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ON COMBINATORIAL PROPERTIES OF TWO CONVEX POLYTOPES VIA ECCENTRICITY BASED TOPOLOGICAL INDICES

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Abstract. Graph theory is the most powerful tools in the mathematics and computer science, also study of descriptors in quantitative structure property relationship (QSPR) and quantitative structure activity relationship (QSAR) studies in the chemistry science. The eccentricity based topological indices are very important for QSPR/QSAR studies, and these values have been studied for different graph types in many articles recently. In this paper, some eccentricity based topological indices of two convex polytopes Q_n and R_n are computed.

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1 Introduction

Graph theory has been studied different areas such as mathematics, information, chemistry sciences, and so on. Especially, it has been the most important mathematical tools for the study the analysis of daily life problems. For example, the mathematical chemistry is that part of theoretical chemistry which is concerned with applications of mathematical methods to chemical problems (Cayley, 1874). A chemical graph is a graph such that each vertex represents an atom of the molecule, and represents covalent bonds between atoms by edges of the corresponding vertices (Balaban et al., 1999; Zhou & Du, 2010; Todeschini & Consonni, 2000). Furthermore, the graph theory has successfully provided chemists with a variety of very useful tools, namely, the topological index. A topological index is a numerical value associated with chemical constitution purporting for the correlation of a chemical structure with various physical properties, chemical reactivity or biological activity, also it has used vulnerability of chemical graphs (Todeschini & Consonni, 2000). Research on the topological indices has been intensively rising recently. There are numerous topological descriptors that have found some applications in theoretical chemistry, especially in QSPR/QSAR research (Balaban et al., 1999; Hwang & Ghosh, 1987; Todeschini & Consonni, 2000).

Let $G = (V(G), E(G))$ be a simple undirected graph of order n and size m. Now, we give some definitions is related to graphs. For any vertex $v \in V(G)$, the *open neighborhood* of v is $N_G(v) = \{u \in V(G)|uv \in E(G)\}$ and *closed neighborhood* of v is $N_G[v] = N_G(v) \cup \{v\}$. The *degree of vertex* v in G denoted by $deg_G(v)$, that is the size of its open neighborhood (West, 2001). The *distance* $d_G(u, v)$ between two vertices u and v in G is the length of a shortest path between them. The eccentricity value of the vertex $u \in V(G)$ denoted by $\varepsilon_G(u)$ is

$\varepsilon_G(u) = max_{v\in V(G)} d_G(u,v)$, that is the largest between vertex u and any other vertex v of G (Buckley & Harary, 1990).

The first topological index is the *Wiener index* denoted by $W(G)$ in chemical graph theory and is defined by the chemist Wiener (1947). The Wiener index aims to sum of the half of distances between every pair of vertices of G and it was defined as follows:

$$W(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} d_G(v_i, v_j). \tag{1}$$

Then, a lot of topological indices were introduced after defining the Wiener index. Now, the eccentricity-based topological indices terminology will be given.

In Gupta et al. (2000) introduced new topological index namely *connective eccentricity* index denoted by $\xi^{ce}(G)$ for the graph G. It was defined with as follows:

$$\xi^{ce}(G) = \sum_{u\in V(G)} \left(\frac{deg_G(u)}{\varepsilon_G(u)}\right). \tag{2}$$

The *eccentric connectivity* index $\xi^c(G)$ was defined by Sharma et al. (1997). The eccentric connectivity index was denoted by $\xi^c(G)$ for the any graph G, also was defined as follows:

$$\xi^{c}(G) = \sum_{u\in V(G)} \left(deg_G(u)\varepsilon_G(u)\right). \tag{3}$$

The *modified eccentric connectivity* index $\xi_c(G)$ was defined in Ashrafi et al. (2011) as follows:

$$\xi_{c}(G) = \sum_{u\in V(G)} \left(\delta_G(u)\varepsilon_G(u)\right), \tag{4}$$

where $\delta_G(u) = \sum_{v\in N_G(u)} deg_G(v)$, that is the sum of degrees of vertices which is the vertex u neighbor's, furthermore it was studied in Berberler & Berberler (2015).

The *total eccentricity* index $\xi(G)$ was presented by Farooq & Malik (2015), which was defined as follows:

$$\xi(G) = \sum_{u\in V(G)} \left(\varepsilon_G(u)\right). \tag{5}$$

The *first Zagreb index* and the *second Zagreb index* of graphs were defined by Gutman & Trinajstic (1972). Then the *first*, *second* and *third Zagreb eccentricity* indices $M_1^*(G)$, $M_1^{**}(G)$ and $M_2^*(G)$ were defined by Vukicevic & Graovac (2010) and Ghorbani & Hosseinzadeh (2012), respectively.

