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Extremal values on the general degree-eccentricity index of trees of fixed maximum degree

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Abstract

For a connected graph G and $a, b \in \mathbb{R}$, the general degree-eccentricity index is defined as $\mathrm{DEI}_{a,b}(G) = \sum_{v \in V(G)} d_G^a(v)\mathrm{ecc}_G^b(v)$, where $V(G)$ is the vertex set of G, $d_G(v)$ is the degree of a vertex v and $\mathrm{ecc}_G(v)$ is the eccentricity of v in G, i.e. the maximum distance from v to another vertex of the graph. This index generalizes several well-known 'topological indices' of graphs such as the eccentric connectivity index. We characterize the unique trees with the maximum and the minimum general degree-eccentricity index among all n-vertex trees with fixed maximum degree for the cases $a \geq 1, b \leq 0$ and $0 \leq a \leq 1, b \geq 0$. This complements previous results on the general degree-eccentricity index for various classes of trees.

1 Introduction

In organic chemistry, topological indices of graphs have been found to be useful in chemical documentation, isomer discrimination, structure-property relationships, structure-activity (SAR) relationships, and pharmaceutical drug design. Eccentricity-based indices have shown very good correlations with respect to both physical and biological properties of chemical substances [3]. They provide excellent predictive power for pharmaceutical properties, for example, for predicting the anti-HIV activity of chemical substances [1].

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For $a, b \in \mathbb{R}$, the general degree-eccentricity index is defined for a connected graph G as

$$\mathrm{DEI}_{a,b}(G) = \sum_{v \in V(G)} d_G^a(v) \mathrm{ecc}_G^b(v),$$

where $\mathrm{ecc}_G(v)$ is the eccentricity of v, that is, the greatest distance between v and another vertex of G.

Several important eccentricity-based indices are special cases of this general index:

- $\mathrm{DEI}_{a,1}(G)$ is the general eccentric connectivity index introduced in [8],
- $\mathrm{DEI}_{1,1}(G)$ is the classical eccentric connectivity index,
- $\mathrm{DEI}_{1,-1}(G)$ is the connective eccentricity index,
- $\mathrm{DEI}_{0,1}(G)$ is the total eccentricity index and
- $\mathrm{DEI}_{0,2}(G)$ is the first Zagreb eccentricity index of G.

Mathematical properties of eccentricity-based indices have been studied due to the extensive applications of these indices. Let us briefly review some results on eccentricity-based topological indices of graphs.

Morgan, Mukwembi and Swart [7] obtained sharp lower and upper bounds on the eccentric connectivity index for trees with given order and diameter. Zhou and Du [11] found sharp upper bounds for this invariant, and bounds for trees with given maximum degree were obtained in [2].

Upper bounds on the connective eccentricity index for graphs of given order and matching number were given by Xu et al. [10], a lower bound for graphs of given order and clique number was proved by Wang et al. [9]. In [8], sharp upper and lower bounds on the general eccentric connectivity index of trees with prescribed order and diameter/number of pendant vertices were given.

In [5], Masre and Vertrik introduced and studied the general degree-eccentricity index of a graph; in particular, they proved a sharp upper bound on this index for graphs of given order for the case $a > 0, b < 0$, and a sharp lower bound for the case $a < 0, b > 0$. In [6], the same authors studied the general degree-eccentricity index for trees of various kinds. In particular, they proved upper and lower bounds on $\mathrm{DEI}_{a,b}$ for trees of given order for the cases $0 < a < 1, b > 0$ and $a > 1, b < 0$. This line of investigation was continued in [4] where similar questions with regards to trees with given diameter are studied.

In this short note we continue the investigation of the general degree-eccentricity index for trees with a particular focus on trees with given maximum degree. First we give a short proof for the following theorem, which is a slight generalization of a main result of [6]. Denote by S_n the star $K_{1,n-1}$ on n vertices, and by P_n the path on n vertices. Our first result is the following, which is slightly more general than the result in [6].

Theorem 1.1. *Let T be a tree of order n.*

(i) For $a \geq 1$ and $b \leq 0$, $DEI_{a,b}(P_n) \leq DEI_{a,b}(T) \leq DEI_{a,b}(S_n)$.

