Extremal Trees with Respect to Dominance Order

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Abstract. Let $(T_i)_{i\geq 0}$ be a sequence of trees such that T_{i+1} arises by deleting the b_i vertices of degree ≤ 1 from T_i. We determine those trees of given degree sequence or maximum degree for which the sequence $b_0, b_1, ...$ is maximum or minimum with respect to the dominance order. As a consequence we also determine trees of given degree sequence or maximum degree that are of maximum or minimum Balaban index.

Keywords. Dominance order; tree; Balaban index

1 Introduction

For some $p \geq 0$ let $x_0 \geq x_1 \geq ... \geq x_p \geq 0$ and $y_0 \geq y_1 \geq ... \geq y_p \geq 0$ be real numbers such that $\sum_{i=0}^{p} x_i = \sum_{i=0}^{p} y_i$. If $\sum_{i=0}^{k} x_i \leq \sum_{i=0}^{k} y_i$ for all $0 \leq k \leq p$, we write

$$(x_0, x_1, ..., x_p) \preceq (y_0, y_1, ..., y_p).$$

The partial order induced by '$\preceq$' on the set of partitions of $x_0 + x_1 + ... + x_p$ where the summands are rearranged in non-increasing order is usually refered to as the *dominance order*. It is a classical result (cf. e.g. Theorem 108 in [10]) that $(x_0, x_1, ..., x_p) \preceq (y_0, y_1, ..., y_p)$ holds if and only if $\sum_{i=0}^{p} g(x_i) \leq \sum_{i=0}^{p} g(y_i)$ for all continuous and convex functions g.

A tree $T = (V(T), E(T))$ is a connected graph without cycles with vertex set $V(T)$ and edge set $E(T)$. The degree of some vertex $u \in V(T)$ is denoted by $d(u, T)$. Let

$$V_{\leq 1}(T) = \{u \in V(T) \mid d(u, T) \leq 1\},$$

i.e. if $|V(T)| \geq 2$, then $V_{\leq 1}(T)$ is exactly the set of *endvertices* of the tree T and if $|V(T)| = 1$, then $V_{\leq 1}(T) = V(T)$. Starting from a given tree T we define a sequence of trees as follows. Let $T_0 = T$ and for $i \geq 1$ let $T_i = T_{i-1} - V_{\leq 1}(T_{i-1})$. Let $n_i(T) = |V(T_i)|$ and $b_i(T) = |V_{\leq 1}(T_i)| = n_i(T) - n_{i+1}(T)$ for $i \geq 0$.

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It is easy to see that $n_i(T) \geq 2$ implies $b_i(T) \geq 2$ and thus $b_i(T) = 0$ for $i \geq n_0(T) + 1$. Furthermore, since the deletion of an endvertex from a tree can only lead to at most one new endvertex, we have $b_i(T) \geq b_{i+1}(T)$ for $i \geq 0$.

Hence $b_0(T) + b_1(T) + ... + b_{n_0(T)}(T) = n_0(T) = |V(T)|$ represents a partition of $|V(T)|$, where the summands are in non-increasing order. Let $\mathbf{b}(T) = (b_0(T), b_1(T), ..., b_{n_0(T)}(T))$. In this note we determine those trees T of given degree sequence or maximum degree for which $\mathbf{b}(T)$ is maximum or minimum with respect to dominance order among all trees of the same degree sequence or maximum degree.

We have been motivated by the so-called *Balaban index* $\mathcal{B}$ defined for a tree T as $\mathcal{B}(T) = \sum_{i \geq 0} b_i(T)^2$. The Balaban index is one of the *molecular descriptors* cf. [5] which are studied in chemistry in order to capture chemically relevant properties of molecules using graph-theoretical invariants derived from the graphs representing the molecular structure. Such parameters have recently received growing attention from mathematicians cf. e.g. [2, 3, 4, 6, 7, 8, 9] and [12]. Balaban showed in [1] that $\mathcal{B}$ correlates well with the octane number of certain compounds.

Since $x \mapsto x^2$ is continuous and convex, the trees T for which $\mathbf{b}(T)$ is maximum or minimum with respect to the dominance order are also of maximum or minimum Balaban index.

For an ingenious application of the dominance order to the Wiener index which is another chemical descriptor see [11].

2 Degree sequence

It is well-known that the positive integers $d_1 \leq d_2 \leq ... \leq d_n$ are the degree sequence of a tree T if and only if $0 = 2 + \sum_{u \in V(T)} (d_i - 2)$. Therefore, if $n \geq 2$ and the tree T has degree sequence $d_1 \leq d_2 \leq ... \leq d_n$, then the number $b_0(T)$ of its endvertices equals

$$b_0(T) = 2 + \sum_{d_i \geq 3} (d_i - 2).$$

Our argument relies on the following two observations.

Lemma 2.1 *If T is a tree with degree sequence $d_1 \leq d_2 \leq ... \leq d_n$ where $n \geq 2$, then for $k \geq 1$*

$$\sum_{i=0}^{k} b_i(T) \quad \leq \quad \max \left\{ l \,\middle|\, \sum_{i=1}^{l} (d_i - 1) \leq \sum_{i=0}^{k-1} b_i(T) \right\}. \qquad (1)$$

Proof: Let $l_1 = \sum_{i=0}^{k} b_i(T)$ and $l_2 = \max\left\{l \,\middle|\, \sum_{i=1}^{l}(d_i - 1) \le \sum_{i=0}^{k-1} b_i(T)\right\}$.

