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THE INDEX OF TREES WITH SPECIFIED MAXIMUM DEGREE

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Abstract Let $\mathcal{T}(n,\Delta)$ be the set of all trees on n vertices with a given maximum degree Δ. In this paper we identify in $\mathcal{T}(n,\Delta)$ the tree whose index, i.e. the largest eigenvalue of the adjacency matrix, has the maximum value.

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1. INTRODUCTION

There are many papers in literature where the largest eigenvalue (or the *index*) of simple graphs is being considered (see [2] for more details). One special class of graphs, which attracts much attention among various researchers, consists of trees. Within the trees of fixed order, trees with maximum (or minimum) indices are already identified; they are stars (respectively paths) - see, for example, [9].

Further efforts were focused on some special classes of trees (say, for trees of some fixed form, or trees with some prescribed invariants). Recall, trees having a perfect matching, or a prescribed size of maximal matchings, were considered in [18, 8]; coloured constrained trees were investigated in [4]; trees with a fixed diameter were examined in [7, 15, 13]; trees with a fixed number of pendant vertices were considered in [17], and so on.

Recall, a *chemical tree* is a tree with a maximum (vertex) degree at most four. Recently, chemical trees were considered by M. Fischermann et al. in [5]. They have conjectured (on the basis of computer search) that in the class of trees with fixed order and maximal degree the trees with maximal index coincide with trees with minimal Wiener index. (The problem related to the minimal Wiener index has been solved in [6].) Here, prompted by their investigations and the conjecture, we will focus our attention on trees with a specified maximum degree.

Let $\mathcal{T}(n, \Delta)$ be the set of all trees on n vertices and the maximum degree Δ. We will identify in $\mathcal{T}(n, \Delta)$ the tree(s) having maximum index. (An upper bound for the index of trees with maximum degree Δ and arbitrary order is given in [14].)

For the basic notions and terminology on spectral graph theory the readers are referred to [1] (see also, [3]). To make the paper more self-contained, we will give here only a few basic facts. The *spectrum* of a graph is the spectrum of its adjacency matrix. The largest eigenvalue (note, all of them are real) is called the *index* (or spectral radius) of the graph. In the case of connected graphs, the positive eigenvector corresponding to the index is referred to as the *principal eigenvector*. The index of a (connected) graph G will be denoted by μ $(= \mu_G)$, and the corresponding principal eigenvector by $\mathbf{x}$ $(= \mathbf{x}_G)$. In sequel, we will consider $\mathbf{x}$ as an n-tuple $(x_1, x_2, \ldots, x_n)$, or interchangeably as a mapping $\mathbf{x} : V(G) \to \mathbf{R}^n$ (here $n = |V(G)|$). With this notation, we have that $\mu x_i = \sum_{j \sim i} x_j$ for any vertex i of G; here $\sim$ denotes that the corresponding vertices are adjacent. The latter condition represents an *eigenvalue equation* for the i-th vertex.

2. BASIC TOOLS

In order to identify the tree(s) in the set $\mathcal{T}(n, \Delta)$ with maximum index, we will need some results on graph perturbations (see, for example, [3]). As it will become apparent very soon, it suffices for us to exhibit how the index of some graph is changed after performing only two simple perturbations: (i) a rotation of an edge and (ii) a local switching.

(i) Let $e = rs$ be an edge of a graph G, and assume that vertex r is non-adjacent to t. The *rotation* (around r) consists of a deletion of the edge e followed by an addition of the edge $e' = rt$.

Theorem 1.1 *Let G' be a graph obtained from a connected graph G of order n by the rotation defined as above. Let $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ be the principal eigenvector of G. Then the following holds:*

$$\textit{if } x_t \geq x_s \textit{ then } \mu_{G'} > \mu_G.$$

(ii) Let $e = st$ and $f = uv$ be two edges of a graph G, and assume that vertices s and v, and t and u are non-adjacent. The *local switching* (with respect to e and f) consists of a deletion of edges e and f, followed by an addition of edges $e' = sv$ and $f' = tu$. It can be easily seen that local switching preserves degrees. Another remarkable fact is that any two graphs of the same order and with the same degree sequence can be obtained from one to another by local switchings in turns (see, for example, [16] p. 45).

