International Mathematical Forum, Vol. 7, 2012, no. 6, 273 - 280

The Edge Version of Eccentric Connectivity Index

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Abstract

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. The eccentric connectivity index of G, denoted by $\xi^c(G)$, is defined as $\sum_{v\in V(G)} deg(v)ec(v)$, where $deg(v)$ is the degree of a vertex v and $ec(v)$ is its eccentricity. In this paper, we propose the edge version of the above index, the *edge eccentric connectivity index* of G, denoted by $\xi^c_e(G)$, which is defined as $\xi^c_e(G) = \sum_{f\in E(G)} deg(f)ec(f)$, where $deg(f)$ is the degree of an edge f and $ec(f)$ is its eccentricity. Various upper and lower bounds are obtained for this index of connected graphs in terms of order, size, girth and the first Zagreb index of G, respectively.

Keywords: Eccentric connectivity index; edge eccentric connectivity index; bounds

Mathematics Subject Classification: 05C12; 05A15; 05A20; 05C05

1. Introduction

The study of the quantitative structure-activity relationship (QSAR) aims to rapidly and effectively predict the physico-chemical, pharmacological and toxicological properties of a compound directly from its molecular structure. In chemistry, a molecular graph represents the topology of a molecule. One can model a molecule by a graph by using the points to represent the atoms, and the edges to symbolize the covalent bonds. So, it is natural for scholars to study relevant properties of these graph models. During this process, a number of graph invariants are proposed. The parameters derived from this graph-theoretic model of a chemical structure are being used not only in QSAR studies pertaining to molecular design and pharmaceutical drug design, but

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also in the environmental hazard assessment of chemicals. During the past several decades, many such graph invariant ‘topological indices’ have been raised and extensively studied, such as, Wiener index, Randić index, Hosoya index, and so on.

More recently, a new topological index, *eccentric connectivity index*, has been investigated. This topological model has been shown to give a high degree of predictability of pharmaceutical properties, and may provide leads for the development of safe and potent anti-HIV compounds. We encourage the reader to consult papers [1–9] for some applications and papers [10–15] for the mathematical properties of this topological index.

In this paper, we introduce the concept of the edge eccentric connectivity index. We investigate the edge eccentric connectivity index of connected graphs. Upper and lower bounds are obtained for the edge eccentric connectivity index of connected graphs.

Now, we introduce some notation and terminology. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. Let $deg_G(v)$ denote the degree of the vertex v in G. If $deg_G(v) = 1$, then v is said to be a *pendent vertex*. An edge incident to a pendent vertex is said to be a *pendent edge*. Let S_n and C_n be the star and cycle on n vertices, respectively. For two vertices u and v in $V(G)$, we denote by $d_G(u, v)$ the distance between u and v, i.e., the length of the shortest path connecting u and v. The *eccentricity* of a vertex v in $V(G)$, denoted by $ec_G(v)$, is defined to be

$$ec_G(v) = \max\{d_G(v, w) | w \in V(G)\}.$$

The *diameter* of a graph G is then defined to be $\max\{ec_G(v) | v \in V(G)\}$. The *eccentric connectivity index*, $\xi^c(G)$, of a graph G is defined as

$$\xi^c(G) = \sum_{v \in V(G)} deg(v) ec(v).$$

Let $f = uv$ be an edge in $E(G)$. Then the degree of the edge f is defined to be $deg_G(u) + deg_G(v) - 2$. For two edges $f_1 = u_1v_1, f_2 = u_2v_2$ in $E(G)$, the distance between f_1 and f_2, denoted by $d_G(f_1, f_2)$, is defined to be

$$d_G(f_1, f_2) = \min\{d_G(u_1, u_2), d_G(u_1, v_2), d_G(v_1, u_2), d_G(v_1, v_2)\}.$$

The *eccentricity* of an edge f, denoted by $ec_G(f)$, is defined as

$$ec_G(f) = \max\{d_G(f, e) | e \in E(G)\}.$$

The *edge eccentric connectivity index* of G, denoted by $\xi^c_e(G)$, is defined as

$$\xi^c_e(G) = \sum_{f \in E(G)} deg_G(f) ec_G(f).$$

We will omit the subscript G when the graph is clear from the context.

2. Main results

In this section, we shall investigate the edge eccentric connectivity index of a connected graph G.

Firstly, we establish a simple relation between the edge eccentric connectivity index of a connected graph and the eccentric connectivity index of its line graph.

Theorem 1. *Let G be a connected graph and $L(G)$ be its line graph. Then*

$$\xi_e^c(G) = \xi^c(L(G)) - 2m(L(G)),$$

where $m(L(G))$ is the number of edges in $L(G)$.

