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ABC_4 and GA_5 indices of para-line graph of some convex polytopes

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Abstract In this paper, we will compute Fourth atom-bond connectivity index $ABC_4(G)$ and Fifth geometric-arithmetic connectivity index $GA_5(G)$, by considering G as para-line graph of some convex polytopes.

Keywords Topological indices, line graph, subdivision, convex polytopes.

AMS 2010 subject classifications 05C90, 05C35, 05C12.

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1. Introduction

In the field of chemistry, graph theory has been applied to a wide range of research areas: synthetic chemistry, quantum chemistry, thermochemistry etc. Graph theory has provided the chemist with a variety of very useful tools. Some of the graph theory concepts corresponds to the terms in chemistry e.g. point as an atom, line as a covalent bond, degree as atom valency and path as chemical substructure etc. Topological representation of an object tells us about the number of elements composing it and their connectivity (see [3]). Topological indices are invariant under graph isomorphisms. They have significant role in the quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) investigations (see [4, 6, 15, 35, 39]).

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G) \subseteq V(G) \times V(G)$. Let $p = |V(G)|$, the order of G and $q = |E(G)|$, the size of G. The degree d_v of any vertex v is defined as the number of vertices joining to that vertex v and the degree d_e of an edge $e \in E(G)$ is defined as the number of its adjacent vertices in $V(L(G))$, where $L(G)$ is the line graph whose vertices are the edges of G and they are adjacent if and only if they have a common end point in G. In structural chemistry, line graph of a graph G is very useful. The first topological index on the basis of line graph was introduced by Bertz in 1981 (see [5]). For more details on line graph see the articles [12, 14, 16, 17, 18, 21]. The subdivision $S(G)$ of a graph G can be obtained by replacing each edge of G by a path of length 2, or we can say by inserting an additional vertex between each pair of vertices of G. The line graph of subdivision is known as para-line graph. For more details on the topological indicies of para-line graphs we refer to the articles [22],–,[40].

Convex polytopes are fundamental geometric objects. The beauty of their theory is nowadays complemented by their importance for many other mathematical subjects, ranging from integration theory, algebraic topology, and algebraic geometry to linear and combinatorial optimization (see [11]). Also people are paying attention in finding

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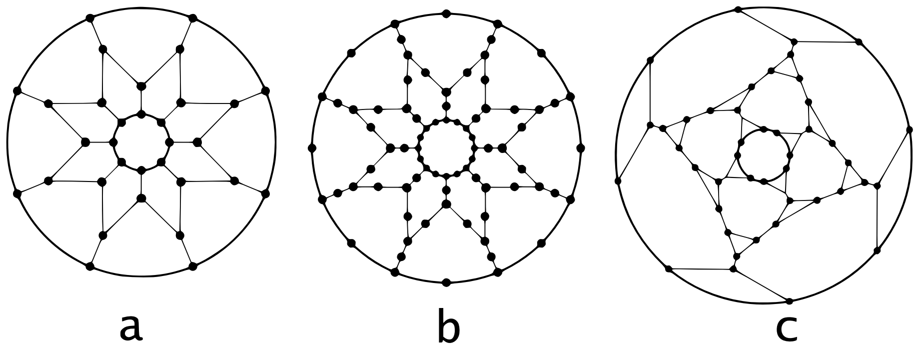

Figure 1. (a) Convex Polytope D_8, (b) Subdivision of D_8, (c) Para-line graph of D_4.

metric dimension and labeling of convex polytopes (see [1, 2, 19, 20]). From these motivational work, we take a step in finding the topological indices of para-line graph of some convex polytopes.

Lemma 1
Let G be a graph with $u, v \in V(G)$ and $e = uv \in E(G)$. Then:

$$d_e = d_u + d_v - 2.$$

Using above lemma, we can find the degree of a vertex of line graph.

Lemma 2
[13] Let G be a graph of order p and size q, then the line graph $L(G)$ of G is a graph of order q and size $\frac{1}{2}M_1(G) - q$.

1.1. Para-line graphs of convex polytopes D_n, Q_n and R_n

In this section we will discuss the combinatorial aspects of subdivision of some convex polytopes and their para-line graphs.

1.2. Convex polytope D_n

Consider the graph of convex polytope D_n as defined in [1]. The convex polytope D_n for $n = 8$ is shown in Figure 1-a.

1.2.1. Subdivision of Convex polytope D_n We obtain the graph $S(D_n)$ by replacing each edge of D_n by a path of length 2. The subdivision of D_n for $n = 8$ is shown in Figure 1-b. Using Lemma 2, the total number of edges are $12n$. Also $|V(S(D_n))| = 10n$ in which $6n$ vertices have degree 2 and $4n$ vertices have degree 3.

