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THE WIENER INDEX OF STARLIKE TREES AND A RELATED PARTIAL ORDER

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Abstract

Let $\Gamma = (b_1, b_2, \ldots, b_n)$ be a partition of the integer $n-1$. A starlike tree is a tree in which exactly one vertex has degree greater than two. An n-vertex starlike tree is fully determined by the length b_i, $i = 1, 2, \ldots, m$, of its branches, hence by the partition Γ. The Wiener index of such a starlike tree is denoted by $W(\Gamma)$.

Two partitions Γ and Γ' (of the same integer) are partially ordered as $\Gamma \lhd \Gamma'$ iff $\sum_{i=1}^{k} b_i \leq \sum_{i=1}^{k} b'_i$ for all k. We show that $\Gamma \lhd \Gamma'$ implies $W(\Gamma) < W(\Gamma')$.

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1. INTRODUCTION

A tree in which exactly one vertex has degree greater than two is said to be starlike.

Let T be a starlike tree on n vertices. We denote its maximal vertex degree by m, $m \geq 3$, and the length (= number of edges = number of vertices) of its branches by $b_1, b_2, \ldots, b_m$. By convention, $b_1 \geq b_2 \geq \cdots \geq b_m$.

Because $b_1 + b_2 + \cdots + b_m = n - 1$, the structure of the starlike tree T is fully determined by the partition $\Gamma = (b_1, b_2, \ldots, b_m)$ of $n-1$. In view of this a starlike tree will be denoted by $T(\Gamma)$ or $T(b_1, b_2, \ldots, b_m)$. If $b_1 = b_2 = \cdots = b_m = 1$ then $m = n - 1$ and the respective tree is the simple star on n vertices. Three examples are given below, of which the third is a simple star:

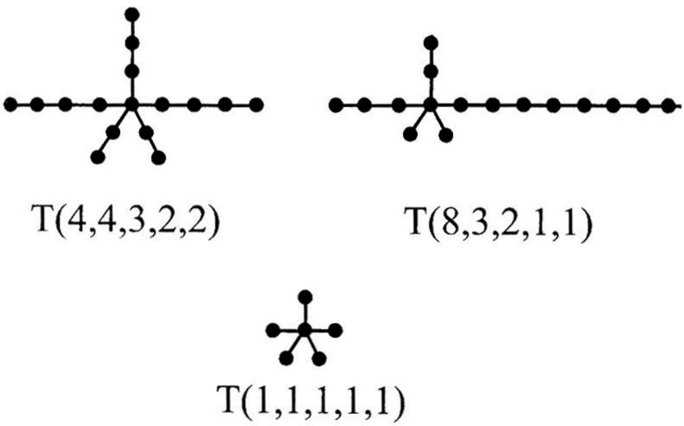
Recently, the Randić (connectivity) index χ [1] of starlike trees was studied [2] and the following formula was deduced

$$\chi = \frac{n-1}{2} - \frac{\sqrt{2}}{2}\left[\left(\sqrt{2}-1\right)m - \sqrt{m}\right] - \frac{\sqrt{2}-1}{2}\left(1 - \sqrt{\frac{2}{m}}\right)S \qquad (1)$$

where S is the number of branches of length one. Eq. (1) implies:

Proposition 1. For fixed m, χ is a monotonically decreasing function of S. For fixed S, χ is a monotonically decreasing function of m.

Proposition 2. Among n-vertex starlike trees the star ($m = n-1$, $b_1 = b_2 = \cdots = b_m = 1$) has minimal Randić index. Among n-vertex starlike trees the maximum value of χ is attained by any such tree with $m = 3$ and $S = 0$.



Formula (1) and Propositions 1 and 2 provide a complete ordering of starlike trees with regard to their Randić indices. These results motivated us to seek for regularities in the ordering of starlike trees with regard to other topological indices. In this paper we report some findings related to the Wiener index.

2. THE WIENER INDEX OF A STARLIKE TREE

The Wiener index [3] of a graph is equal to the sum of distances (= length of shortest paths) between all pairs of vertices of that graph. For details of the theory of this much-studied topological index see, for instance, Vol. 35 of MATCH.

The Wiener index of a starlike tree $T(b_1, b_2, \ldots, b_m) = T(\Gamma)$ will be denoted by $W(b_1, b_2, \ldots, b_m)$ or $W(\Gamma)$.

