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Eccentric Connectivity Index: Extremal Graphs and Values

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ABSTRACT

Eccentric connectivity index has been found to have a low degeneracy and hence a significant potential of predicting biological activity of certain classes of chemical compounds. We present here explicit formulas for eccentric connectivity index of various families of graphs. We also show that the eccentric connectivity index grows at most polynomially with the number of vertices and determine the leading coefficient in the asymptotic behavior.

Keywords: Eccentric connectivity index, Extremal graph.

1 INTRODUCTION

One of the most serious problems affecting the use of topological descriptors in mathematical chemistry is their degeneracy — the fact that there are two or more graphs with same value of given descriptor. The recently considered eccentric connectivity index and its derivatives were found to exhibit quite low degeneracy. This fact, along with simplicity of required computations, makes them potentially very useful for predicting various properties of many classes of chemical compounds. Indeed, they have been found to perform better than several other standard topological descriptors [3,7,8,9,11]. In spite of the growing number of papers concerned with their particular applications, their basic mathematical properties have not been studied until very recently. Then two papers appeared reporting various upper and lower bounds on the eccentric connectivity index for trees subject to certain constraints [13,5]. It was found that the extremal values of the eccentric connectivity index among all trees on a given number of vertices are attained on paths and stars. It was also shown that the stars are extremal among all graphs. The main goal of this paper is to further this line of research by going beyond the trees. Along the way we first give explicit formulas for the values of the eccentric connectivity index for several families of graphs in terms of their size, and then prove that the eccentric connectivity index grows no faster than a cubic polynomial in the number of vertices. We determine the coefficient of the leading term and show that the bound is asymptotically sharp by constructing a family of graphs for which the leading term of the cubic bound is attained. We also offer an alternative proof of the extremality result for general trees. The paper is concluded by indicating some possible directions for future research.

2 DEFINITIONS AND PRELIMINARIES

All graphs in this paper are finite, simple and connected. For terms and concepts not defined here we refer the reader to any of several standard monographs such as, e.g., [4] or [12].

Let G be a graph on n vertices. We denote the vertex and the edge set of G by $V(G)$ and $E(G)$, respectively. For two vertices u and v of $V(G)$ we define their **distance** $d(u,v)$ as the length of any shortest path connecting u and v in G. For a given vertex u of $V(G)$ its **eccentricity** $\varepsilon(u)$ is the largest distance between u and any other vertex v of G. Hence, $\varepsilon(u) = \max_{v\in V(G)} d(u,v)$. The maximum eccentricity over all vertices of G is called the **diameter** of G and denoted by $D(G)$; the minimum eccentricity among the vertices of G is called the **radius** of G and denoted by $R(G)$. The set of vertices whose eccentricity is equal to the radius of G is called the **center** of G. It is well known that each tree has either one or two vertices in its center. The **eccentric connectivity index** $\xi(G)$ of a graph G is defined as

$$\xi(G) = \sum \delta_u \varepsilon(u),$$

where δ_u denotes the degree of vertex u, i.e., the number of its neighbors in G.

A graph G is **vertex-transitive** if its automorphism group is transitive. For a vertex-transitive graph G its center coincides with $V(G)$. Since a vertex-transitive graph is necessarily regular, we have a particularly simple expression for the eccentric connectivity index of a vertex transitive graph.

Proposition 1. Let G be a vertex-transitive graph on n vertices of degree δ. Then

$$\xi(G) = n\delta R(G).$$

■

As a consequence, we obtain explicit formulas for the eccentric connectivity indices of several familiar classes of graphs.

Corollary 2.

(1) $\xi(K_n) = n(n-1)$;

(2) $\xi(C_n) = 2n\left\lfloor \frac{n}{2} \right\rfloor$;

(3) $\xi(\Pi_m) = 6m\left\lfloor \frac{m}{2}+1 \right\rfloor$;

(4) $\xi(A_m) = 8m\left\lfloor \frac{m}{2}+1 \right\rfloor$;

(5) $\xi(Q_m) = m^2 2^m$.

Here K_n, C_n, Π_m, A_m and Q_m denote the complete graph on n vertices, the cycle on n vertices, the m–sided prism, the m–sided antiprism, and the m–dimensional hypercube, respectively.

■

The following results can be easily obtained by a straightforward computation.

Proposition 3. Let $K_{m,n}$ be a complete bipartite graph on $m+n$ vertices. For $m,n \geq 2$, we have $\xi(K_{m,n}) = 4mn$. In particular, $\xi(K_{m,n}) = 4n^2$ for $n \geq 2$.