Theorem 1.2 *Let G' be a graph obtained from a connected graph G of order n by the local switching defined as above. Let $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ be the principal eigenvector of G. Then the following holds:*

> *if $(x_s - x_u)(x_v - x_t) \geq 0$ then $\mu_{G'} \geq \mu_G$, with equality for the indices if and only if $x_s = x_u$ and $x_v = x_t$.*

Remark These two theorems can be found in [3] in the weaker forms. The forms given above are recently (along with the proofs) obtained in [13]. □

3. MAIN RESULTS

When considering a class of trees $\mathcal{T}(n, \Delta)$, we will assume that $\Delta > 2$ (for $\Delta = 2$ there exists just one tree, namely a path, and then our problem becomes trivial). For short, let T_M be a tree from $\mathcal{T}(n,\Delta)$ whose index attains the maximum value. By $\mathbf{x}$ we will denote the principal eigenvector of T_M. In the following lemmas we focus our attention on some basic properties of T_M.

Lemma 3.1 *At most one vertex of T_M has degree non-equal to 1 or Δ.*

Proof Assume to the contrary, and let s and t be the vertices of T_M such that $1 < deg(s), deg(t) < \Delta$. Let $\mathbf{x}$ be the principal eigenvector of T_M and assume, without loss generality, that $\mathbf{x}(s) \leq \mathbf{x}(t)$.

Assume first that s and t are non-adjacent. Let r be a vertex adjacent to s which does not lye on the unique path between s and t. Then we can rotate the edge rs (around r) to the position of the non-edge rt, to get again a tree from $\mathcal{T}(n,\Delta)$. But then, by Theorem 1.1, the index of the tree just obtained is greater than that of T_M, a contradiction.

We next assume that s and t are adjacent. Let r be any vertex, other than t, adjacent to s. We can now rotate the edge rs (around r) to the position of the non-edge rt, to get again a tree from $\mathcal{T}(n,\Delta)$ (note, rt is a non-edge, since otherwise there will be a triangle in T_M). But then, by Theorem 1.1, the index of the tree just obtained is greater than that of T_M, a contradiction.

This completes the proof. $\square$

Lemma 3.2 *If each vertex in T_M is of degree 1 or Δ, then $n \equiv 2(mod(\Delta - 1))$; otherwise, if there exists a vertex (in T_M) of degree d, $1 < d < \Delta$, then $n \equiv d + 1(mod(\Delta - 1))$.*

Proof Let k be the number of vertices in T_M which are of degree Δ. Assume first that each vertex of T_M is of degree 1 or Δ. Then, $k\Delta + n - k = 2(n-1)$, and therefore $n = k(\Delta - 1) + 2$. Otherwise, assume (by Lemma 3.1) that there is the unique vertex in T_M of degree $d \neq 1, \Delta$. Then, as above, $k\Delta + d + (n - k - 1) = 2(n - 1)$, and therefore $n = k(\Delta - 1) + d + 1$. This completes the proof. $\square$

In the next few lemmas we will consider the components of $\mathbf{x}$.

Lemma 3.3 *If s and t are two vertices of T_M such that $deg(s) > deg(t)$ then $\mathbf{x}(s) > \mathbf{x}(t)$.*

Proof Assume to the contrary that $deg(s) > deg(t)$, but $\mathbf{x}(s) \leq \mathbf{x}(t)$. Let r be a vertex of T_M adjacent to s, but non-adjacent to t. Notice that such a vertex must exist. To see this, take that r is not on the unique path between

s and t; note also that $deg(s) > 1$ ensures the existence of r, as required. We will next rotate the edge rs (around r) to the position of the non-edge rt (notice that r cannot be adjacent to both s and t, since r does not belong to the unique path between s and t; otherwise, there would exist a cycle in T_M). Notice that after this rotation the obtained graph is again a tree from $\mathcal{T}(n, \Delta)$. By Theorem 1.2, the index of this tree is greater than the index of T_M, a contradiction. This completes the proof. $\square$

