ON THE ECCENTRIC CONNECTIVITY INDEX OF CERTAIN MOLECULAR GRAPHS

SAEID ALIKHANI[*], ROSLAN HASNI[a], MOHAMMAD A. IRANMANESH
Department of Mathematics, Yazd University, 89195-741, Yazd, Iran
[a]*School of Mathematical Sciences, Universiti Sains Malaysia,11800 Penang, Malaysia*

The eccentric connectivity index of a molecular graph G is defined as $\zeta(G)=\sum_{u\in V(G)} deg(v)ecc(v)$, where $ecc(v)$ is defined as the length of a maximal path connecting v to another vertex of G. In this paper we obtain some formulas for computing of this index for some specific graphs.

(Received January 27, 2011; Accepted April 4, 2011)

Keywords: Eccentric connectivity index, Eccentric connectivity polynomial, graph

1. Introduction

A simple graph $G=(V,E)$ is a finite nonempty set $V(G)$ of objects called vertices together with a (possibly empty) set $E(G)$ of unordered pairs of distinct vertices of G called edges. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds.

If $x, y \in V(G)$ then the *distance* $d(x, y)$ between x and y is defined as the length of a minimum path connecting x and y. The *eccentric connectivity index* of the molecular graph G, $\xi^c(G)$, was proposed by Sharma, Goswami and Madan [8]. It is defined as $\xi^c(G)=\sum_{u\in V(G)} deg_G(u)ecc(u)$, where $deg_G(x)$ denotes the degree of the vertex x in G and $ecc(u)=Max\{d(x,u) \mid x\in V(G)\}$, for details see [3,5,6]. The radius and diameter of G are defined as the minimum and maximum eccentricity among vertices of G, respectively. The eccentric connectivity polynomial of a graph G is $ECP(G,x)=\sum_{v\in V(G)} deg(v)x^{ecc(v)}$, (see [12]). Therefore the eccentric connectivity index is the first derivative of $ECP(G,x)$ evaluated at $x=1$ (see [7]).

The *corona* of two graphs G_1 and G_2, as defined by Frucht and Harary in [4], is the graph $G=G_1\circ G_2$ formed from one copy of G_1 and $|V(G_1)|$ copies of G_2, where the ith vertex of G_1 is adjacent to every vertex in the ith copy of G_2. The corona $G\circ K_1$, in particular, is the graph constructed from a copy of G, where for each vertex $v\in V(G)$, a new vertex v' and a pendant edge vv' are added. The *join* of two graphs G_1 and G_2, denoted by $G_1\vee G_2$ is a graph with vertex set $V(G_1)\cup V(G_2)$ and edge set $E(G_1)\cup E(G_2)\cup\{uv \mid u\in V(G_1)$ and $v\in V(G_2)\}$.

[*]Corresponding author: alikhani@yazduni.ac.ir

A graph is an *empty graph* if contain no edges. The empty graph of order n is denoted by O_n.

In Section 2 we compute the eccentric connectivity polynomial for specific graphs denoted by $G(m)$ and $G_1(m)G_2$. In Section 3 we compute the eccentric connectivity polynomial for corona and join of two graphs. Using our results, we study the eccentric connectivity index of these kind of graphs.

2. Eccentric connectivity index of some specific graphs

In this section we consider two certain graphs with specific construction and compute their eccentric connectivity indexes.

Let P_{m+1} be a path with vertices labeled by $y_0, y_1, \dots, y_m$, for $m \geq 0$ and let G be any graph. Denote by $G_{v_0}(m)$ (or simply $G(m)$, if there is no likelihood of confusion) a graph obtained from G by identifying the vertex v_0 of G with an end vertex y_0 of P_{m+1} (see Figure 0). For example, if G is a path P_2, then $G(m) = P_2(m)$ is the path P_{m+2}. Also, we denote the graph obtained from graphs G_1 and G_2 by adding a path P_m from a vertex in G_1 to a vertex of G_2, by $G_1(m)G_2$. (Fig. 1).

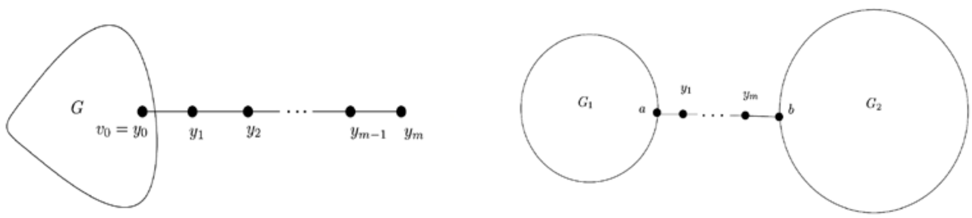

Fig. 1. Graphs $G(m)$ and $G_1(m)G_2$, respectively.

Theorem 1 . *The eccentric connectivity index of $G_{v_0}(m)$ is*

$$\zeta(G(m)) = \sum_{u \in V(G)} deg(u) Max\{d(u, v_0) + m + 1, ecc(u)\}.$$

Proof. It is easy to see that the eccentricity of a vertex u in a graph $G_{v_0}(m)$ is $Max\{d(u, v_0) + m + 1, ecc(u)\}$. Therefore we have the result by definition of eccentricity index. ■

We state and prove the following theorem which is about the eccentric connectivity index of $G_1(m)G_2$:

Theorem 2 . *The eccentric connectivity polynomials of $G_1(m)G_2$ is*

$$\xi(G_1(m)G_2) = \sum_{u \in V(G_1)} deg(u) Max\{d(u,a) + ecc_2(b) + m + 1, ecc_1(u)\} + \sum_{u \in V(G_2)} deguMax\{d(u,b) + ecc_1(a) + m + 1, ecc_2(u)\},$$

where a,b are two vertices of $G_1(m)G_2$ in Figure 1.

