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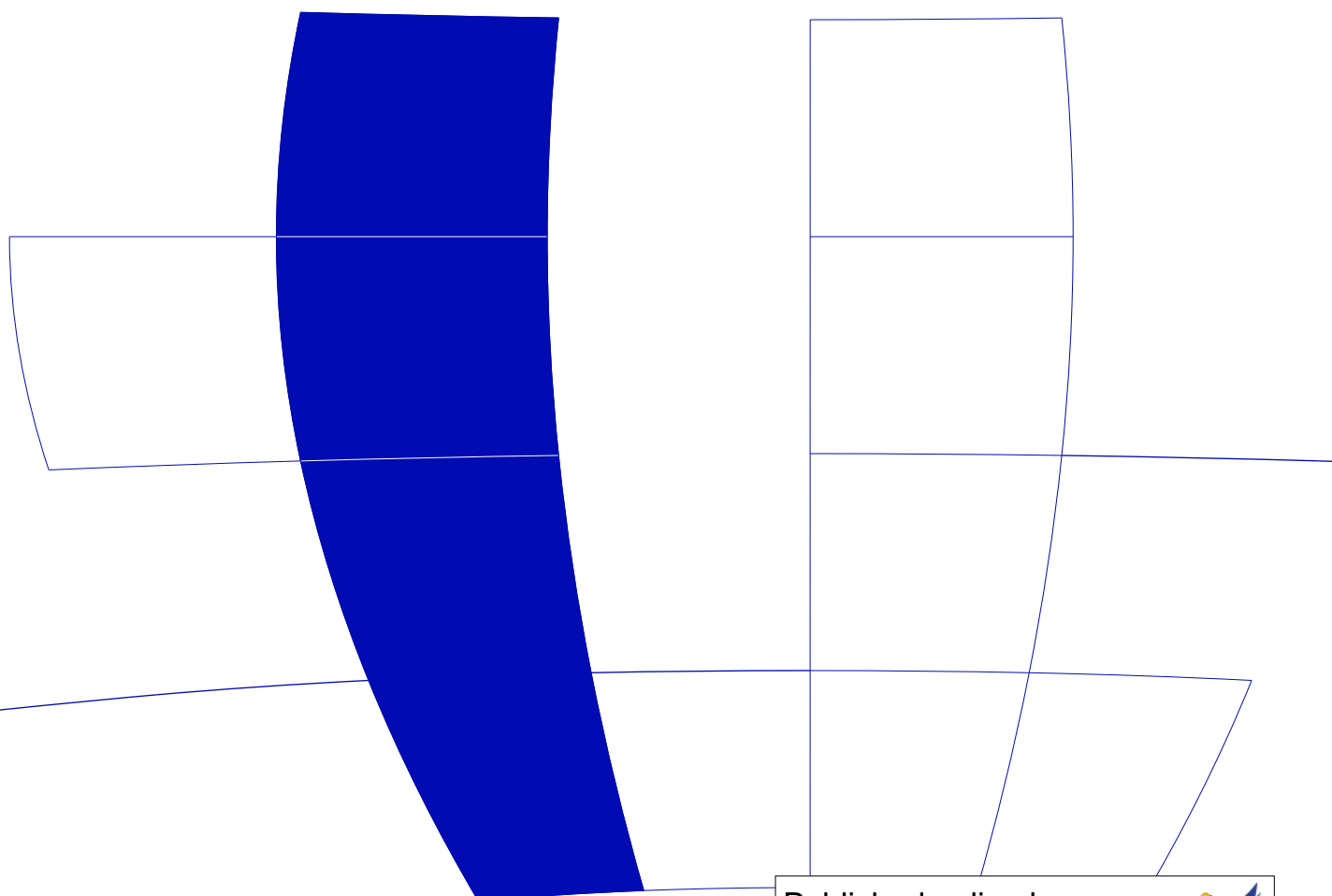
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Largest Laplacian Eigenvalue and Degree Sequences of Trees

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Abstract

We investigate the structure of trees that have greatest maximum eigenvalue among all trees with a given degree sequence. We show that in such an extremal tree the degree sequence is non-increasing with respect to an ordering of the vertices that is obtained by breadth-first search. This structure is uniquely determined up to isomorphism. We also show that the maximum eigenvalue in such classes of trees is strictly monotone with respect to majorization.