■

The case of the complete bipartite graph $K_{m,n}$ when one of the classes of bipartition is of size 1 is treated separately. In order to facilitate the comparison with other trees on n vertices, we find it more convenient to state the result as follows.

Proposition 4. Let $S_n = K_{1,n-1}$ be a star on $n \geq 3$ vertices. Then $\xi(S_n) = 3(n-1)$.

■

The results of Propositions 3 and 4 and the first two cases of Corollary 2 were obtained in [13].

Proposition 5. Let W_n and B_n denote the graphs of the pyramid and the bipyramid with n–gonal base. Then $\xi(W_n) = 7n$ and $\xi(B_n) = 12n$.

■

(The pyramid graph W_n is also known as the wheel graph on n spokes.)

The last result of this section is concerned with paths on n vertices. It was also, in a slightly different way, reported in [13].

Proposition 6. Let P_n be a path on n vertices. Then

$$\xi(P_n) = \begin{cases} \frac{3}{2}(n-1)^2 & \textit{for n odd}; \\ \frac{3}{2}n(n-2)+2 & \textit{for n even.} \end{cases}$$

■

The above result can be written in a more compact form.

Proposition 7. Let P_n be a path on n vertices. Then

$$\xi(P_n) = 6\left\lfloor \frac{n-1}{2} \right\rfloor \left\lceil \frac{n-1}{2} \right\rceil + 1 + (-1)^n .$$

■

3 EXTREMAL TREES

It was proved in [13] that the path on n vertices and the star on n vertices are extremal with respect to the eccentric connectivity index among all trees on n vertices. In this section we offer an alternative proof of this fact based on the concept of remote vertices.

Let T_n be a tree on n vertices. A vertex $v \in V(T_n)$ is **remote** if the eccentricity of some other vertex of T_n is achieved on v, i.e., if $\varepsilon(u) = d(u,v)$ for some vertex $u \neq v$. A remote vertex v is **strictly remote** if there is a vertex $u \in V(T_n)$ such that ε (u) = $d(u,v) > d(u,w)$ for all vertices $w \in V(T_n)$, $w \neq v$. For a remote vertex v we denote by $Z(v)$ the set of all vertices whose eccentricity is attained on v. The cardinality of $Z(v)$ we denote by $\zeta(v)$.

Lemma 8. Let w be an interior vertex of T_n . Then w is not remote.

Proof Let v be a vertex from $Z(w)$ and $\varepsilon(v) = d(v,w)$ is the length of the unique path P in T_n connecting v and w. This path contains exactly one of $\delta_w \geq 2$ edges incident with w. By adding to P any of the remaining $\delta_w - 1$ edges incident with w, say the edge wu, we obtain a path P' that is longer than P. Further, $d(v,u) = d(v,w) + 1 > \varepsilon(v)$, a contradiction with the supposed remoteness of w.

■

Hence, any remote vertex is necessarily a leaf. The converse is not true – there are leaves that are not remote. However, any tree must contain at least two remote leaves.

Lemma 9. Every tree on $n \geq 2$ vertices contains at least two remote leaves.

Proof Let u be an interior vertex of a tree T_n on n vertices. The eccentricity $\varepsilon(u)$ is attained on a leaf v_1 of T_n. Further, $\varepsilon(v_1)$ is attained on some other vertex v_2, and v_2 is a leaf. Hence, both v_1 and v_2 are remote, and since each tree on $n > 1$ vertices has at least two leaves, the claim follows.

■

The existence of non–remote, or at least non-strictly remote leaves will be crucial for our main result.

Lemma 10. Let $T_n \neq P_n$ be a tree on n vertices. Then there is a leaf v in T_n which is not strictly remote.

Proof Since $T_n \neq P_n$, there is an interior vertex w of degree $\delta_w \geq 3$. Also, the number k of leaves of T_n is at least three. Let us denote those leaves by $v_1, \cdots, v_k$, and let v_p be such that $d(w,v_p) \leq d(w,v_i)$ for all $i \neq p$. Let us suppose that v_p is strictly remote. Then there is a leaf v_q such that $d(v_q,v_p) > d(v_q,v_i)$ for all $i \neq p$. There is exactly one path P in T_n connecting v_q and v_p, and this path either contains vertex w or not. The two possibilities are shown in Fig. 1 a) and b), respectively. If P contains w, then the path P_i from v_q

