On the maximal eccentric connectivity indices of graphs

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Abstract. For a connected simple graph G, the eccentricity ec(v) of a vertex v in G is the distance from v to a vertex farthest from v, and d(v) denotes the degree of a vertex v. The eccentric connectivity index of G, denoted by $\xi^{c}(G)$, is defined as $\sum_{v \in V(G)} d(v)ec(v)$. In this paper, we will determine the graphs with maximal eccentric connectivity index among the connected graphs with n vertices and m edges $(n \le m \le n+4)$, and propose a conjecture on the graphs with maximal eccentric connectivity index among the connected graphs with n vertices and m edges $(m \ge n+5)$.

§1 Introduction and notation

For a connected simple graph G, we define the distance d(u, v) between two vertices u and v as the length of the shortest path connecting u and v in G. The eccentricity ec(v) of a vertex v in a connected graph G is the distance between v and a vertex farthest from v. The diameter Diam(G) of G is the maximum eccentricity among the vertices of G. The eccentric connectivity index of G [5], denoted by $\xi^{c}(G)$, is defined as

$$\xi^{c}(G) = \sum_{v \in V(G)} ec(v)d(v) = \sum_{uv \in E(G)} \omega_{G}(uv),$$

where $\omega_G(uv)$ denotes the weight of edge uv in G and equals ec(u) + ec(v).

As a novel, distance-cum-adjacency topological descriptor, the eccentric connectivity index provides excellent correlations with regard to both physical and biological properties of chemical substances. The simplicity amalgamated with high correlating ability of this index can be easily exploited in QSPR/QSAR studies (see [2, 5]). Recently, many results on the eccentric connectivity index have been obtained for various classes of graphs, see, for example, [1,3,4,6]. Let $d_{n,m} = \left\lfloor \frac{2n+1-\sqrt{17+8(m-n)}}{2} \right\rfloor$, and $E_{n,m}$ be the graph obtained from a path $P_{d_{n,m}+1} =$

 $v_0v_1 \ldots v_{d_{n,m}}$ by joining each vertex of $K_{n-d_{n,m-1}}$ to both $v_{d_{n,m}}$ and $v_{d_{n,m-1}}$, and by joining

Received: 2012-03-25.

MR Subject Classification: 05C12, 05A15, 05A20, 05C05.

Keywords: Eccentric connectivity index, diameter, distance.

Digital Object Identifier(DOI): 10.1007/s11766-014-3023-7.

Supported by China Postdoctoral Science Foundation (2012M520815 and 2013T60411), and the National Natural Science Foundation of China (11001089).

 $m-n+1-\binom{n-d_{n,m}}{2}$ vertices of $K_{n-d_{n,m-1}}$ to $v_{d_{n,m-2}}$. Clearly, $E_{n,n-1} \cong P_n$. In this paper, we will show that for $8 \le n \le m \le n+2$ and $14 \le n+3 \le m \le n+4$, $E_{n,m}$ is the unique graph with maximal eccentric connectivity index among the connected graphs with n vertices and m edges, respectively. Finally, we conjecture that $n+5 \le m \le n(n-1)/2$ and $d_{n,m} \ge 3$, $E_{n,m}$ is the graph with maximal eccentric connectivity index among the connected graphs with n vertices and m edges.

§2 Main results

Let $T_{n,i}$ be the tree obtained from $P_{n-1} = v_0 v_1 \dots v_{n-2}$ by attaching a pendent vertex v_{n-1} to v_i , where $1 \le i \le \lfloor \frac{n-2}{2} \rfloor$. Let $T_a^{n,p}$ be the tree obtained by attaching a and p-a pendent vertices respectively to the two end vertices of the path P_{n-p} for $1 \le a \le \lfloor \frac{p}{2} \rfloor$, and let $T^{n,p} = \{T_a^{n,p} | 1 \le a \le \lfloor \frac{p}{2} \rfloor, 2 \le p \le n-2\}.$

Lemma 2.1. [6] Among the trees on n vertices with at least p pendent vertices, any tree $T \in T^{n,p}$ reaches the maximal value on the eccentric connectivity index. Moreover, P_n , $T_{n,1}$ and $T_{n,2}$ are respectively the only trees with the first three maximal eccentric connectivity indices.

