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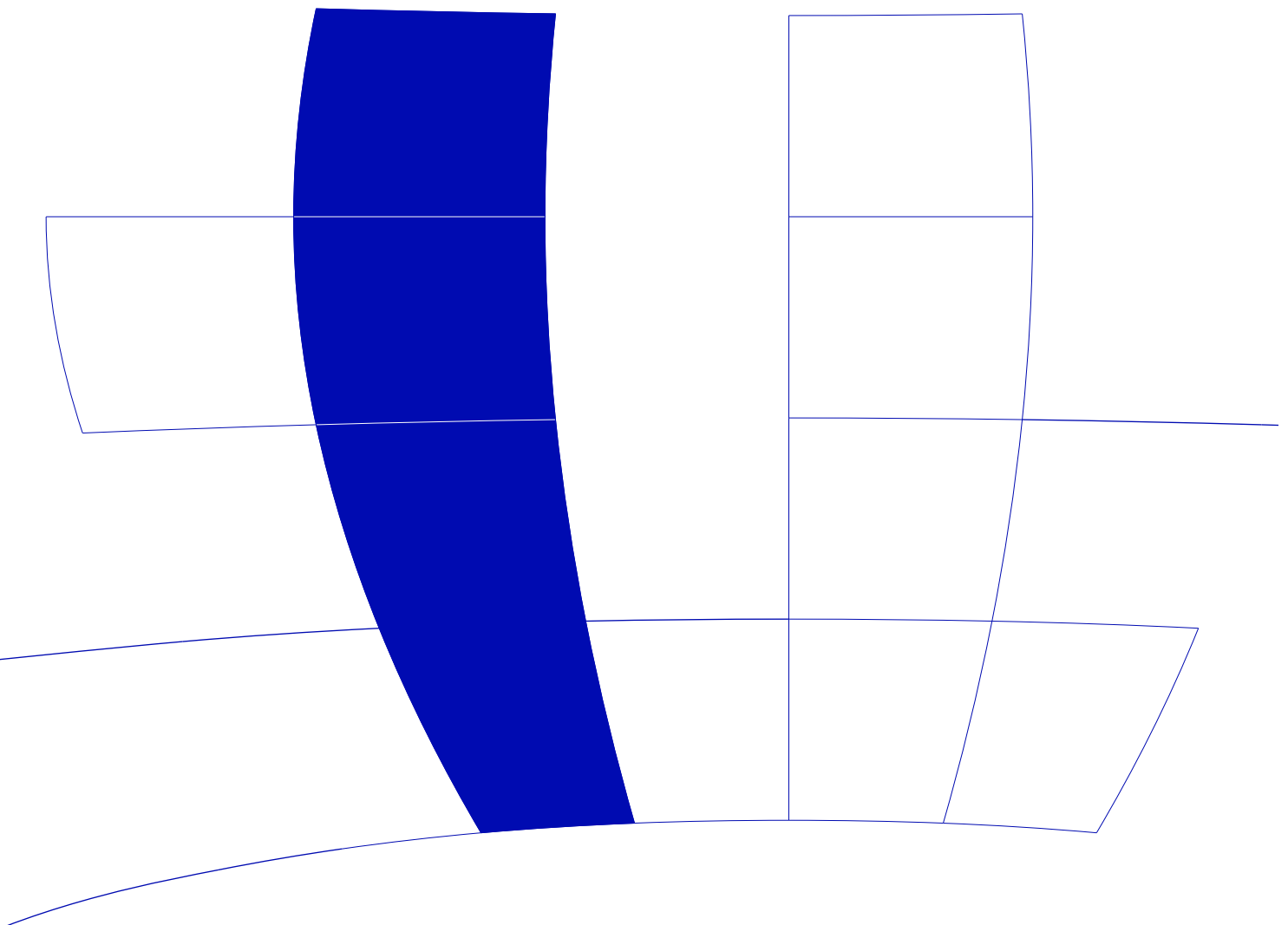
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Algebraic Connectivity and Degree Sequences of Trees

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Abstract

We investigate the structure of trees that have minimal algebraic connectivity among all trees with a given degree sequence. We show that such trees are caterpillars and that the vertex degrees are non-decreasing on every path on non-pendant vertices starting at the characteristic set of the Fiedler vector.