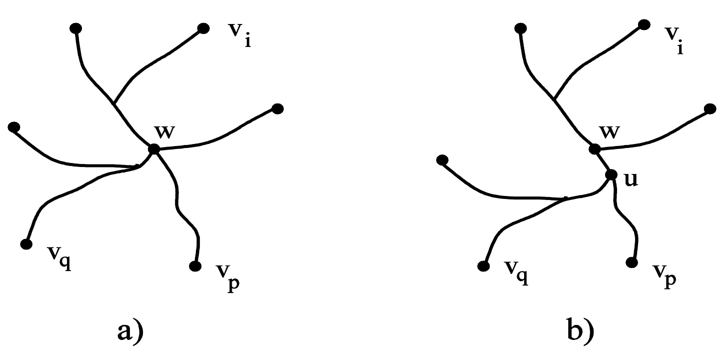

Figure 1: With the proof of Lemma 10.

to any of v_i, $i \neq p$, is at least as long as the path from v_q to v_p, since the sub-path from w to v_i is at least as long as the sub–path of P from w to v_p. This is in contradiction with the supposed strict remoteness of vertex v_p. If P does not contain w, it must contain a vertex, say u, from the path connecting w and v_p. Again, by concatenating the paths from v_q to u, from u to w, and from w to any of v_i, we obtain a path from v_q to v_i , $i \neq p$, longer than P This implies that $\varepsilon(v_q) > d(v_q, v_p)$, a contradiction with the fact that v_p is strictly remote.

■

We now take a tree T_n on n vertices and transform it in the following way. Let v be a leaf of T_n that is not strictly remote. It is attached to an internal vertex w. Let $\varepsilon(v)$ is achieved on a leaf z_1. Then $\varepsilon(z_1) \geq \varepsilon(v)$, since v is not strictly remote. Let z_2 is a leaf such the $\varepsilon(z_1) = d(z_1, z_2)$. Then $\varepsilon(z_2) \geq \varepsilon(z_1) \geq \varepsilon(v)$. By detaching vertex v from w and attaching it to z_2 we obtain a tree T'_n on the same number of vertices. We say that the vertex v is pivotal for the above transformation. The procedure is illustrated in Fig. 2.

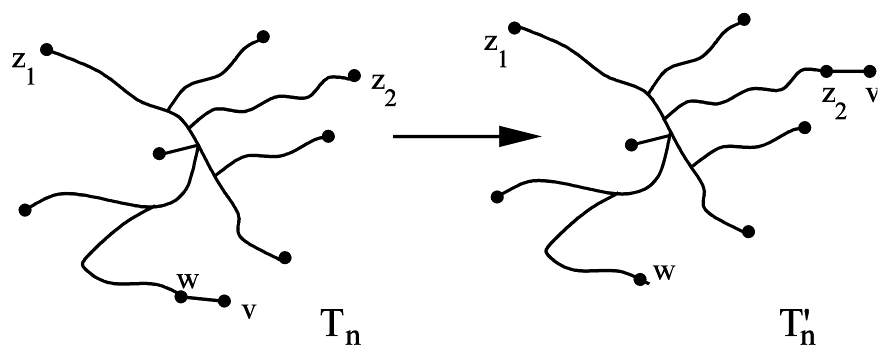

Figure 2: The eccentric connectivity index increasing transformation

We claim that the described transformation with any non-strictly remote pivotal leaf increases the eccentric connectivity index.

Proposition 11.

$$\zeta(T'_n) > \zeta(T_n).$$

Proof The eccentric connectivity index of a graph G is computed by summing the contributions of the form $\delta_u \varepsilon(u)$ over all vertices u of G. Since v is not strictly remote, no vertex of T_n will suffer a decrease of its eccentricity when v is detached from w. The degree of vertex v is equal to one in both T_n and T'_n; however, its eccentricity in T_n is equal to $\varepsilon(z_2) + 1$, hence exceeding its eccentricity in T_n. (Remember that $\varepsilon(z_2) \geq \varepsilon(v)$ in T_n.) The only contribution in T'_n that is smaller than the corresponding contribution in T_n is the one of vertex w, since its degree decreased by one. Hence, the difference of the contributions of vertex w to $\xi(T'_n)$ and $\xi(T_n)$, respectively, is $\varepsilon(w)$. But this decrease is more than compensated for by the increased contribution of vertex z_2: its contribution will increase by $\varepsilon(z_2) \geq \varepsilon(v) > \varepsilon(w)$, due to the increased degree of z_2 in T'_n. Finally, there is additional increase by one of the eccentricities of all $\zeta(z_2) > 0$ vertices of $Z(z_2)$. Hence, the total sum of all contributions $\delta_u \varepsilon(u)$ of all vertices in T_n strictly exceeds the sum of corresponding contributions to $\xi(T'_n)$, and the claim follows.