The *first Zagreb eccentricity* index was defined as follows:

$$M_1^*(G) = \sum_{uv\in E(G)} \left(\varepsilon_G(u) + \varepsilon_G(v)\right). \tag{6}$$

The *second Zagreb eccentricity* index was defined as follows:

$$M_1^{**}(G) = \sum_{u\in V(G)} \left((\varepsilon_G(u))^2\right). \tag{7}$$

The *third Zagreb eccentricity* index was defined as follows:

$$M_2^*(G) = \sum_{uv\in E(G)} \left(\varepsilon_G(u)\varepsilon_G(v)\right). \tag{8}$$

In Ilic (2012), the *average eccentricity index* denoted by $avec(G)$ was defined for any graph G as follows:

$$avec(G) = \frac{1}{|V(G)|}\left(\sum_{u\in V(G)} (\varepsilon_G(u))\right). \tag{9}$$

The *eccentricity based geometric-arithmetic* index denoted by $GA_4(G)$ was defined for any graph G in Ghorbani & Khaki (2012) as follows:

$$GA_4(G) = \sum_{uv\in E(G)} \left(\frac{2\sqrt{\varepsilon_G(u)\varepsilon_G(v)}}{\varepsilon_G(u)+\varepsilon_G(v)}\right). \tag{10}$$

A new version of the ABC index namely $ABC_5(G)$ was defined for any graph G in Farahani (2013) as follows:

$$ABC_5(G) = \sum_{uv\in E(G)} \left(\sqrt{\frac{\varepsilon_G(u)+\varepsilon_G(v)-2}{\varepsilon_G(u)\varepsilon_G(v)}}\right). \tag{11}$$

The eccentricity based topological connectivity indices are the distance-related topological invariants whose potential of predicting biological activity of the certain classes of chemical compounds made them very attractive for use in QSAR/QSPR studies. The some topological indices and some eccentricity based topological indices were studied in some papers, the readers can see them in Ilic & Gutman (2011); Aslan (2015); Aslan & Kurkcu (2015); Aslan (2015); Imran et al. (2018); Durgut & Turaci (2021); Idrees et al. (2019); Akhter et al. (2019); Hayat & Imran (2014); Turaci & Okten (2015); Gao et al. (2018); Kutucu & Turaci (2017); Turaci & Durgut (2021).

This paper is organized as follows: In Section 2, the definitions of two convex polytopes Q_n and R_n are given. Then, exact solutions of some eccentricity based topological indices are given for Q_n and R_n in Section 3. Finally, in Section 4, we present our conclusions.

2 Two Convex Polytopes Q_n and R_n

In this section, two polytopes are determined according to combinatorial aspects. Firstly, we give definitions of two convex polyopes denoted by Q_n and R_n. Then, the vertex and edge partitions of these polytopes are given. The some topological indices of convex polytopes were studied in Asif et al. (2020); Sohail et al. (2018); Nazeer et al. (2016); Foruzanfar et al. (2018); Turaci & Durgut (2022).

2.1 The convex polytope Q_n

The graph of convex polytope Q_n consists of 3-sided faces, 4-sided faces, 5-sided faces and n-sided faces as defined in Baca (1992), where $|V(Q_n)| = 4n$ and $|E(Q_n)| = 7n$. The convex polytope Q_8 is shown in Figure 1.

2.2 The convex polytope R_n

The graph of convex polytope R_n is obtained as a combination of the graph of a prism and the graph of antiprism as defined in Baca (1992), where $|V(R_n)| = 3n$ and $|E(R_n)| = 6n$. The convex polytope R_8 is shown in Figure 2.