(ii) For $0 \leq a \leq 1$ and $b \geq 0$, $DEI_{a,b}(S_n) \leq DEI_{a,b}(T) \leq DEI_{a,b}(P_n)$.

As we shall see, if $a \notin \{0, 1\}$ or $b \neq 0$, then equalities in the lower and upper bounds in (i) and (ii) hold if and only if T is isomorphic to P_n and S_n, respectively.

Denote by $B_{n,d}$ the tree of order n obtained from a path with $n-d+1$ vertices by adding $d-1$ pendant vertices to one endpoint of the path, and by $V_{n,d}$ the complete $(d-1)$-ary tree, that is, a $(d-1)$-ary tree where every level is completely filled except the last one, but the children of the last level fill this level consecutively. For trees with fixed maximum degree we prove the following.

Theorem 1.2. *Let T be a tree with maximum degree d and order n.*

(i) For $a \geq 1$ and $b \leq 0$, $DEI_{a,b}(B_{n,d}) \leq DEI_{a,b}(T) \leq DEI_{a,b}(V_{n,d})$.

(ii) For $0 \leq a \leq 1$ and $b \geq 0$, $DEI_{a,b}(V_{n,d}) \leq DEI_{a,b}(T) \leq DEI_{a,b}(B_{n,d})$.

Similarly to Theorem 1.1, we shall prove that if $a \notin \{0, 1\}$ and $b \neq 0$, then equalities in the lower and upper bounds in (i) and (ii) hold if and only if T is isomorphic to $V_{n,d}$, and to $B_{n,d}$, respectively.

We further remark that for the case when $a, b \geq 1$, we cannot prove any general upper and lower bounds. For instance, it is intuitively clear that for large n, if a is substantially larger than b, then having large degrees is beneficial for maximizing $\mathrm{DEI}_{a,b}$, so $V_{n,d}$ should be extremal with respect to maximizing $\mathrm{DEI}_{a,b}$, while $B_{n,d}$ should give the smallest value of $DEI_{a,b}$. On the other hand, if b is much larger than a, then the converse should hold.

Finally, let us mention that for $a, b \geq 1$ a similar phenomenon naturally should hold for trees of large order, but then with respect to the graphs S_n and P_n as in Theorem 1.1.

In Section 2 we prove Theorems 1.1 and 1.2, and in Section 3 we give some conclusions and further problems.

2 Proofs of the main results

We shall use standard graph theory notation and terminology. The *order* of a graph is its number of vertices. The notation $G \cong H$ means that G and H are isomorphic.

The shortest path between any two vertices of greatest distance in a connected graph G is called a *diametral path*. A vertex of a path P which is adjacent to an endpoint of the path is called a *near-extremal vertex* of P.

The neighbor set of a vertex v in G is denote by $N_G(v)$, and the distance between two vertices u, v in G is denoted by $d_G(u, v)$. We denote the degree of a vertex v in G by $d_G(v)$.

We shall need the following lemma from [8].

Lemma 2.1. *[8] Let $1 \leq x < y$ and $c > 0$. For $a > 1$ and $a < 0$, we have*

$$(x + c)^a - x^a < (y + c)^a - y^a.$$

If $0 < a < 1$, then

$$(x + c)^a - x^a > (y + c)^a - y^a.$$

Let us now prove Theorem 1.1.

Proof of Theorem 1.1. We shall prove part (ii) of the theorem. Then we explain how part (i) can be proved using similar arguments.

Let us first prove the lower bound in (ii). So assume that $0 \leq a \leq 1, b \geq 0$ and let us show that S_n is extremal with respect to having minimum value of $\mathrm{DEI}_{a,b}$ for trees of order n. The proof is by contradiction. Suppose that T is a tree of order n with minimum value of $\mathrm{DEI}_{a,b}$ among trees of order n, and that T is not isomorpic to S_n. Moreover, among all such trees that minimizes $\mathrm{DEI}_{a,b}$, we assume that T is a tree where a near-extremal vertex of a diametral path has largest degree.

