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Paper

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Semiregular Trees with Minimal Index

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Abstract

A semiregular tree is a tree where all non-pendant vertices have the same degree. Belardo et al. (MATCH Commun. Math. Chem. 61(2), pp. 503–515, 2009) have shown that among all semiregular trees with a fixed order and degree, a graph with index is a caterpillar. In this technical report we provide a different proof for this theorem. Furthermore, we give counter examples that show this result cannot be generalized to the class of trees with a given (non-constant) degree sequence.

Key words: adjacency matrix, eigenvectors, spectral radius, Perron vector, tree
1991 MSC: 05C35, 05C75, 05C05, 05C50

1 Introduction

Let $G(V, E)$ be a simple connected undirected graph with vertex set $V(G)$ and edge set $E(G)$. The spectral radius or *index* of G is the largest eigenvalue of its adjacency matrix $A(G)$ of G. It is well known that a tree with given order has maximal index radius if and only if it is a star, and it has minimal index if and only if it is a path. However, it has only recently been shown that within the class of trees with a given degree sequence, extremal graphs have a ball-like structure where vertices of highest degrees are located near the center. Such trees can easily be found using a breadth-first search algorithm, see [2].

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In this paper we are interested in trees with minimal index. Recall that a vertex of degree 1 is called a *pendant* vertex (or *leaf*) of a tree. We call a tree G *d-semiregular* when all of its non-pendant vertices have degree d. We denote the class of d-semiregular trees with n vertices by $\mathcal{T}_{d,n}$. Note that this class is non-empty only if $n \equiv 2 \mod (d-1)$. We assume throughout the paper that $d \geq 3$ (otherwise $G \in \mathcal{T}_{2,n}$ is simply a path with n vertices). Recall that a *caterpillar* is a tree where the subtree induced by all of its non-pendant vertices is a path. We denote the uniquely defined caterpillar in $\mathcal{T}_{d,n}$ by $C_{d,n}$. Recently Belardo et al. [1] have investigated d-semiregular trees with small index. They characterized all d-semiregular trees with given order that have minimal index.

Theorem 1 ([1]) *A tree G has smallest index in class $\mathcal{T}_{d,n}$ if and only if it is a caterpillar $C_{d,n}$.*

In this technical report we give a different proof for this theorem based on local perturbations of trees and inequalities between the corresponding Rayleigh quotients. We have already used this approach to show the analogous results for the Laplacian spectral radius of semiregular trees, see [3]. The presented proof is essentially the same but with the eigenvalue equation and the Rayleigh quotient for the adjacency matrix instead of that for the Laplacian.

If the given degree sequence is not constant, then the structure of extremal trees is more complicated. Section 3 gives an example of an extremal graph that is not a caterpillar.

2 Proof of Theorem 1

Let $\mu(G)$ denote the largest eigenvalue of $A(G)$. As G is connected, $A(G)$ is irreducible and thus $\mu(G)$ is simple and there exists a unique positive eigenvector f_0 with $||f_0|| = 1$ by the Perron-Frobenius Theorem (see, e.g., [4]). We refer to such an eigenvector as the *Perron vector* of G. Remind that f_0 fulfills the eigenvalue equation

$$\mu f_0(v) = \sum_{uv \in E} f_0(u) . \tag{1}$$

Moreover, by the Rayleigh-Ritz Theorem f_0 maximizes the Rayleigh quotient for non-zero vectors f on $V(G)$ defined as

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

In particular, for any positive function f with $||f|| = 1$ we find

$$\mu(G) = 2 \sum_{uv \in E} f_0(u) f_0(v) \geq 2 \sum_{uv \in E} f(u) f(v) \tag{3}$$

where equality holds if and only if $f = f_0$. Recall that $\mu(G) > 1$ if $G \neq K_1, K_2$ and that every pendant vertex of G is a strict local minimum of f_0.