Key words: graph Laplacian, largest eigenvalue, spectral radius, eigenvector, tree, degree sequence, majorization

1 Introduction

The *Laplacian* matrix $L(G)$ of a graph $G = (V, E)$ with vertex set V and edge set E is given as

$$L(G) = D(G) - A(G) \,, \tag{1}$$

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where $A(G)$ denotes the adjacency matrix of G and $D(G)$ is the diagonal matrix whose entries are the vertex degrees, i.e., $D_{vv} = d(v)$, where $d(v)$ denotes the degree of vertex v. We write L for short if there is no risk of confusion.

The Laplacian L is symmetric and all its eigenvalues are non-negative. These eigenvalues have been intensively investigated, see e.g. [8] for a comprehensive survey. In particular the largest eigenvalue, denoted by $\lambda(G)$ throughout the paper, is of importance. In literature there exist many bounds on the largest eigenvalue of a graph; in Brankov et al. [4] some of them are collected and it is shown how these can be derived in a systematic way.

Here we are interested in the structure of trees which have largest maximum eigenvalue among all trees with a given degree sequence. We call such trees *extremal trees*. We show that for such trees the degree sequence is non-increasing with respect to an ordering of the vertices that is obtained by breadth-first search. We also show that the largest maximum eigenvalue in such classes of trees is strictly monotone with respect to some partial ordering of degree sequences. (Similar results hold for the spectral radius of trees with given degree sequence [2].)

The paper is organized as follows: The results of this paper are stated in Section 2. In Section 3 we prove these theorems by means of a technique of rearranging graphs which has been developed in [1, 3] for the problem of minimizing the first Dirichlet eigenvalue within a class of trees.

2 Degree Sequences and Largest Eigenvalue

Let $d(v)$ denote the degree of vertex v. We call a vertex v with $d(v) = 1$ a *pendant vertex* of a graph (or *leaf* in case of a tree). Recall that a sequence $\pi = (d_0, \ldots, d_{n-1})$ of non-negative integers is called *degree sequence* if there exists a graph G for which $d_0, \ldots, d_{n-1}$ are the degrees of its vertices. In particular, π is a tree sequence, i.e. a degree sequence of some tree, if and only if every $d_i > 0$ and $\sum_{i=0}^{n-1} d_i = 2(n-1)$. We refer the reader to [7] for relevant background on degree sequences. We introduce the following class for which we can characterize extremal graphs with respect to the maximum eigenvalue.

$$\mathcal{T}_\pi = \{G \text{ is a tree with degree sequence } \pi\}.$$

For this characterization of extremal trees in $\mathcal{T}_\pi$ we introduce an ordering of the vertices $v_0, \ldots, v_{n-1}$ of a graph G by means of breadth-first search: Select a vertex $v_0 \in G$ and create a sorted list of vertices beginning with v_0; append all neighbors $v_1, \ldots, v_{d(v_0)}$ of v_0 sorted by decreasing degrees; then append

all neighbors of v_1 that are not already in this list; continue recursively with $v_2, v_3, \ldots$ until all vertices of G are processed. In this way we build layers where each v in layer i is adjacent to some vertex w in layer $i-1$ and vertices u in layer $i+1$. We then call the vertex w the *parent* of v and v a child of w.

