Bulletin T.CXXVII de l'Académie Serbe des Sciences et des Arts - 2003
Classe des Sciences mathématiques et naturelles
Sciences mathématiques, № 28

ON THE COEFFICIENTS OF THE LAPLACIAN CHARACTERISTIC POLYNOMIAL OF TREES

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(Presented at the 1st Meeting, held on February 28, 2003)

A b s t r a c t. Let the Laplacian characteristic polynomial of an n-vertex tree T be of the form $\psi(T,\lambda) = \sum\limits_{k=0}^{n} (-1)^{n-k}\, c_k(T)\, \lambda^k$. Then, as well known, $c_0(T) = 0$ and $c_1(T) = n$. If T differs from the star (S_n) and the path (P_n), which requires $n \geq 5$, then $c_2(S_n) < c_2(T) < c_2(P_n)$ and $c_3(S_n) < c_3(T) < c_3(P_n)$. If $n = 4$, then $c_3(S_n) = c_3(P_n)$.

AMS Mathematics Subject Classification (2000): 05C05, 05C12, 05C50
Key Words: Laplacian spectrum, Laplacian characteristic polynomial, Trees, Distance (in graph), Wiener number

1. *Introduction*

Let G be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$. The adjacency matrix $A(G)$ of G is a square matrix of order n whose (i,j)-entry is unity if the vertices v_i and v_j are adjacent, and is zero otherwise. The degree d_i of the vertex v_i is the number of first neighbors of this vertex. By $D(G)$ we denote the square matrix of order n whose i-th diagonal element is equal to d_i and whose off–diagonal elements are zero. By I_n we denote the unit matrix of order n .

The Laplacian matrix of the graph G is $L(G) = D(G) - A(G)$. The characteristic polynomial of the Laplacian matrix, $\psi(G,\lambda) = \det(\lambda I_n - L(G))$, is said to be the Laplacian characteristic polynomial of the graph G. In what follows we write it in the coefficient form as

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

If so, then $c_k(G) \geq 0$ for all k and for all G.

The connection between the coefficients of the Laplacian characteristic polynomial and the structure of the respective graph was established by Kel'mans long time ago [1, p. 38]:

$$c_k(G) = \sum_{F \in \mathcal{F}_k(G)} \gamma(F), \tag{1}$$

where F is a spanning forest and the summation goes over the set $\mathcal{F}_k(G)$ of all spanning forests of G, possessing exactly k components, and where $\gamma(F)$ is the product of the number of vertices of the components of F.

Clearly, $\mathcal{F}_0(G) = \emptyset$, which is consistent with the fact that $c_0(G) = 0$ for all graphs G.

In this work we are concerned with trees, i.e., connected and acyclic graphs. If T is an n-vertex tree, then for $k \geq 1$, the elements of $\mathcal{F}_k(T)$ are obtained by deleting $k-1$ distinct edges from T. This, in particular, means that

$$|\mathcal{F}_k(T)| = \binom{n-1}{k-1} \ . \tag{2}$$

Some immediate consequences of formulas (1) and (2) are:

$$c_1(T) = n \tag{3}$$
$$c_n(T) = 1 \tag{4}$$
$$c_{n-1}(T) = 2(n-1) \tag{5}$$

and [9]:

$$c_{n-2}(T) = 2\,n^2 - 5\,n + 3 - \frac{1}{2}\sum_{i=1}^{n} d_i^2 \tag{6}$$

$$c_{n-3}(T) = \frac{1}{3}\left[4\,n^3 - 18\,n^2 + 24\,n - 10 + \sum_{i=1}^{n} d_i^3 - 3(n-2)\sum_{i=1}^{n} d_i^2\right] . \tag{7}$$

The n-vertex star, denoted by S_n , is the n-vertex tree with maximum $(= n - 2)$ number of vertices of degree one. The n-vertex path, denoted by P_n is the n-vertex tree with minimum $(= 2)$ number of vertices of degree one.