We use the following approach for proving Theorem 1: For any tree G in $\mathcal{T}_{d,n}$ we construct a positive function f such that $\mathcal{R}_G(f) \geq \mathcal{R}_{C_{d,n}}(f_0)$ where f_0 denotes the Perron vector of the caterpillar $C_{d,n}$. Then we find $\mu(G) \geq \mathcal{R}_G(f) \geq \mathcal{R}_{C_{d,n}}(f_0) = \mu(C_{d,n})$ and we are done when either one of the inequalities is strict or f does not fulfill the eigenvalue equation (1). Vector f is constructed by starting with Perron vector f_0 on $C_{d,n}$ and rearranging the edges of the caterpillar until we arrive at G. f and f_0 have then the same valuations but different Rayleigh quotients.

First we summarize the notion used for our construction: We write $u \sim v$ if the vertices u and v are adjacent, i.e., if $uv \in E(G)$. $d_G(v)$ denotes the degree of v in G, while $d^\star_G(v)$ is the number of non-pendant vertices that are adjacent to v. For two adjacent non-pendant vertices $v \sim u$ the *branch* B_{vu} is the subtree induced by v and all vertices of the component of $G\backslash\{vu\}$ that contains u. The length $\ell(B_{vu})$ of a branch is the number of its non-pendant vertices. We call a vertex v with $d^\star_G(v) \geq 3$ a *branching point* of G, and a non-pendant vertex v with $d^\star_G(v) = 1$ a *bud* of G. We call a branch with exactly one branching point v^* (and exactly one bud vertex) a *proper branch*. A positive function f on G is called *unimodal* with maximum $\hat{v}$ if it is monotonically non-increasing on every path in G starting at $\hat{v}$ and non-constant except (possibly) on just one edge incident to $\hat{v}$.

The atomic steps of our rearrangement are *switching* of edges which have already been used by various authors, e.g., [5]: Let P be the path $u_1^\circ v_1 \ldots v_2 u_2$ in $G \in \mathcal{T}_{d,n}$ where u_1° is a pendant vertex, $d^\star_G(u_2) \geq 2$ and $v_1 \neq v_2$. Then we get a new tree $G' \in \mathcal{T}_{d,n}$ by replacing edges $v_1 u_1^\circ$ and $v_2 u_2$ by the respective edges $v_1 u_2$ and $v_2 u_1^\circ$, see Fig. 1. For a unimodal function f on G with $f(v_1) \geq f(v_2)$ we construct a function f' on G' by $f'(u_1^\circ) = \min(f(u_1^\circ), f(u_2))$, $f'(u_2) = \max(f(u_1^\circ), f(u_2))$, and $f'(x) = f(x)$ for all other vertices. Notice that switching does not change the number of pendant and non-pendant vertices.

Lemma 2 *Let $G \in \mathcal{T}_{d,n}$ and f be a unimodal function on G with maximum $\hat{v}$. Construct G' and f' as described above. If $f(v_1) \geq f(v_2)$, then f' is again unimodal with maximum $\hat{v}$ and $\mathcal{R}_{G'}(f') \geq \mathcal{R}_G(f)$. The inequality is strict if and only if either $f(v_1) > f(v_2)$ and $f(u_1^\circ) < f(u_2)$, or $f(u_1^\circ) > f(u_2)$.*

Proof. Unimodality of f and $f(v_1) \geq f(v_2)$ imply $f(v_2) > f(u_2)$ and $f(v_1) \geq f(u_1^\circ)$. Assume first that $f(u_1^\circ) \leq f(u_2)$. Then $f'(x) = f(x)$ for all $x \in V(G)$ and by switching edges $v_1 u_1^\circ$ with $v_2 u_2$ with $v_1 u_2$ and $v_2 u_1^\circ$ and we find (for