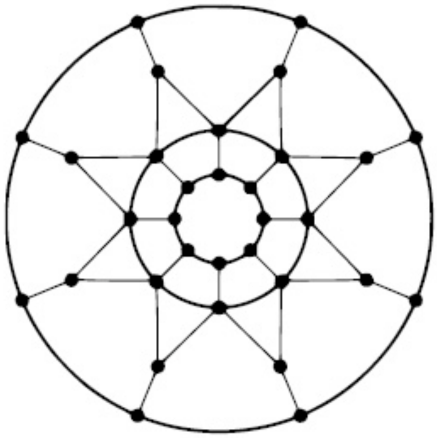

Figure 1: The convex polytope Q_8

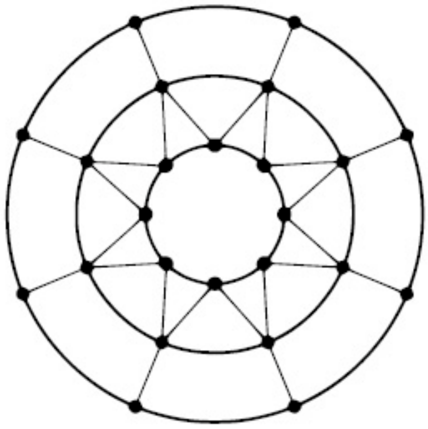

Figure 2: The convex polytope R_8

2.3 The vertex and edge partitions of the convex polytopes Q_n and R_n

Let $n \geq 5$. We partition $V(G)$ into subsets based on the degrees of vertices, sum of the degrees of neighbors of vertices, the eccentricity values of vertices and frequencies of vertices in G which is isomorphic to Q_n and R_n, respectively. The vertex partition of Q_n and R_n with respect to degrees and eccenticity values are shown in Tables 1, 2, 3 and 4. Let $uv \in E(G)$. We partition $E(G)$ into subsets based on the degrees of end vertices, the eccentricity values of end vertices and frequencies of vertices in G which is isomorphic to Q_n and R_n, respectively. These edge partitions of the graphs Q_n and R_n are shown in Tables 5, 6, 7 and 8. The vertex and edge partitions of the convex polytopes Q_n and R_n have been obtained by using the C programming language. The obtained tables can be seen in **Appendix A**.

3 Vertex eccentricity-based topological indices of the convex polytopes Q_n and R_n

In this section, we compute some eccentricity-based topological indices of the convex polytopes Q_n and R_n. By using the MAPLE program results of following theorems have been obtained.

Theorem 1. *Let Q_n be a convex polytope of order 4n and size 7n, where $n \geq 5$. Then,*

$$\textbf{(a)}\ \xi^{ce}(Q_n) = \begin{cases} \frac{28n^2+116n}{n^2+8n+15} & \text{, if } n \text{ is odd;} \\ \frac{28n^2+88n}{n^2+6n+8} & \text{, if } n \text{ is even.} \end{cases}$$

(b) $\xi^c(Q_n) = 7n^2 + \frac{47}{2}n + (\frac{7}{2}n)(-1)^{n+1}$.

(c) $\xi_c(Q_n) = 26n^2 + 85n + (13n)(-1)^{n+1}$.

(d) $\xi(Q_n) = 2n^2 + 7n + (n)(-1)^{n+1}$.

(e) $M_1^*(Q_n) = 7n^2 + \frac{47}{2}n + (\frac{7}{2}n)(-1)^{n+1}$.

(f) $M_1^{**}(Q_n) = \begin{cases} n^3 + 8n^2 + 17n & \text{, if } n \text{ is odd;} \\ n^3 + 6n^2 + 10n & \text{, if } n \text{ is even.} \end{cases}$

(g) $M_2^*(Q_n) = \begin{cases} \frac{7}{4}n^3 + \frac{27}{2}n^2 + \frac{107}{4}n & \text{, if } n \text{ is odd;} \\ \frac{7}{4}n^3 + 10n^2 + 15n & \text{, if } n \text{ is even.} \end{cases}$

(h) $avec(Q_n) = \begin{cases} \frac{n+4}{2} & \text{, if } n \text{ is odd;} \\ \frac{n+3}{2} & \text{, if } n \text{ is even.} \end{cases}$

(i) $GA_4(Q_n) = \begin{cases} 5n + \frac{2n}{n+4}\sqrt{n^2 + 8n + 15} & \text{, if } n \text{ is odd;} \\ 5n + \frac{2n}{n+3}\sqrt{n^2 + 6n + 8} & \text{, if } n \text{ is even.} \end{cases}$

(j) $ABC_5(Q_n) = \begin{cases} \frac{4n}{n+5}\sqrt{n+3} + \frac{6n}{n+3}\sqrt{n+1} + 4n\sqrt{\frac{n+2}{n^2+8n+15}} & \text{, if } n \text{ is odd;} \\ \frac{4n}{n+4}\sqrt{n+2} + \frac{6n}{n+2}\sqrt{n} + 4n\sqrt{\frac{n+1}{n^2+6n+8}} & \text{, if } n \text{ is even.} \end{cases}$

