ON THE ECCENTRIC CONNECTIVITY INDEX OF CERTAIN MOLECULAR GRAPHS

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The eccentric connectivity index of a molecular graph \( G \) is defined as
\[ \zeta(G) = \sum_{u \in V(G)} deg_G(v) \text{ecc}(v), \]
where \( \text{ecc}(v) \) 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 this index for some specific graphs.

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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 \( G \), \( \zeta^C(G) \), was proposed by Sharma, Goswami and Madan\(^8\). It is defined as
\[ \zeta^C(G) = \sum_{u \in V(G)} deg_G(u) \text{ecc}(u), \]
where \( deg_G(x) \) denotes the degree of the vertex \( x \) in \( G \) and \( \text{ecc}(u) = \max\{d(x, u) \mid x \in V(G)\} \), 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 \( ECP(G, x) = \sum_{v \in V(G)} deg(v)x^{\text{ecc}(v)} \), (see\(^1\)),\(^2\),\(^12\)). 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 \( E(G_1) \cup E(G_2) \cup \{uv \mid u \in V(G_1) \text{ and } v \in V(G_2)\} \).

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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 \( y_0, y_1, \ldots, y_m \), for \( m \geq 0 \) and let \( G \) be any graph. Denote by \( G_{y_0}(m) \) (or simply \( G(m) \), if there is no likelihood of confusion) a graph obtained from \( G \) by identifying the vertex \( y_0 \) 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).

![Graphs G(m) and G_1(m)G_2](image)

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

**Theorem 1.** The eccentric connectivity index of \( G_{y_0}(m) \) is

\[
\zeta(G(m)) = \sum_{u \in V(G)} \deg(u)\max\{d(u, y_0) + m + 1, ecc(u)\}.
\]

**Proof.** It is easy to see that the eccentricity of a vertex \( u \) in a graph \( G_{y_0}(m) \) is \(\max\{d(u, y_0) + m + 1, ecc(u)\}\). 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

\[
\xi(G_1(m)G_2) = \sum_{u \in V(G_1)} \deg(u)\max\{d(u, a) + ecc_2(b) + m + 1, ecc_1(u)\} + \\
\sum_{u \in V(G_2)} \deg(u)\max\{d(u, b) + ecc_1(a) + m + 1, ecc_2(u)\}
\]

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
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

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

$$= \sum(deg(v) + n_2)x^{ecc(v)} + \sum(deg(v) + 1)x^{ecc(v)} + 2$$

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

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 $ECP(G_1 \lor G_2)$:

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

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

Proof. We observe that when we construct $G_1 \lor G_2$, 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:

$$ECP(G_1 \lor G_2) = \sum_{v \in V(G_1 \lor G_2)} deg(v)x^{ecc(v)}$$
\[
= \sum_{v \in G_1} (\text{deg}(v) + n)x^2 + \sum_{w \in G_2} (\text{deg}(w) + m)x^2 \\
= x^2(2mn + \sum_{v \in V(G_1)} \text{deg}(v) + \sum_{w \in V(G_2)} \text{deg}(w)).
\]

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 eccentric 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
\[
\zeta^C(G_1 \odot G_2) = 2(e_1 + e_2 + m) + mn + (n + 1) \sum_{v \in V(G_1)} \text{ecc}(v),
\]
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
\[
\zeta^C(G_1 \vee G_2) = 2(2mn + \sum_{v \in V(G_1)} \text{deg}(v) + \sum_{w \in V(G_2)} \text{deg}(w)).
\]

**References**