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SOME TOPOLOGICAL INDICES VALUES OF THE CONVEX POLYTOPE D_n AND ITS SUBDIVISION GRAPH $S(D_n)$

Tufan Turaci

Faculty of Engineering, Department of Computer Engineering, Pamukkale University, 20160 Denizli, Turkiye

Abstract. Graph theory has been studied different areas such as computer science, information, mathematics, natural sciences, and so on. Especially, it has been the most important mathematical analysis tools for the study the analysis of chemistry science. For example, the studies of descriptors in quantitative structure property relationship (QSPR) and quantitative structure activity relationship (QSAR) studies in the chemistry science have been used graph theory tecniques. Furtermore, topological indices have been also used to determine combinatorial properties of chemical graphs. In this paper, exact values of some eccentricity-based topological indices of the convex polytope D_n and its subdivision graph $S(D_n)$ have been determined.

Keywords: Graph theory, convex polytopes, subdivision graphs, eccentricity, topological indices.
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Corresponding author: Tufan Turaci, Faculty of Engineering, Department of Computer Engineering, Pamukkale University, 20160 Denizli-Turkey, e-mail: *tturaci@pau.edu.tr*
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1 Introduction

The graph theory is a branch of mathematical chemistry, that is it uses graph theory to mathematical modeling of chemical structures. A molecule or chemical compound can be represented graphically by a chemical graph, also known as a molecular graph. In a chemical graph, an atom of the molecule is represented by a vertex, and also the covalent bonds between atoms is represented by an edge. A topological index is a number that assists in understanding various physical characteristics, chemical reactivities, and boiling activities of a chemical compound by characterizing the whole molecular graph structure (Hayat et al., 2024). Graph theory is used to study of descriptors in quantitative structure property relationship (QSPR) and quantitative structure activity relationship (QSAR) studies in the chemistry science (Balaban et al., 1999; Hwang & Ghosh, 1987; Todeschini & Consonni, 2000). For example, the mathematical chemistry is that part of theoretical chemistry which is concerned with applications of mathematical methods to chemical problems (Cayley, 1874).

Let $G = (V(G), E(G))$ be a simple graph of order n and size m. 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

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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). There are many distance-based parameters in graph theory, such as eccentricity-based topological indices or network centrality measures (Aytac, 2020; Aytac et al., 2019; Aytac & Ozturk, 2020).

The concept of topological indices is very important in chemical graph theory. This theory applies graph theory in mathematical modeling of chemical structure. The first topological index is the *Wiener index* denoted by $W(G)$ in chemical graph theory and is defined by the chemist H. Wiener. The Wiener index has been closely correlated with the boiling points of alkane molecules (Wiener, 1947). The Wiener index aims to sum of the half of distances between every pair of vertices of G and it has been defined as follows:

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

After the definition of the Wiener index, many topological indices based on the degrees and eccentiricity values of graphs have been defined.The eccentricity-based topological indices are used as an important tool to the prediction of physico-chemical, pharmacological and toxicological properties of a compound directly from its molecular structure (Imran et al., 2018). The definitions of some important eccentricity-based topological have been given following.

The *connective eccentricity* index $\xi^{ce}(G)$ has been defined by Gupta et al. (2000) for the molecular graph G. The definiton of this index has been 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 $\xi^c(G)$ has been defined by Sharma et al. (1997). The eccentric connectivity index has been denoted by $\xi^c(G)$ for the any graph G, also it has been defined as follows:

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

In Ashrafi et al. (2011), the *modified eccentric connectivity* index $\xi_c(G)$ has been defined 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 has been further studied in Berberler & Berberler (2015).

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

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

The degre-based Zagreb indices and eccentricity-based Zagreb indices have been used a lot of study in chemistry science. The *first Zagreb index* and the *second Zagreb index* of graphs have been defined by Gutman et al. in Gutman & Trinajstic (1972). Then the *first*, *second* and *third Zagreb eccentricity* indices $M_1^*(G)$, $M_1^{**}(G)$ and $M_2^*(G)$ have been defined by Vukicevic et al. in Vukicevic & Graovac (2010) and Ghorbani et al. in Ghorbani & Hosseinzadeh (2012), respectively.

The *first Zagreb eccentricity* index has been 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 has been defined as follows:

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

The *third Zagreb eccentricity* index has been defined as follows:

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

The *average eccentricity index* $avec(G)$ has been defined in Ilic (2012) for any graph G. The definiton of $avec(G)$ has been 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 $GA_4(G)$ has been defined for any graph G in Ghorbani & Khaki (2012) as follows:

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

The fifth version of the atom bond connectivity index namely $ABC_5(G)$ has been 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 (Imran et al., 2018). Some papers about eccentricity-based topological indices can been seen by readers in Ilic & Gutman (2011); Aslan (2015); Aslan & Kurkcu (2015); Aslan (2015); Imran et al. (2018); Durgut & Turaci (2023); Idrees et al. (2019); Akhter et al. (2019); Hayat & Imran (2014); Turaci & Okten (2015); Gao et al. (2018); Kutucu & Turaci (2017); Turaci & Durgut (2022); Aytac & Vatansever (2023).