Lemma 3.4 *There exists a vertex c in T_M such that each leaf of T_M is at distance $h-1$ or h (for some h) from c.*

Proof Let c be a vertex of T_M such that $\mathbf{x}(c) = \max_{v \in V(T_M)} \mathbf{x}(v)$, i.e. c is a vertex with maximum weight (with respect to $\mathbf{x}$). Assume now to the contrary, and let u_1 and v_0 be the leaves at distances $d(u_1, c) = p$ and $d(v_0, c) = q$ such that $q - p \geq 2$. Let $u_2, u_3, \ldots, u_p, c$ and $v_1, v_2, \ldots, v_{q-1}, c$ be the vertices on the unique paths from u_1 and v_0 to c, respectively. Let $e_i = u_i u_{i+1}$, while $f_i = v_i v_{i+1}$ $(i = 1, 2, \ldots)$. Consider now the local switching of edges e_i and f_i, where new edges are $u_i v_{i+1}$ and $v_i u_{i+1}$. Then, T_M is transformed to a tree T^i, for each i.

Now, by Theorem 1.2, we always have $(\mathbf{x}(u_i) - \mathbf{x}(v_i))(\mathbf{x}(v_{i+1}) - \mathbf{x}(u_{i+1})) \leq 0$; otherwise, the index of T^i becomes greater than the index of T_M. A specific situation can occur when $(\mathbf{x}(u_i) - \mathbf{x}(v_i))(\mathbf{x}(v_{i+1}) - \mathbf{x}(u_{i+1})) = 0$. If only one of these two factors is equal to zero, then the index of T^i is again greater than the index of T_M (cf. Theorem 1.2). So, it remains that either $(\mathbf{x}(u_i) - \mathbf{x}(v_i))(\mathbf{x}(v_{i+1}) - \mathbf{x}(u_{i+1})) < 0$ or that both of these two factors are zero. With this in mind, we next have:

$$(\mathbf{x}(u_1) - \mathbf{x}(v_1))(\mathbf{x}(v_2) - \mathbf{x}(u_2)) \leq 0, \tag{1}$$

$$(\mathbf{x}(u_2) - \mathbf{x}(v_2))(\mathbf{x}(v_3) - \mathbf{x}(u_3)) \leq 0, \tag{2}$$

$$\cdots \tag{3}$$

Since $deg(u_1) < deg(v_1)$, we get $\mathbf{x}(u_1) < \mathbf{x}(v_1)$ (by Lemma 3.3). But then from (1) we get $\mathbf{x}(u_2) < \mathbf{x}(v_2)$; next from (2) we get $\mathbf{x}(u_3) < \mathbf{x}(v_3)$, and so on. Since $p < q$, at some step we obtain $\mathbf{x}(c) < \mathbf{x}(v_k)$ for some k, a contradiction. So, c is the vertex as required, and $|q - p| \leq 1$ for any two leaves.

This completes the proof. $\square$

Remark The vertex c as specified in Lemma 3.4 belongs to the center of T_M. To see this, we will show that $rad(T_M) = h$ (here we assume, without loss of generality, that $ecc(c) = h$). Firstly, it is easy to see that only a vertex adjacent to c can have an eccentricity less than $h+1$. Next, among these vertices (i.e. neighbours of c), there is at most one vertex with eccentricity less than $h+1$. If such a vertex exists then its eccentricity is h as well, but its weight need not be equal to the weight of c (as can be seen by examples). So, in further we will assume that c is a vertex (of T_M) with maximum weight, and as well, one of the "central" vertices. $\square$

Lemma 3.5 *Let u_0 $(= c)$ be a root of T_M, while u_k an arbitrary leaf. Let $u_0, u_1, u_2, \ldots, u_k$ be a path (in T_M) starting from u_0 and terminating in u_k. Then*

$$\mathbf{x}(u_0) \geq \mathbf{x}(u_1) > \mathbf{x}(u_2) > \cdots > \mathbf{x}(u_{k-1}) > \mathbf{x}(u_k).$$