Key words: algebraic connectivity, graph Laplacian, tree, degree sequence, Fiedler vector, Dirichlet matrix

1 Introduction

Let $G(V, E)$ be a simple (finite) undirected graph with vertex set V and edge set E . The total number of vertices is denoted by n . The *Laplacian* of G is the matrix

$$L(G) = D(G) - A(G), \quad (1)$$

where $A(G)$ denotes the adjacency matrix of the graph 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. For graphs with weights $w(e)$ for each edge $e \in E$ the Laplacian is defined analogously where the adjacency matrix contains the edge weights

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and the diagonal entries of $D(G)$ are the sums of the weights of the edges at the vertices of G , i.e. $D_{vv} = \sum_{e=vu \in E} w(e)$.

The Laplacian L is symmetric and all its eigenvalues are non-negative. The first eigenvalue is always 0. The second smallest eigenvalue, denoted by $\alpha(G)$ in the following, has become quite popular and is called the *algebraic connectivity* of G by Fiedler [10]. It allows some conclusions about the connectedness of the graph. A graph G is connected if and only if $\alpha(G) \neq 0$. Moreover, $\alpha(G)$ is a lower bound for the vertex and edge connectivities of G . Hence properties of the algebraic connectivity has been investigated in the literature. In particular many upper and lower bounds have been shown. We refer to the recent survey by de Abreu [8] and the references cited therein. Other authors have ordered trees by their algebraic connectivity [17] or characterize extremal graphs, i.e., graphs that have minimal algebraic connectivity among all graph within particular graph class. Godsil and Royle [13] assume that *graphs with small values of $\alpha(G)$ tend to be elongated graphs of large diameter with bridges*. For example, for trees on n vertices with a fixed diameter the algebraic connectivity is minimized for paths with stars of (almost) equal size attached to both ends, see [9]. Cubic graphs with minimal algebraic connectivity look like a “string of pearls”, see [4]. Belhaiza et al. [2] used the AGX-system which raised the conjecture that the connected graphs $G \neq K_n$ with minimal algebraic connectivity are all so called (n, p, t) -path-complete graphs.

In this note we are interested in the structure of trees which have minimal algebraic connectivity among all trees with a given degree sequence. (Recall that a sequence $\pi = (d_0, \dots, d_{n-1})$ of non-negative integers is called *degree sequence* if there exists a graph G for which d_0, \dots, d_{n-1} are the degrees of its vertices. We refer the reader to [16] for relevant background on degree sequences.) We call a degree sequence for a tree a *tree sequence*. We show that such a tree is a *caterpillar*, i.e., a tree in which the removal of all pendant vertices (vertices of degree 1) gives a path. For further characterization we use a result of Fiedler [11] about eigenvectors of the second smallest eigenvalue which are called *Fiedler vectors*: The subgraph induced by non-positive vertices of any Fiedler vector (i.e., vertices with non-positive valuation) and the subgraph induced non-negative vertices are both connected. Such connected subgraphs are called *weak nodal domains* [3, 7] (in analogy to eigenfunctions of the Laplace-Beltrami operator on manifolds [5, 6]), or *Perron components* [15]. The two nodal domains of a Fiedler vector of a tree are either separated by an edge (*characteristic edge*) or there is a single vertex (*characteristic vertex*) where the Fiedler vector vanishes [11]. On each of these nodal domains we can declare a Dirichlet matrix whose first eigenvalue is exactly the algebraic connectivity of the original graph. Thus we arrive at the following necessary condition.

Theorem 1 *Let T be a tree that has minimal algebraic connectivity among all trees with given degree sequence $\pi = (d_0, \dots, d_{n-1})$. Then T is a caterpillar. Moreover, if P is the path induced by all non-pendant vertices of T with non-negative (non-positive) valuation, then its degree sequence is monotone with a minimum at the characteristic vertex or edge.*

Remark 1 *It is an open problem how the degree sequence π has to be partitioned for the two nodal domains to obtain a tree with minimum algebraic connectivity. We ran some computational experiments but could not detect any general pattern.*

For the proof of this theorem we use the concept of *geometric nodal domains* and *Dirichlet matrix* introduced in [3]. This concept is described in Sect. 2. We then can use perturbation of trees to obtain results for the first Dirichlet eigenvalue for each of the two nodal domains of the Fiedler vector (Sect. 3) which are then used to proof the theorem in Sect 4. Our approach is related to the concept of *Perron components* and “*bottleneck*” *matrix* introduced in [15]. Thus it could also be used to verify the results of [14] (e.g., their Thm. 5 can be deduced from Lemma 4 below).