Theorem 2.1. Let G be a graph with n vertices and n edges, that is, G is a unicyclic graph, where $n \ge 6$. Then $\xi^c(G) \le \xi^c(E_{n,n})$, with equality if and only if $G \cong E_{n,n}$.

Proof. Let G be a unicyclic graph on n vertices. Then $Diam(G) \leq n-2$ and $\omega(e) \leq 2n-4$ for any edge $e \in E(G)$. If $G \not\cong C_n$, then we can always find an edge e of G such that G-e is a tree with at least three pendent vertices. By Lemma 2.1 we have $\xi^c(G) \leq \xi^c(G-e) + \omega(e) \leq$ $\xi^c(T_{n,1}) + 2n - 4 = \xi^c(E_{n,n})$. Note that $\omega(e) = 2n - 4$ implies $G \cong E_{n,n}$, thus the equality holds if and only if $G \cong E_{n,n}$.

Suppose that $G \cong C_n$, where $n \ge 6$. If n is even, then we have $\xi^c(C_n) = n^2 < \frac{3(n-2)^2}{2} + 4n - 9 = \xi^c(E_{n,n})$; if n is odd, then $\xi^c(C_n) = n^2 - n < \frac{3(n-2)^2+1}{2} + 4n - 9 = \xi^c(E_{n,n})$. The result now follows.

Let $Q_{n,n}$ be the tree obtained from $P_{n-1} = v_0 v_1 \dots v_{n-2}$ by joining an isolated vertex v_{n-1} to both v_{n-2} and v_{n-4} .

Lemma 2.2. Let G be a unicyclic graph on n vertices, $n \ge 6$ and $G \not\cong E_{n,n}$. Then $\xi^c(G) \le \xi^c(Q_{n,n})$, with equality if and only if $G \cong Q_{n,n}$.

Proof. By applying an argument similar to the proof of Theorem 2.1, we can show that the result is true for the case $G \cong C_n$. Suppose that G is not a cycle on n vertices. Let g(G) be the length of the unique cycle in G. If $g(G) \ge 5$, then $Diam(G) \le n-3$ and there exists an edge e in the unique cycle of G such that $G - e \not\cong P_n, T_{n,1}, T_{n,2}$, and

$$\xi^{c}(G) \leq \xi^{c}(G-e) + \omega(e) \leq \xi^{c}(T_{n,2}) + 2n - 6 < \xi^{c}(T_{n,2}) + 2n - 5 = \xi^{c}(Q_{n,n}).$$

If g(G) = 4 and $n \ge 7$, then $Diam(G) \le n-2$ and there is an edge e such that G - e is a tree such that $G - e \not\cong P_n, T_{n,1}$. Clearly, there exists no edge of weight 2n - 4 in G. Then

$$\xi^{c}(G) \leq \xi^{c}(G-e) + \omega(e) \leq \xi^{c}(T_{n,2}) + 2n - 5 = \xi^{c}(Q_{n,n}),$$

with equality only if $G - e \cong T_{n,2}$ and $\omega(e) = 2n - 5$. These imply that $G \cong Q_{n,n}$. By simple computation we can also obtain the result for n = 6.

If g(G) = 3, and $G \not\cong E_{n,n}$, then there is an edge e such that $G - e \not\cong P_n, T_{n,1}$. If $Diam(G) \leq n-3$, similarly, the result follows. If Diam(G) = n-2, then G is the graph obtained from $P_{n-1} = v_0v_1 \dots v_{n-2}$ by joining an isolated vertex v_{n-1} to both v_i and v_{i+1} , where $1 \leq i \leq n-4$. Then

 $\xi^{c}(Q_{n,n}) - \xi^{c}(G) = 4n - 12 - \omega(v_{i}v_{n-1}) - \omega(v_{i+1}v_{n-1}) \ge 4n - 12 - (2n - 7) - (2n - 6) > 0.$ These complete the proof.

Theorem 2.2. Let G be a connected graph with n vertices and n+1 edges, where $n \ge 6$. Then $\xi^{c}(G) \le \xi^{c}(E_{n,n+1})$, with equality if and only if $G \cong E_{n,n+1}$.