Proof The first and the last inequality in this chain are true (by assumptions, or by Lemma 3.3). We take here that $k > 2$, since otherwise there is nothing to prove. Now, assume to the contrary, i.e. that for some i $(1 \leq i < k)$ $\mathbf{x}(u_i) \leq \mathbf{x}(u_{i+1})$ holds. But then, since T_M has the maximal index, we must have (by Theorem 1.2) that $(\mathbf{x}(u_{i-1}) - \mathbf{x}(u_{i+2}))(\mathbf{x}(u_{i+1}) - \mathbf{x}(u_i)) \leq 0$. Therefrom we get $\mathbf{x}(u_{i-1}) \leq \mathbf{x}(u_{i+2})$. In the same way we get $\mathbf{x}(u_{i-2}) \leq \mathbf{x}(u_{i+3})$, and so forth. At some step we will encounter that $u_{i-s} = u_0$ or $u_{i+s+1} = u_k$. But this is a contradiction. If $u_{i-s} = u_0$ occurs, we get a tree with more than two central vertices; if $u_{i+s+1} = u_k$, then the conclusion follows from Lemma 3.3 (since u_k is a leaf). This completes the proof. $\square$

The next lemma directly follows from the previous one.

Lemma 3.6 *If u is a vertex of T_M of degree d such that $1 < d < \Delta$, then u is at distance $h-1$ from c.*

Proof Assume to the contrary that u is at distance k from c, where $k \neq h-1$. Since $k \neq h$, we can assume that $k \leq h-2$. Consider any maximal path starting at c, passing through u and terminating in r (which is, of course, a leaf). Then, we can rotate a hanging edge incident to r (around r) to make it a hanging edge at u. But then, by Theorem 1.1 (and Lemma 3.5), we get a contradiction, in fact a tree whose index is greater than the index of T_M. This completes the proof. $\square$

Consider now the partition

$$V(T_M) = V_0(c) \,\dot\cup\, V_1(c) \,\dot\cup\, \cdots \,\dot\cup\, V_{h-1}(c) \,\dot\cup\, V_h(c),$$

where $V_k(c) = \{u \mid d(c,u) = k\}$ $(k = 0, 1, \ldots, h-1, h)$. It will be called the *distance partition* of the vertex set of T_M with respect to c. The next lemma is a slight generalization of Lemma 3.5. It is noteworthy to mention that we will not need it in attempting to prove our main result, but we include it here only to gain attention on one interesting phenomenon.

Lemma 3.7 *If $u \in V_i(c)$ and $v \in V_j(c)$, where $i < j$, then $\mathbf{x}(u) \geq \mathbf{x}(v)$.*

Proof Assume first that c is not on the unique path between u and v. Then the proof follows from Lemma 3.5. We next assume that c is on the unique path between u an v. If so, assume to the contrary, and let $\mathbf{x}(u) < \mathbf{x}(v)$. Without loss of generality, we can also take that j is the largest possible. If v is a leaf, but not u we are done (by Lemma 3.3). So, assume next that both u and v are leaves. But then $i = j - 1$ (by Lemma 3.4). Proceeding as in the proof of Lemma 3.4, let $u_0 = u, u_1, \ldots$ be the vertices on the unique path between u and c; also, let $v_0 = v, v_1, \ldots$ be the vertices on the unique path between v and c. Then by performing the local switching on the edges u_iu_{i+1} and v_iv_{i+1} $(i = 0, 1, \ldots)$ as in the proof of Lemma 3.4 we arrive at the condition $\mathbf{x}(c) \leq \mathbf{x}(v_{j-1})$. If $\mathbf{x}(c) < \mathbf{x}(v_{j-1})$ we are done (in fact we get a contradiction). So consider the situation when $\mathbf{x}(c) = \mathbf{x}(v_{j-1})$. By tracing backwards the chain of conditions stemming from Theorem 1.2, namely the conditions $\mathbf{x}(u_i) = \mathbf{x}(v_i)$, we arrive at the condition $\mathbf{x}(u_1) = \mathbf{x}(v_1)$. But then we get a contradiction $\mathbf{x}(u_0) = \mathbf{x}(v_0)$ (by applying eigenvalue equations for vertices u and v). Consequently, it follows that v has a neighbor, say v', belonging to $V_{j+1}(c)$. On the other hand, u has a neighbor, say u', belonging to V_{i+1} (as can be argued by Lemma 3.6). Making use of Theorem 1.2, we have that $(\mathbf{x}(u') - \mathbf{x}(v'))(\mathbf{x}(v) - \mathbf{x}(u)) < 0$. But then, we get that $\mathbf{x}(u') < \mathbf{x}(v')$, a contradiction to the choice of v. This completes the proof. □