Let $u \in V_{\le 1}(T_{k'})$ for some $0 \le k' \le k$. If $k' = 0$, then let $V_u = \emptyset$ and if $k' \ge 1$, then let V_u denote a set of $(d(u,T) - 1)$ neighbours of u in $\bigcup_{i=0}^{k'-1} V_{\le 1}(T_i)$. (Note that such a set always exists and that there are exactly $(d(u,T) - 1)$ such neighbours provided $|V_{\le 1}(T_{k'})| \ge 2$.)

Clearly, $V_u \cap V_{u'} = \emptyset$ for all $u, u' \in \bigcup_{i=0}^{k} V_{\le 1}(T_i)$ with $u \ne u'$. This implies

$$\begin{aligned}\sum_{i=0}^{k-1} b_i(T) &= \left|\bigcup_{i=0}^{k-1} V_{\le 1}(T_i)\right| \\ &\ge \sum_{u \in \bigcup_{i=0}^{k} V_{\le 1}(T_i)} |V_u| \\ &= \sum_{u \in \bigcup_{i=0}^{k} V_{\le 1}(T_i)} (d(u,T) - 1) \\ &\ge \sum_{i=1}^{l_1}(d_i - 1).\end{aligned}$$

This immediately implies $l_1 \le l_2$ and the proof is complete. □

Lemma 2.2 *For $n, b_0 \ge 2$ let $1 = d_1 = d_2 = \dots = d_{b_0} < d_{b_0+1} \le d_{b_0+2} \le \dots \le d_n$ be integers. Let b_1 be such that*

$$b_0 + b_1 = \max\left\{l \,\middle|\, \sum_{i=1}^{l}(d_i - 1) \le b_0\right\}.$$

Let

$$d'_j = \begin{cases} 1 & , j = 1, 2, \dots, b_1 \\ d_{b_0+j} - \left(b_0 - \sum_{i=1}^{b_0+b_1}(d_i - 1)\right) & , j = b_1 + 1 \\ d_{b_0+j} & , j = b_1 + 2, b_1 + 3, \dots, n - b_0. \end{cases}$$

Then $d_1 \le d_2 \le \dots \le d_n$ is the degree sequence of a tree if and only if $d'_1 \le d'_2 \le \dots \le d'_{n-b_0}$ is the degree sequence of a tree.

Proof: Since

$$\sum_{j=1}^{n-b_0}(d'_j - 2)$$

$$
\begin{aligned}
&= -b_1 + \left(d_{b_0+b_1+1} - \left(b_0 - \sum_{i=1}^{b_0+b_1} (d_i - 1) \right) - 2 \right) + \sum_{i=b_0+b_1+2}^{n} (d_i - 2) \\
&= \sum_{i=1}^{b_0+b_1} (d_i - 2) + (d_{b_0+b_1+1} - 2) + \sum_{i=b_0+b_1+2}^{n} (d_i - 2) \\
&= \sum_{i=1}^{n} (d_i - 2),
\end{aligned}
$$

the desired result follows. □

We proceed to the main result of this section.

Proposition 2.3 *Let T be a tree with degree sequence $d_1 \leq d_2 \leq ... \leq d_n$, where $n \geq 2$.*

(i) $\mathrm{b}(T') \preceq \mathrm{b}(T)$ *for all trees T' with degree sequence $d_1 \leq d_2 \leq ... \leq d_n$ if and only if*

$$
b_k(T) = \begin{cases} 2 + \sum\limits_{d_i \geq 3} (d_i - 2) & , k = 0 \\ \max \left\{ l \,\middle|\, \sum\limits_{i=1}^{l} (d_i - 1) \leq \sum\limits_{i=0}^{k-1} b_i(T) \right\} - \sum\limits_{i=0}^{k-1} b_i(T) & , k \geq 1. \end{cases} \tag{2}
$$

(ii) $\mathrm{b}(T) \preceq \mathrm{b}(T')$ *for all trees T' with degree sequence $d_1 \leq d_2 \leq ... \leq d_n$ if and only if*

$$
b_k(T) = \begin{cases} 2 + \sum\limits_{d_i \geq 3} (d_i - 2) & , k = 0 \\ 2 & , 1 \leq k \leq \lfloor \frac{n_0(T) - b_0(T)}{2} \rfloor \\ 2 \left(\frac{n_0(T) - b_0(T)}{2} - \left\lfloor \frac{n_0(T) - b_0(T)}{2} \right\rfloor \right) & , k = \lfloor \frac{n_0(T) - b_0(T)}{2} \rfloor + 1. \end{cases} \tag{3}
$$

Proof: Since the term on the right side of (1) is non-decreasing in $\sum_{i=0}^{k-1} b_i(T)$, the '*if*-part of (i) follows immediately. The '*if*-part of (ii) is trivial.