Eqs. (3)–(5) imply that all n-vertex trees have equal Laplacian coefficients c_1 , c_n , and c_{n-1} . In view of Eqs. (6) and (7), it is easy to verify that for any n-vertex tree, different from S_n and P_n ,

$$c_{n-2}(S_n) < c_{n-2}(T) < c_{n-2}(P_n) \tag{8}$$

$$c_{n-3}(S_n) < c_{n-3}(T) < c_{n-3}(P_n) \ . \tag{9}$$

Recall that trees different from S_n and P_n exist only for $n \geq 5$.

In this work we show that among n-vertex trees, the star and the path are extremal also with respect to the Laplacian coefficients c_2 and c_3 . i.e., we demonstrate the validity of:

Theorem 1. *Let T be an n-vertex tree, different from S_n and P_n . Then the inequalities*

$$c_2(S_n) < c_2(T) < c_2(P_n) \tag{a}$$

and

$$c_3(S_n) < c_3(T) < c_3(P_n) \tag{b}$$

are obeyed for all T and all $n \geq 5$.

2. *The Second Laplacian Coefficient and the Wiener Number*

The Wiener number $W(G)$ of a (connected) graph G is equal to the sum of distances between all pairs of vertices of G [2, 3]:

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v|G) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} d(u,v|G) \tag{10}$$

where $d(u,v|G)$ denotes the distance (= number of edges in a shortest path) between the vertices u and v .

For the Wiener number of a tree T the following result is long known [10]:

$$W(T) = \sum_{e \in E(T)} n_1(e|T)\, n_2(e|T) \tag{11}$$

with $n_1(e|T)$ and $n_2(e|T)$ denoting the number of vertices of T , lying on the two sides of the edge e , and with summation going over all edges of T .

Now, $n_1(e|T)$ and $n_2(e|T)$ are just the number of vertices of the two components of the subgraph $T-e$, and $T-e$ is just a spanning forest of T, possessing two components. In view of this, the product $n_1(e|T)\,n_2(e|T)$ can be identified with $\gamma(T-e)$. Consequently, the right–hand side of Eq. (11) can be identified with the the right–hand side of Eq. (1) for $k=2$, namely with $\sum\limits_{F\in\mathcal{F}_2(T)}\gamma(F)$. We thus arrive at the noteworthy conclusion that the second coefficient of the Laplacian characteristic polynomial (a linear–algebra–based quantity) coincides with the Wiener number (a metric–based quantity), i.e.,

$$c_2(T)=W(T)\ . \tag{12}$$

Relation (12) was known already to Merris, Mohar and McKay in the late 1980s [5, 6, 7, 8]. Combining it with the long–known inequalities [4]

$$W(S_n)\le W(T)\le W(P_n)$$

we readily arrive at statement (a) of Theorem 1.

To these authors' knowledge, until now part (a) of Theorem 1 has not been stated in the mathematical literature. Yet, it is a direct consequence of two previously known results, and thus cannot be considered as something new and original. Inequalities (a) have been included into Theorem 1 in order to stress their analogy to inequalities (b), and also to provide a motivation for the conjecture formulated at the end of this paper.

For completeness, we mention that

$$c_2(S_n)=W(S_n)=(n-1)^2 \qquad \text{and} \qquad c_2(P_n)=W(P_n)=\binom{n+1}{3}\ . \tag{13}$$

3. *Proving Part (b) of Theorem 1*

Preparations

Let G be a connected graph and u its vertex. Denote by $d(u|G)$ the sum of the distances between u and all other vertices of G.

Lemma 2. *If u is a terminal vertex of the path P_n, then $d(u|P_n)=\binom{n}{2}$.*

P r o o f. The distances between u and the other vertices of P_n are $1,2,\ldots,n-1$. □

Lemma 3. *Let e be an edge of the graph G, connecting the vertices r and s. If G is connected, but $G-e$ disconnected, composed of components*

R and S, such that $r \in V(R)$ and $s \in V(S)$ (see Fig. 1), then

$$W(G) = W(R) + W(S) + |R|\, d(s|S) + |S|\, d(r|R) + |R|\,|S|,$$

where $|R|$ and $|S|$ stand for the number of vertices of R and S, respectively.