Remark In the general case, in contrast to Lemma 3.5, we cannot put $\mathbf{x}(u) > \mathbf{x}(v)$ instead of $\mathbf{x}(u) \geq \mathbf{x}(v)$. This will be explained later. □

From the above lemmas it follows that T_M is a tree which satisfies:

(i) it is a rooted tree with c (the center of T_M) as the root;

(ii) its height with respect to c is equal to h $(= h(T_M))$;

(iii) each leaf is at distance $h - 1$ or h from c;

(iv) each vertex, except possibly one, is of degree 1 or Δ;

(v) the vertex of degree d $(1 < d < \Delta)$, if any, is at distance $h-1$ from c.

Notice also (as follows from above) that a tree T_M with the height at most 2, is determined by (i)-(v) up to isomorphism. So, assume that further on $h(T_M)$ is greater than 2.

Recall now that a rooted tree is a *balanced tree* if all vertices at any (but fixed) distance from the root have the same degree; see, for example, [11], p. 106. So, such a tree (of height h) can be described by h parameters $p_0, p_1, \ldots, p_{h-1}$, where p_i is the degree of any vertex at i-th layer. If T is a balanced tree with the above parameters, we write $T = T(p_0, p_1, \ldots, p_{h-1})$. So, T_M is an induced subgraph of

$$T(\overbrace{\Delta, \Delta, \ldots, \Delta}^{h}),$$

which can be abbreviated to $T(h, \Delta)$. Thus, for T_M we have

$$T(h-1, \Delta) \subset T_M \subseteq T(h, \Delta);$$

here $\subseteq$ denotes the fact that the first graph is an induced subgraph of the second one. Actually, T_M can be obtained from $T(h-1, \Delta)$ by attaching the appropriate number of bouquets with $\Delta - 1$ edges to the vertices on the $(h-1)$-th layer, and possibly only one bouquet with $d-1$ edges to one vertex on the same layer.

We will now precise the structure of T_M (as suggested by our computer experiments with *Mathematica*). For this aim, consider $T(h-1, \Delta)$ and traverse it (starting from its root) in a depth-first search (DFS) manner (see, for example, [12]). Then the vertices from the layers are labeled in order as they were encountered (for the first time) by the DFS. After this step, we add bouquets (of sizes as above) to the vertices from the last layer in $T(h-1, \Delta)$ respecting the order in which they were encountered - that means the vertices first encountered first get the bouquets. This tree will be denoted by $B(n, \Delta)$. We next give some further explanations.

Let u be any vertex of T_M other than c. Denote by T^u a subtree hanging at u, i.e. it contains u and all vertices v for which u belongs to the unique path between v and c. We can classify trees T^u as follows: (i) L-type (*large trees*) - balanced with height $h - d(c, u)$; (ii) M-type (*medium trees*)- non-balanced with height $h - d(c, u)$; (iii) S-type (*small trees*)- balanced with height $h - 1 - d(c, u)$. Now, if T_M is not a balanced tree, then the trees T^u for $u \in V_1(c)$ are all but possibly one of type L or S. If T^{u_1} for $u_1 \in V_1(c)$

is a tree of type M, then its subtrees T^u for $u \in V_2(c)$ are all but one of type L or S. If T^{u_2} for $u_2 \in V_2(c)$ is a tree of type M, then its subtrees are all but one of types L or S, and so forth. In the final stage, all subtrees are of type L or S. Consequently, there are no two subtrees of type M whose roots are on the same layer; otherwise, that situation will be referred to as a *failure.*