Let $P = u_0 u_1 \dots u_k$ be a diametral path in T. Among such paths in T, we assume that P is the one where a near-extremal vertex has largest degree. Since T is not isomorphic to S_n, $k \geq 3$. Furthermore, assume that u_1 has larger (or equal) degree than u_{k-1}.

Consider the tree $T' = T - u_{k-1}u_k + u_1 u_k$. In T', every vertex has at most the same eccentricity as in T, and u_1 and u_{k-1} have the same eccentricity in T and T'. Moreover, $d_{T'}(u_1) = d_T(u_1) + 1$ and $d_{T'}(u_{k-1}) = d_T(u_{k-1}) - 1$, and all other vertices have the same degree in T' as in T. Thus,

$$d^a_{T'}(u_1) + d^a_{T'}(u_{k-1}) \leq d^a_T(u_1) + d^a_T(u_{k-1}) \tag{1}$$

by Lemma 2.1. It follows that $\mathrm{DEI}_{a,b}(T') \leq \mathrm{DEI}_{a,b}(T)$, and T' has a diametral path where a near-extremal vertex has larger degree than in T, which contradicts the choice of T. Hence, $T \cong S_n$.

Let us now turn to the upper bound in (ii). Suppose that $0 \leq a \leq 1, b \geq 0$ and let us show that P_n is extremal with respect to having maximum value of $\mathrm{DEI}_{a,b}$ for trees of order n. The proof is again by contradiction. Suppose that T is a tree of order n that maximizes $\mathrm{DEI}_{a,b}$ and that T is not isomorphic to P_n. Moreover, among all such trees that maximize $\mathrm{DEI}_{a,b}$, we assume that T is a tree with a longest diametral path.

Let $P = u_0 u_1 \dots u_k$ be a diametral path in T, and suppose that there is a vertex u_p on P with degree at least 3. Let $x \notin V(P)$ be a vertex that is adjacent to u_p and consider the tree $T' = T - u_p x + u_0 x$. In T', every vertex has at least as large eccentricity as in T, and u_0 has greater eccentricity than u_p in T. Moreover, $2 = d_{T'}(u_0) = d_T(u_0) + 1$ and $d_{T'}(u_p) = d_T(u_p) - 1 \geq 2$, and all other vertices have the same degree in T' as in T. Thus,

$$d^a_{T'}(u_0) + d^a_{T'}(u_p) \geq d^a_T(u_0) + d^a_T(u_p) \tag{2}$$

by Lemma 2.1. It follows that $\mathrm{DEI}_{a,b}(T') \geq \mathrm{DEI}_{a,b}(T)$, and T' has a diametral path that is longer than the one in T. This is a contradiction, and we conclude that $T \cong P_n$.

Now, the proofs of the lower and upper bounds in (i) are completely analogous to the proofs of the upper and lower bounds of (ii), respectively, so we omit the details here. □

Let us now check that if $a \notin \{0, 1\}$ or $b \neq 0$, then we have equality in the upper and lower bounds in Theorem 1.1 if and only if T is isomorphic to S_n or P_n, respectively. We shall be content with verifying this for part (ii); for (i) the argument is completely analogous.

Regarding the lower bound, we have equality in (1) precisely when $a = 0$ or $a = 1$. Moreover, continuing this process of "moving" pendant vertices as in the proof of Theorem 1.1 will eventually decrease the length of the diametral path and thus yield a smaller value of $\mathrm{DEI}_{a,b}$ if $b > 0$. Hence, for the lower bound in (ii), equality holds if and only if $T \cong S_n$ for the case when $a \notin \{0, 1\}$ or $b \neq 0$.

As for the upper bound, we have equality in (2) precisely when $a = 0$ or $a = 1$. Moreover, since T' has greater diameter than T, $\mathrm{DEI}_{a,b}(T') < \mathrm{DEI}_{a,b}(T)$ unless $b = 0$. In conclusion, for the case when $a \notin \{0, 1\}$ or $b \neq 0$, equality holds in the upper bound in (ii) if and only if $T \cong P_n$.

Next, we turn to the proof of Theorem 1.2.

Proof of Theorem 1.2. We shall be content with proving part (i). As in the proof of Theorem 1.1, the proof of part (ii) is analogous and we omit it.