2 Nodal Domains and Dirichlet Matrix

A *graph with boundary* $G(V_0 \cup \partial V, E_0 \cup \partial E)$ consists of a (non-empty) set of interior vertices V_0 , boundary vertices ∂V , interior edges E_0 that connect interior vertices, and boundary edges ∂E that join interior vertices with boundary vertices. There are no edges between two boundary vertices. The *Dirichlet matrix* L_0 is the matrix obtained from the graph Laplacian L by deleting all rows and columns that correspond to boundary vertices. This definition is motivated by the concept of *geometric realization* of a graph, see [3, 12]. The first Dirichlet eigenvalue $\nu(G)$ is strictly positive. If the graph induced by the interior vertices is connected, then $\nu(G)$ is simple and there exists an eigenvector which is strictly positive at all interior vertices.

When a Fiedler vector f of a tree has a characteristic vertex v_0 then each of the two weak nodal domains can be seen as a graph with v_0 as its boundary vertex. Then the algebraic connectivity $\alpha(G)$ is exactly the first Dirichlet eigenvalue of each nodal domain, with the Fiedler vector restricted to the respective interior vertices as their eigenvectors (see also [1]). In the other case when the two nodal domains of the Fiedler vector are separated by a characteristic edge $e = uw$, we split this edge of weight 1 into edges $e_1 = uv_0$ and $e_2 = v_0w$ with weights $w_1 = |f(w) - f(u)|/|f(u)|$ and $w_2 = |f(w) - f(u)|/|f(w)|$ by inserting a new vertex v_0 . (In the geometric realization of a graph edges of weight w correspond to arcs of length $1/w$.) By this procedure the algebraic connectivity remains

unchanged and v_0 becomes the characteristic vertex of the Fiedler vector of the new graph [3, Lemma 3.14]. In either case we construct two graphs with boundary whose first Dirichlet eigenvalues coincide with $\alpha(G)$. We call these graphs the *geometric nodal domains* of G . Thus we can prove our theorem by looking at the first Dirichlet eigenvalue of its nodal domains.

Remark 1 *The concept of geometric nodal domains is defined analogously for arbitrary eigenfunctions of connected graphs.*

The Rayleigh quotient associated to the Laplacian matrix L is defined by

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

The following result characterizes the first Dirichlet eigenvalue $\nu(G)$ and the algebraic connectivity $\alpha(G)$ of some graph G . It immediately follows from the Courant-Fisher Theorem.

Proposition 1 *For a graph with boundary $G(V_0 \cup \partial V, E_0 \cup \partial E)$ we have*

$$\nu(G) = \min_{f \in \mathbb{R}^{|V_0|}, f \neq 0} \mathcal{R}_{L_0}(f) \quad (3)$$

Moreover, $f \neq 0$ is an eigenvector of the first Dirichlet eigenvalue $\nu(G)$ of L_0 if and only if $\mathcal{R}_{L_0}(f) = \nu(G)$.

For a graph $G(V, E)$ we have

$$\alpha(G) = \min_{f \in \mathbb{R}^{|V|}, f \neq 0, \sum f(v)=0} \mathcal{R}_L(f) \quad (4)$$

Moreover, $f \neq 0$ is an eigenvector of the second Laplacian eigenvalue $\alpha(G)$ (i.e. a Fiedler vector) if and only if $\sum_{v \in V} f(v) = 0$ and $\mathcal{R}_L(f) = \alpha(G)$.

3 First Dirichlet Eigenvalues of Rooted Trees

Geometric nodal domains of Fiedler vectors of trees are rooted trees T_0 where its root v_0 is its only boundary vertex. One of its boundary edges has weight w_0 with $1/w_0 \in (0, 1]$ whereas all other (boundary and interior) edges have weight 1. The following lemma immediately follows from [11, Thm. (3,14)].

