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Unicyclic Graphs and Their Zagreb Indices: A Subdivision Approach

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ABSTRACT: The first Zagreb index $M_1(G)$ of a graph G is equal to the sum of squares of the degree of vertices, and the second Zagreb index $M_2(G)$ is the sum of the products of the degrees of pairs of adjacent vertices of G. This paper uses the subdivision concept to study the Zagreb indices and coindices of the line graph and line cut-vertex graph of a particular class of unicyclic graphs, called cycle-star graph.

Keywords: First Zagreb index, second Zagreb index, first Zagreb coindex, second Zagreb coindex, subdivision graph, cycle-star graph.

Contents

1. Introduction

A graph $G = (V, E)$ consists of a vertex set $V(G)$ and an edge set $E(G)$, with $|V(G)| = n$ and $|E(G)| = m$. The n and m, represent the order and size of G, respectively, and are important for describing and measuring the fundamental properties of graphs. The notation uv is used to denote an edge between two vertices, u and v. An important concept in graph theory is the degree of a vertex in a graph G. The degree of a vertex v, denoted as $d_G(v)$, is the number of edges in G that are incident to v.

In chemical graph theory, the first and second Zagreb indices are among the most well-known and extensively studied topological indices. These indices are used to describe the topological structure of chemical substances, particularly organic molecules. Since their introduction in [4], these indices have been further developed in [5]. The fundamental properties of $M_1(G)$ and $M_2(G)$ are given in [7,14].

The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of a graph G are defined, respectively, as

$$M_1 = M_1(G) = \sum_{st \in E(G)} [d_G(s) + d_G(t)]$$

$$M_2 = M_2(G) = \sum_{st \in E(G)} d_G(s) \cdot d_G(t)$$

Several results and studies have been conducted concerning the Zagreb indices (M_1 and M_2) and their applications in various fields, particularly in chemical graph theory and chemo-informatics [2,3,6,8,9]. Some historical details about the Zagreb indices can be seen in [10].

In 2008, Došlić [1] introduced the concept of the first Zagreb coindex as an extension or complement to the existing Zagreb indices. The first Zagreb coindex, denoted by $\overline{M_1}$, is a topological index that is defined based on the same principles as the original Zagreb indices.

$$\overline{M_1} = \overline{M_1}(G) = \sum_{st \notin E(G)} [d_G(s) + d_G(t)] \tag{1.1}$$

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The second Zagreb coindex, denoted by $\overline{M_2}$, is defined analogously to the second Zagreb index (M_2).

$$\overline{M_2} = \overline{M_2}(G) = \sum_{st \notin E(G)} d_G(s) \cdot d_G(t) \tag{1.2}$$

In expressions (1.1) and (1.2) for the first and second Zagreb coindex, it is assumed that the vertices u and v represent distinct vertices in the graph G.

Let $S(G)$ denote the subdivision graph of a graph G, which is done by inserting new vertices into its edges. This process effectively subdivides each edge in G by replacing each edge with a path of length two. The concept of the cycle-star graph was first introduced in [18]. A *cycle-star graph*, written $CS_{k,n-k}$, is a graph consisting of two parts: a cycle of length k and $n-k$ leaf vertices, each connected to a single vertex of the cycle. Therefore, all cycle-star graphs $CS_{k,n-k}$ are unicyclic graphs, meaning they are connected graphs that contain exactly one cycle. An example of a cycle-star graph is shown in Figure 1.

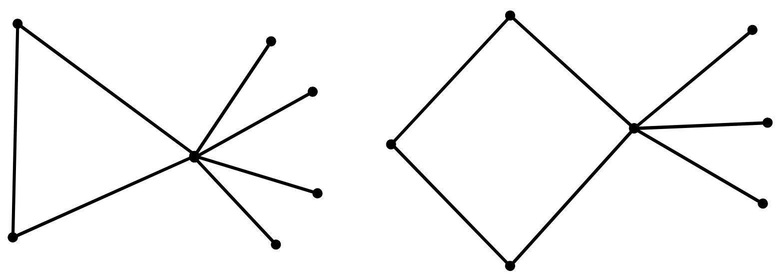

Figure 1: The cycle-star graphs $CS_{3,4}$ and $CS_{4,3}$

Because cycle–star graphs can serve as idealized models for certain organic molecular structures, they are of interest in mathematical chemistry. These graphs provide simplified representations of organic compounds, which mainly consist of carbon atoms bonded with hydrogen and other heteroatoms, and are useful for theoretical analysis rather than exact molecular depiction.

