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Topological Indices of the Line Graph of Subdivision Graph of Complete Bipartite Graphs

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Abstract: Topological index is a number associated with molecular graph and this number correlate certain physico-chemical properties of chemical compounds. In the study of QSAR/QSPR, topological indices such as, Randić index, Zagreb index, general sum-connectivity index, atom-bond connectivity (ABC) index and geometric-arithmetic (GA) index are exploited to estimate the bioactivity of chemical compounds. In this paper, we compute generalized Randić , first and second Zagreb, first and second multiple Zagreb, hyper Zagreb, general sum connectivity index, ABC and GA indices of the line graph of subdivision graph of complete bipartite graphs. Moreover, we also give an explicit formula for ABC_4 and GA_5 indices of the line graph of subdivision graph of complete bipartite graphs.

Keywords: Zagreb indices, degree, complete bipartite graph, line graph, subdivision graph.

1 Introduction

During past few decades, role of Graph theory has increased considerably in Chemistry. Topological indices basically attach a number to a molecular graph which gives a lot of useful information about that organic compound. The significance of topological index is usually associated with quantitative structures property relationship (QSPR) and quantitative structure activity relationship (QSAR) (see [25]). First topological index was introduced in 1947 by famous chemist Harold Wiener [26], known as Wiener index now a day. During 90's a large number of other topological indices came into existence and revolutionized the world of chemistry.

Several physicochemical properties such as molecular weight, density, boiling point, heats of vaporization, vapor pressure, molar volume, equalized electronegativity, infrared group frequency, isomer shift, quadruple splitting, edge shift, molar refraction, dipole movements, van der wall volume, proton-ligand formation and polarizability of organic compounds can be modeled using topological indices, see [24,31,32,33,34,35,36,37,38,39,40]. A number of graphs are composed of simpler graphs that serve as their basic building blocks. Due to this, a large number of chemists and mathematicians have been paying their attentions to study the properties of subdivision graphs of well-known families of graphs. In this paper, we have observed that the complete bipartite graph $K_{n,m}$ can be constructed from simpler star graphs S_m and hence use this idea to calculate the topological indices of this family.

A bipartite graph, also known as bi-graph, consists of a set of vertices which is decomposed into two disjoint sets such that no two vertices within the same set are adjacent. A cyclic graph is bipartite if and only if its cycles are of even length, a well-known result. In particular, all acyclic (having no cycles) graphs are bipartite. A complete bipartite graph is a bipartite graph such that every pair of graph vertices in the two sets are adjacent. If there are n and m vertices in the two sets, the complete bipartite graph is denoted by $K_{(n,m)}$.

In 2011, Ranjini et al. calculated the explicit expressions for the Shultz indices of the subdivision graphs of the tadpole, wheel, helm and ladder graphs [27].

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They also studied the Zagreb indices of the line graphs of the tadpole, wheel and ladder graphs with subdivision in [28]. In 2015, Su and Xu calculated the general sum-connectivity indices and co-indices of the line graphs of the tadpole, wheel and ladder graphs with subdivision in [30]. In [29], Nadeem et al. computed ABC4 and GA5 indices of the line graphs of the tadpole, wheel and ladder graphs by using the notion of subdivision

2 Basic concepts and terminology

A graph $G=(V,E)$ with vertex set V and edge set E is connected if there is a connection among any pair of vertices of G. A chemical graph is a graph whose vertices denote atoms and edges denote bonds among these atoms. The degree of a vertex v denoted by d_v is the number of vertices attached to the vertex v. In a chemical graph G, $d_v \leq 4$ for all $v \in V(G)$. Let us review some important topological indices:

The first degree based topological index is Randić index [19] denoted by $R_{\frac{1}{2}}(G)$ and is defined as:

$$R_{\frac{1}{2}}(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

Bolloas and Erdos in [2] defined independently the concept of general Randić index R_α. The general Randić index R_α is defined as,

$$R_\alpha = \sum_{uv\in E(G)} (d_u d_v)^\alpha \tag{1}$$

The so-called sum-connectivity index is a recent invention by Bo Zhou and Nenad Trinajstic [3] and it's defined as

$$SCI(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u + d_v}}.$$

In 2010, the general sum-connectivity index $\chi_\alpha(G)$ was introduced in [4]:

$$\chi_\alpha(G) = \sum_{uv\in E(G)} (d_u + d_v)^\alpha. \tag{2}$$

In 1972, *I. Gutman* [11] introduced one of the oldest topological index based on degree of vertices of the graph G named as *first Zagreb index*. The first Zagerb $(M_1(G))$ and *second Zagreb* $M_2(G)$ is defined as

$$M_1(G) = \sum_{v\in V(G)} d(v)^2 = \sum_{uv\in E(G)} [d(u)+d(v)] \tag{3}$$

$$M_2(G) = \sum_{uv\in E(G)} [d(u)\times d(v)] \tag{4}$$

where $d(u)$ is the degree of the vertex u in the graph G.