Lemma 2 *Let T_0 be a tree with a single boundary vertex v_0 and f a non-negative eigenvector corresponding to the first Dirichlet eigenvalue $\nu(T_0)$. Then on every simple path starting at v_0 , f is either strictly increasing or constant zero.*

A *branch* at vertex u of a tree with root v_0 is a maximal subtree of $G \setminus \{u\}$ that does not contain v_0 .

Lemma 3 *If a tree T_0 has minimal first Dirichlet eigenvalue among all rooted trees with given degree sequence, then T_0 is a caterpillar where at most one neighbors of its root is not a pendant vertex.*

Proof. Let T_0 have minimal first Dirichlet eigenvalue, i.e., $\nu(T_0) \leq \nu(T'_0)$ for all rooted trees T'_0 with the same degree sequence. Assume first that there is only one boundary edge xv_0 , then $\nu(T_0)$ is simple and there exists an eigenvector f with $f(v_0) = 0$ and $f(u) > 0$ for all $u \neq v_0$. Now suppose T_0 is not a caterpillar with the proposed property. Then there exist two simple paths $(v_0, \dots, v_{i-1}, x_i, \dots, x_j)$ and $(v_0, \dots, v_{i-1}, y_i, \dots, y_k)$ where $x_i \neq y_i$, $j, k > i$, and where x_j and y_k are pendant vertices. By Lemma 2, f is strictly increasing on each of these. Without loss of generality we assume $f(x_j) > f(y_i)$. Otherwise we have $f(x_i) < f(x_j) \leq f(y_i) < f(y_k)$ and we exchange the role of the two paths. Now we construct a new graph T'_0 by rearranging edges in T_0 . Replace all edges $y_i t$ where $t \neq v_{i-1}$ by edges $x_j t$. Notice that this rearrangement does not change the degree sequence. We construct a new vector f' such that $f'(u) = \max(f(u), f(x_j))$ for all vertices u that are in a branch at y_i in T_0 , and $f'(u) = f(u)$ for all others. Notice that $\sum_{v \in V} f'(v)^2 \geq \sum_{v \in V} f(v)^2$ and $\sum_{uv \in E'} w(uv)(f'(u) - f'(v))^2 < \sum_{uv \in E} w(uv)(f(u) - f(v))^2$ and thus $\nu(T'_0) \leq \mathcal{R}_L(f') < \mathcal{R}_L(f) = \nu(T_0)$, a contradiction to our assumption that T_0 has minimal first Dirichlet eigenvalue.

For the case where T_0 has two or more boundary edges then $T_0 \setminus \{v_0\}$ consists of several branches at root v_0 . There exists an eigenvector f that is positive on exactly one of these and zero on all others. Then all these other branches must be pendant vertices, since otherwise we could apply the same rearrangement of edges and obtain a tree T'_0 with the same degree sequence and strictly smaller first Dirichlet eigenvalue. \square

The *trunk* of a rooted caterpillar T_0 is a longest path starting at root v_0 . Notice that the trunk is terminated by v_0 and a pendant vertex (its *head*). Let $h(v)$ denote the geodetic distance between vertex v and root v_0 (*height*). Now construct a new rooted graph T'_0 by one of the following perturbations:

- (P1) Replace edge wv_i by an edge wv_j , where $w (\neq v_0)$ is a pendant vertex, and v_i and v_j are trunk vertices with $h(v_i) < h(v_j)$;
- (P2) insert a vertex w and add a new edge wv_j to one of the trunk vertices $v_j (\neq v_0)$.

Notice that in both cases the trunk of T'_0 is longer than that of T_0 if v_j is the head of the trunk of T_0 .