Definition 1 (BFD-ordering) *Let $G(V, E)$ be a connected graph with root v_0. Then a well-ordering $\prec$ of the vertices is called* breadth-first search order- ing with decreasing degrees *(BFD-ordering for short) if the following holds for all vertices $v, w \in V$:*

(B1) if $w_1 \prec w_2$ then $v_1 \prec v_2$ for all children v_1 of w_1 and v_2 of w_2;
(B2) if $v \prec u$, then $d(v) \geq d(u)$.

We call connected graphs that have a BFD-ordering of its vertices a BFD- graph *(see Fig. 1 for an example).*
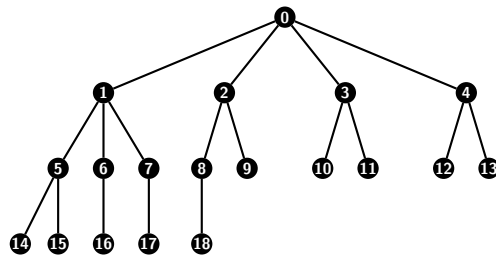

Fig. 1. A BFD-tree with degree sequence $\pi = (4^2, 3^4, 2^3, 1^{10})$

Every graph has for each of its vertices v an ordering with root v that satisfies (B1). This can be found by a breadth-first search as described above. However, not all trees have an ordering that satisfies both (B1) and (B2); consider the tree in Fig. 2.
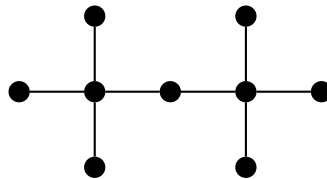

Fig. 2. A tree with degree sequence $\pi = (4^2, 2^1, 1^6)$ where no BFD-ordering exists.

Theorem 2 *A tree G with degree sequence π is extremal in class $\mathcal{T}_\pi$ if and only if it is a BFD-tree. G is then uniquely determined up to isomorphism. The BFD-ordering is consistent with the corresponding eigenvector f of G in such a way that $|f(u)| > |f(v)|$ implies $u \prec v$.*

For a tree with degree sequence π a sharp upper bound on the largest eigen- value can be found by computing the corresponding BFD-tree. Obviously find- ing this tree can be done in $O(n)$ time if the degree sequence is sorted.

We define a partial ordering on degree sequences $\pi = (d_0, \ldots, d_{n-1})$ and $\pi' = (d'_0, \ldots, d'_{n'-1})$ with $n \leq n'$ and $\pi \neq \pi'$ as follows: we write $\pi \lhd \pi'$ if and only if $\sum_{i=0}^{j} d_i \leq \sum_{i=0}^{j} d'_i$ for all $j = 0, \ldots n - 1$ (recall that the degree sequences are non-increasing).

Theorem 3 *Let π and π' be two distinct degree sequences of trees with $\pi \lhd \pi'$. Let G and G' be extremal trees in the classes $\mathcal{T}_\pi$ and $\mathcal{T}_{\pi'}$, respectively. Then we find for the corresponding maximum eigenvalues $\lambda(G) < \lambda(G')$.*

We get the following well-known results as immediate corollaries.

Corollary 4 *A tree T is extremal in the class of all trees with n vertices if and only if it is the star $K_{1,n-1}$.*

Corollary 5 ([5, Thm. 2.2]) *A tree G is extremal in the class of all trees with n vertices and k leaves if and only if it is a star with paths of almost the same lengths attached to each of its k leaves.*

Proof of Cor. 4 and 5. The tree sequences $\pi_n = (n - 1, 1, \ldots, 1)$ and $\pi_{n,k} = (k, 2, \ldots, 2, 1, \ldots, 1)$ are maximal w.r.t. ordering $\lhd$ in the respective classes of all trees with n vertices and all trees with n vertices and k pendant vertices. Thus the statement immediately follows from Theorems 2 and 3. $\square$

3 Proof of the Theorems

We denote the largest eigenvalue of a graph G by $\lambda(G)$. We denote the number of vertices of a graph G by $n = |V|$ and the geodesic path between two vertices u and v by P_{uv}.