In 2012, *Ghorbani* et. al [8] defined new versions of Zagreb indices of a graph G. These are named as *first multiple Zagreb index* $PM_1(G)$, *second Zagreb index* $PM_2(G)$ and these indices are defined as

$$PM_1(G) = \prod_{uv\in E(G)} [d(u)+d(v)] \tag{5}$$

$$PM_2(G) = \prod_{uv\in E(G)} [d(u)\times d(v)] \tag{6}$$

Recently, Shirdel et al. [20] proposed the *hyper-Zagreb index* as

$$HM(G) = \sum_{uv\in E(G)} [d(u)+d(v)]^2 \tag{7}$$

Hundreds of research papers have been published on Zagreb indices few are mention here [1,7,9,10,16,23]. The widely used connectivity topological index is atom-bond connectivity (ABC) index introduced by Estrada et al. in [6]. The ABC index of graph G is defined as

$$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}. \tag{8}$$

D. Vukicevic and B. Furtula introduced the geometric arithmetic (GA) index in [22] and defined as

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}. \tag{9}$$

The fourth version of ABC index is proposed by *Ghorbani* [12] et al.

$$ABC_4(G) = \sum_{uv\in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} \tag{10}$$

Graovac et al. [13] introduced the fifth version of GA index and defined as

$$GA_5(G) = \sum_{uv\in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v} \tag{11}$$

3 Constuction of line graph of subdivision graph of complete bipartite graph and main results

We need some terminology and need to understand a construction of graphs in order to calculate the topological indices. By subdivision of a graph G, we mean a graph obtained from G by replacing each edge of G with P_2, i.e. path of length 2. We shall denote by $S(G)$, the subdivision graph of G. The line graph $L(G)$ of a

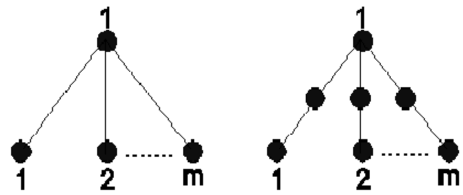

Fig. 1: $K_{n,m}$.

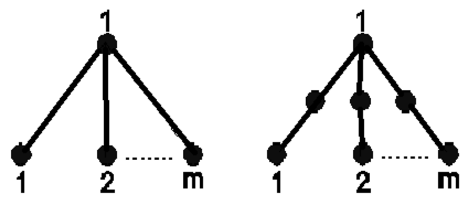

Fig. 2: S_m and $L(S_m)$.

graph G is the graph whose vertices are exactly the edges of the graph G and two vertices are adjacent in $L(G)$ if and only if they have common vertex in the graph G.

Complete bipartite graphs constitute an important and large family of graphs. A complete bipartite graph G is a graph whose vertex set $V(G)$ can be partitioned into two non-empty sets V_1 and V_2 in such a way that every vertex in V_1 is adjacent to every vertex in V_2, no vertex in V_1 is adjacent to a vertex in V_1 and no vertex in V_2 is adjacent to a vertex in V_2. Throughout this paper, we shall assume $|V_1| = n$ and $|V_2| = m$ and we shall denote the complete bipartite graph as $K_{n,m}$ (see Figure 1). In some sense, we can think of this graph as it is composed of the n stars graphs S_m. The star graph S_m and its line graph $L(S_m)$ are shown in the figure. Let us now examine the line graph of the subdivision graph of the star graph, i.e. $L(S(S_m))$. It is an easy exercise to note that this graph consists of a complete graph K_m along with one edge attached to each vertex as shown in the Figure 2. It has been observed that when we construct the line graph of the subdivision graph of the complete bipartite graph, i.e. $L(S(K_{n,m}))$ we obtain n graphs of the form $L(S(S_m))$ (see Figure 3) connected with each other.

