TREES WITH GIVEN DEGREE SEQUENCE IN S-ORDER

HUA WANG AND SHUAI YUAN

ABSTRACT. In this note we consider the lexicographical ordering by spectral moments of trees with given degree sequence. Such questions have been studied for a variety of different categories of trees. Particularly, the last tree in this ordering among trees with given degree sequence was recently identified in two independent manuscripts. The characterization of the first such trees, however, remains open. We make some progress on this question in this note, by making use of the interpretation of the spectral moment in terms of numbers of paths and the product of adjacent vertex degrees, the first trees are characterized with the additional condition that the nonleaf vertex degrees are different from each other. We also comment on the case when there are repetitions in the vertex degrees.

1. INTRODUCTION

For a graph G with $|V(G)| = n$ and adjacency matrix $A(G)$, let

$$\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G)$$

be the eigenvalues of $A(G)$ in non-increasing order. The k-th *spectral moment* of G, denoted by $S_k(G)$, is defined as

$$\sum_{i=1}^{n} (\lambda_i(G))^k$$

for $k = 0, 1, \ldots, n-1$. The sequence of spectral moments of G

$$S(G) = (S_0(G), S_1(G), \ldots, S_{n-1}(G))$$

introduces a natural lexicographical ordering of graphs on given number of vertices, called the *S-order.* That is, a graph G_1 appears earlier in the S-order than a graph G_2 if and only if from some k,

$$S_i(G_1) = S_i(G_2)$$

for $0 \leq i \leq k$ and

$$S_{k+1}(G_1) < S_{k+1}(G_2).$$

S-order has been used in producing graph catalogs [3] and has been extensively studied for different categories of graphs such as trees, unicyclic

This work was partially supported by grants from the Simons Foundation (#245307).

graphs, and bicyclic graphs [4, 14, 15]. In particular, trees received much attention in recent years. The S-order among trees with given maximum degree [7], trees with given diameter [13], quasi-trees [8] have been explored. Most recently, the S-order in a more general setting, i.e., among trees with given *degree sequence* (the non-increasing sequence of internal vertex degrees), is considered [1, 6]. The last such tree is characterized. Through comparisons of such extremal trees with different degree sequences, the authors of [1, 6] also obtained extremal results on other categories of trees. To find the first such tree among trees with a given degree sequence, however, seem to be a different question and was left open.

In this note, we aim to characterize the first trees in S-order among trees with given degree sequence, with the additional constraint that the nonleaf vertices have different degrees. We call such trees the *alternating greedy trees*, defined in the form of the algorithm to construct such a tree. This concept has only appeared (to our best knowledge) in the study of the Randić index [12] and was not formally defined.

Definition 1 (Alternating greedy trees). *Given the degree sequence*

$$\{d_1, d_2, \ldots, d_m\},$$

the alternating greedy tree is constructed through the following recursive algorithm:

(i) If $m-1 \leq d_m$, then the alternating greedy tree is simply obtained by a tree rooted at r with d_m children with degrees

$$d_1, \ldots, d_{m-1} \text{ and } \underline{1, \ldots, 1}_{(d_m - m + 1)} \text{ 1's;}$$

(ii) Otherwise, $m-1 \geq d_m + 1$. We produce a subtree T_1 rooted at r with $d_m - 1$ children with degrees

$$d_1, \ldots, d_{d_m - 1};$$

(iii) Consider the alternating greedy tree S with degree sequence

$$\{d_{d_m}, \ldots, d_{m-1}\},$$

let v be a leaf with the smallest neighbor degree. Identify the root of T_1 with v.

As an example (Figures 1, 2, 3), for the given degree sequence

$$\{8, 7, 6, 6, 5, 5, 3, 3, 3, 2\}:$$

- T_1 is constructed with degrees $\{8, 2\}$ (as in (ii)), leaving the degree sequence $\{7, 6, 6, 5, 5, 3, 3, 3\}$ (as in (iii)) with the corresponding alternating greedy tree S_1;
- To construct S_1, T_2 is formed with degrees $\{7, 6, 3\}$, leaving the degree sequence $\{6, 5, 5, 3, 3\}$ with the corresponding alternating greedy tree S_2;

- To construct S_2, T_3 is formed with degrees $\{6, 5, 3\}$, leaving the degree sequence $\{5, 3\}$ to provide us the trivial S_3 (as in (i));
- Attaching T_3 to S_3 (as in (iii)) yields S_2. Then attaching T_2 to S_2 yields S_1. In the final step, it is obvious that the two choices for attaching T_1 to S_1 yield two different such alternating greedy trees. Consequently, unlike the greedy trees, alternating greedy trees are not necessarily unique.