The Rayleigh quotient of the graph Laplacian L of a vector f on V is the fraction

$$\mathcal{R}_G(f) = \frac{\langle f, Lf \rangle}{\langle f, f \rangle} = \frac{\sum_{uv \in E}(f(u) - f(v))^2}{\sum_{v \in V} f(v)^2}. \tag{2}$$

By the Rayleigh-Ritz Theorem we find the following well-known property for the spectral radius of G.

Proposition 6 ([6]) *Let $\mathcal{S}$ denote the set of unit vectors on V. Then*

$$\lambda(G) = \max_{f \in \mathcal{S}} \mathcal{R}_G(f) = \max_{f \in \mathcal{S}} \sum_{uv \in E} (f(u) - f(v))^2.$$

Moreover, if $\mathcal{R}_G(f) = \lambda(G)$ for a function $f \in \mathcal{S}$, then f is the Laplacian eigenvector corresponding to the maximum eigenvalue $\lambda(G)$ of $L(G)$.

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Notice that every eigenvector f corresponding to the maximum eigenvalue must fulfill the eigenvalue equation

$$Lf(x) = d(x)f(x) - \sum_{yx \in E} f(y) = \lambda f(x) \quad \text{for every } x \in V. \tag{3}$$

Trees are a special case of bipartite graphs. Hence the following observation is important.

Proposition 7 ([9]) *Let $G(V_1 \cup V_2, E)$ be a connected graph with bipartition $V_1 \cup V_2$ and $n = |V_1 \cup V_2|$ vertices. Then there is an eigenfunction f corresponding to the maximum eigenvalue of $L(G)$, such that f is positive on V_1 and negative on V_2.*

The main techniques for proving our theorems is *rearrangement* of edges. We need two types of rearrangement steps that we call *switching* and *shifting*, resp., in the following.

Lemma 8 (*Switching*) *Let $T \in \mathcal{T}_\pi$ and let u_1v_1, $u_2v_2 \in E(T)$ be edges such that the path $P_{v_1v_2}$ neither contains u_1 nor u_2. Then by replacing edges u_1v_1 and u_2v_2 by the respective edges u_1v_2 and u_2v_1 we get a new tree T' which is also contained in $\mathcal{T}_\pi$. Furthermore for every eigenvector f corresponding to the maximum eigenvalue $\lambda(T)$ we find $\lambda(T') \geq \lambda(T)$ whenever $|f(u_1)| \geq |f(u_2)|$ and $|f(v_2)| \geq |f(v_1)|$. The inequality is strict if one of the latter two inequalities is strict.*

Proof. Since $P_{v_1v_2}$ neither contains u_1 nor u_2 by assumption, T' is again a tree. Since switching of two edges does not change degrees, T' also belongs to class $\mathcal{T}_\pi$. Let f be an eigenvector corresponding to the maximum eigenvalue $\lambda(T)$ with $||f|| = 1$. Without loss of generality we assume that $f(v_1) > 0$. To verify the inequality we have to compute the effects of removing and inserting edges on the Rayleigh quotient. We have to distinguish between two cases:

(1) $f(v_1)$ and $f(u_2)$ have different signs. Then by Prop. 7 and our assumptions $0 < f(v_1) \leq f(v_2)$ and $f(u_1) \leq f(u_2) < 0$. Thus

$$\begin{aligned}
\lambda(T') - \lambda(T) &\geq \langle f, L(T')f \rangle - \langle f, L(T)f \rangle \\
&= \left[(f(u_1) - f(v_2))^2 + (f(v_1) - f(u_2))^2 \right] \\
&\quad - \left[(f(v_1) - f(u_1))^2 + (f(u_2) - f(v_2))^2 \right] \\
&= 2(f(u_1) - f(u_2))(f(v_1) - f(v_2)) \\
&\geq 0 \ .
\end{aligned}$$