P r o o f. Let $x \in V(R)$ and $y \in V(S)$. Then $d(x, y|G) = d(x, r|R) + d(s, y|S) + 1$. Now, bearing in mind the definition (10) of the Wiener number, we obtain

$$\begin{aligned}
W(G) &= \sum_{\{x,x'\} \subseteq V(R)} d(x, x'|G) + \sum_{\{y,y'\} \subseteq V(S)} d(y, y'|G) + \sum_{x \in V(R)} \sum_{y \in V(S)} d(x, y|G) \\
&= W(R) + W(S) + \sum_{x \in V(R)} \sum_{y \in V(S)} [d(x, r|R) + d(s, y|S) + 1] \\
&= W(R) + W(S) + \left[\sum_{x \in V(R)} d(x, r|R)\right] \left[\sum_{y \in V(S)} 1\right] \\
&+ \left[\sum_{x \in V(R)} 1\right] \left[\sum_{y \in V(S)} d(s, y|S)\right] + \left[\sum_{x \in V(R)} 1\right] \left[\sum_{y \in V(S)} 1\right].
\end{aligned}$$

Lemma 3 follows now from

$$\sum_{x \in V(R)} d(x, r|R) = d(r|R)$$

$$\sum_{y \in V(S)} 1 = |S|$$

$$\sum_{x \in V(R)} 1 = |R|$$

$$\sum_{y \in V(S)} d(s, y) = d(s|S) \; . \quad \square$$

Consider a special case of the graph G described in Lemma 3: Let $S = P_k$ and let s be a terminal vertex of P_k. Denote this graph by R_k, see Fig. 1. Then by combining Lemmas 2 and 3, and bearing in mind that

$W(P_k) = \binom{k+1}{3}$, we have

$$W(R_k) = W(R) + \binom{k+1}{3} + |R| \binom{k}{2} + k\,[|R| + d(r|R)] \ . \tag{14}$$

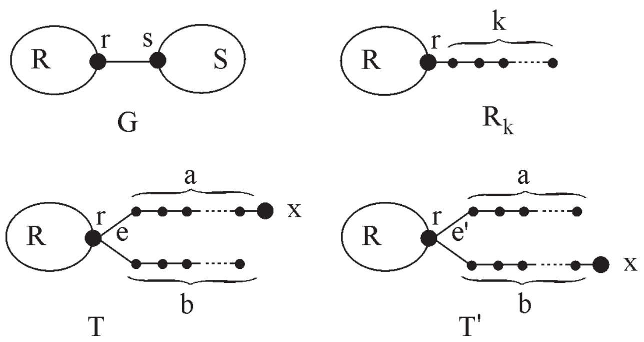

Fig 1. The structure and labeling of vertices and edges of graphs G and R_k , considered in Lemma 3 and Eq. (14), and of the trees T and T' , considered in Lemmas 4 and 5.

An Auxiliary Result

Let R be a tree on $|R|$ vertices, $|R| \geq 2$. Let T and T' be trees whose structure is depicted in Fig. 1. Hence, both T and T' possess $|R|+a+b+1$ vertices. If $a = b$, then T and T' are isomorphic. Therefore, in what follows we shall assume that $a \neq b$. Further, without loss of generality, we assume that $a+1 \leq b$.