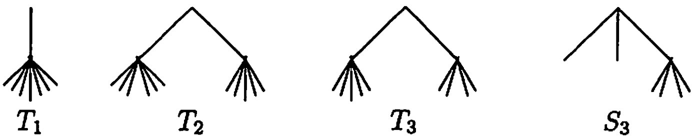

FIGURE 1. Construction of T_1, T_2, T_3, and S_3

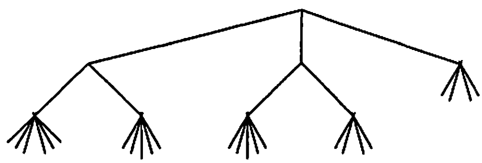

FIGURE 2. The alternating greedy tree S_1 from T_2, T_3 and S_3.

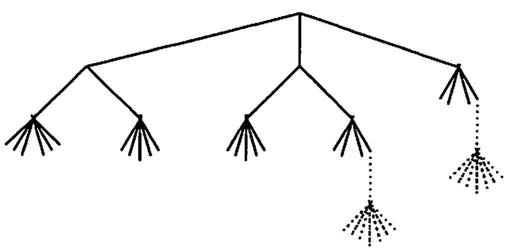

FIGURE 3. The alternating greedy trees T or T' from T_1 and S_1.

Theorem 1.1. *Among trees of given degree sequence $\{d_1, d_2, \ldots, d_m\}$, where $d_i \neq d_j$ for $1 \leq i \neq j \leq m$ (hereforth referred to as a "distinct" degree sequence), the first tree in S-order must be an alternating greedy tree.*

As commented in [12] and from Definition 1, it is easy to see that the following fact, established in Section 2, implies the extremality of the alternating greedy trees.

Lemma 1.2. *For a tree T with given (distinct) degree sequence that appear the first in the S-order and a longest path $P(v_0, v_{t+1}) = v_0 v_1 \dots v_t v_{t+1}$ in T. For $i \leq \frac{t+1}{2}$, we must have*

$$deg(v_i) \leq deg(v_{t+1-i}) < deg(v_k) \text{ for } i < k < t+1-i \tag{1}$$

if i is even; and

$$deg(v_i) > deg(v_{t+1-i}) > deg(v_k) \text{ for } i < k < t+1-i \tag{2}$$

if i is odd.

Remark 1. *In fact, applying conditions (1) and (2) on all paths of a tree forces the neighbors of leaves to have the largest degrees, the vertices at distance two from the leaves to have the smallest degrees, etc. More specifically, denote by L_k the set of vertices whose closest leaves are at distance k (i.e., L_0 is the set of leaves, L_1 are neighbors of leaves, etc.), Lemma 1.2 implies that:*

- *The largest degrees are assigned to vertices in L_1;*
- *The smallest degrees are assigned to vertices in L_2;*
- *The remaining largest degrees are assigned to vertices in L_3;*
- ...

This is exactly how we construct an alternating greedy tree with a given degree sequence. Hence, to prove Theorem 1.1, we only need to show Lemma 1.2.

2. Proof of Lemma 1.2

First note the following beautiful result that represents the spectral moment of a graph with the number of closed walks.

Lemma 2.1. [2] *The k-th spectral moment of G is equal to the number of closed walks of length k.*

When trees are under consideration, closed walks of length ≤ 6 simply result from paths of length ≤ 3. Consequently, for a tree T with given degree sequence, it is easy to see that $S_k(T)$ is a constant for $k = 0, 1, 2, 3, 4, 5$ and

$$S_6(T_1) - S_6(T_2) = 6\left(\phi_{T_1}(P_4) - \phi_{T_2}(P_4)\right)$$

for two trees T_1 and T_2, where $\phi_T(P_4)$ is the number of P_4 in T. One can see, for example, [6] and the references thereof for more detailed analysis on the k-th spectral moment of trees.

Note that a P_4 in a tree T must have its "middle" edge on some edge $uv \in E(T)$, with $(deg(u)-1)(deg(v)-1)$ choices for the two end vertices of this P_4. Therefore, we have

$$\phi_T(P_4) = \sum_{uv \in E(T)} (deg(u)-1)(deg(v)-1) =: \mathcal{R}(T). \tag{3}$$

Since all trees with a given degree sequence share the same $S_k(T)$ for $0 \leq k \leq 5$ but not for $k = 6$, by the definition, the first trees in S-order are exactly the ones whose $S_6(T)$ is minimized. Therefore, to show Lemma 1.2, it suffices to show that minimizing (3) implies (1) and (2).

First of all, since v_0 and v_{t+1} are both leaves, we have

$$1 = deg(v_0) = deg(v_{t+1}) < deg(v_k)$$

for any $0 < k < t+1$. Hence (1) holds for $i = 0$.