We first prove the upper bound in (i). Suppose that T is an extremal tree for the upper bound. We prove by contradiction that T must be isomorphic to $V_{n,d}$.

Let $P = u_0u_1 \dots u_k$ be a diametral path in T, and set $r = \lfloor k/2 \rfloor$. Without loss of generality, we assume that among the trees of order n that maximize $\mathrm{DEI}_{a,b}$, T has a shortest diametral path. Moreover, among all such trees, we assume that T is the one where u_r has the largest degree; in turn, among all such graphs we choose T to be the one with the largest number of vertices of largest degree among the vertices adjacent to u_r; etc. for the vertices of distance s to u_r, $s = 2, 3, \dots$.

If there are vertices x and y such that $d(x, u_r) > d(y, u_r)$ and $d_T(x) > d_T(y)$, then let $x_1, \dots, x_l$, where $l = \min\{d - d_T(y), d_T(x) - 2\}$, be l neighbors of x not on P. Consider the graph

$$T' = T - \{xx_1, \dots, xx_l\} + \{yx_1, \dots, yx_l\}.$$

Every vertex in T' has smaller or equal eccentricity as in T. Moreover, $d_{T'}(y) \geq d_T(x)$, $d_{T'}(x) \leq d_T(y)$ and $d_{T'}(y) - d_T(x) = d_T(y) - d_{T'}(x)$, so

$$d^a_{T'}(y) + d^a_{T'}(x) \geq d^a_T(y) + d^a_T(x)$$

by Lemma 2.1. Hence, $\mathrm{DEI}_{a,b}(T') \geq \mathrm{DEI}_{a,b}(T)$, which contradicts the choice of T, and we can conclude that there are no vertices $x, y \in V(T)$ such that $d(x, u_r) > d(y, u_r)$ and $d_T(x) > d_T(y)$.

Next, we prove that there cannot be any vertex x in T of degree at most $d-1$ and a pendant vertex v such that $d_T(u_r, v) > d_T(u_r, x) + 1$. Let x be a vertex of degree at most $d-1$ with shortest distance to u_r, and assume that there is a pendant vertex v of T such that $d_T(u_r, v) > d_T(u_r, x) + 1$. Suppose v is adjacent to w in T. Consider the tree $T'' = T - vw + xv$. Then every vertex of T'' has smaller or equal eccentricity than in T. Moreover, since $d_T(w) \leq d_T(x)$ (by the argument in the preceding paragraph),

$$d^a_{T''}(x) + d^a_{T''}(w) \geq d^a_T(x) + d^a_T(w)$$

by Lemma 2.1. Thus $\mathrm{DEI}_{a,b}(T'') \geq \mathrm{DEI}_{a,b}(T)$, which again contradicts the choice of T, so there cannot be any vertex x in T of degree at most $d-1$ and a pendant vertex v such that $d_T(u_r, v) > d_T(u_r, x) + 1$.

From the preceding paragraphs, we conclude that all vertices in T have degree d, except the ones in the last and second to last layer of T, if we view T as a d-ary tree with root u_r. It remains to prove that all vertices in the second to last layer have degree 1 or d, except for at most one vertex. So suppose that there are two vertices x and y such that $d(x, u_r) = d(y, u_r)$ and $d > d_T(x) \geq d_T(y) > 1$. Similar calculations as before shows that "moving" pendant vertices from the vertex y to the vertex x yields a tree T' with $\mathrm{DEI}_{a,b}(T') \geq \mathrm{DEI}_{a,b}(T)$. We omit these details and conclude that $T \cong V_{n,d}$.

Next, we prove the lower bound in (i). Suppose that T is an extremal tree for the lower bound. We prove by contradiction that T must be isomorphic to $B_{n,d}$. We assume that T is an extremal graph with as large diameter as possible, and among all these graphs we assume that T is one where a near-extremal vertex of a diametral path has as large degree as possible.