For any tree T the Wiener index can be calculated by means of the Doyle–Graver formula ([4], see also [5, 6]):

$$W(T) = \binom{n+1}{3} - \sum_{u} \sum_{i<j<k} n_i \, n_j \, n_k$$

where the first summation goes over all vertices u of degree greater than two, and where $n_1, n_2, n_3, \ldots$ denote the number of vertices in the branches attached to the vertex u. Applied to starlike trees the Doyle–Graver formula yields

$$W(b_1, b_2, \ldots, b_m) = \binom{n+1}{3} - \sum_{1 \le i<j<k \le m} b_i \, b_j \, b_k \ . \tag{2}$$

In particular, for $m = 3$:

$$W(b_1, b_2, b_3) = \binom{n+1}{3} - b_1 \, b_2 \, b_3$$

for $m = 4$:

$$W(b_1, b_2, b_3, b_4) = \binom{n+1}{3} - b_1 \, b_2 \, b_3 - b_1 \, b_2 \, b_4 - b_1 \, b_3 \, b_4 - b_2 \, b_3 \, b_4$$

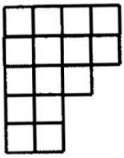
etc.

3. THE RUCH–SCHÖNHOFER–SNAPPER PARTIAL ORDERING OF PARTITIONS

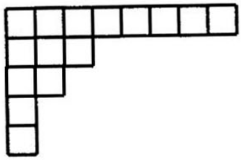
In connection with the representations of the symmetric group a partial ordering of partitions was conceived independently by Ruch and Schönhofer [7, 8] and Snapper [9] (see also [10]).

Let $\Gamma = (b_1, b_2, \ldots, b_m)$ and $\Gamma' = (b'_1, b'_2, \ldots, b'_{m'})$ be two different partitions of the same integer, i. e., $b_1 + b_2 + \cdots + b_m = b'_1 + b'_2 + \cdots + b'_{m'}$. Then Γ' is said to dominate Γ, denoted by $\Gamma \lhd \Gamma'$, if for all $k = 1, 2, \ldots, \min\{m, m'\}$, $\sum_{i=1}^{k} b_i \leq \sum_{i=1}^{k} b'_i$. If neither $\Gamma \lhd \Gamma'$ nor $\Gamma' \lhd \Gamma$, then the partitions Γ and Γ' are not comparable (with regard to the relation $\lhd$). For instance, $\Gamma = (2,2,2)$ and $\Gamma' = (3,1,1,1)$ are not comparable, as well as $\Gamma = (4,4,1)$ and $\Gamma' = (5,2,2)$.

Partitions may be visualized by means of Young diagrams, in which boxes are arranged in rows, so that b_i boxes come in the i-th row, $i = 1, 2, \ldots, m$. For instance, the partitions $\Gamma_a = (4,4,3,2,2)$ and $\Gamma_b = (8,3,2,1,1)$ are presented as:



Γ_a



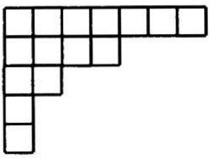
Γ_b

Now, a partition Γ' dominates the partition Γ if the Young diagram of Γ can be obtained from the Young diagram of Γ' by moving boxes downwards [7, 8].

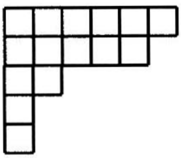
For instance, $\Gamma_a \lhd \Gamma_b$, because of the sequence

$$\Gamma_b \to \Gamma_c \to \Gamma_d \to \Gamma_e \to \Gamma_f \to \Gamma_a$$

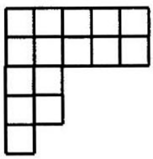
in which one box is moved downwards in each step. Note that such a sequence is not unique, but at least one must exist between any two comparable partitions.



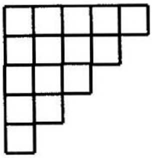
Γ_c



Γ_d



Γ_e



Γ_f

4. THE MAIN RESULT

Theorem 1. Let $T(\Gamma)$ and $T(\Gamma')$ be two non-isomorphic starlike trees with equal number of vertices. If $\Gamma \lhd \Gamma'$ then $W(\Gamma) < W(\Gamma')$.

Proof. Theorem 1 is a straightforward consequence of Eq. (2) and Corollary 2.1 of Theorem 2, which will be proven in the subsequent section. □

By means of Theorem 1 we can order some starlike trees with respect to their Wiener numbers (if Γ and Γ' are comparable), but not all starlike trees (when Γ and Γ' are not comparable). Note that if Γ and Γ' are not comparable, then the respective Wiener indices may be different (e.g. for $\Gamma = (7,4,1,1)$ and $\Gamma' = (8,2,2,1)$ for which $W(\Gamma) = 67$ and $W(\Gamma') = 68$) or equal (e.g. for $\Gamma = (8,4,1,1)$ and $\Gamma' = (9,2,2,1)$ for which $W(\Gamma) = W(\Gamma') = 76$).

Corollary 1.1. Among n-vertex starlike trees the star has the minimum Wiener index. Among n-vertex starlike trees the maximum value of W is attained by the tree with $m = 3$ and branch-lengths differing as little as possible, i. e.:

$$\begin{aligned} b_1 = b_2 = b_3 &\quad \text{if} \quad n-1 \equiv 0 \pmod 3 \\ b_1 = b_2 + 1 = b_3 + 1 &\quad \text{if} \quad n-1 \equiv 1 \pmod 3 \\ b_1 = b_2 = b_3 + 1 &\quad \text{if} \quad n-1 \equiv 2 \pmod 3 \,. \end{aligned}$$

Theorem 1 and Corollary 1.1 should be compared with Propositions 1 and 2.