The Zagreb indices of unicyclic graphs have recently attracted considerable attention. Related research includes studies on the maximal hyper-Zagreb index of unicyclic graphs with a specified order and matching number [20], general multiplicative Zagreb indices of unicyclic graphs [13], and Zagreb eccentricity indices of unicyclic graphs [19]. However, there has been no attempt to study the Zagreb indices of the intersection graph on the vertex set of unicyclic graphs. In this paper, we compute the Zagreb indices and coindices of a class of unicyclic graphs called the cycle-star graph, and we examine the line graph and line cut-vertex graph of the subdivision graph of these graphs. Readers are recommended to refer to the paper [15] for more information about Zagreb indices and coindices of graphs using graph operators. For definitions and notations not introduced here, the readers are referred to [11].

The structure of this paper is as follows. Section 2 presents the Zagreb indices and coindices of the line graph of the subdivision graph of the cycle-star graph $CS_{k,n-k}$. Section 3 covers the Zagreb indices and coindices of the line-cut vertex graph of the subdivision graph of the cycle-star graph $CS_{k,n-k}$. Section 4 concludes with recommendations for further study. The paper concludes with a list of references.

2. Zagreb indices of the line graph of the subdivision graph of the cycle-star graph $CS_{k,n-k}$

In particular, unless otherwise specified, the parameters $k \geq 3$ and $n-k \geq 1$ are considered for every cycle-star graph $CS_{k,n-k}$.

From a given graph, a variety of graph operators (also known as graph-valued functions) can be used to create a new graph. One such graph operator is the line graph of a graph G. The *line graph* of a graph G, written $L(G)$, is the graph whose vertices are the edges of G. Two vertices of $L(G)$ are adjacent whenever the corresponding edges of G share a vertex in common. The study of [17] focused on analyzing the Zagreb indices and coindices of the subdivision graph line graphs.

In the next theorem, the line graph of the subdivision graph of the cycle-star graph is determined.

Theorem 2.1 *Let G be the line graph derived from the subdivision graph of the cycle-star graph $CS_{k,n-k}$. Then $M_1(G) = n^3 + (6-3k)n^2 + (3k^2 - 12k + 13)n - k^3 + 6k^2 - 5k$; and*

$$M_2(G) = \frac{1}{2}\left(n^4 + (7-4k)n^3 + (6k^2 - 21k + 20)n^2 - (4k^3 - 21k^2 + 40k - 32)n\right) + \frac{1}{2}\left(k^4 - 7k^3 + 20k^2 - 16k\right).$$

Proof: Let $G = L(S(CS_{k,n-k}))$. Then the graph G comprises $2n$ vertices, of which there are $2k-2$ vertices degree 2; $n-k+2$ vertices are of degree $n-k+2$; and $n-k$ vertices are of degree 1. Thus,

$$\begin{aligned} M_1(G) &= 4(2k-2) + (n-k+2)(n-k+2)^2 + (n-k) \\ &= n^3 + (6-3k)n^2 + (3k^2 - 12k + 13)n - k^3 + 6k^2 - 5k. \end{aligned}$$

To find $M_2(G)$, we first find the size of G. The size of G is

$$|E(G)| = \frac{(n-k+2)(n-k+1)}{2} + 2k - 1 + n - k = \frac{1}{2}[n^2 + k^2 + 5n - 2nk - k].$$

In other words, $E(G)$ contains $2k-3$ edges where both end vertices have degree 2; 2 edges where end vertices have degree 2 and $n-k+2$; $n-k$ edges where end vertices have degree 1 and $n-k+2$; and the remaining $\frac{(n-k+2)(n-k+1)}{2}$ edges where end vertices have degree $n-k+2$. Thus,

$$M_2(G) = (8k-12) + (4n - 4k + 8) + (n-k)(n-k+2) + \frac{(n-k+2)(n-k+1)}{2}(n-k+2)^2$$
$$= \frac{1}{2}\left(n^4 + (7-4k)n^3 + (6k^2 - 21k + 20)n^2 - (4k^3 - 21k^2 + 40k - 32)n\right) + \frac{1}{2}\left(k^4 - 7k^3 + 20k^2 - 16k\right).$$

□

An example of Theorem 2.1 is shown in Figure 2.