Let $P = u_0 u_1 \dots u_k$ be such a diametral path in T. Suppose first that there is a vertex not on P of degree at least two. Then there is such a vertex x which is adjacent to $s \geq 1$ pendant vertices $y_1, \dots, y_s$. Consider the graph

$$T' = T - \{xy_1, \dots, xy_s\} + \{u_0 y_1, \dots, u_0 y_s\}.$$

Every vertex in T' has equal or larger eccentricity than in T. Moreover, $d_{T'}(u_0) = d_T(x)$ and $d_{T'}(x) = d_T(u_0)$, and all other vertices have the same degree in T' than in T. Hence, $\mathrm{DEI}_{a,b}(T') \leq \mathrm{DEI}_{a,b}(T)$ and T' has a longer path than T, a contradiction.

Suppose now that only pendant vertices in T are adjacent to vertices in P, and that there is a vertex u_p distinct from u_1, u_{k-1} with degree at least 3 in T. If u_p is the only vertex of degree d in P then we consider the tree T'' obtained from T by joining $d - d_T(u_{k-1})$ pendant vertices adjacent to u_p to u_{k-1} instead, and removing the edges between u_p and these adjacent pendant vertices. As in the preceding paragraph, $\mathrm{DEI}_{a,b}(T'') \leq \mathrm{DEI}_{a,b}(T)$, which contradicts the choice of T.

Assume now instead that there are several vertices of degree d in P. Furthermore, we assume that u_p has smallest degree among the vertices in T with degrees in $\{3, \ldots, d\}$ that are distinct from u_{k-1} and u_1. Let y be a pendant vertex adjacent to u_p. We form the new tree $T'' = T - u_{p-1}u_p + u_{p-1}y$ from T. Every vertex in T'' has at least the same eccentricity as in T. Moreover, $d_{T'}(u_p) = d_T(u_p) - 1$ and $d_{T'}(y) = d_T(y) + 1 = 2$, and every other vertex has the same degree in T' as in T. Thus

$$d^a_{T'}(u_p) + d^a_{T'}(y) \leq d^a_T(u_p) + d^a_T(y)$$

by Lemma 2.1. This implies that $\mathrm{DEI}_{a,b}(T'') \leq \mathrm{DEI}_{a,b}(T)$, which is a contradiction to the choice of T. It follows that the only vertices of T that may have degree greater than 2 are u_{k-1} and u_1.

Now, if both these vertices have degree at least 3, then assume that u_{k-1} has smaller degree than u_1. Let y be a pendant vertex adjacent to u_{k-1}, and consider the tree $T^{(3)} = T - u_{k-1}y + u_k y$. Then every vertex in $T^{(3)}$ has at least the same eccentricity as in T. Moreover, $d_{T^{(3)}}(u_k) = 2 = d_T(u_k) + 1$ and $d_{T^{(3)}}(u_{k-1}) = d_T(u_{k-1}) - 1$, so

$$d^a_{T^{(3)}}(u_{k-1}) + d^a_{T^{(3)}}(u_k) \leq d^a_T(u_{k-1}) + d^a_T(u_k)$$

by Lemma 2.1. Since all other vertex degrees are the same in T and $T^{(3)}$, $\mathrm{DEI}_{a,b}(T^{(3)}) \leq \mathrm{DEI}_{a,b}(T)$, which again contradicts the choice of T.

This implies that there is only one vertex in T that has degree greater than 2, which in fact has degree d, and we conclude that T must be isomorphic to $B_{n,d}$. $\square$

Let us now prove that if $a > 1$ and $b < 0$, then we have strict inequalities in (i) in Theorem 1.2 if T is not isomorphic to $B_{n,d}$ or $V_{n,d}$, respectively. The corresponding statement for part (ii) can be proved similarly and is omitted.

Consider the proof of the upper bound in (i). In the third paragraph of the proof, we have that $\mathrm{DEI}_{a,b}(T') = \mathrm{DEI}_{a,b}(T)$ only if $b = 0$. Moreover, the same clearly holds for the trees T'' and T considered in the fourth paragraph of the proof. Thirdly, as for the trees T' and T considered in the fifth paragraph of the proof we have that $\mathrm{DEI}_{a,b}(T') = \mathrm{DEI}_{a,b}(T)$ only holds if $a = 1$. In conclusion, if $a > 1$ and $b < 0$, then we have strict inequality in the upper bound in part (i) in Theorem 1.2 if T is not isomorphic to $V_{n,d}$, respectively.