In order to prove the '*only if*-part of (i) (or (ii)), we have to prove the existence of a tree T with degree sequence $d_1 \leq d_2 \leq ... \leq d_n$ such that (2) (or (3)) holds.

For (i) this follows easily by induction using Lemma 2.2. For (ii) there is obviously a caterpillar with the desired property, i.e. T_1 is a path. □

3 Maximum degree

Let T be a tree of order $n \geq 0$ and maximum degree at most $\Delta \geq 2$. It is an easy exercise to verify that

$$b_0(T) \quad \leq \quad f_\Delta(n) := \begin{cases} \left\lfloor \frac{(\Delta-2)n+2}{\Delta-1} \right\rfloor & , n \geq 3 \\ n & , n \leq 2. \end{cases} \tag{4}$$

Furthermore, $b_0(T) \geq 2$, if $n \geq 2$ and $b_0(T) \geq \Delta$, if T has maximum degree Δ. Obviously, the function f_Δ is non-decreasing in n. Furthermore, one easily checks that $n \leq m$ implies $n - f_\Delta(n) \leq m - f_\Delta(m)$.

If T is a tree of order n and maximum degree at most Δ such that $b_i(T) = f_\Delta(n_i(T))$ for all $i \geq 0$ and T' is an arbitrary tree of order n and maximum degree at most Δ, then (4) implies $b_0(T) \geq b_0(T')$ and, by induction, for $k \geq 1$

$$\begin{aligned}
\sum_{i=0}^{k} b_i(T) &= \sum_{i=0}^{k-1} b_i(T) + b_k(T) \\
&= \sum_{i=0}^{k-1} b_i(T) + f_\Delta\left(n - \sum_{i=0}^{k-1} b_i(T)\right) \\
&= n - \left(\left(n - \sum_{i=0}^{k-1} b_i(T)\right) - f_\Delta\left(n - \sum_{i=0}^{k-1} b_i(T)\right)\right) \\
&\geq n - \left(\left(n - \sum_{i=0}^{k-1} b_i(T')\right) - f_\Delta\left(n - \sum_{i=0}^{k-1} b_i(T')\right)\right) \\
&= \sum_{i=0}^{k-1} b_i(T') + f_\Delta\left(n - \sum_{i=0}^{k-1} b_i(T')\right) \\
&\geq \sum_{i=0}^{k-1} b_i(T') + b_k(T') = \sum_{i=0}^{k} b_i(T').
\end{aligned}$$

We proceed to the results of this section.

Proposition 3.1 *Let T be a tree of order $n \geq 0$ and maximum degree at most $\Delta \geq 2$.*

Then $\mathbf{b}(T') \preceq \mathbf{b}(T)$ for all trees T' of order n and maximum degree at most Δ if and only if $b_i(T) = f_\Delta(n_i(T))$ for all $i \geq 0$.

Proof: The '*if*'-part follows from the above inequalities. For the '*only if*'-part, we construct a tree $T(n, \Delta)$ of order n and maximum degree at most Δ with $b_i(T(n, \Delta)) = f_\Delta(n_i(T(n, \Delta)))$ for all $i \geq 0$.

Let $V(T(n,\Delta)) = \{u_1, u_2, ..., u_n\}$ for $n \geq 1$. Let $E(T(1,\Delta)) = \emptyset$. For $i \geq 2$, let $E(T(i,\Delta)) = E(T(i-1,\Delta)) \cup \{u_i u_{i'}\}$ such that $i' = \min\{j \mid 1 \leq j \leq i-1 \text{ and } d(u_j, T(i-1,\Delta)) < \Delta\}$. It is straightforward to check that $T(n,\Delta)$ has the desired properties. □

Proposition 3.2 *Let T be a tree of order $n \geq \Delta + 1$ and maximum degree exactly $\Delta \geq 2$.*

Then $\mathbf{b}(T) \preceq \mathbf{b}(T')$ for all trees T' of order n and maximum degree exactly Δ if and only if

$$b_k(T) = \begin{cases} \Delta & , k = 0 \\ 2 & , 1 \leq k \leq \lfloor \frac{n-\Delta}{2} \rfloor \\ 2\left(\frac{n-\Delta}{2} - \lfloor \frac{n-\Delta}{2} \rfloor\right) & , k = \lfloor \frac{n-\Delta}{2} \rfloor + 1. \end{cases}$$

Proof: Since a tree of maximum degree Δ has at least Δ endvertices, the '*if*-part follows. The '*only if*-part follows by considering the tree that arises by attaching $(\Delta - 1)$ new endvertices to one endvertex of the path $P_{n-\Delta+1}$ of order $n - \Delta + 1$. □

Finally, we want to point out that $\mathbf{b}(P_n) \preceq \mathbf{b}(T) \preceq \mathbf{b}(K_{1,n-1})$ for all trees T of order n, $\mathbf{b}(P_n) = \mathbf{b}(T)$ if and only if $P_n = T$ and $\mathbf{b}(T) = \mathbf{b}(K_{1,n-1})$ if and only if $T = K_{1,n-1}$, where P_n and $K_{1,n-1}$ denote the path and the star of order n, respectively.

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