The proof of Lemma 1.2 follows in an inductive manner on i. Assume now that (1) and (2) hold for $i = 0, \ldots, i_0$, we consider the case when i_0 is even and show (2) for $i = i_0 + 1$, the case for odd i_0 is similar.

Let $\mathcal{D}$ denote the set of degrees of the vertices v_j, $i_0 + 1 \leq j \leq t - i_0$. If

$$deg(v_{i_0+1}) = \max \mathcal{D} \tag{4}$$

and

$$deg(v_{t-i_0}) = \max(\mathcal{D} - \{deg(v_{i_0+1})\}) \tag{5}$$

both hold, we have

$$deg(v_{i_0+1}) > deg(v_{t+1-(i_0+1)}) > deg(v_k)$$

for $i_0 + 1 \leq k \leq t + 1 - (i_0 + 1)$. This is exactly (2) for $i = i_0 + 1$.

Suppose now (for contradiction) that T minimizes $\mathcal{R}(.)$ and at least one of (4) and (5) is not true. Without loss of generality, assume that (4) does not hold. Then there exists an s, $i_0 + 1 < s \leq t - i_0$, such that

$$deg(v_s) > deg(v_{i_0+1}).$$

Note that, by applying inductive hypothesis (1) to $i = i_0$, we must have

$$deg(v_{s+1}) > deg(v_{i_0}).$$

Consider the tree

$$T' = (T/\{v_{i_0}v_{i_0+1}, v_s v_{s+1}\}) \cup \{v_{i_0}v_s, v_{i_0+1}v_{s+1}\} \tag{6}$$

obtained from T by reversing the segment $v_{i_0+1} \ldots v_s$ and the pendant components (Figure 4).

Under this operation, the contribution

$$(deg(u)-1)(deg(v)-1)$$

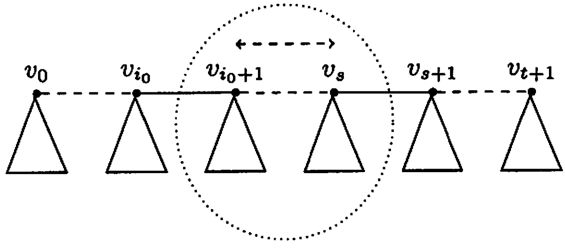

FIGURE 4. Constructing T' from T

to (3) stays the same for any edge uv except for $v_{i_0}v_{i_0+1}$, v_sv_{s+1}, $v_{i_0}v_s$ and $v_{i_0+1}v_{s+1}$. Thus

$$\begin{aligned}
&\mathcal{R}(T') - \mathcal{R}(T)\\
=&(deg(v_{i_0}) - 1)(deg(v_s) - 1) + (deg(v_{i_0+1}) - 1)(deg(v_{s+1}) - 1)\\
&\quad - (deg(v_{i_0}) - 1)(deg(v_{i_0+1}) - 1) - (deg(v_s) - 1)(deg(v_{s+1}) - 1)\\
=&(deg(v_{i_0} - deg(v_{s+1})) \cdot (deg(v_s) - deg(v_{i_0+1}))\\
<&0,
\end{aligned}$$

contradicting the minimality of T with respect to $\mathcal{R}(.)$.

Therefore, one can conclude that for any tree T with given degree sequence, $\mathcal{R}(T)$ (and hence $\phi(T)$) is only minimized when (1) and (2) are satisfied for any longest path in the tree.

Remark 2. *The constraint that all nonleaf vertex degrees are pairwise different is not absolutely necessary. With a little more technical details, one can show that the same conclusion holds if none of the vertex degrees are repeated more than twice. We provide the rather simple argument here with slightly stronger constraint and comment on the case when the vertex degrees are repeated "many" times in the next section.*

Also note that, reiterating our argument in the inductive step will provide an algorithm that will always generate a tree T' with smaller $\mathcal{R}(.)$. Such an algorithm terminates in finite steps as we either reach the conclusion or decrease the value of $\mathcal{R}(.)$ in every step.

3. ON DEGREE SEQUENCES WITH REPEATED DEGREES

With repeated degrees, conditions (1) and (2) are no longer necessary conditions for achieving the minimum $\mathcal{R}(.)$. For instance, on a longest path with internal vertex degrees $\{4, 4, 4, 4, 3, 2, 2\}$, both of the following arrangements obtain the same minimum contribution to $\mathcal{R}(.)$ from edges on this path:

- $(deg(v_0), \ldots, deg(v_9)) = (1, 4, 2, 4, 3, 4, 2, 4, 1)$;

- $(deg(v_0), \ldots, deg(v_9)) = (1, 4, 3, 4, 2, 4, 2, 4, 1)$.