Lemma 4 *Let T_0 a rooted tree and construct a new tree T'_0 as described above. Then $\nu(T'_0) < \nu(T_0)$.*

Proof. Let f be a nonnegative eigenfunction to the first Dirichlet eigenvalue $\nu(T_0)$. For case (P1) we construct function f' on T'_0 by $f'(v) = f(v)$ for all $v \neq w$ and $f'(w) = \max(f(w), f(v_j))$. By Lemma 2, f is strictly increasing on the trunk of T . Thus we find analogously to the proof of Lemma 3, $\nu(T'_0) \leq \mathcal{R}_L(f') < \mathcal{R}_L(f) = \nu(T_0)$ as proposed. For case (P2) we set $f'(v) = f(v)$ for all $v \neq w$ and $f'(w) = f(v_j) > 0$ and thus $\sum_{v \in V} f'(v)^2 > \sum_{v \in V} f(v)^2$ and the statement follows. \square

Lemma 5 *A tree T_0 has minimal first Dirichlet eigenvalue among all rooted trees with given degree sequence if and only if T_0 is a caterpillar where the degrees are non-decreasing on the path starting at root v_0 and induced by all non-pendant vertices of T_0 .*

Proof. By Lemma 3, T_0 is a caterpillar. Let $(v_0, v_1, \dots, v_k, v_{k+1})$ be the trunk of T_0 . If T_0 does not have increasing degrees, then there exist vertices v_i and v_j , $i < j$, in this path with $2 \leq d(v_j) < d(v_i)$. Thus we can replace $c = d(v_j) - d(v_i)$ edges and get a new graph T'_0 with the same degree sequence as T_0 . By Lemma 4, $\nu(T_0) < \nu(T'_0)$, a contradiction to our assumptions. \square

4 Proof of the Theorems

We now show our result by gluing two rooted trees together.

Lemma 6 *Let T_1 and T_2 be two trees with one boundary vertex. Construct a new tree T without boundary by identifying the boundary vertices of these trees and turning the new vertex into an interior vertex. Then $\alpha(T) \leq \max(\nu(T_1), \nu(T_2))$. The inequality is strict if $\nu(T_1) \neq \nu(T_2)$.*

Proof. We assume without loss of generality that $\nu(T_1) \geq \nu(T_2)$. Let V_1 and V_2 denote the respective vertex sets and f_1 and f_2 be corresponding non-negative Dirichlet eigenvectors such that $\sum_{v \in V_1} f_1(v) = \sum_{w \in V_2} f_2(w)$. Construct a vector f on T by $f(v) = f_1(v)$ for all $v \in V_1$ and $f(u) = -f_2(u)$ for $u \in V_2$. Notice that for positive numbers $x, y, a, b > 0$ we find $\frac{x+a}{y+b} \leq \frac{x}{y}$ if and only if $\frac{a}{b} \leq \frac{x}{y}$ and that either both or none of the equalities hold. Then we find by Proposition 1

$$\begin{aligned}
\alpha(T) &= \min_{\sum g(v)=0} \mathcal{R}_L(g) \\
&\leq \mathcal{R}_L(f) = \frac{\sum_{uv \in E} w(uv)(f(u) - f(v))^2}{\sum_{v \in V} f(v)^2} \\
&= \frac{\sum_{uv \in E_1} w(uv)(f_1(u) - f_1(v))^2 + \sum_{uv \in E_2} w(uv)(f_2(u) - f_2(v))^2}{\sum_{v \in V_1} f_1(v)^2 + \sum_{v \in V_2} f_2(v)^2} \\
&\leq \frac{\sum_{uv \in E_1} w(uv)(f_1(u) - f_1(v))^2}{\sum_{v \in V_1} f_1(v)^2} = \nu(T_1) .
\end{aligned}$$

Moreover, $\alpha(T) < \nu(T_1)$ whenever $\nu(T_1) > \nu(T_2)$ and thus the second statement follows. \square

Proof of Theorem 1. Assume T has minimal algebraic connectivity $\alpha(T)$ and let T_1 and T_2 be its the two geometrical nodal domains. Then $\nu(T_1) = \nu(T_2) = \alpha(T)$. Both subtrees must be caterpillars as described in Lemma 5. Otherwise, if (say) T_1 does not have this property we could replace it by a tree T'_1 with the same corresponding edge weights as in T_1 and with $\nu(T'_1) < \alpha(T)$. Consequently we could construct a new tree graph T' with the same degree sequence as in T but with $\alpha(T') < \alpha(T)$ by Lemma 6, a contradiction. Thus the statement follows. \square

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