(2) $f(v_1)$ and $f(u_2)$ have the same sign. Then $0 < f(v_1) \leq -f(v_2)$ and $0 < f(u_2) \leq -f(u_1)$. We define a new function f' such that $f'(x) = f(x)$ for all x that belong to the same component of $T \setminus \{v_1u_1, v_2u_2\}$ as v_1 and v_2,

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and $f'(x) = -f(x)$ otherwise. Thus

$$\begin{aligned}
\lambda(T') - \lambda(T) &\geq \langle f', L(T')f' \rangle - \langle f, L(T)f \rangle \\
&= \left[(f'(u_1) - f'(v_2))^2 + (f'(v_1) - f'(u_2))^2 \right] \\
&\quad - \left[(f(v_1) - f(u_1))^2 + (f(u_2) - f(v_2))^2 \right] \\
&= 2(f(u_1) + f(u_2))(f(v_1) + f(v_2)) \\
&\geq 0 \, .
\end{aligned}$$

Therefore in both cases $\lambda(T') \geq \lambda(T)$. If $|f(u_1)| > |f(u_2)|$ or $|f(v_2)| > |f(v_1)|$ then the eigenvalue equation (3) would not hold for v_1 or u_2. Thus f (and f', resp.) is not an eigenfunction corresponding to $\lambda(T')$ and thus $\lambda(T') > \mathcal{R}_{T'}(f') \geq \lambda(T)$ as claimed. $\square$

Lemma 9 (*Shifting*) *Let $T \in \mathcal{T}_\pi$ and $u, v \in V(T)$. Assume we have edges $ux_1, \ldots, ux_k \in E(T)$ such that none of the x_i is in P_{uv}. Then we get a new graph T' by replacing all edges $ux_1, \ldots, ux_k$ by the respective edges $vx_1, \ldots, vx_k$. If f is an eigenvector with respect to $\lambda(T)$, then we find $\lambda(T') > \lambda(T)$ whenever $|f(u)| \leq |f(v)|$.*

Proof. Assume without loss of generality that $f(u) > 0$. Then we have two cases: $f(v)$ and $f(u)$ have the same sign. Then by our assumptions $f(v) \geq f(u) > 0$ and $f(x_i) < 0$ for all $i = 1, \ldots, k$, and we find

$$\begin{aligned}
\lambda(T') - \lambda(T) &\geq \langle f, L(T')f \rangle - \langle f, L(T)f \rangle \\
&= \sum_{i=1}^{k} \left[(f(x_i) - f(v))^2 - (f(x_i) - f(u))^2 \right] \\
&= 2(f(u) - f(v)) \sum_{i=1}^{k} f(x_i) + k(f(v)^2 - f(u)^2) \\
&\geq 0 \, .
\end{aligned}$$

Now if $\lambda(T') = \lambda(T)$ then f also must be an eigenvector of T' by Prop. 6. Thus the eigenvalue equation (3) for vertex u and v in T and T' implies that $f(x_i) = 0$ for all i, a contradiction. The second case where $f(v)$ and $f(u)$ have different signs is shown by means of a function f' analogously to the proof of Lemma 8. $\square$

Lemma 10 *Let T be extremal in class $\mathcal{T}_\pi$ and f an eigenvector corresponding to $\lambda(T)$. If $|f(v)| > |f(u)|$, then $d(v) \geq d(u)$.*

Proof. Suppose that $|f(v)| > |f(u)|$ for some vertices $u, v \in V(T)$ but $d(v) < d(u)$. Then we construct a new graph $T' \in \mathcal{T}_\pi$ by shifting $k = d(u) - d(v)$ edges in T. For this purpose we can choose any k of the $d(u) - 1$ edges that are not contained in P_{uv}. Let $x_1 u, \ldots, x_k u$ be these edges which are replaced by $x_1 v, \ldots, x_k v$. Thus we can apply Lemma 9 and obtain $\lambda(T') > \lambda(T)$, a

contradiction to our assumption. $\square$

Lemma 11 *Each class $\mathcal{T}_\pi$ contains a BFD-tree T that is uniquely determined up to isomorphism.*