Proof. The values of $\xi^{ce}(Q_n)$, $\xi^c(Q_n)$, $\xi_c(Q_n)$, $\xi(Q_n)$, $M_1^{**}(Q_n)$ and $avec(Q_n)$ can be obtained by the Formulas 2, 3, 4, 5, 7, 9 and using the vertex partitions of Q_n as shown the Tables 1 and 2. Similarly, the values of $M_1^*(Q_n)$, $M_2^*(Q_n)$, $GA_4(Q_n)$ and $ABC_5(Q_n)$ can be obtained by the Formulas 6, 8, 10, 11 and using the edge partitions of Q_n as shown the Tables 5 and 6. □

Theorem 2. *Let R_n be a convex polytope of order 3n and size 6n, where $n \geq 5$. Then,*

(a) $\xi^{ce}(R_n) = \begin{cases} \frac{24n^2+44n}{n^2+4n+3} & \text{, if } n \text{ is odd;} \\ \frac{24n}{n+2} & \text{, if } n \text{ is even.} \end{cases}$

(b) $\xi^c(R_n) = 6n^2 + \frac{25}{2}n + (\frac{1}{2}n)(-1)^{n+1}$.

(c) $\xi_c(R_n) = 25n^2 + 52n + (2n)(-1)^{n+1}$.

(d) $\xi(R_n) = \frac{3}{2}n^2 + \frac{13}{4}n + (\frac{1}{4}n)(-1)^{n+1}$.

(e) $M_1^*(R_n) = 6n^2 + \frac{25}{2}n + (\frac{1}{2}n)(-1)^{n+1}$.

(f) $M_1^{**}(R_n) = \begin{cases} \frac{3}{4}n^3 + \frac{7}{2}n^2 + \frac{19}{4}n & \text{, if } n \text{ is odd;} \\ \frac{3}{4}n^3 + 3n^2 + 3n & \text{, if } n \text{ is even.} \end{cases}$

(g) $M_2^*(R_n) = \begin{cases} \frac{3}{2}n^3 + \frac{13}{2}n^2 + 7n & \text{, if } n \text{ is odd;} \\ \frac{3}{2}n^3 + 6n^2 + 6n & \text{, if } n \text{ is even.} \end{cases}$

(h) $avec(R_n) = \frac{1}{2}n + \frac{13}{12} + (\frac{1}{12})(-1)^{n+1}$.

(i) $GA_4(R_n) = \begin{cases} 3n + \frac{3n}{n+2}\sqrt{n^2 + 4n + 3} & \text{, if } n \text{ is odd;} \\ 6n & \text{, if } n \text{ is even.} \end{cases}$

(j) $ABC_5(R_n) = \begin{cases} \frac{4n}{n+3}\sqrt{n+1} + \frac{2n}{n+1}\sqrt{n-1} + 6n\sqrt{\frac{n}{n^2+4n+3}} & \text{, if } n \text{ is odd;} \\ \frac{12n}{n+2}\sqrt{n} & \text{, if } n \text{ is even.} \end{cases}$

Proof. The values of $\xi^{ce}(R_n)$, $\xi^{c}(R_n)$, $\xi_c(R_n)$, $\xi(R_n)$, $M_1^{**}(R_n)$ and $avec(R_n)$ can be obtained by the Formulas 2, 3, 4, 5, 7, 9 and using the vertex partitions of R_n as shown the Tables 3 and 4. Similarly, the values of $M_1^{*}(R_n)$, $M_2^{*}(R_n)$, $GA_4(R_n)$ and $ABC_5(R_n)$ can be obtained by the Formulas 6, 8, 10, 11 and using the edge partitions of R_n as shown the Tables 7 and 8. □

4 Conclusion

In this paper, we have studied and computed some eccenricity-based topological indices for two convex polytopes Q_n and R_n. The research work can be continued to derive new architectures from the convex polytopes Q_n and R_n for future works. Also, the eccentricity-based topological indices can be computed for other convex polytopes, their's subdivisions and line graphs for future works.

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Appendix A. The tables of vertex and edge partitions of the polytopes Q_n and R_n.

Table 1: The partitions of vertices in $G \cong Q_n$ for n is odd.