Lemma 3.8 *For any two subtrees (of T_M), attached at vertices from the same layer, there are no failures.*

Proof Assume to the contrary that there exists a failure. Let u' and v' be the vertices (from the same layer) giving rise to a failure. Then there is a path from u' to some vertex, say u_2, from the $(h-2)$-th layer for which T^{u_2} is of type M. Similarly, there is a path from v' to some vertex, say v_2, from the $(h-2)$-th layer for which T^{v_2} is of type M. Assume first that u_1 and v_1 are the vertices of $V_{h-1}(c)$ chosen so that u_1 is adjacent to u_2 and $deg(u_1) = 1$, while v_1 is adjacent to v_2 and $deg(v_2) > 1$. If so, by Theorem 1.2 (and Lemma 3.3), and since T_M has the maximum index, we get $\mathbf{x}(v_2) > \mathbf{x}(u_2)$. Conversely, we next take that $deg(u_1) > 1$, while $deg(v_1) = 1$. But then, in the same way, we get $\mathbf{x}(u_2) > \mathbf{x}(v_2)$, a contradiction. This completes the proof. □

Collecting the above results, we immediately get our main result.

Theorem 3.9 *There is a unique graph in $\mathcal{T}(n, \Delta)$ (for each n and Δ) with the largest index; it is equal to $B(n, \Delta)$.*

Proof We start from the first layer. If there are no subtrees of type M whose roots are at the first layer, we are done ($T_M = B(n, \Delta)$). Otherwise, there is a unique subtree T^{u_1} of type M, with $u_1 \in V_1(c)$. We then proceed with the second layer focusing our attention only to the neighbours of u_1. If there are no subtrees of type M whose roots are the observed vertices of the second layer we are done ($T_M = B(n, \Delta)$). Continuing in this way, and using (repeatedly) Lemma 3.8, we will get a tree which is equal to $B(n, \Delta)$. Note, in each step subtrees of type L can be relocated to the left, next subtrees of type S can be relocated to the right, while those of type M are kept in the middle. This is in accordance with DFS strategy used in constructing the graphs $B(n, \Delta)$. This completes the proof. □

Example Assume first that $n = 37$ and $\Delta = 3$. Then the corresponding maximal graph is shown in Fig. 1. Its center consists of one vertex (top one).

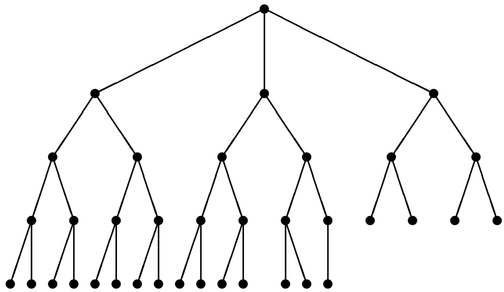

Fig. 1: A tree with maximum index in $\mathcal{T}(37, 3)$.

Assume now that $n = 26$ and $\Delta = 4$. Then the corresponding maximal graph is shown in Fig. 2. Its center consists of two (adjacent) vertices (middle ones).

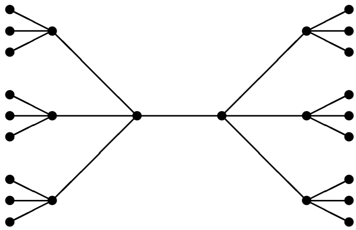

Fig. 2: A tree with maximum index in $\mathcal{T}(26, 4)$.

In this situation, we have a tree which is balanced in the sense that all vertices at any (but fixed) distance from the center are of the same degree. With such trees, if we take one of the central vertices as a root we can have that two vertices from different layers have the same weight (with respect to the principal eigenvector); see also the remark after Lemma 3.7. $\square$

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