Proof. Obviously, $L(G)$ is connected. Note that $deg_G(f) = deg_{L(G)}(f)$ and $ec_G(f) = ec_{L(G)}(f) - 1$. Thus, we have

$$\xi_e^c(G) = \sum_{f \in L(G)} deg_{L(G)}(f)(ec_{L(G)}(f) - 1) = \xi^c(L(G)) - 2m(L(G)).$$

$\square$

Corollary 1. *For the n-vertex star S_n, we have $\xi_e^c(S_n) = 0$.*

Proof. Since $L(S_n)$ is a complete graph on $n-1$ vertices. Then $\xi_e^c(S_n) = \xi^c(K_{n-1}) - (n-1)(n-2) = 0$ by Theorem 1. $\square$

Corollary 2. *For any connected graph G, $\xi_e^c(G)$ and $\xi^c(L(G))$ are of the same parity.*

Morgan *et al.* [10] proved that among all connected graphs, the star S_n is the graph with the minimum eccentric connectivity index. For the edge eccentric connectivity index, we obtain a similar conclusion as follows.

Theorem 2. *Let G be a connected graph. Then $\xi_e^c(G) \geq 0$ with the equality if and only if $G \cong S_n$ or C_3.*

Proof. For a connected graph G, we clearly have $\xi_e^c(G) \geq 0$. If $G \cong S_n$ or C_3, then $\xi_e^c(G) = 0$ by Corollary 1.

Now, let $\xi_e^c(G) = 0$. If $G \ncong S_n, C_3$, then there exists an edge f in $E(G)$ such that $ec(f) \geq 1$. But then $\xi_e^c(G) \geq deg(f)ec(f) > 0$, a contradiction. $\square$

The *lollipop graph $LOP_{n,d}$* is a graph obtained from the complete graph K_{n-d} and the path P_d by joining one end-vertex of P_d to each vertex of K_{n-d}.

Lemma 1 ([10]). *Let G be a connected graph of order n and diameter d. Then $\xi^c(G) \leq d(n-d)^2 + O(n^2)$, and the bound is attained at $LOP_{n,d}$.*

Let $B_{n,d}$ denote the tree obtained from the path P_d by attaching to one of its end-vertices $n-d$ pendent edges.

Theorem 3. *Let G be a connected graph of size m and diameter d. Then*

$$\xi_e^c(G) \leq d(m-d)^2 + O(m^2),$$

and the bound is attained at $B_{m+1,d}$.

Proof. Let G be a connected graph of size m and diameter d. If G has a diametrical path lying within one cycle of G, then the diameter of $L(G)$ is also d. Otherwise, $L(G)$ has diameter $d-1$. Note that $L(G)$ has m vertices. So, by Lemma 1, we obtain

$$\xi^c(L(G)) \leq d(m-d)^2 + O(m^2)$$

or

$$\xi^c(L(G)) \leq (d-1)(m-d+1)^2 + O(m^2) = (d-1)(m-d)^2 + O(m^2).$$

In either case, we have

$$\xi^c(L(G)) \leq d(m-d)^2 + O(m^2).$$

It then follows from Theorem 1 that

$$\xi^c_e(G) \leq d(m-d)^2 + O(m^2) - 2m(L(G)).$$

Since G is a connected, $L(G)$ is a connected graph of order m. Then $m(L(G)) \geq m-1$. Hence

$$\xi^c_e(G) \leq d(m-d)^2 + O(m^2) - 2(m-1) = d(m-d)^2 + O(m^2).$$

Since $L(B_{m+1,d}) = LOP_{m,d}$, $B_{m+1,d}$ attains the upper bound by Theorem 1 and Lemma 1. This completes the proof. □

Corollary 3. *Let G be a connected graph of size m. Then*

$$\xi^c_e(G) \leq \max\{\psi(\lfloor\frac{m}{3}\rfloor), \psi(\lceil\frac{m}{3}\rceil)\} + O(m^2),$$

and the bound is attained at $B_{m+1,\lfloor\frac{m}{3}\rfloor}$ *or* $B_{m+1,\lceil\frac{m}{3}\rceil}$.

Proof. Let $\psi(x) = x(m-x)^2$. Then $\psi' = (x-m)^2 + 2x(x-m) = 3x^2 - 4mx + m^2 = (3x-m)(x-m)$, $\psi'' = 6x - 4m$. Also, $\psi''|_{x=\frac{m}{3}} = 2m - 4m < 0$. Note that d is an integer. Then

$$\psi(d) \leq \max\{\psi(\lfloor\frac{m}{3}\rfloor), \psi(\lceil\frac{m}{3}\rceil)\}.$$

Therefore, $\xi^c_e(G) \leq \psi(d) + O(m^2) \leq \max\{\psi(\lfloor\frac{m}{3}\rfloor), \psi(\lceil\frac{m}{3}\rceil)\} + O(m^2)$. Clearly, the bound is attained at $B_{m+1,\lfloor\frac{m}{3}\rfloor}$ or $B_{m+1,\lceil\frac{m}{3}\rceil}$. □

The first *Zagreb index* of a graph G, denoted by $M_1(G)$, is defined as $\sum\limits_{u\in V(G)} (deg_G(u))^2$. We have

Theorem 4. *Let G be a connected graph of order n and size m. Then*

$$M_1(G)r - 2mr \leq \xi_e^c(G) \leq M_1(G)d - 2md, \tag{1}$$

where the equalities hold in both sides of (1) if and only if $G \cong C_n$ or S_n, $r = \min\{ec_G(f)|f \in E(G)\}$ and $d = \max\{ec_G(f)|f \in E(G)\}$, respectively.