Lemma 4. If T and T' are the above specified trees (see Fig. 1), then for all $a \geq 0$ and $b \geq 0$,

$$c_3(T') - c_3(T) = (b-a) \left[W(R) - d(r|R) + \frac{|R|-1}{6}\,(b-a-1)(b-a+1) \right] \ . \tag{15}$$

P r o o f. According to Eq. (1), since T and T' are trees,

$$c_3(T) = \sum_{f,g \in E(T)} \gamma(T-f-g) \qquad \text{and} \qquad c_3(T') = \sum_{f',g' \in E(T')} \gamma(T'-f'-g')$$

where f and g as well as f' and g' are distinct edges. In view of the structure of T and T' (see Fig. 1), it is easily seen that for any pair of edges f, g one can find a pair of edges f', g', such that $\gamma(T - f - g) = \gamma(T' - f' - g')$, except is one of the edges f, g coincides with edge e, and one of the edges f', g' coincides with edge e', see Fig. 1. Bearing this in mind we have

$$c_3(T') - c_3(T) = \sum_{f' \in E(T')} \gamma(T' - e' - f') - \sum_{f \in E(T)} \gamma(T - e - f) \ . \tag{16}$$

Now, $T - e$ consists of two components: P_{a+1} and R_b. Therefore, because the edge f belongs either to P_{a+1} or to R_b,

$$\begin{aligned}\sum_{f \in E(T)} \gamma(T - e - f) &= \sum_{f \in E(P_{a+1})} \gamma(P_{a+1} - f \cup R_b) + \sum_{f \in E(R_b)} \gamma(P_{a+1} \cup R_b - f) \\ &= (|R| + b) \sum_{f \in E(P_{a+1})} \gamma(P_{a+1} - f) + (a+1) \sum_{f \in E(R_b)} \gamma(R_b - f)\end{aligned}$$

which, in view of formula (11), results in

$$\sum_{f \in E(T)} \gamma(T - e - f) = (|R| + b)\, W(P_{a+1}) + (a+1)\, W(R_b) \ .$$

By an analogous reasoning,

$$\sum_{f' \in E(T')} \gamma(T' - e' - f') = (|R| + a)\, W(P_{b+1}) + (b+1)\, W(R_a) \ .$$

By substituting the above two expressions back into (16), and by taking into account Eq. (14), we obtain

$$\begin{aligned}c_3(T') - c_3(T) &= [(|R| + a)\, W(P_{b+1}) + (b+1)\, W(R_a)] \\ &- [(|R| + b)\, W(P_{a+1}) + (a+1)\, W(R_b)] \\ &= (|R| + a) \binom{b+2}{3} - (|R| + a) \binom{a+2}{3} \\ &+ (b+1) \left[W(R) + \binom{a+1}{3} + |R| \binom{a}{2} + a\,[|R| + d(r|R)] \right] \\ &- (a+1) \left[W(R) + \binom{b+1}{3} + |R| \binom{b}{2} + b\,[|R| + d(r|R)] \right] \ .\end{aligned}$$

Lemma 4 follows now after a lengthy, but elementary, calculation. $\square$

Lemma 5. If T and T' are the same trees as in Lemma 4, then $c_3(T) = c_3(T')$ if $|R| = 2$ and $a = b - 1$. If either $a + 1 < b$ or $|R| > 2$ or both, then $c_3(T) < c_3(T')$.

P r o o f. Lemma 5 is an immediate consequence of Lemma 4. If $|R| = 2$, then $R = P_2$ and, consequently, $W(R) = d(r|R) = 1$, i.e., $W(R) - d(r|R) = 0$. If, in addition, $b - a - 1 = 0$ then the entire right–hand side of Eq. (15) is equal to zero.

If, however, $|R| > 2$, then the Wiener number of R is necessarily greater than $d(r|R)$, implying that the right–hand side of (15) is positive–valued. Even if $W(R) = d(r|R)$, but $a + 1 < b$, the right–hand side of (15) is positive. $\square$

Completing the Proof

Let G be an n-vertex graph and F its spanning forest consisting of k components. Then $\gamma(F)$ is equal to the product of k positive integers whose sum is equal to n. The smallest possible value of such a product is equal to $n-k+1$, namely when the respective k integers are $n-k+1, 1, 1, \ldots, 1$.