For example if we take $n = 3$ and $m = 5$ then the line graph of the subdivision graph of the complete bipartite graph $K_{3,5}$ is shown in the Figure 4. Note that there are $3 - L(S(S_5))$ which are attached with each other as shown

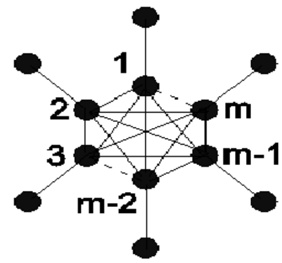

Fig. 3: $L(S(S_m))$.

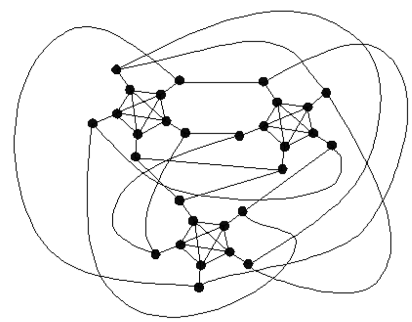

Fig. 4: $L(S(K_{3,5}))$.

in the Figure 4. Here note that the degrees of the vertices are either 3 or 5. Similar pattern has been observed in general case. It has also been observed that there are mC_2^n edges among these $n - L(S(S_m)$ graphs. As each $L(S(S_m))$ consists of $m + C_2^m$ edges and there are n such graphs so the total number of edges in $L(S(K_{n,m}))$ will be $mC_2^n + nC_2^m + mn$. On the other hand, as there are mn edges in $K_{n,m}$ so there will be $2mn$ edges in $S(K_{n,m})$ and hence $2mn$ vertices in its line graph.

Let G be a molecular graph and $e = u,v$ is an edge of G. Then we define the degree vector associated to the edge e to be (d_u, d_v). The above construction shows that degrees of vertices of the line graph of subdivision graph of complete bipartite graph $L(S(K_{n,m}))$ can be m or n only, so the possible degree vectors in this graph can be $(m,m),(n,n)$ or (n,m) only. The following tables summarize this data

Table 1: Edge partition of the line graph of subdivision graph of $K_{n,m}$ based on degree of end vertices.

Degree vector (d_u, d_v)	(m,m)	(n,n)	(m,n)
Number of edges	nC_2^m	mC_2^n	nm

Now we are ready to compute the Randic (R_α), first and second Zagreb, first and second multiple Zagreb, Hyper Zagreb, sum connectivity, atom-bond connectivity ABC and geometric-arithmetic GA indices of the line graph of subdivision graph of complete bipartite graphs.

Theorem 1. *The general Randic index R_α and the general sum connectivity index χ_α of the line graph of subdivision graph of complete bipartite graph $L(S(K_{n,m}))$ is*

$$R_\alpha(L(S(K_{n,m}))) = \frac{1}{2}(n(m-1)m^{2\alpha+1} + 2n^{\alpha+1}m^{\alpha+1} + m(n-1)n^{2\alpha+1})$$

$$\chi_\alpha(L(S(K_{n,m}))) = 2^{\alpha-1}n(m-1)m^{\alpha+1} + mn(m+n)^\alpha + 2^{\alpha-1}m(n-1)n^{(\alpha+1)}$$

Proof. As above construction reveals that $L(L(S(K_{n,m})))$ contains $2mn$ vertices and $n(C_2^m + m) + \frac{(mn(n-1))}{2}$ edges. Now there are nC_2^m edges whose both vertices have degree as (m,m), there are nm edges whose degree vector is (n,m) and remaining $\frac{mn(n-1)}{2}$ edges have (n,n) as the degree vector. Thus, by using the definition we obtain the required result.

If we put $\alpha = 1$ in the formulas of general Randic index, we get $R_1(L(S(K_{n,m}))) = \frac{1}{2}(n(m-1)m^3 + 2n^2m^2 + m(n-1)n^3)$. Similarly using $\alpha = 1$ in the formula of general sum connectivity index , we get $SCI(L(S(K_{n,m}))) = n(m-1)m^2 + mn(m+n) + m(n-1)n^2$.

Corollary. The classical Randic index will be $nm + \sqrt{nm} - \frac{n+m}{2}$

Note that $\sqrt{nm}$ and $\frac{n+m}{2}$ represents the geometric and arithmetic means of n,m respectively.