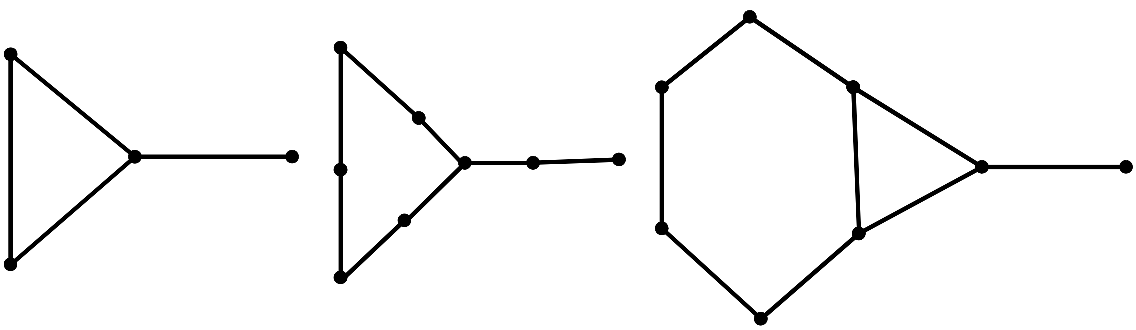

Figure 2: The cycle-star graph $CS_{3,1}$; $S(CS_{3,1})$; $L(S(CS_{3,1}))$

For $G = L(S(CS_{3,1}))$ of Figure 2, using Theorem 2.1,

$$M_1(G) = 64 + 16(6-9) + 4(27 - 36 + 13) - 27 + 54 - 15 = 44.$$

$$M_2(G) = \frac{1}{2}(256 + 64(7-12) + 16(54 - 63 + 20) - 4(108 - 189 + 120 - 32)) + \frac{1}{2}(81 - 189 + 180 - 48) = 54.$$

We now provide the expressions for the first and second Zagreb coindices of the line graph of the subdivision graph of the cycle-star graph.

The following two results [8] are the comprehensive set of relationships between the first and second Zagreb index and coindex of a graph.

Theorem 2.2 *Let G be a graph with n vertices and m edges. Then* $\overline{M_1}(G) = 2m(n-1) - M_1(G)$.

Theorem 2.3 *Let G be a graph with n vertices and m edges. Then* $\overline{M_2}(G) = 2m^2 - \frac{1}{2}M_1(G) - M_2(G)$.

Using Theorem 2.2 and Theorem 2.3, we have the following result.

Theorem 2.4 *Let G be the line graph of the subdivision graph of the cycle-star graph $CS_{k,n-k}$. Then* $\overline{M_1}(G) = n^3 + (3-k)n^2 - (k^2 - 12k + 18)n + k^3 - 7k^2 + 6k$.

Proof: Let $G = L(S(CS_{k,n-k}))$. The order and size of G are $2n$ and $\frac{1}{2}[n^2+k^2+5n-2nk-k]$, respectively. By Theorem 2.1, $M_1(G) = n^3 + (6-3k)n^2 + (3k^2 - 12k + 13)n - k^3 + 6k^2 - 5k$. Then Theorem 2.2 implies that

$$\overline{M_1}(G) = (n^2 + k^2 + 5n - 2nk - k)(2n-1) - (n^3 + (6-3k)n^2 + (3k^2 - 12k + 13)n - k^3 + 6k^2 - 5k).$$

Since $(n^2 + k^2 + 5n - 2nk - k)(2n-1) = 2n^3 + 2nk^2 + 10n^2 - 4n^2k - 2nk - n^2 - k^2 - 5n + 2nk + k$,

$$\overline{M_1}(G) = n^3 + (3-k)n^2 - (k^2 - 12k + 18)n + k^3 - 7k^2 + 6k.$$

□

Theorem 2.5 *Let G be the line graph of the subdivision graph of the cycle-star graph $CS_{k,n-k}$. Then* $\overline{M_2}(G) = n^3 + \frac{n^2}{2}(2k-1) - \frac{n}{2}(10k^2 - 42k + 45) + \frac{1}{2}(6k^3 - 25k^2 + 21k)$.