Proof. According to the definition of the edge eccentricity connectivity index, we have

$$\xi_e^c(G) = \sum_{f=uv \in E(G)} (deg_G(u) + deg_G(v) - 2)ec_G(f).$$

So

$$r \sum_{f=uv \in E(G)} (deg_G(u)+deg_G(v)-2) \leq \xi_e^c(G) \leq d \sum_{f=uv \in E(G)} (deg_G(u)+deg_G(v)-2),$$

that is,

$$M_1(G)r - 2mr \leq \xi_e^c(G) \leq M_1(G)d - 2md,$$

by the fact that

$$M_1(G) = \sum_{f=uv \in E(G)} (deg_G(u) + deg_G(v)).$$

The equalities hold in the left- and right-hand sides of (1) if and only if for each $f \in E(G)$, $ec_G(f) = r$ and $ec_G(f) = d$, respectively. That is, $G \cong S_n$ or C_n. $\square$

Theorem 5. *Let G be a connected k-regular graph of order n. Then*

$$nk(k-1)r \leq \xi_e^c(G) \leq nk(k-1)d, \tag{2}$$

where the equalities hold in both sides of (2) if and only if $G \cong C_n$, $r = \min\{ec_G(f)|f \in E(G)\}$ and $d = \max\{ec_G(f)|f \in E(G)\}$, respectively.

Proof. Note that for a k-regular graph G, G has $\frac{nk}{2}$ edges. By the definition of the edge eccentric connectivity index, we have

$$\xi_e^c(G) = \sum_{f=uv \in E(G)} (2k-2)ec_G(f).$$

So

$$(2k-2)\frac{nk}{2}r \leq \xi_e^c(G) = (2k-2) \sum_{f=uv \in E(G)} ec_G(f) \leq (2k-2)\frac{nk}{2}d,$$

that is,

$$nk(k-1)r \leq \xi_e^c(G) \leq nk(k-1)d.$$

The equalities hold in the left- and right-hand sides of (2) if and only if for each $f \in E(G)$, $ec_G(f) = r$ and $ec_G(f) = d$, respectively. Note that G is a k-regular graph. Thus, the equalities hold in the left- and right-hand sides of (2) if and only if $G \cong C_n$, that is, G is a 2-regular graph. □

Theorem 6. *Let G be a connected graph of order n. Then*

$$\xi_e^c(G) \leq d\sqrt{M_1(L(G))},$$

where the equality holds if and only if $G \cong C_n$ or S_n, $M_1(L(G)) = \sum_{f\in E(G)} (deg_G(f))^2$ and $d = \max\{ec_G(f) | f \in E(G)\}$, respectively.

Proof. According to the definition of the edge eccentricity connectivity index, we have

$$\begin{aligned} \xi_e^c(G) &= \sum_{f=uv\in E(G)} deg_G(f)ec_G(f) \leq \sqrt{\sum_{f\in E(G)} (deg_G(f))^2}\sqrt{\sum_{f\in E(G)} (ec_G(f))^2} \\ &\leq d\sqrt{\sum_{f\in E(G)} (deg_G(f))^2} \\ &= d\sqrt{\sum_{f\in V(L(G))} (deg_G(f))^2} \\ &= d\sqrt{M_1(L(G))}, \end{aligned}$$

where the equality holds if and only if $\frac{ec_G(f)}{deg_G(f)}$ is a constant and $ec_G(f) = d$, that is, $G \cong C_n$ or S_n. This completes the proof. □

Theorem 7. *Let G be a connected graph of size m and girth g. Then*

$$\xi_e^c(G) \geq (\lfloor \frac{g}{2} \rfloor - 1)(M_1(G) - 2m),$$

where the equality holds if and only if $G \cong C_m$.

Proof. Suppose that the grith of G is g and C_g is a cycle in G. Then $ec_G(f) \geq \lfloor \frac{g-2}{2} \rfloor = \lfloor \frac{g}{2} \rfloor - 1$ for any edge f in G. So we have

$$\begin{aligned} \xi_e^c(G) &= \sum_{f=uv\in E(G)} deg_G(f)ec_G(f) \\ &\geq (\lfloor \frac{g}{2} \rfloor - 1) \sum_{f=uv\in E(G)} deg_G(f) \\ &= (\lfloor \frac{g}{2} \rfloor - 1) \sum_{f=uv\in E(G)} [(deg_G(u) + deg_G(v)) - 2] \\ &= (\lfloor \frac{g}{2} \rfloor - 1) \left(\sum_{f=uv\in E(G)} (deg_G(u) + deg_G(v)) - 2m \right) \\ &= (\lfloor \frac{g}{2} \rfloor - 1)(M_1(G) - 2m). \end{aligned}$$

where the equality holds if and only if for any edge f, there exists $ec_G(f) = \lfloor \frac{g}{2} \rfloor - 1$, that is, $G \cong C_m$. This completes the proof. $\square$

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Received: August, 2011