Furthermore, the convex polytopes which are geometric graphs have been studied in many different studies. The readers can be seen these studies in Asif et al. (2020); Sohail et al. (2018); Nazeer et al. (2016); Foruzanfar et al. (2018); Turaci (2022); Turaci & Durgut (2023); Hayat et al. (2024). In this paper, some important eccentricity-based topological indices have been determined for the convex polytope D_n and its subdivision graph $S(D_n)$.

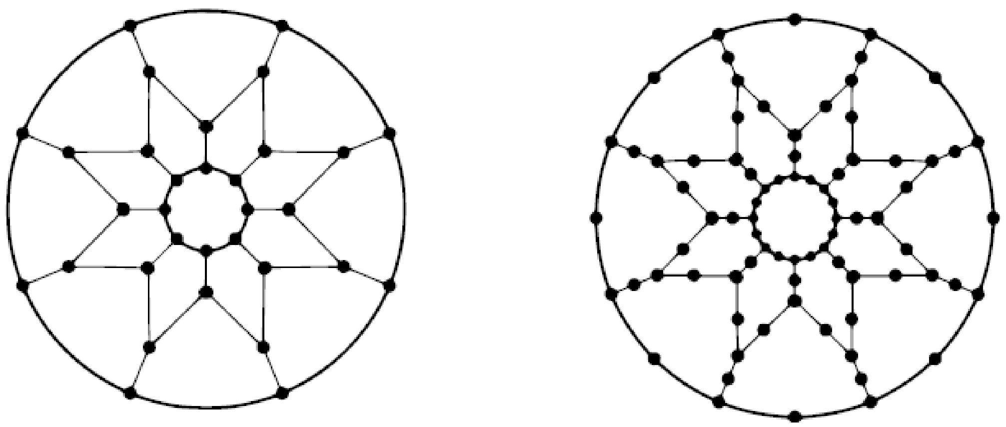
This paper is organized as follows: In Section 2, the definitions of the convex polytope D_n and its subdivision $S(D_n)$ have been given. Then, exact solutions of some eccentricity based topological indices have been presented for D_n and $S(D_n)$ in Section 3. Finally, the conclusion of paper has been given in Section 4.

2 The Convex Polytope D_n and Its Subdivision Graph $S(D_n)$

In this section, the convex polytope D_n is determined according to combinatorial aspects. Firstly, the definition of the convex polytope D_n and the definition of subdivision of the convex polytope D_n denoted by $S(D_n)$ have been given. Then, the vertex and edge partitions of the convex polytope D_n and $S(D_n)$ have been given.

2.1 The Definitions of Convex Polytope D_n and Its Subdivision Graph $S(D_n)$

The graph of convex polytope D_n consists of 5-sided faces and n-sided faces as defined in Baca (1988), where $|V(D_n)| = 4n$ and $|E(D_n)| = 6n$. The subdivision $S(D_n)$ by inserting an additional vertex between each pair of adjacent vertices of D_n. We have $|V(S(D_n))| = 10n$ and $|E(S(D_n))| = 12n$. The polytope D_8 and its subdivision $S(D_8)$ are shown in Figure 1.



(a) **(b)**

Figure 1: **(a)** The convex polytope D_8 **(b)** the subdivision graph $S(D_8)$

2.2 The Vertex and Edge Partitions of the Convex Polytope D_n and Its Subdivision Graph $S(D_n)$

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 D_n and $S(D_n)$, respectively. The vertex partition of D_n and $S(D_n)$ 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 D_n and $S(D_n)$, respectively. These edge partitions of the graphs D_n and $S(D_n)$ are shown in Tables 5, 6, 7 and 8. The vertex and edge partitions of the convex polytopes D_n and $S(D_n)$ 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 polytope D_n and Its Subdivision Graph $S(D_n)$

In this section, some eccentricity-based topological indices of the convex polytopes D_n and its subdivision graph $S(D_n)$ have been presented. All results of following theorems have been obtained by MAPLE programming language.

Theorem 1. *Let D_n be a convex polytope of order 4n and size 6n, where $n \geq 5$. Then,*

(a) $\xi^{ce}(D_n) = \frac{24n}{n+\frac{9}{2}+(\frac{1}{2})(-1)^{n+1}}$.

(b) $\xi^{c}(D_n) = 6n^2 + 27n + (3n)(-1)^{n+1}$.

(c) $\xi_{c}(D_n) = 6n^2 + 81n + (9n)(-1)^{n+1}$.

(d) $\xi(D_n) = 2n^2 + 9n + (n)(-1)^{n+1}$.

(e) $M_1^{*}(D_n) = 6n^2 + 27n + (3n)(-1)^{n+1}$.