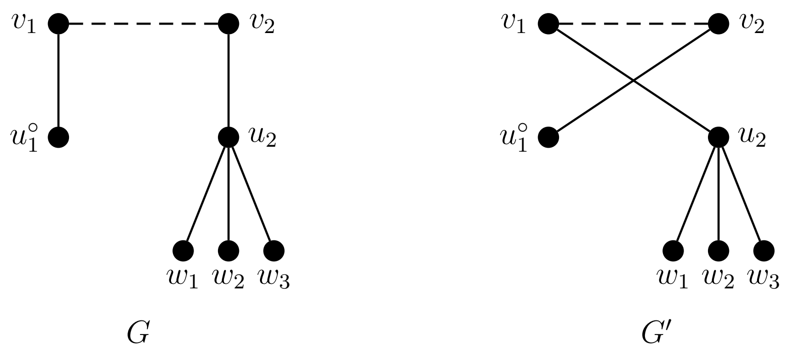

Fig. 1. Switching edges $v_1u_1^\circ$ and v_2u_2 with edges v_1u_2 and $v_2u_1^\circ$. (Dashed lines are paths in G and G', respectively, and need not be edges. Vertices and edges that are not involved are omitted.)

$||f|| = 1$)

$$\begin{aligned}\mathcal{R}_{G'}(f') - \mathcal{R}_G(f) &= 2 \sum_{xy\in E'\setminus E} f'(x)f'(y) - 2 \sum_{uv\in E\setminus E'} f(u)f(v) \\ &= 2\left(f(u_1^\circ)f(v_2) + f(u_2)f(v_1) - f(u_1^\circ)f(v_1) - f(u_2)f(v_2)\right) \\ &= 2\left(f(u_1^\circ) - f(u_2)\right)\cdot\left(f(v_2) - f(v_1)\right) \geq 0\end{aligned}$$

where the inequality is strict whenever $f(v_1) > f(v_2)$ and $f(u_1^\circ) < f(u_2)$.

If $f(u_1^\circ) > f(u_2)$ we have $f'(u_1^\circ) = f(u_2)$, $f'(u_2) = f(u_1^\circ)$, and $f'(x) = f(x)$ otherwise. Let w_j, $j = 1, \ldots, d_G(u_2) - 1$, be the neighbors of u_2 not equal to v_2. Then

$$\begin{aligned}\mathcal{R}_{G'}(f') - \mathcal{R}_G(f) &= 2\sum_{w_j} f'(u_2)f'(w_j) - 2\sum_{w_j} f(u_2)f(w_j) \\ &= 2\sum_{w_j}(f(u_1^\circ) - f(u_2))f(w_j) \geq 0\end{aligned}$$

where the inequality is strict whenever $f(u_1^\circ) > f(u_2)$.

Unimodality for f' follows from the fact that monotonicity of f on paths in G that start at v_1 or v_2 is preserved at the corresponding paths in G'. $\square$

Now if a tree G has no branching point, then it is necessarily a caterpillar. Otherwise, there is a branching point v^* with (at least) two proper branches $B_{v^*u_2}$ and $B_{v^*x_1}$, see Fig. 2. Let v_2 be the bud of $B_{v^*x_1}$ and $u_1^\circ \sim v_2$ a pendant vertex. Then we can switch edges v^*u_2 and $v_2u_1^\circ$ with $v^*u_1^\circ$ and v_2u_2 and obtain a d-semiregular tree G' with $d^\star_{G'}(v^*) = d^\star_G(v^*) - 1 \geq 2$ and $d^\star_{G'}(v_2) = d^\star_G(v_2) + 1 = 2$ while $d^\star(x)$ remains unchanged for all other non-pendant vertices x. Hence the number of buds and consequently the number of proper branches is by reduced by 1. We call such a rearrangement a *branch reduction* for G with *reduction point* v^*. We call the set of vertices in $B_{v^*u_2} \cup B_{v^*x_1}$ the *fork* of the branch reduction. A branch reduction is called *minimal* if its fork is minimal among all possible branch reductions.