■

Now we can prove the result on extremal trees.

Theorem 12. Let T_n be a tree on n vertices, $T_n \neq P_n$, $T_n \neq S_n$. Then

$$\xi(S_n) < \xi(T_n) < \xi(P_n).$$

Proof The right hand side inequality follows from Proposition 11. For any tree $T_n \neq P_n$ it is always possible to construct a tree T'_n on n vertices with $\xi(T'_n) > \xi(T_n)$. By iterating the above procedure one will always end with P_n. To see that the procedure indeed stops, one should notice that vertex v becomes strictly remote in T'_n; hence, it cannot be pivotal in the next iteration. Further, if w was an interior vertex of degree $\delta_w \geq 3$ in T_n, then the number of leaves in T_n that are not strictly remote is decreased by one. If w was an interior vertex of degree 2 in T_n, it becomes a leaf in T'_n, and it is not strictly remote. Hence we repeat the procedure taking w as the pivotal leaf. After a finite number of steps we will reach an interior vertex of degree greater than two, and at this point the number of non-strictly remote leaves will drop by one. Hence, the iterations stop after a finite number of steps and the algorithm terminates with the only tree without non-strictly remote vertices i.e., with P_n.

The left hand side inequality follows by considering a transformation that is, in a sense, inverse to the one described above. For a given tree $T_n \neq S_n$ on n vertices one takes a remote leaf, say v, detaches it from its neighbor u, and attaches it to an interior vertex w of the largest degree in T_n, thus obtaining a tree T''_n on the same number of vertices. It can be shown that the increased contribution of vertex w to $\xi(T''_n)$ is more than offset by the decreased contributions of vertices u, v, and any vertices of $Z(v)$ if v was strictly remote in T_n. The reasoning is analogous to the one used in establishing the right hand side inequality, and we omit the details.

■

4 EXTREMAL GRAPHS

It can be inferred from the previous section that the eccentric connectivity index of a tree is at least linear and at most quadratic in the number of vertices. Then, none of the eccentric connectivity indices of Corollary 2 is more than quadratic in the number of vertices. Moreover, from case (5) of Corollary 2 one can see that the eccentric connectivity index of the m–dimensional hypercube Q_m is asymptotically proportional to $n\ (log\ n)^2$, where $n = 2^m$ is the number of vertices of Q_m. By considering a regular dendrimer one can show that the growth rates of the type $n\ log\ n$ are also possible among the trees. Hence, the question arises: Are the growth rates of the eccentric connectivity index on trees representative for all graphs?

On the lower end of the span the answer is affirmative. It was shown in [13] that the n-vertex star has the smallest eccentric connectivity index among all connected graphs on n vertices. Furthermore, in the same paper it was established that the linear growth rate of the eccentric connectivity index can be also achieved on graphs with cycles.

The upper edge of the possible range of the eccentric connectivity index is more interesting. It is not difficult to see that the eccentric connectivity index of any graph must be bounded by a cubic polynomial in the number of vertices. Both the diameter and the degree are bounded from above by n-1 and the summation over all vertices results in a factor bounded by n. So, for any graph G on n vertices we have $\xi(G) = O(n^3)$. In the rest of this section we prove that this upper bound is actually achieved. Furthermore, we find the leading coefficient and we prove that the bound is asymptotically sharp.

Theorem 13. Let G be a connected graph on n vertices. Then the maximum possible value of the eccentric connectivity index of G is given by

$$\xi(G) = \frac{4}{27}n^3 + o(n^2).$$

Proof Let us consider a complete graph on $\left\lfloor \frac{2n}{3} \right\rfloor$ vertices and identify one of its vertices with an end-vertex of a path on $n - \left\lfloor \frac{2n}{3} \right\rfloor + 1$ vertices. We denote the obtained graph by L_n and call it a **lollipop** on n vertices. An example is shown in Fig. 3.