Proof. We observe that the eccentricity of a vertex u in a graph G_1 is

$Max\{d(u,a)+ecc_2(b)+m+1, ecc_1(u)\}$. Also the eccentricity of a vertex u in a graph G_2 is $Max\{d(u,b)+ecc_1(a)+m+1, ecc_2(u)\}$. So we have the result by definition of eccentricity index. ■

3. The eccentricity index of corona and join of two graphs

In this section we consider the corona and the join of two graphs, and compute their eccentricity connectivity polynomials. Using our results, we obtain formulas for eccentricity index of corona and join of two graphs.

Theorem 3 . *Let G_1 and G_2 be two graphs of order n_1 and n_2, respectively. Then*

$$ECP(G_1 \circ G_2, x) = x(ECP(G_1, x) + ECP(G_2, x)) + x[(n_2 + x)\sum_{v \in G_1} x^{ecc(v)}].$$

Proof. In the corona of two graphs G_1 and G_2, the degree of each vertices of G_1 increase by n_2 and the eccentricity of these vertices increase by one. Also the degree of each vertices of G_2 increase by one and the eccentricity of these vertices increase by two. Therefore we have

$$\begin{aligned}ECP(G_1 \circ G_2) &= \sum_{v \in V(G_1 \circ G_2)} deg(v).x^{ecc(v)}\\ &= \sum (deg(v)+n_2)x^{ecc(v)+1} + \sum (deg(v)+1)x^{ecc(v)+2}\\ &= x(ECP(G_1, x) + ECP(G_2, x)) + x[(n_2 + x)\sum_{v \in G_1} x^{ecc(v)}].\end{aligned}$$ ■

Let us denote graph $H \circ K_1$ simply by H^*. We have the following corollary:

Corollary 1 . *Suppose that H is a graph of order n. Then*

$$ECP(H^*, x) = x(ECP(H, x)) + x[(1+x)\sum_{v \in H} x^{ecc(v)}].$$

Proof. It suffices to put $G_2 = K_1$ in Theorem 3. Since $ECP(K_1, x) = 0$, we have the result. ■

The following theorem give us the formula for $ECP(G_1 \vee G_2)$:

Theorem 4 . *Suppose that G_1 and G_2 are two graphs with orders m and n, respectively. Then we have*

$$ECP(G_1 \vee G_2) = x^2(2mn + \sum_{v \in V(G_1)} deg(v) + \sum_{w \in V(G_2)} deg(w)).$$

Proof. We observe that when we construct $G_1 \vee G_2$, the degree of each vertices in G_1 increase by n and the degree of each vertices in G_2 increase by m. Also observe that the eccentricity for every vertex is two. Therefore by definition of eccentric connectivity polynomial we have:

$$ECP(G_1 \vee G_2) = \sum_{v \in V(G_1 \vee G_2)} deg(v).x^{ecc(v)}$$

$$= \sum_{v \in G_1} (deg(v) + n)x^2 + \sum_{w \in G_2} (deg(w) + m)x^2$$

$$= x^2(2mn + \sum_{v \in V(G_1)} deg(v) + \sum_{w \in V(G_2)} deg(w)). \qquad \blacksquare$$

As an example, by applying Theorem 4 for $G_1 = O_n$ and $G_2 = O_m$, we have the following corollary for complete bipartite graphs (see [1]).

Corollary 2 . *If* $m, n \geq 2$, *then the eccentricity connectivity polynomial of* $K_{m,n}$ *is* $ECP(K_{m,n}, x) = 2mnx^2$.

Since the eccentric connectivity index is the first derivative of $ECP(G, x)$ evaluated at $x = 1$, then we have the following theorem.

Theorem 5 . *Let* G_1 *and* G_2 *be two graphs of orders* m *and* n, *respectively. Then*

$$\zeta^c(G_1 \circ G_2) = 2(e_1 + e_2 + m) + mn + (n+1) \sum_{v \in V(G_1)} ecc(v),$$

where e_1 and e_2 are the number of edges of G_1 and G_2, respectively.

Theorem 6 . *Let* G_1 *and* G_2 *be two graphs of orders* m *and* n, *respectively. Then we have*

$$\zeta^c(G_1 \vee G_2) = 2(2mn + \sum_{v \in V(G_1)} deg(v) + \sum_{w \in V(G_2)} deg(w)).$$

References

[1] S. Alikhani, M.A. Iranmanesh, Digest Journal of nanomaterials and biostructures, **6**(1), 253 (2011).
[2] A.R. Ashrafi, M. Ghorbani and M. Hemmasi, Digest Journal of Nanomaterials and Biostructures **4**(3), 483 (2009).
[3] Shubo Chen, Weijun Liu, and Fangli Xia, J. Comput. Theor. Nanosci. **8**, 17 (2011).
[4] R. Frucht and F. Harary, Aequationes Math. 4, 322-324 (1970).
[5] I. Gutman, O.E. Polansky, Mathematical Concepts in Organic Chemistry, Springer-Verlag, New York, (1986).
[6] M. A. Johnson, G.M. Maggiora, Concepts and Applications of Molecular Similarity, Wiley Interscience, New York, (1990).
[7] M.J. Morgan, et al., Discrete Mathematics (2010), doi:10.1016/j.disc.2009.12.013.
[8] V. Sharma, R. Goswami, A. K. Madan, J. Chem. Inf. Comput. Sci. **37**, 273 (1997).