The former is what conditions (1) and (2) claim while the latter is not. Consider, for instance, the two trees T and T' in Figure 5 with the same degree sequence, we have $S_k(T) = S_k(T')$ for $0 \leq k \leq 7$. Simple calculations (by making use of Lemma 2.1) shows that $S_8(T) > S_8(T')$ and hence T' appears earlier in the S-order than T (an alternating greedy tree).

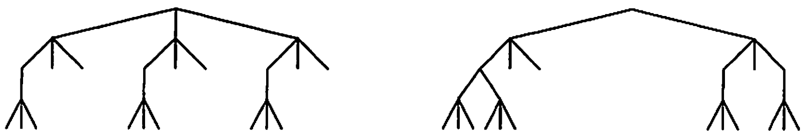

FIGURE 5. Trees T (left) and T' (right) with degree sequence $\{4, 4, 4, 4, 4, 4, 3, 2, 2, 2\}$

Note that the tree T', while being non-isomorphic to T, is still an alternating greedy tree as shown in Figure 6. Thus, although we cannot establish Theorem 1.1 through Lemma 1.2 when repeated degrees are present, it is still possible that the first tree in S-order has to be an alternating greedy tree. But the study of $S_k(.)$ for $k \geq 8$ appears to be much more complicated and a novel idea may be needed.

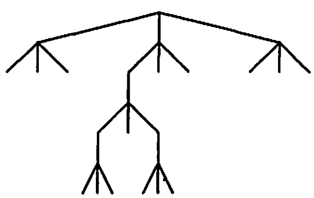

FIGURE 6. T' is an alternating greedy tree

Question 3.1. *With repeated vertex degrees, is it still true that the first tree in S-order has to be an alternating greedy tree?*

4. Concluding remarks

We show that the first tree in S-order among trees with given (distinct) degree sequence must be an alternating greedy tree. Making use of the fundamental representation of the spectral moments with number of paths, the question is somewhat reduced to finding minimal sum of products of adjacent vertex degrees, one that is very similar to the study of the *Randić index* and *weight* of trees [5, 9, 10]. Part of a recent paper on the number of walks in graphs has also done similar analysis [11].

However, because of the nature of S-order, more subtle argument will be needed to answer the question when the nonleaf degrees are repeated. We briefly commented on this question.

Acknowledgment

We thank the referees for pointing out our mistakes and offering many helpful suggestions.

References

[1] E. Andriantiana, S. Wagner, Spectral moments of trees with given degree sequence, to appear.

[2] D. Cvetković, M. Doob, H. Sachs, Spectra of Graphs–Theory and Applications, *Academic Press,* New York, 1980.

[3] D. Cvetković, M. Petrić, A table of connected graphs on six vertices, *Discrete Math.* **50** (1984) 37–49.

[4] D. Cvetković, P. Rowlinson, Spectra of unicyclic graphs, *Graph Combin.* **3** (1987) 7–23.

[5] C. Delorme, O. Favaron, D. Rautenbach, On the Randić index, *Discrete Math.* **257** (2002) 29–38.

[6] S. Li, Y. Song, On the spectral moment of trees with given degree sequence, to appear.

[7] X.-F. Pan, X.L. Hu, X.G. Liu, H.Q. Liu, The spectral moments of trees with given maximum degree, *Applied Mathematics Letters* **24** (2011) 1265–1268.

[8] X.-F. Pan, X. Liu, H.Q. Liu, On the spectral moment of quasi-trees, *Linear Algebra and its Applications* **436** (2012) 927–934.

[9] M. Randić, On characterization of molecular branching, *J. Amer. Chem. Soc.* **97** (1975) 6609–6615.

[10] D. Rautenbach, A note on trees of maximum weight and restricted degrees, *Discrete Math.* **271** (2003) 335–342.

[11] H. Täubig, J. Weihmann, S. Kosub, R. Hemmecke, E. Mayr, Inequalities for the Number of Walks in Graphs, *Algorithmica,* to appear.

[12] H. Wang, Extremal trees with given degree sequence for the Randić index, *Discrete Math.* **308** (2008) 3407-3411.

[13] Y.P. Wu, H.Q. Liu, Lexicographical ordering by spectral moments of trees with a prescribed diameter, *Linear Algebra and its Applications* **433** (2010) 1707–1713.

[14] Y.P. Wu, H.Q. Liu, Ordering unicyclic graphs with respect to spectral moment, to appear.

[15] Y.P. Wu, Q. Fan, On the lexicographical ordering by spectral moments of bicyclic graphs, to appear.

Hua Wang, Department of Mathematical Sciences, Georgia Southern University, Statesboro, GA 30460, USA

E-mail address: hwang@georgiasouthern.edu

Shuai Yuan, Department of Mathematical Sciences, Georgia Southern University, Statesboro, GA 30460, USA

E-mail address: sy00504@georgiasouthern.edu