Corollary 1.2. Among n-vertex starlike trees with a fixed value of m, the tree with $S = m - 1$, i. e., $b_2 = b_3 = \cdots = b_m = 1$ has minimum Wiener index. Among n-vertex starlike trees with a fixed value of m, the maximum value of W is attained by the tree whose branch-lengths differ as little as possible, i. e., $b_1 - b_m \leq 1$.

5. AN AUXILIARY RESULT

Consider a partition $\Gamma = (b_1, b_2, \ldots, b_m)$ and define a polynomial

$$P(\Gamma, x) = \prod_{i=1}^{m}(x + b_i) = x^m + c_1(\Gamma)\, x^{m-1} + c_2(\Gamma)\, x^{m-2} + \cdots + c_m(\Gamma) .$$

It is easy to see that the coefficients $c_k(\Gamma)$, $k = 1, 2, \ldots, m$, satisfy the relation

$$c_k(\Gamma) = \sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq m} b_{i_1} b_{i_2} \cdots b_{i_k} . \tag{3}$$

It is consistent to define $c_k(\Gamma) = 0$ for $k > m$.

Theorem 2. Let $\Gamma = (b_1, b_2, \ldots, b_m)$ and $\Gamma' = (b'_1, b'_2, \ldots, b'_{m'})$ be two different partitions of the same integer. If $\Gamma \lhd \Gamma'$, then the (strict) inequality $c_k(\Gamma) > c_k(\Gamma')$ holds for all $k = 2, 3, \ldots, \max\{m, m'\}$,.

Proof. We first consider the case when the Young diagram of Γ is obtained by moving downwards a single box of the Young diagram of Γ'. Let the box from the p-th row be moved into the q-th row, $p < q$. Then $b'_p = x$, $b'_q = y$, $b_p = x - 1$, $b_q = y + 1$ and $b_r = b'_r$ for $r \neq p, q$. It must be $b_p \geq b_q$ and therefore $x - 1 \geq y + 1$, i. e., $x - y - 1 > 0$.

Now, for $k \geq 2$ the terms $b'_{i_1} b'_{i_2} \cdots b'_{i_k}$, occuring on the right-hand side of Eq. (3) and pertaining to the partition Γ', can be divided into four types:

type 1: terms containing neither b'_p nor b'_q;

type 2: terms containing both b'_p and b'_q;

type 3: terms containing b'_p, but not b'_q;

type 4: terms containing b'_q, but not b'_p.

The same classification applies to the terms $b_{i_1} b_{i_2} \cdots b_{i_k}$, pertaining to the partition Γ.

In the case of Γ' the sum of terms of type 1 is a positive-valued number B_1, independent of x and y, depending on b'_r, $r \neq p, q$. Analogously, the sums of the terms of type 2, 3, and 4 are equal to $xy\, B_2$, $x\, B_3$, and $y\, B_3$, respectively, where also B_2 and B_3 are positive numbers independent of x and y, depending on b'_r, $r \neq p, q$. Thus $c_k(\Gamma')$ is equal to $B_1 + xy\, B_2 + (x+y)B_3$.

In the case of the partition Γ, in view of the fact that $b_r = b'_r$ for $r \neq p, q$, the sums of the terms of type 1, 2, 3, and 4 are equal to B_1, $(x-1)(y+1)B_2$, $(x-1)B_3$, and $(y+1)B_3$, respectively. Therefore

$$\begin{aligned} c_k(\Gamma) &= B_1 + (x-1)(y+1)B_2 + (x-1+y+1)B_3 \\ &= B_1 + xy\, B_2 + (x+y)B_3 + (x-y-1)B_2 \\ &= c_k(\Gamma') + (x-y-1)B_2 \\ &> c_k(\Gamma') \, . \end{aligned}$$

By this we have shown that Theorem 2 holds if only one box needs to be moved downwards.

If, however, the transformation of the Young diagram of Γ' into the Young diagram of Γ requires the moving of several boxes, this can be done by a sequence of single-box transformations. Consequently, Theorem 2 holds for any two comparable partitions Γ and Γ'. □

For the proof of Theorem 1 we need a special case of Theorem 2:

Corollary 2.1. If $\Gamma \lhd \Gamma'$ for two distinct partitions Γ and Γ', then $c_3(\Gamma) > c_3(\Gamma')$, i. e.,

$$\sum_{1 \leq i<j<k \leq m} b_i\, b_j\, b_k \;>\; \sum_{1 \leq i<j<k \leq m'} b'_i\, b'_j\, b'_k \,.$$

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