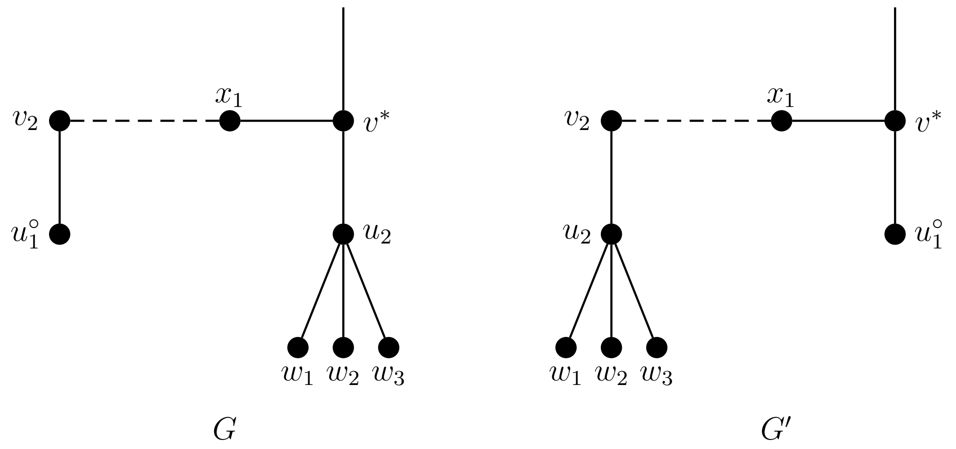

Fig. 2. Branch reduction: branch $B_{v^* u_2}$ in G has been replaced by a leaf in G'. (Dashed lines are paths in G and G', respectively, and need not be edges. Further details omitted.)

We can repeat such steps until a caterpillar remains. Thus we arrive at the following

Lemma 3 *For every tree $G \in \mathcal{T}_{d,n}$ there exists a sequence of branch reductions*

$$G = G_t \to G_{t-1} \to \cdots \to G_1 \to G_0 = C_{d,n} \tag{4}$$

that transforms G into caterpillar $C_{d,n}$.

The switchings of these branch reductions can be reverted. Thus we obtain a sequence of graph rearrangements that transforms $C_{d,n}$ back into tree G,

$$C_{d,n} = G_0 \to G_1 \to \cdots \to G_{t-1} \to G_t = G \; .$$

Notice that caterpillar $C_{d,n}$ is symmetric about either a central vertex v_c or a central edge e_c (depending whether the number of vertices in the trunk is even or odd). This also holds for Perron vector f_0, since otherwise we could create a different Perron vector by reflecting the values of f_0 at v_c and e_c, respectively.

Lemma 4 *The Perron vector f_0 of $C_{d,n}$ is unimodal with maximum in v_c or e_c.*

Proof. Let $v_1, \ldots, v_k$ denote the non-pendant vertices of $C_{d,n}$ such that $v_i \sim v_{i+1}$, and let $v_0 \sim v_1$ and $v_{k+1} \sim v_k$ be two pendant vertices. By (1) we find $\mu f_0(v_i^\circ) = f_0(v_i)$ for all pendant vertices v_i° adjacent to v_i and thus

$$\left(\mu - \frac{d-2}{\mu}\right) f_0(v_i) = f_0(v_{i-1}) + f_0(v_{i+1}) \qquad \text{for all } i = 1, \ldots, k.$$

Since f_0 must obtain its maximum on the trunk, there is some vertex v_j

that satisfies $\left(\mu - \frac{d-2}{\mu}\right) f_0(v_j) = f_0(v_{j-1}) + f_0(v_{j+1}) < 2f_0(v_j)$, and hence $\left(\mu - \frac{d-2}{\mu}\right) < 2$. Now suppose f_0 is not strictly monotone on a path starting at a maximum of f_0. Then there exists a saddle point v_s of f_0, that is, $\left(\mu - \frac{d-2}{\mu}\right) f_0(v_s) = f_0(v_{s-1}) + f_0(v_{s+1}) \geq 2f_0(v_s)$, and thus $\left(\mu - \frac{d-2}{\mu}\right) \geq 2$, a contradiction. □

Now let $C_{d,n} = G_0 \to G_1$ be the inverse of the last branch reduction in sequence (4) with reduction point v^*. Then G_1 has three proper branches $B_{v^*v_1}$, $B_{v^*v_2}$, and $B_{v^*v_3}$ with respective lengths $\ell_1 \geq \ell_2 \geq \ell_3$.