Let us now turn to the lower bound in the proof of part (i) of Theorem 1.2. In the second paragraph of the proof, we compare T' and T, and get that $\mathrm{DEI}_{a,b}(T') \leq \mathrm{DEI}_{a,b}(T)$ and equality holds only if $b = 0$. Then the tree T'' is formed and we clearly have $\mathrm{DEI}_{a,b}(T'') = \mathrm{DEI}_{a,b}(T)$ precisely when $b = 0$ and $a = 1$. Finally, in the second to last paragraph a tree $T^{(3)}$ is defined, and we have $\mathrm{DEI}_{a,b}(T^{(3)}) = \mathrm{DEI}_{a,b}(T)$ precisely when $a = 1$. We conclude that if $a > 1$ and $b < 0$, then we have equality in the lower bound in part (i) of Theorem 1.2 if and only if $T \cong B_{n,d}$.

3 Conclusion and Open Problems

In this paper, we have obtained upper and lower bounds on the general degree-eccentricity index

$$\mathrm{DEI}_{a,b}(G) = \sum_{v \in V(G)} d_G^a(v)\mathrm{ecc}_G^b(v),$$

for n-vertex trees T with a fixed maximum degree for the cases when $a \geq 1, b \leq 0$ and $0 \leq a \leq 1, b \geq 1$. Our results complement previous results on trees of general order and trees with given diameter [4, 5] (as well as other families of trees considered in [4, 5]).

Moreover, we have noted that for the case when $a, b \geq 1$, it is not possible to prove general upper and lower bounds for $\mathrm{DEI}_{a,b}$. However, it remains to consider the general degree-eccentricity index for other values of a and b. For instance, we have the following open problem.

Problem 3.1. *Determine upper and lower bounds on $DEI_{a,b}(T)$ for trees T of given order and maximum degree, when $a < 0, b > 0$.*

Naturally, this question can be studied for the more general family of trees with given order, as well as more restricted families obtained by fixing other graph invariants as well.

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References

[1] H. Dureja, S. Gupta, A. K. Madan, Predicting anti-HIV-1 activity of 6-arylbenzonitriles: computational approach using superaugmented eccentric connectivity topochemical indices, *J. Mol. Graph. Model.* 26 (2008), 1020–1029.

[2] A. Ilić, I. Gutman, Eccentric connectivity index of chemical trees, *MATCH Commun. Math. Comput. Chem.* 65 (2021), 731–744.

[3] V. Kumar, S. Sardana, A. K. Madan, Predicting anti-HIV activity of 2, 3-diaryl-1, 3-thiazolidin-4-ones: computational approach using reformed eccentric connectivity index, *J. Mol. Model.* 10 (2004), 399–407.

[4] M. Masre, On General Degree-Eccentricity Index For Trees with Fixed Diameter and Number of Pendant Vertices, *Iranian J. Math. Chem.* 14 (2023), 19–32.

[5] M. Masre, T. Vetrík, On the general degree-eccentricity index of a graph, *Afr. Mat.* 32 (2021), 495–506.

[6] M. Masre, T. Vetrík, General Degree-Eccentricity Index of Trees, *Bull. Malays. Math. Sci. Soc.* 44 (2021), 2753–2772.

[7] M. J. Morgan, S. Mukwembi, H. C. Swart, On the eccentric connectivity index of a graph, *Discrete Math.* 311 (2021), 1229–1234.

[8] T. Vetrík, M. Masre, Generalized eccentric connectivity index of trees and unicyclic graphs, *Discrete Appl. Math.* 284 (2020), 301–315.

[9] X. Wang, L. Tang, X. Chen, M. Li, Y. La, On the connective eccentricity index of graphs with fixed clique number, *Ars Combin.* 138 (2018), 105–117.

[10] K. Xu, K.C. Das, H. Liu, Some extremal results on the connective eccentricity index of graphs, *J. Math. Anal. Appl.* 433 (2016), 803–917.

[11] B. Zhou, Z. Du, On eccentric connectivity index, *MATCH Commun. Math. Comput. Chem.* 63 (2010), 181–198.

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