(f) $M_1^{**}(D_n) = \begin{cases} n^3 + 10n^2 + 25n & \text{, if } n \text{ is odd;} \\ n^3 + 8n^2 + 16n & \text{, if } n \text{ is even.} \end{cases}$

(g) $M_2^{*}(D_n) = \begin{cases} \frac{3}{2}n^3 + 15n^2 + \frac{75}{2}n & \text{, if } n \text{ is odd;} \\ \frac{3}{2}n^3 + 12n^2 + 24n & \text{, if } n \text{ is even.} \end{cases}$

(h) $avec(D_n) = \frac{n+\frac{9}{2}+(\frac{1}{2})(-1)^{n+1}}{2}$.

(i) $GA_4(D_n) = 6n$.

(j) $ABC_5(D_n) = \begin{cases} \frac{12n}{n+5}\sqrt{n+3} & \text{, if } n \text{ is odd;} \\ \frac{12n}{n+4}\sqrt{n+2} & \text{, if } n \text{ is even.} \end{cases}$

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

Theorem 2. *Let $S(D_n)$ be a graph which is the subdivision of the convex polytope D_n of order 10n and size 12n, where $n \geq 5$. Then,*

(a) $\xi^{ce}(S(D_n)) = \begin{cases} \frac{24n}{n+5} & \text{, if } n \text{ is odd;} \\ \frac{24n^3+240n^2+584n}{n^3+15n^2+74n+120} & \text{, if } n \text{ is even.} \end{cases}$

(b) $\xi^{c}(S(D_n)) = 24n^2 + 120n$.

(c) $\xi_{c}(S(D_n)) = 60n^2 + 300n$.

(d) $\xi(S(D_n)) = 10n^2 + 50n$.

(e) $M_1^{*}(S(D_n)) = 24n^2 + 120n$.

(f) $M_1^{**}(S(D_n)) = 10n^3 + 100n^2 + 252n + (2n)(-1)^{n}$.

(g) $M_2^{*}(S(D_n)) = 12n^3 + 120n^2 + 300n$.

(h) $avec(S(D_n)) = n + 5$.

(i) $GA_4(S(D_n)) = \begin{cases} 12n & \text{, if } n \text{ is odd;} \\ 4n + \frac{8n}{2n+9}\sqrt{n^2+9n+20} + \frac{8n}{2n+11}\sqrt{n^2+11n+30} & \text{, if } n \text{ is even.} \end{cases}$

$$(j)\ ABC_5(S(D_n)) = \begin{cases} \frac{12n}{n+5}\sqrt{2n+8} & , \text{if } n \text{ is odd;} \\ \frac{4n}{n+5}\sqrt{2n+8} + 4n\sqrt{\frac{2n+7}{n^2+9n+20}} + 4n\sqrt{\frac{2n+9}{n^2+11n+30}} & , \text{if } n \text{ is even.} \end{cases}$$

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

4 Conclusion

In this paper, some eccenricity-based topological indices for a convex polytope D_n and its subdivision graph $S(D_n)$ have been computed. The research work can be continued to derive new architectures from the convex polytope D_n for future works. Furthermore, the eccentricity-based topological indices can be computed for different convex polytopes and their's subdivision graphs for future works.

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Appendix A. The tables of vertex and edge partitions of the polytope D_n and Its Subdivision Graph $S(D_n)$.

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

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

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

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

Table 3: The partitions of vertices in $G \cong S(D_n)$ for n is odd.

Type of vertices	$deg_G(u)$	**Frequency**	$\delta_G(u)$	$\varepsilon_G(u)$
1	3	$4n$	6	n+5
2	2	$6n$	6	n+5

Table 4: The partitions of vertices in $G \cong S(D_n)$ for n is even.

Type of vertices	$deg_G(u)$	**Frequency**	$\delta_G(u)$	$\varepsilon_G(u)$
1	3	$4n$	6	n+5
2	2	n	6	n+5
3	2	n	6	n+4
4	2	$2n$	6	n+6
5	2	n	6	n+4
6	2	n	6	n+5

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

Type of edges	$(deg_G(u), deg_G(v))$	**Frequency**	$(\varepsilon_G(u), \varepsilon_G(v))$
1	(3,3)	$6n$	$\left(\frac{n+5}{2}, \frac{n+5}{2}\right)$

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

Type of edges	$(deg_G(u), deg_G(v))$	**Frequency**	$(\varepsilon_G(u), \varepsilon_G(v))$
1	(3,3)	$6n$	$\left(\frac{n+4}{2}, \frac{n+4}{2}\right)$

Table 7: The partitions of edges in $G \cong S(D_n)$ for n is odd.

Type of edges	$(deg_G(u), deg_G(v))$	**Frequency**	$(\varepsilon_G(u), \varepsilon_G(v))$
1	(2,3)	$12n$	$(n+5, n+5)$

Table 8: The partitions of edges in $G \cong S(D_n)$ for n is even.

Type of edges	$(deg_G(u), deg_G(v))$	**Frequency**	$(\varepsilon_G(u), \varepsilon_G(v))$
1	(2,3)	$4n$	$(n+5, n+5)$
2	(2,3)	$4n$	$(n+4, n+5)$
3	(2,3)	$4n$	$(n+6, n+5)$