Lemma 5 *Let k denote the number of non-pendant vertices of $C_{d,n}$. Assume that no proper branch of G_1 contains more trunk vertices than the union of the remaining two branches, i.e., $\ell(B_{v^*v_i}) \leq \lceil \frac{k+1}{2} \rceil$ for all proper branches of G_1. Then there exists a unimodal function f_1 on G_1 with maximum in branching point v^* such that $\mathcal{R}_{G_1}(f_1) \geq \mathcal{R}_{G_0}(f_0) = \mu(C_{d,n})$.*

Proof. Let v_0 be either v_c or incident to e_c. By symmetry and Lemma 4, v_0 is a maximum of f_0 and $C_{d,n}$ has two branches $B_o = B_{v_0v_1}$ and $B_e = B_{v_0v_2}$ of length $\ell_o = \lceil \frac{k+1}{2} \rceil$ and $\ell_e = \lfloor \frac{k+1}{2} \rfloor$, respectively. Let $v_1, \ldots, v_k$ denote the remaining trunk vertices of $C_{d,n}$, enumerated such that $f_0(v_i) \geq f_0(v_{i+1})$ for all $i = 0, \ldots, k-1$ and all vertices with odd (even) index belong to B_o (B_e). By Lemma 4, $f_0(v_i) > f_0(v_{i+2})$ for all $i = 1, \ldots, k-2$.
Now we rearrange the vertices of $G_0 = C_{d,n}$ in a spiral-like way to obtain G_1:

1. Switch edges $v_0u_0^\circ$ and v_1v_3 with v_0v_3 and $v_1u_0^\circ$, where $u_0^\circ \sim v_0$ is a pendant vertex. By Lemma 2, we obtain a tree $T_1 \in \mathcal{T}_{d,n}$ and a unimodular function g_1 on T_1 with $\mathcal{R}_{T_1}(g_1) \geq \mathcal{R}_{G_0}(f_0)$.
2. Start with $S = \{1, 2, 3\}$ and $R = \{4, 5, \ldots, k\}$.
3. Let i and m be the least indices in S and R, respectively, and j be the least index in $S \setminus \{i\}$. Then $v_j \sim v_m$ and $g_i(v_i) \geq g_i(v_j)$. Let l_1, l_2, and l_3 be the length of the branches $B_{v_0v_1}$, $B_{v_0v_2}$, and $B_{v_0v_3}$ in T_i.
4. If $\{l_1, l_2, l_3\} = \{\ell_1, \ell_2, \ell_3\}$, then set $f_1 = g_i$ and stop.
5. If $l_b = \ell_1$ for some $b \in \{1, 2, 3\}$, then remove the indices of the corresponding vertices from S and R and goto Step 3.
6. Switch edges $v_iu_i^\circ$ and v_jv_m with v_iv_m and $v_ju_i^\circ$, where $u_i^\circ \sim v_i$ is a pendant vertex. By Lemma 2, we obtain a tree $T_j \in \mathcal{T}_{d,n}$ and a unimodular function g_j on T_j with $\mathcal{R}_{T_j}(g_j) \geq \mathcal{R}_{T_i}(g_i)$.
7. Replace $S \leftarrow (S \cup \{m\}) \setminus \{i\}$ and $R \leftarrow R \setminus \{m\}$ and goto Step 3.

It is straightforward to show that this procedure creates G_1 and that $\mathcal{R}_{G_1}(f_1) \geq \mathcal{R}_{G_0}(f_0)$. □

All remaining steps in sequence (4) are simpler to handle.

Lemma 6 *Let $G_i \to G_{i+1}$ be the inverse of a branch reduction in sequence*

(4) with reduction point v^*, for an $i = 1, \ldots, t-1$. Assume f_i is a unimodal function on G_i such that its maximum $\hat{v}$ is either in v^* or not contained in the fork of the branch reduction. Then there exists a unimodal function f_{i+1} in G_{i+1} with maximum $\hat{v}$ and $\mathcal{R}_{G_{i+1}}(f_{i+1}) \geq \mathcal{R}_{G_i}(f_i)$.