Now, if T is an n-vertex tree, then each of its k-component spanning forests is obtained by deleting from T a $(k-1)$-tuple of distinct edges. In the case of the star S_n each of its k-component spanning forests consists of k isolated vertices and a copy of S_{n-k+1}. The γ-value of each of these spanning forests is minimal, equal to $n - k + 1$. If $k \neq 1, n-1, n$, then any other n-vertex tree has a k-component spanning forest whose γ-value exceeds $n - k + 1$. An exception is the 4-vertex path, considered below, cf. Eq. (17).

Bearing the above in mind, as well as Eqs. (1) and (2), we arrive at

Theorem 6. *If T is an n-vertex tree, $n \geq 5$, different from S_n, then*

$$\begin{aligned} c_1(T) &= c_1(S_n) = n \\ c_{n-1}(T) &= c_{n-1}(S_n) = 2(n-1) \\ c_n(T) &= c_n(S_n) = 1 \end{aligned}$$

whereas for $2 \leq k \leq n-2$,

$$c_k(T) > c_k(S_n) = \binom{n-1}{k-1}(n-k+1) . \quad \square$$

Clearly, the left–hand side inequalities (a) and (b) in Theorem 1 are special cases of Theorem 6.

In order to complete the proof of Theorem 1 we have to verify also the right–hand side of inequality (b). To do this consider the transformation $T \to T'$ of the trees specified in Lemmas 4 and 5, see Fig. 1. If $a+1 \leq b$, then this transformation increases the third Laplacian coefficient, except when $|R| = 2$ and $a+1 = b$, when the value of c_3 remains the same.

Repeating the transformation $T \to T'$ $a+1$ times, the entire a-branch of T will be transferred to the b-branch and the degree of the vertex r diminished by one. Repeating such transformations sufficiently many times we will ultimately arrive at the path P_n. With a single exception (discussed below) such a multi–step transformation will necessarily increase the value of c_3, implying that for any n-vertex tree T, different from P_n, $c_3(P_n) > c_3(T)$.

The single exception is the case $|R| = 2$, $a = 0$, $b = 1$. Then $T = S_4$ and $T' = P_4$. In this case, according to Lemma 5, the transformation $T \to T'$ does not increase the value of the third Laplacian coefficient, and we thus have

$$c_3(S_4) = c_3(P_4) \ . \tag{17}$$

Because S_4 and P_4 are the only 4-vertex trees, the exception (17) does not effect the validity of the right–hand side inequality (b).

Thus we demonstrated that for $n \geq 5$ the path P_n has maximum c_3-value among all n-vertex trees.

This proves the right–hand side of inequality (b).

The proof of Theorem 1 has thus been completed. $\square$

By the above considerations we also proved

Theorem 7. *Among n-vertex trees, $n \geq 1$, $n \neq 4$, the unique tree with minimum third Laplacian coefficient is the star S_n, and the unique tree with maximum third Laplacian coefficient is the path P_n. Exceptionally, for $n = 4$, $S_n \neq P_n$, but $c_3(S_n) = c_3(P_n)$.* $\square$

In analogy to Eq. (13),

$$c_3(S_n) = \frac{1}{2}\,(n-1)(n-2)^2 \qquad \text{and} \qquad c_3(P_n) = \binom{n+2}{5} \ .$$

4. *Conclusion: A Conjecture*

Summarizing Theorem 1 and Eqs. (3), (4), (5), (8), and (9), we see that the inequalities

$$c_k(S_n) \leq c_k(T) \leq c_k(P_n) \tag{18}$$

hold for all values of n, and for all n-vertex trees T, provided $k = 1, 2, 3, n-3, n-2, n-1$, and n.

Conjecture. The inequalities (18) hold for all values of n , $n \geq 1$, for all n-vertex trees T, and for all values of k , $1 \leq k \leq n$.

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