cap E(U)$. It is clear that no matching N in $\mathcal{N}_k^u$ is of type 0, because every matching of type 1 corresponds to a matching of S (which N does not since $u_p\hat{v}_1 = u_0\hat{v}_1$ and the edge of U incident with u_0 are both in N), and every matching of type 2 contains the edge $u_0\hat{u}_1$.

The set $\mathcal{N}_k^u$ contains precisely $\binom{n-3-d}{k-1-d}$ matchings, and for distinct vertices u, w, the matchings are distinct, $\mathcal{N}_k^u \cap \mathcal{N}_k^w = \emptyset$. This gives rise to $\sum_{d=1}^{k-1} n_d \binom{n-3-d}{k-1-d}$ additional k-matchings of S', which we were to prove. □

Let us observe that the estimate for the difference $c_k(T') - c_k(T)$ in Theorem 2.2 is just the "first-order estimate" and that the method of our proof easily reveals additional k-matchings of S' (except in some very specific cases).

3 The transformation σ

Let u_0 be a vertex of a tree T of degree $p+1$. Suppose that $u_0u_1, \dots u_0u_p$ are pendant edges incident with u_0, and that v_0 is the neighbor of u_0 distinct from $u_1, \ldots, u_p$. Then we form a tree $T' = \sigma(T, u_0)$ by removing the edges $u_0u_1, \ldots u_0u_p$ from T and adding p new pendant edges $v_0v_1, \ldots v_0v_p$ incident with v_0. We say that T' is a *σ-transform* of T.

Proposition 3.1 *Every tree which is not a star contains a vertex u_0 such that $p = \deg_T(u_0) - 1$ neighbors of u_0 are leaves of T, while the remaining neighbor of u_0 is not a leaf. Consequently, every tree can be transformed into a star by a sequence of σ-transformations.*

Proof. Let us consider a longest path S in T. Clearly, S connects two leaves x and y and the vertex u_0 adjacent to x has the required property. The second part of the proposition is easily proved by induction on the number of leaves of the tree since every σ-transformation increases the number of leaves by one. □

Theorem 3.2 *Let $T' = \sigma(T, u_0)$ be a σ-transform of a tree T of order $n = |T|$. For $d = 2, \ldots, k$, let n_d be the number of vertices in $T - u_0$ that are at distance d from u_0 in T. Then*

$$c_k(T) \geq c_k(T') + \sum_{d=2}^{k} n_d\, p \binom{n-2-d}{k-d} \quad \textit{for} \;\; 2 \leq k \leq n-2$$

and $c_k(T) = c_k(T')$ for $k \in \{0, 1, n-1, n\}$.

Proof. The last claim was already argued before, so let us assume that $2 \leq k \leq n-2$. Again, we will compare k-matchings in $S = S(T)$ and in $S' = S(T')$. We denote by $\hat{u}_i$ ($1 \leq i \leq p$) and $\hat{v}_0$ the vertices of S and S' which subdivide edges u_0u_i and u_0v_0, respectively.

The edges of S and S' are in the natural bijective correspondence, and it is easy to see that a k-matching M' of S' is also a k-matching of S unless $\hat{v}_0u_0 \in M'$ and $v_0\hat{v}_i \in M'$ for some $1 \leq i \leq p$. In the latter case, a k-matching of S is obtained by replacing the edge $\hat{v}_0u_0$ of M' by the edge $\hat{v}_0v_0$.

Similarly as in the proof of Theorem 2.2, we shall prove that there exist k-matchings of S that are not counted in the above 1-1 correspondence $M' \mapsto M$. We refer to the notation introduced in that proof.

Let us consider the $(n-1)$-matching M_0 of S such that the vertex u_0 is not covered by the edges in M_0. Let u be a vertex of T that is at distance $d \geq 2$ from u_0. In S', there is a path U of length $2d-2$ joining v_0 with u. Every second edge on this path belongs to M_0. For $i = 1, \ldots, p$, let us now form an $(n-2)$-matching $M_i^u = ((M_0 + E(U)) \cup \{u_0\hat{u}_i\}) \setminus \{v_0\hat{v}_0, \hat{u}_i u_i\}$. Finally, let $\mathcal{N}_k^u$ be the set of all k-matchings contained in some M_i^u which contain the edges $u_0\hat{u}_i$ and all $d-1$ edges of $M_i^u \cap E(U)$. It is clear that no matching N in $\mathcal{N}_k^u$ appears under the above correspondence $M' \mapsto M$, because every such M either corresponds to a matching of S' (which N does not), or contains the edge $v_0\hat{v}_0$.

The set $\mathcal{N}_k^u$ contains precisely $p\binom{n-2-d}{k-d}$ matchings, and for distinct pairs u, w, the matchings are distinct, $\mathcal{N}_k^u \cap \mathcal{N}_k^w = \emptyset$. This gives rise to $\sum_{d=1}^{k} n_d\, p\binom{n-2-d}{k-d}$ additional k-matchings of S, which we were to prove. □

4 Wiener index

As observed in the introduction, the Wiener index $W(T)$ of an n-vertex tree T is equal to the $(n-2)$nd Laplacian coefficient, $W(T) = c_{n-2}(T)$. It is a simple exercise to show that Theorems 2.2 and 3.2 can be made more explicit for this special coefficient:

Theorem 4.1 *Let $T' = \pi(T, u_0, P, Q)$ be a π-transform of a tree T of order $n = |T|$, and let $T'' = \sigma(T, u_0)$ be a σ-transform of T. If $p = |P| - 1$ and $q = |Q| - 1$, then*

$$W(T') - W(T) = c_{n-2}(T') - c_{n-2}(T) = pq(n-p-q).$$

If $r = \deg_T(u_0) - 1$, then

$$W(T) - W(T'') = c_{n-2}(T) - c_{n-2}(T'') = r(n-r-1).$$

Ordering of trees based on their Wiener index has a long history and is in almost ideal correlation with several combinatorial properties and, notably, also with some physical properties of substances whose molecular graphs correspond to such trees, see, e.g. [2, 8]. Theorem 4.1 suggests a refinement of this order. Namely, trees with the same Wiener index should be ordered (lexicographically) according to the values of other Laplacian coefficients. Of course, Laplacian-cospectral trees [1, 4] will be indistinguishable.

Another partial ordering among classes of Laplacian-cospectral trees of the same order n may be of interest. We can say that $T \preceq T'$ if $c_i(T) \leq c_i(T')$ for $i = 1, \ldots, n$. Theorems 2.2 and 3.2 show that this poset has a unique minimal and a unique maximal element. It would be interesting to know what is the height (the maximum length of a chain) and how large is the width (the maximum size of an antichain) of this poset.

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