Proof: By Theorem 2.1, $M_1(G) = n^3 + (6-3k)n^2 + (3k^2 - 12k + 13)n - k^3 + 6k^2 - 5k$;
$M_2(G) = \frac{1}{2}[n^4 + (7-4k)n^3 + (6k^2 - 21k + 20)n^2 - (4k^3 - 21k^2 + 40k - 32)n + k^4 - 7k^3 + 20k^2 - 16k]$.
Then Theorem 2.3 implies that $\overline{M_2}(G) = \frac{1}{2}\left(n^2 + k^2 + 5n - 2nk - k\right)^2 - \frac{1}{2}M_1(G) - M_2(G)$.

Since, $(n^2+k^2+5n-2nk-k)^2 = n^4+(10-4k)n^3+(6k^2-22k+25)n^2-(4k^3-14k^2+10k)n+k^4-2k^3+k^2)$,

$$\overline{M_2}(G) = n^3 + \frac{n^2}{2}(2k-1) - \frac{n}{2}(10k^2 - 42k + 45) + \frac{1}{2}(6k^3 - 25k^2 + 21k).$$

□

3. Zagreb indices of the line cut-vertex graph of the subdivision graph of the cycle-star graph $CS_{k,n-k}$

The notion of line cut-vertex graph of a graph was introduced by Kulli et al. [12]. The *line cut-vertex graph* of a graph G, denoted by $L_c(G)$, is the graph whose vertices are the edges and cut-vertices of G. Two vertices of $L_c(G)$ are adjacent whenever the corresponding edges of G share a common vertex, or one vertex corresponds to an edge e_i of G the other corresponds to a cut-vertex c_j of G such that e_i is incident with c_j.

In the next theorem, the line cut-vertex of the subdivision graph of the cycle-star graph is determined.

Theorem 3.1 *Let G be the line cut-vertex graph of the subdivision graph of the cycle-star graph $CS_{k,n-k}$. Then,*
$M_1(G) = n^3 + (11-3k)n^2 + (3k^2 - 22k + 40)n - k^3 + 11k^2 - 32k + 14$; *and*

$$M_2(G) = \frac{1}{2}(n^4 + k^4 + (13-4k)n^3 + (6k^2 - 37k + 56)n^2 - (4k^3 - 35k^2 + 96k - 80)n) - \frac{11}{2}k^3 + 22k^2 - 34k + 9.$$

Proof: Let $G = L_c(S(CS_{k,n-k}))$. The subdivision graph $S(CS_{k,n-k})$ contains $2n$ vertices and $2n$ edges. Thus, the line cut-vertex graph of $S(CS_{k,n-k})$ consists of $3n-k+1$ vertices, where $2k-2$ vertices of are of degree 2; $2(n-k)$ vertices are degree 2; 2 vertices are of degree $n-k+3$; 1 vertex is of degree $n-k+2$, and the remaining $n-k$ vertices are of degree $n-k+4$. Thus,

$$\begin{aligned}M_1(G) &= 4(2k-2) + 4(2n-2k) + 2(n-k+3)^2 + (n-k+2)^2 + (n-k)(n-k+4)^2 \\ &= n^3 + (11-3k)n^2 + (3k^2-22k+40)n - k^3 + 11k^2 - 32k + 14.\end{aligned}$$

Now, the size of G is

$$|E(G)| = \frac{(n-k+3)(n-k+2)}{2} + 3(n-k) + 2k - 1 = \frac{1}{2}(n^2 + k^2 + 11n - 7k - 2nk + 4).$$

In other words, $E(G)$ contains $2k-3$ edges whose end vertices have degree 2; $n-k$ edges whose end vertices have degree 2; 2 edges whose end vertices have degree 2 and $n-k+3$; $2(n-k)$ edges whose end vertices have degree 2 and $n-k+4$; 2 edges whose end vertices have degree n and $n-1$; $n-k$ edges whose end vertices have degree $n-1$ and $n-k+4$; 1 edge whose end vertices have degree $n-k+3$; $2(n-k)$ edges whose end vertices have degree $n-k+3$ and $n-k+4$; and the remaining $\frac{(n-k)(n-k-1)}{2}$ edges whose end vertices have degree $n-k+4$. Thus,

$$\begin{aligned}M_2(G) =& 4(2k-3) + 4(n-k) + 4(n-k+3) + 2(n-k)(2n-2k+8) + 2n(n-1) + \\ & (n-k)(n-1)(n-k+4) + (n-k+3)^2 + 2(n-k)(n-k+3)(n-k+4) + \\ & \frac{(n-k)(n-k-1)}{2}(n-k+4)^2 \\ =& \frac{1}{2}(n^4 + k^4 + (13-4k)n^3 + (6k^2-37k+56)n^2 - (4k^3-35k^2+96k-80)n) - \\ & \frac{11}{2}k^3 + 22k^2 - 34k + 9.\end{aligned}$$