Proof. The inverse of the branch reduction is performed by switching edges $v^*u_1^\circ$ and v_2u_2 with edges v^*u_2 and $v_2u_1^\circ$, see Fig. 2. From unimodality we can conclude that f_i restricted to the fork of the branch reduction, $B_{v^*u_2} \cup B_{v^*x_1}$, attains its maximum in v^*. In particular we have $f_i(v^*) \geq f_i(v_2)$. Hence the assumptions of Lemma 2 hold and the result follows. $\square$

Notice that the condition of Lemma 6 is always satisfied when f_i attains it maximum in a branching point of G_i.

Proof of Theorem 1. Suppose that G is not a caterpillar. Let $C_{d,n} = G_0 \to G_1 \to \cdots \to G_{t-1} \to G_t = G$ be a sequence of inverses of *minimal* branch reductions. Let k again denote the number of non-pendant vertices of $C_{d,n}$. Assume first that the longest branch in G_1 has length $\ell \leq \lceil \frac{k+1}{2} \rceil$. Then by Lemma 5 we can construct a unimodal function f_1 on G_1 which attains its maximum in the branching point. By applying Lemma 6 for all remaining inverse branch reductions we get a unimodal function f on G with $\mathcal{R}_G(f) \geq \mu(C_{d,n})$.

Assume now that there is a proper branch in G_1 with length $\ell > \lceil \frac{k+1}{2} \rceil$. Then the fork of the minimal branch reduction contains less than $\lfloor \frac{k+1}{2} \rfloor$ non-pendant vertices and thus $\hat{v}$ must be contained in the remaining branch of G_1. Hence by Lemma 6 we get a unimodal function f_1 on G_1 where its maximum $\hat{v}$ is located on the longest proper branch of G_1. Notice that for all subsequent inverse minimal branch reductions $G_i \to G_{i+1}$, each fork must have less than $\lfloor \frac{k+1}{2} \rfloor$ non-pendant vertices and thus cannot contain maximum $\hat{v}$. Therefore we find a unimodal function f on G with $\mathcal{R}_G(f) \geq \mu(C_{d,n})$ by Lemma 6.

At last we have to note that equality $\mathcal{R}_G(f) = \mu(C_{d,n})$ only holds if none of the inequalities in Lemmata 2 and 5 is strict, which implies that f_0 is constant on $C_{d,n}$, a contradiction to Lemma 4. $\square$

3 Non-semiregular trees

Let $\mathcal{T}_\pi$ denote the class of trees with degree sequence π. Then we can again ask for the structure of trees with minimal index in $\mathcal{T}_\pi$. The naïve conjecture states: *If a tree G has minimal index in class $\mathcal{T}_\pi$, then G is a caterpillar.* Unfortunately, computational experiments have shown that this conjecture is false. We performed an exhaustive search on trees on up to 20 vertices using

Wolfram's Mathematica and Royle's *Combinatorial Catalogues* [6] and found several counter examples, see Figure 3.

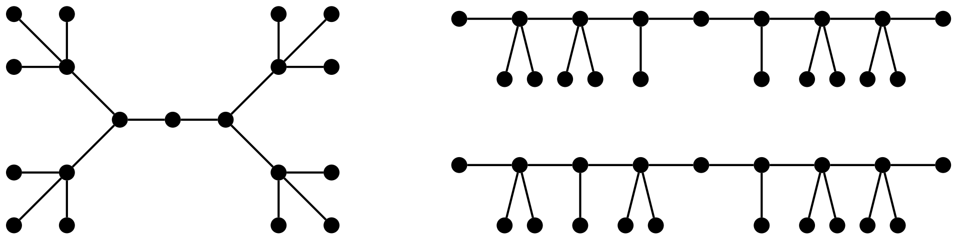

Fig. 3. Three of the extremal trees with degree sequence $\pi = (4^4, 3^2, 2, 1^{12})$; all have spectral radius $\mu(G) = \sqrt{6}$.

Unfortunately we were not able to detect a general pattern. Our observations could be summarized in the following way:

- Extremal trees need not be unique (up to isomorphism). Figure 3 gives an example.
- None of the extremal trees has to be a caterpillar.
- Buds have largest degree in each proper branch of an extremal tree.
- Degrees need not be monotone along the trunk of a proper branch.

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