1.2.2. Para-line graph of Convex polytope D_n The para-line graph $L(S(D_n))$ of D_n for $n = 4$ is shown in Figure 1-c. Using Lemma 2, the total number of edges are $18n$. Also $|V(L(S(D_n)))| = 12n$ and all vertices are of degree 3.

1.3. Convex polytope Q_n

Consider the graph of convex polytope Q_n as defined in [2]. The convex polytope Q_n for $n = 8$ is shown in Figure 2-a.

1.3.1. Subdivision of Convex polytope Q_n We obtain the graph $S(Q_n)$ by replacing each edge of Q_n by a path of length 2. The subdivision of Q_n for $n = 8$ is shown in Figure 2-b. Using Lemma 2, the total number of edges are $14n$. Also $|V(S(Q_n))| = 11n$ in which $7n$ vertices have degree 2, $3n$ vertices have degree 3 and n vertices have degree 5.

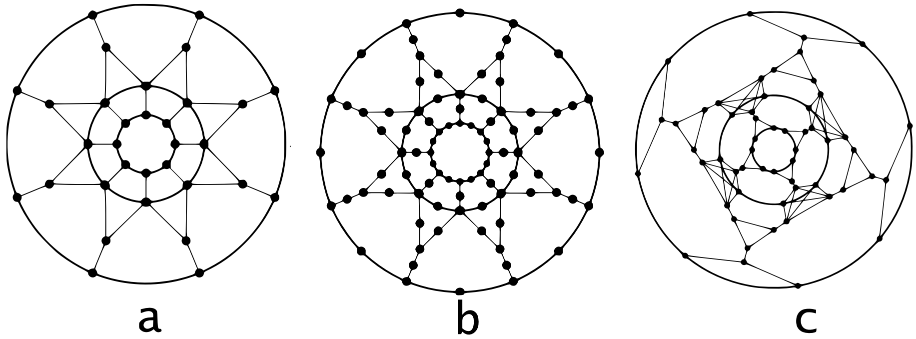

Figure 2. (a) Convex Polytope Q_8, (b) Subdivision of Q_8, (c) Convex polytope R_4.

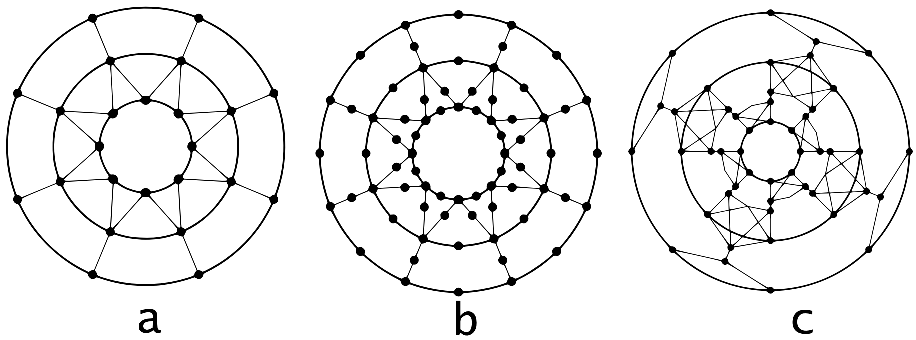

Figure 3. (a) Convex polytope R_8, (b) Subdivision of R_8, (c) Para-line graph of R_4.

1.3.2. Para-line graph of Convex polytope Q_n The para-line graph $L(S(Q_n))$ of Q_n for $n = 4$ is shown in Figure 2-c. Using Lemma 2, the total number of edges are $26n$. Also $|V(L(S(Q_n)))| = 14n$ in which $9n$ vertices have degree 3 and $5n$ vertices have degree 5.

1.4. Convex polytope R_n

Consider the graph of convex polytope R_n as defined in [2]. The convex polytope R_n for $n = 8$ is shown in Figure 3-a.

1.4.1. Subdivision of Convex polytope R_n We obtain the graph $S(R_n)$ by replacing each edge of R_n by a path of length 2. The subdivision of R_n for $n = 8$ is shown in Figure 3-b. Using Lemma 2, the total number of edges are $12n$. Also $|V(S(R_n))| = 9n$ in which $6n$ vertices have degree 2, n vertices have degree 3, n vertices have degree 4 and n vertices have degree 5.

1.4.2. Para-line graph of Convex polytope R_n The para-line graph $L(S(R_n))$ of R_n for $n = 4$ is shown in Figure 3-c. Using Lemma 2, the total number of edges are $25n$. Also $|V(L(S(Q_n)))| = 12n$ in which $3n$ vertices are of degree 3, $4n$ vertices are of degree 4 and $5n$ vertices are of degree 5.