Proof. Let G be a graph on n vertices with n + 1 edges and exactly two cycles. Then we know that $Diam(G) \leq n - 3$ and there exists an edge e in a cycle such that G - e has two pendent vertices, thus G - e is not isomorphic to $E_{n,n}$ and $Q_{n,n}$, and by Theorem 2.2, we have

$$\xi^{c}(G) \leq \xi^{c}(G-e) + \omega(e) < \xi^{c}(Q_{n,n}) + 2n - 6 = \xi^{c}(E_{n,n+1}).$$

Let G have three cycles, then there is an edge e such that $G - e \not\cong E_{n,n}$. If Diam(G) = n-2, then G is obtained from $P_{n-1} = v_0 v_1 \dots v_{n-2}$ by joining an isolated vertex v_{n-1} with v_{i-1}, v_i and v_{i+1} , where $1 \leq i \leq \lfloor \frac{n-2}{2} \rfloor$. If i = 1, then $G \cong E_{n,n+1}$. Let $i \geq 2$. It is easy to prove that $\xi^c(G) < \xi^c(E_{n,n+1})$. If $Diam(G) \leq n-3$, by Theorem 2.2 we have

$$\xi^{c}(G) \le \xi^{c}(G-e) + \omega(e) \le \xi^{c}(Q_{n,n}) + 2n - 6 = \xi^{c}(E_{n,n+1}).$$

If $G - e \cong Q_{n,n}$, then Diam(G) < Diam(G - e). Thus $\xi^c(G) < \xi^c(G - e) + \omega(e)$ and $\xi^c(G) < \xi^c(E_{n,n+1})$. If $G - e \not\cong Q_{n,n}$, then by Lemma 2.2 we have that $\xi^c(G - e) < \xi^c(Q_{n,n})$. Thus $\xi^c(G) < \xi^c(E_{n,n+1})$.

Theorem 2.3. Let G be a connected graph with n vertices and n+2 edges, where $n \ge 8$. Then $\xi^{c}(G) \le \xi^{c}(E_{n,n+2})$, with equality if and only if $G \cong E_{n,n+2}$.

Proof. If G has a spanning tree T with at least four pendent vertices, and let e_1, e_2, e_3 be the edges not in T, that is, $T + e_1 + e_2 + e_3 = G$. Note that $Diam(G) \le n - 3$, by Lemma 2.1 we have

$$\xi^{c}(G) \leq \xi^{c}(T) + \omega(e_{1}) + \omega(e_{2}) + \omega(e_{3}) \leq \xi^{c}(T_{1}^{n,4}) + 3(2n-6) = \xi^{c}(E_{n,n+2}).$$

It is easy to prove that the above equality holds if and only if $G \cong E_{n,n+2}$.

Suppose that all spanning trees of G have at most three pendent vertices. If $G - e_1$ has two edge-disjoint cycles for any edge e_1 of a cycle in G, then we can always find edges e_2, e_3 such that $G - e_1 - e_2 - e_3$ is a spanning trees with at least four pendent vertices, this is a contradiction. Then for any edge e_1 in a cycle of $G, G - e_1$ must have exactly three cycles, and ZHANG Jian-bin, et al.

G has exactly a non-trivial block (the block has at least three edges) that is showed in Fig.1.



Fig.1. Graphs H_1 and H_2 .

Clearly, $H_2 - e_1 - e_2 - e_3$ have four pendent vertices, then $G - e_1 - e_2 - e_3$ must contain at least four pendent vertices and the non-trivial block of G is not isomorphic to H_2 . If $G \not\cong H_1$, then G can be obtained from H_1 by planting many trees to it. Suppose that there is a tree planting to a vertex but not u_1 of P^4 in Fig.1, we choose three edges e_1, e_2, e_3 respectively at the path P^1, P^2, P^3 in Fig.1. Then $G - e_1 - e_2 - e_3$ have four pendent vertices, that is a contradiction. Thus it must be $G \cong H_1$ and $Diam(G) \leq \lfloor \frac{n}{2} \rfloor$. For $n \geq 8$, we have $\xi^c(G) \leq 2(n+2)\lfloor \frac{n}{2} \rfloor < \lfloor \frac{3(n-3)^2+1}{2} \rfloor + 10n - 32 = \xi^c(E_{n,n+2})$.

Theorem 2.4. Let G be a connected graph with n vertices and m edges, where $n \ge 11$ and m = n + 3. Then $\xi^c(G) \le \xi^c(E_{n,m})$, with equality if and only if $G \cong E_{n,m}$.