Type of vertices	$deg_G(u)$	**Frequency**	$\delta_G(u)$	$\varepsilon_G(u)$
1	3	n	11	$\frac{n+5}{2}$
2	5	n	19	$\frac{n+3}{2}$
3	3	n	13	$\frac{n+3}{2}$
4	3	n	9	$\frac{n+5}{2}$

Table 2: The partitions of vertices in $G \cong Q_n$ for n is even.

Type of vertices	$deg_G(u)$	**Frequency**	$\delta_G(u)$	$\varepsilon_G(u)$
1	3	n	11	$\frac{n+4}{2}$
2	5	n	19	$\frac{n+2}{2}$
3	3	n	13	$\frac{n+2}{2}$
4	3	n	9	$\frac{n+4}{2}$

Table 3: The partitions of vertices in $G \cong R_n$ for n is odd.

Type of vertices	$deg_G(u)$	**Frequency**	$\delta_G(u)$	$\varepsilon_G(u)$
1	4	n	18	$\frac{n+3}{2}$
2	5	n	21	$\frac{n+1}{2}$
3	3	n	11	$\frac{n+3}{2}$

Table 4: The partitions of vertices in $G \cong R_n$ for n is even.

Type of vertices	$deg_G(u)$	**Frequency**	$\delta_G(u)$	$\varepsilon_G(u)$
1	4	n	18	$\frac{n+2}{2}$
2	5	n	21	$\frac{n+2}{2}$
3	3	n	11	$\frac{n+2}{2}$

Table 5: The partitions of edges in $G \cong Q_n$ for n is odd.

Type of edges	$(deg_G(u), deg_G(v))$	**Frequency**	$(\varepsilon_G(u), \varepsilon_G(v))$
1	(3,3)	$2n$	$\left(\frac{n+5}{2}, \frac{n+5}{2}\right)$
2	(3,5)	n	$\left(\frac{n+5}{2}, \frac{n+3}{2}\right)$
3	(5,5)	n	$\left(\frac{n+3}{2}, \frac{n+3}{2}\right)$
4	(3,5)	$2n$	$\left(\frac{n+3}{2}, \frac{n+3}{2}\right)$
5	(3,3)	n	$\left(\frac{n+5}{2}, \frac{n+3}{2}\right)$

Table 6: The partitions of edges in $G \cong Q_n$ for n is even.

Type of edges	$(deg_G(u), deg_G(v))$	**Frequency**	$(\varepsilon_G(u), \varepsilon_G(v))$
1	(3,3)	$2n$	$\left(\frac{n+4}{2}, \frac{n+4}{2}\right)$
2	(3,5)	n	$\left(\frac{n+4}{2}, \frac{n+2}{2}\right)$
3	(5,5)	n	$\left(\frac{n+2}{2}, \frac{n+2}{2}\right)$
4	(3,5)	$2n$	$\left(\frac{n+2}{2}, \frac{n+2}{2}\right)$
5	(3,3)	n	$\left(\frac{n+4}{2}, \frac{n+2}{2}\right)$

Table 7: The partitions of edges in $G \cong R_n$ for n is odd.

Type of edges	$(deg_G(u), deg_G(v))$	**Frequency**	$(\varepsilon_G(u), \varepsilon_G(v))$
1	(4,4)	n	$\left(\frac{n+3}{2}, \frac{n+3}{2}\right)$
2	(4,5)	$2n$	$\left(\frac{n+3}{2}, \frac{n+1}{2}\right)$
3	(5,5)	n	$\left(\frac{n+1}{2}, \frac{n+1}{2}\right)$
4	(3,5)	n	$\left(\frac{n+3}{2}, \frac{n+1}{2}\right)$
5	(3,3)	n	$\left(\frac{n+3}{2}, \frac{n+3}{2}\right)$

Table 8: The partitions of edges in $G \cong R_n$ for n is even.

Type of edges	$(deg_G(u), deg_G(v))$	**Frequency**	$(\varepsilon_G(u), \varepsilon_G(v))$
1	(4,4)	n	$\left(\frac{n+2}{2}, \frac{n+2}{2}\right)$
2	(4,5)	$2n$	$\left(\frac{n+2}{2}, \frac{n+2}{2}\right)$
3	(5,5)	n	$\left(\frac{n+2}{2}, \frac{n+2}{2}\right)$
4	(3,5)	n	$\left(\frac{n+2}{2}, \frac{n+2}{2}\right)$
5	(3,3)	n	$\left(\frac{n+2}{2}, \frac{n+2}{2}\right)$