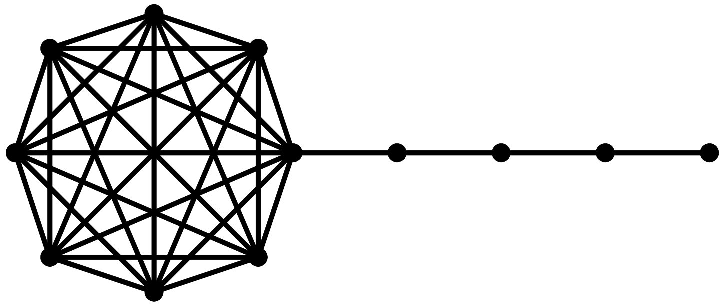

Figure 3: A lollipop on 12 vertices.

Each vertex of $K\left\lfloor \frac{2n}{3} \right\rfloor$ has the eccentricity of at least $\frac{n}{3}$, so their collective contribution to $\xi(L_n)$ is at least

$$\frac{n}{3}\left\lfloor \frac{2n}{3} \right\rfloor\left(\left\lfloor \frac{2n}{3} \right\rfloor - 1\right) = \frac{4}{27}n^3 + o(n^2).$$

The total contribution of vertices in the attached path is quadratic in $n/3$, and hence cannot affect the leading term in the above expression. Hence

$$\xi(L_n) \leq \frac{4}{27}n^3 + o(n^2).$$

We have constructed a graph on n vertices whose eccentric connectivity index is cubic in the number of vertices with the leading coefficient of 4/27. Now we show that no other graph on n vertices can do (much) better.

Let G be an arbitrary graph on n vertices and P a diametral path in G of length n-x. Then each vertex in $V(G) \setminus V(P)$ is connected with at most three vertices of P. (If a vertex $v \in V(G) \setminus V(P)$ is connected with more than three vertices of P, then the distance between the end-vertices of P is less than $n - x$, a contradiction with the fact that P is diametral. Moreover, if a vertex $v \in V(G) \setminus V(P)$ is connected with three vertices of P, then these vertices must be consecutive.) This gives us an upper bound on the number of edges in G.

$$|E(G)| \leq \binom{x}{2} + (n-1-1) + 3(n-x) = \frac{x^2}{2} - \frac{9x}{2} + 4n - 1.$$

Since the eccentricity of any vertex cannot exceed the diameter, and the sum of all degrees is twice the number of edges, we obtain the following upper bound:

$$\xi(G) \leq 2(n-x)\left(\frac{x^2}{2} - \frac{9x}{2} + 4n - 1\right).$$

Consider now the right hand side of the above expression as a function of x,

$$f(x) = 2n\,(4n - 1) + (2 - 17n)\,x + (n + 9)\,x^2 - x^3.$$

By using elementary calculus it follows that $f'(x)$ has two real zeros for all $n \geq 31$ and that $f(x)$ achieves its maximum for $x_2 = \frac{1}{3}(n + 9 + \sqrt{n^2 - 33n + 87})$. The maximum value of $f(x)$ is given by

$$f(x_2) = \frac{1}{27}[2n^3 + 2n^2\sqrt{n^2 - 33n + 87} + 117n^2$$
$$-3n(309 + 22\sqrt{n^2 - 33n + 87}) + 6(270 + 29\sqrt{n^2 - 33n + 87})].$$

Since $\sqrt{n^2 - 33n + 87}$ cannot exceed n for $n \geq 31$, we have

$$f(x_2) \leq \frac{4}{27}n^3 + o(n^2).$$

Hence $\xi(G) \leq \frac{4}{27}n^3 + o(n^2)$ for any graph G on n vertices and the claim follows.

■

5 FURTHER DEVELOPMENTS

We have presented the extremal graphs and extremal values for the eccentric connectivity index, a graph-theoretical descriptor whose potential usefulness in QSAR/QSPR modeling has been empirically confirmed in a number of recent papers. It follows from Theorem 12 that this index behaves well on class of all trees, achieving its extremal values on two trees that are also extremal for several other topological indices. This fact lends some theoretical support to its potential for use in predicting properties and behavior of chemical compounds. We have also determined the maximum order of growth for this index over general graphs. However, much remains to be done. For example, it would be interesting to compute the values of $\xi(G)$ for various classes of linear and reticular polymers. Dendrimers of various types should allow expressing their eccentric connectivity indices in closed forms, and open and closed nanotubes also seem promising in this respect. It would be also interesting to determine the cubic graphs extremal with respect to the eccentric connectivity index. Last, but not the least, it would be interesting to explore various classes of composite graphs and to see which ones admit nice closed formulas for the eccentric connectivity indices.

We have left the derivative indices of the eccentric connectivity index completely out of the scope of this paper [1,6]. Extending the results of further research also to those indices seems the most natural course of future work.

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