Proof. If there is an edge e such that $\omega(e) \leq 2n - 12$ and G - e is connected, then we have $\xi^c(G) \leq \xi^c(G-e) + 2n - 12 \leq \xi^c(E_{n,n+2}) + 2n - 12 = \xi^c(E_{n,n+3}).$

If $G - e \cong E_{n,n+2}$, then G is obtained by adding an edge to $E_{n,n+2}$, and the first inequality above is strict. If $G - e \not\cong E_{n,n+2}$, then by Theorem 2.3 $\xi^c(G - e) < \xi^c(E_{n,n+2})$ and $\xi^c(G) < \xi^c(E_{n,n+3})$. Thus the conclusion is correct for $Diam(G) \le n - 6$.

Let Diam(G) = n - 5. If $n \le 13$, then $\xi^c(G) \le 2(n - 5)m < \left\lfloor \frac{3(n - 3)^2 + 1}{2} \right\rfloor + 12n - 44 = \xi^c(E_{n,n+3}).$

Let $n \ge 14$. Suppose that $v_0v_1 \dots v_{n-7}v_{n-6}v_{n-5}$ is a diametral path of G, and v_{n-4} , v_{n-3} , v_{n-2} , v_{n-1} are the vertices not in the given diametral path. We need to consider two cases:(a) there exists an edge v_iv_{i+1} $(1 \le i \le n-7)$ in a non-trivial block of G (the block has at least three edges) and (b) each edge v_iv_{i+1} for $1 \le i \le n-7$ is a cut edge of G.

Case (a): there exists an edge $v_i v_{i+1}$ $(1 \le i \le n-7)$ in a non-trivial block of G. Let $k \in \{n-4, n-3, n-2, n-1\}$.

If the path $P_{v_iv_k}$ of length $d(v_i, v_k)$ passes a cut vertex in the given diametral path, then $d(v_i, v_k) \leq \max\{d(v_i, v_0), d(v_i, v_{n-5})\}.$

If it does not pass any cut vertex in the given diametral path, then there exists *i* such that $d(v_i, v_k) \leq 10/2 \leq \frac{14-3}{2} \leq \max\{d(v_i, v_0), d(v_i, v_{n-5})\}.$

Thus there is an edge $v_i v_{i+1}$ whose weight is not greater than 2n - 12. From the first part of the theorem, the conclusion is correct.

Case (b): each edge $v_i v_{i+1}$ for $1 \le i \le n-7$ is a cut edge of G. In this case, for any vertex $u, ec(u) = \max\{d(u, v_0), d(u, v_{n-5})\}$, by comparing the sum of the weights of edges in G with

these of $E_{n,m}$, we obtain the result.

Let Diam(G) = n - 4, and $v_0v_1 \dots v_{n-4}$ be a diametral path. Since $n \ge 11$, we can show that $ec(v_i) = \max\{d(v_i, v_0), d(v_i, v_{n-4})\}$ for $0 \le i \le n - 4$ similarly. Then

 $\xi^{c}(G) \leq \xi^{c}(P_{n-3}) + (m-n+4)(2n-8) = \left\lfloor \frac{3(n-4)^{2}+1}{2} \right\rfloor + (m-n+4)(2n-8) < \xi^{c}(E_{n,m}).$

Let Diam(G) = n - 3. Then there are exactly two vertices not in a given diametral path, each of which is adjacent to at least two vertices of the path, and the sum of the weights of edges not in the given diametral path of G is not greater than that of $E_{n,m}$. Thus we complete the proof.

Since $\xi^c(E_{n,n+4}) - \xi^c(E_{n,n+3}) = 2n - 12$ and $d_{n,n+4} = d_{n,n+3} = n - 3$, we can obtain the following theorem similarly.

Theorem 2.5. Let G be a connected graph with n vertices and m edges, where $n \ge 11$ and m = n + 4. Then $\xi^c(G) \le \xi^c(E_{n,m})$, with equality if and only if $G \cong E_{n,m}$.

Finally, we propose

Conjecture 2.1. Let $d_{n,m} \ge 3$. Then $E_{n,m}$ is the unique graph with maximal eccentric connectivity index among all connected graphs with n vertices and m edges.

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