1.5. The edge partitions of para-line graph of convex polytopes w.r.t degree sum

For a vertex $u \in V(G)$, let S_u= $\sum_{uv\in E(G)} d_v$ is the degree sum of u. For $uv \in E(G)$, S_u and S_v is the sum of degrees of all neighbors of vertex u and v in G respectively. We partition $E(G)$ into subsets based on the degree sum of the end vertices of edges in G. The edge partition of $L(S(D_n))$, $L(S(Q_n))$ and $L(S(R_n))$ with respect to degree sum are shown in Tables 1, 2 and 3 respectively.

(S_u, S_v)	Number of edges
$(9,9)$	$18n$

Table 1. The edge partition of para-line graph of D_n w.r.t degree sum

(S_u, S_v)	Number of edges
$(9,9)$	$7n$
$(9,11)$	$4n$
$(11,11)$	n
$(11,13)$	$3n$
$(23,23)$	$11n$

Table 2. The edge partition of para-line graph of Q_n w.r.t degree sum

(S_u, S_v)	Number of edges	(S_u, S_v)	Number of edges
$(9,9)$	$2n$	$(16,16)$	$2n$
$(9,11)$	$2n$	$(16,17)$	$4n$
$(11,23)$	n	$(17,17)$	n
$(23,25)$	$2n$	$(17,24)$	$2n$
$(24,24)$	n	$(23,24)$	$2n$
$(25,25)$	$2n$	$(24,25)$	$4n$

Table 3. The edge partition of para-line graph of R_n w.r.t degree sum

2. Topological Indices of para-line graphs of some Convex Polytopes

In this section we will compute *Fourth Atom-Bond Connectivity Index* and *Fifth Geometric-Arithmetic Index* of the para-line graphs of some convex polytopes discussed in the first section.

2.1. Fourth Atom-Bond Connectivity Index

M. Ghorbani et al. in [7, 8, 9] proposed Fourth Atom-Bond connectivity index as:

$$ABC_4(G) = \sum_{uv\in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}. \tag{1}$$

where S_u is the sum of degrees of all neighbors of vertex u in G. In other words, S_u= $\sum_{uv\in E(G)} d_v$. Similarly for S_v.

2.2. Fifth Geometric-Arithmetic Index

This index was introduced by Graovac et al. in [10] as:

$$GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}. \tag{2}$$

Theorem 1
Let $L(S(D_n))$, $L(S(Q_n))$ and $L(S(R_n))$ are the para-line graphs of convex polytopes D_n, Q_n and R_n respectively then:

$ABC_4(L(S(D_n)))$ = $8n$.
$ABC_4(L(S(Q_n)))$ = $\frac{28}{9}n + \frac{4}{11}n\sqrt{22} + \frac{2}{11}n\sqrt{5} + \frac{12}{253}n\sqrt{506} + \frac{22}{23}n\sqrt{11}$.
$ABC_4(L(S(R_n)))$ = $\frac{8}{9}n + \frac{2}{11}n\sqrt{22} + \frac{4}{253}n\sqrt{506} + \frac{54}{85}n\sqrt{2} + \frac{8}{25}n\sqrt{3} + \frac{1}{24}n\sqrt{46}$
$+\frac{1}{15}n\sqrt{28} + \frac{1}{46}n\sqrt{690} + \frac{1}{34}n\sqrt{442} + \frac{1}{17}n\sqrt{527} + \frac{1}{8}n\sqrt{30}$.

Proof
The Fourth Atom-Bond Connectivity Index can be obtained by using Formula (1) and using edge partitions shown in Tables 1, 2 and 3. □

Theorem 2
Let $L(S(D_n))$, $L(S(Q_n))$ and $L(S(R_n))$ are the para-line graphs of convex polytopes D_n, Q_n and R_n respectively then:

$GA_5(L(S(D_n)) = 18n.$
$GA_5(L(S(Q_n)) = 19n + \frac{6}{5}n\sqrt{11} + \frac{3}{17}n\sqrt{253}.$
$GA_5(L(S(R_n)) = 8n + \frac{3}{5}n\sqrt{11} + \frac{1}{17}n\sqrt{25} + \frac{5}{12}n\sqrt{23} + \frac{89}{49}n\sqrt{6} + \frac{8}{47}n\sqrt{13} + \frac{8}{41}n\sqrt{102}$
$+\frac{32}{33}n\sqrt{17}.$

Proof
The Fifth Geometric-Arithmetic Index can be obtained by using Formula (2) and using edge partitions shown in Tables 1, 2 and 3. □

3. Conclusion

In this paper, we continue the study certain degree based topological indices for the line graph of subdivision graph of 2D-lattice graphs and obtained degree indices "Fourth atom-bond connectivity index $ABC_4(G)$ and Fifth geometric-arithmetic connectivity index $GA_5(G)$" of para-line graph of some convex polytopes.

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