Theorem 2. *Let G be line graph of subdivision graph of complete bipartite graph $K_{n,m}$, then*

$$\begin{aligned}
M_1(G) &= mn(m^2+n^2)\\
M_2(G) &= \frac{mn}{2}(m^3+n^3-(m-n)^2)\\
PM_1(G) &= m^3n^3(m-1)(n-1)(m+n)\\
PM_2(G) &= \frac{m^6n^6}{2}(m-1)(n-1)\\
HM(G) &= mn(2m^3+2n^3-(m-n)^2)
\end{aligned}$$

Proof. The edge partition based on the degree of end vertices is shown in Table 1. We apply Formula 3, 4, 5, 6 and 7 to the Table 1 and get the required indices.

By Similar arguments we can obtain the expressions of ABC and GA indices of line graph of subdivision graph of complete bipartite graph $L(S(K_{n,m}))$.

Theorem 3. *Let G be line graph of subdivision graph of complete bipartite graph $L(S(K_{n,m}))$, then*

$$ABC(G) = \sqrt{\frac{mn}{2}}(\sqrt{n}(m-1) + \sqrt{m}(n-1) + \sqrt{2m+2n-4})$$

$$GA(G) = \frac{mn(m+n-2)}{2} + 2\frac{n^{\frac{3}{2}}m^{\frac{3}{2}}}{n+m}.$$

Let G be a molecular graph and $e = uv$ is an edge of G. Then the sum-degree vector associated to the edge e is (S_u, S_v). The above construction also gives us opportunity to compute S_u and hence the corresponding sum-degree vectors. In $(S(K_(n,m)))$, possibilities for S_u are $m+n(n-1)$ and $n+m(m-1)$ only, for any vertex u. There are three types of sum-degree vectors in the line graph of subdivision graph of complete bipartite graph $L(S(K_(n,m)))$ which are $(n+m(m-1), m+n(n-1)), (n+m(m-1), n+m(m-1))$ and $(m+n(n-1), m+n(n-1))$ and the number of edge corresponding to these sum-degree vectors are mn, nC_2^m and mC_2^n respectively. The following table summarize this data

Table 2: Edge partition of the line graph of subdivision graph of $K_{n,m}$ based on sum-degree of end vertices.

Sum-degree vector (S_u, S_v)	Number of edges
(n+m(m-1),n+m(m-1))	nC_2^m
(m+n(n-1),m+n(n-1))	mC_2^n
(m+n(n-1), n+m(m-1))	nm

Now we compute two important topological indices fourth ABC and fifth GA for line graph of subdivision graph of complete bipartite graph $L(S(K_{n,m}))$. In order to compute these indices, we need an edge partition of $L(S(K_{n,m}))$ based on the degree sum of vertices lying at unit distance from end vertices of each edge. In Table 2 such a partition is shown. In the following theorem, ABC_4 and GA_5 indices of $L(S(K_{n,m}))$ is computed.

Theorem 4. *Let G be line graph of subdivision graph of complete bipartite graph $L(S(K_{n,m}))$, then*

$$\begin{aligned}
ABC_4(G) = &\frac{nm(m-1)}{\sqrt{2}(n+m^2-m)}\sqrt{m^2-m+n-1}\\
&+ \frac{nm(n-1)}{\sqrt{2}(m+n^2-n)}\sqrt{n^2-n+m-1}\\
&+ mn\sqrt{\frac{m^2+n^2-2}{(n+m^2-m)(m+n^2-n)}}
\end{aligned}$$

$$GA_5(G) = \frac{mn(m+n-2)}{2} + \frac{nm\sqrt{(n+m^2-m)(m+n^2-n)}}{n^2+m^2}.$$

Proof. The edge partition based on the degree sum of neighbors of end vertices is shown in Table 2. We apply Formula 10 and 11 to the Table 2 and get the required indices.

4 Conclusion

We have computed degree and sum-degree vectors of all the edges in the line graph of subdivision graph of complete bipartite graph $L(S(K_(n,m)))$. Using that information we have computed the general Randic, first and second Zagreb, first and second multiple Zagreb, Hyper Zagreb, atom-bond connectivity, geometric-arithmetic, fourth version of atom-bond connectivity and fifth version of geometric-arithmetic indices of this family in general.

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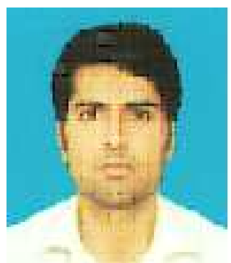

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