Proof. For a given tree sequence the construction of a BFD-tree is straightforward. To show that two BFD-trees T and T' in class $\mathcal{T}_\pi$ are isomorphic we use a function ϕ that maps the vertex v_i in the ith position in the BFD-ordering of T to the vertex w_i in the ith position in the BFD-ordering of T'. By the properties (B1) and (B2) ϕ is an isomorphism, as v_i and w_i have the same degree and the images of neighbors of v_i in the next layer are exactly the neighbors of w_i in the next layer. The latter can be seen by looking on all vertices of T in the reverse BFD-ordering. $\square$

Now let f be an eigenvector corresponding to the maximum eigenvalue $\lambda(T)$ of T. Then we can define an ordering $\prec$ of the vertices of T in such a way that $v_i \prec v_j$ whenever

(i) $|f(v_i)| > |f(v_j)|$ or
(ii) $|f(v_i)| = |f(v_j)|$ and $d(v_i) > d(v_j)$ or
(iii) $|f(v_i)| = |f(v_j)|$, $d(v_i) = d(v_j)$, and there is a neighbor u_i of v_i with $u_i \prec u_j$ for all neighbors u_j of v_j.

Such an ordering can always be constructed recursively starting at a maximum v_0 of $|f(x)|$. If we have already enumerated the vertices in $V_{k-1} = \{v_0, \ldots, v_{k-1}\}$ then the next vertex v_k is the maximum of $V \setminus V_{k-1}$ w. r. t. (i) and (ii). If v_k is not uniquely determined then we look at the respective neighbors that belong to V_{k-1} and select the vertex with the least neighbor (in the ordering of V_{k-1}). It might happen that this is still not uniquely determined or that there are no such neighbors, then we are free to choose any of the qualified vertices.

We enumerate the vertices of T with respect to this ordering, i.e., $v_i \prec v_j$ if and only if $i < j$. In particular, v_0 is a maximum of $|f|$.

Lemma 12 *Let T be extremal in class $\mathcal{T}_\pi$ with corresponding eigenvector f. Then the order $\prec$ defined above is a BFD-ordering.*

Proof. Property (B2) immediately follows from Lemma 10. Let v_0 be the root of T and create another ordering of its vertices by a breadth-first search where the children of a vertex are always sorted by their index. We denote the ith element with respect to this ordering by $v(i)$. We show that both orderings are equivalent, i.e., $v(i) = v_i$. Suppose that there exists an index k where this relation fails and choose k the least index with this property. Then $v(k) = v_m \succ v_k$ and consequently $|f(v_k)| \geq |f(v_m)|$ and $d(v_k) \geq d(v_m)$. Let w_m and w_k be the respective parents of v_m and v_k. Notice that $w_m \prec v_k$ and $w_k \succ w_m$

since $(v_0, \ldots, v_{k-1}, v_m)$ is already a BFD-ordering by our construction. We have the following cases:

(1) $|f(v_k)| > |f(v_m)|$ and the path $P_{w_m w_k}$ does not contain any of the two vertices v_k and v_m. Then we can replace edges $w_k v_k$ and $w_m v_m$ by $w_m v_k$ and $w_k v_m$ and get a new tree T' with $\lambda(T') > \lambda(T)$ by Lemma 8.

(2) $|f(v_k)| > |f(v_m)|$ and v_m is contained in $P_{w_m w_k}$. Then by Lemma 10 $d(v_k) \geq d(v_m) \geq 2$ and there exists a child u_k of v_k. By construction $u_k \succ v_k \succ w_m$. Again we get a new tree T' by replacing edges $w_m v_m$, $u_k v_k$ by the edges $w_m v_k$, $u_k v_m$, with $\lambda(T') > \lambda(T)$. Notice that v_k cannot be in the path $P_{w_m w_k}$.

(3) $|f(v_k)| = |f(v_m)|$ and $d(v_k) > d(v_m)$. Then we can shift $k = d(v_k) - d(v_m)$ children of v_k and get a new tree $T' \in \mathcal{T}_\pi$ with $\lambda(T') > \lambda(T)$ by Lemma 9.

(4) $|f(v_k)| = |f(v_m)|$ and $d(v_k) = d(v_m)$. But then we had $w_k \prec w_m$, a contradiction to (iii) of our ordering.

In either case we get a contradiction to our assumption that T is already extremal. $\square$

Proof of Theorem 2. The result follows immediately from the construction of the ordering $\prec$ and Lemmata 11 and 12. $\square$

Proof of Theorem 3. Let $\pi = (d_0, \ldots, d_{n-1})$ and $\pi' = (d'_0, \ldots, d'_{n'-1})$ be two tree sequences with $\pi \lhd \pi'$ and $n = n'$. By Theorem 2 the maximum eigenvalue becomes the largest one for a tree T within class $\mathcal{T}_\pi$ when T is a BFD-tree. Again f denotes the eigenvector affording $\lambda(T)$. We have to show that there exists a tree $T' \in \mathcal{T}_{\pi'}$ such that $\lambda(T') > \lambda(T)$. Therefore we construct a sequence of trees $T = T_0 \to T_1 \to \cdots \to T_s = T'$ by shifting edges and show that the $\lambda(T_j) > \lambda(T_{j-1})$ for every $j = 1, \ldots, s$. We denote the degree sequence of T_j by $\pi^{(j)}$.

For a particular step in our construction, let k be the least index with $d'_k > d_k^{(j)}$. Let v_k be the corresponding vertex in tree T_j. Since $\sum_{i=0}^{k} d'_i > \sum_{i=0}^{k} d_i^{(j)}$ and $\sum_{i=0}^{n-1} d'_i = \sum_{i=0}^{n-1} d_i^{(j)} = 2(n-1)$ there must exist a vertex $v_l \succ v_k$ with degree $d_l^{(j)} \geq 2$. Thus it has a child u_l. By Lemma 9 we can replace edge $v_l u_l$ by edge $v_k u_l$ and get a new tree T_{j+1} with $\lambda(T_{j+1}) > \lambda(T_j)$. Moreover, $d_k^{(j+1)} = d_k^{(j)} + 1$ and $d_l^{(j+1)} = d_l^{(j)} - 1$, and consequently $\pi^{(j)} \lhd \pi^{(j+1)}$. By repeating this procedure we end up with degree sequence π' and the statement follows for the case where $n' = n$.

Now assume $n' > n$. Then we construct a sequence of trees T_j by the same procedure. However, now it happens that we arrive at some tree T_r where $d'_k > d_k^{(r)}$ but $d_l^{(r)} = 1$ for all $v_l \succ v_k$, i.e., they are pendant vertices. In this case we join a new pendant vertex to v_k. Then $d_k^{(r+1)} = d_k^{(r)} + 1$ and $|\pi^{(r+1)}| = |\pi^{(r)}| + 1$ as we have added a new vertex degree of value 1. Thus

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$\pi^{(r+1)}$ is again a tree sequence with $\pi^{(r)} \lhd \pi^{(r+1)}$. Moreover, $\lambda(T_{r+1}) > \lambda(T_r)$ as $T_{r+1} \supset T_r$. By repeating this procedure we end up with degree sequence π' and the statement of Theorem 3. $\square$

4 Addendum to the Proof

This manuscript has been compiled while M.H. visited Vienna last summer (2007). We applied methods developed in [1] and [2]. Meanwhile Zhang [10] has published the same results. Thus we decided to present our proof to interested readers by this technical report.

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