□

An example of Theorem 3.1 is shown in Figure 3.

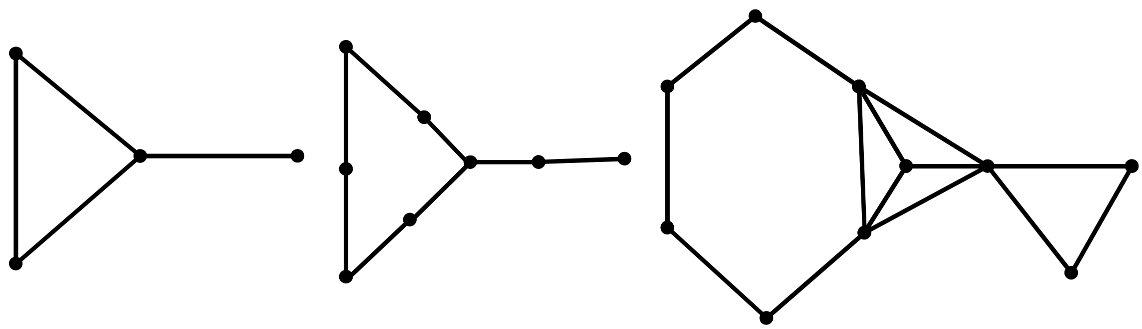

Figure 3: The cycle-star graph $CS_{3,1}$; $S(CS_{3,1})$; $L_c(S(CS_{3,1}))$

For $G = L_c(S(CS_{3,1}))$ of Figure 3, using Theorem 3.1,

$$M_1(G) = 64 + 16(11-9) + 4(27-66+40) - 27 + 99 - 96 + 14 = 90.$$

$$\begin{aligned}M_2(G) =& \frac{1}{2}[256 + 64(13-12) + 16(54-111+56) - 4(108-315+288-80)] + \frac{81}{2} - \frac{(11)(27)}{2} + 198 - 102 + 9 \\ =& 147.\end{aligned}$$

We now provide the expressions for the first and second Zagreb coindices of the line cut-vertex graph of the subdivision graph of the cycle-star graph using Theorem 2.2 and Theorem 2.3.

Theorem 3.2 *Let G be the line cut-vertex graph of the subdivision graph of the cycle-star graph $CS_{k,n-k}$. Then* $\overline{M_1}(G) = 2n^3 + (22-4k)n^2 + (2k^2-10k-28)n - 4k^2 + 28k - 14$.

Proof: The order and size of G are $3n-k+1$ and $\frac{1}{2}(n^2+k^2+11n-7k-2nk+4)$, respectively. By Theorem 3.1, $M_1(G) = n^3 + (11-3k)n^2 + (3k^2-22k+40)n - k^3 + 11k^2 - 32k + 14$. Then Theorem 2.2 implies that

$$\begin{aligned}\overline{M_1}(G) =&(n^2+k^2+11n-7k-2nk+4)(3n-k) - ((n^3+(11-3k)n^2+(3k^2-22k+40)n-\\&k^3+11k^2-32k+14))\\=&(3n^3+(33-7k)n^2+(5k^2-32k+12)n-k^3+7k^2-4k) - ((n^3+(11-3k)n^2+\\&(3k^2-22k+40)n-k^3+11k^2-32k+14))\\=&2n^3+(22-4k)n^2+(2k^2-10k-28)n-4k^2+28k-14.\end{aligned}$$

□

Theorem 3.3 *Let G be the line cut-vertex graph of the subdivision graph of the cycle-star graph $CS_{k,n-k}$. Then*

$$\begin{aligned}\overline{M_2}(G) =&\frac{1}{2}\left(n^2+k^2+11n-7k-2nk+4\right)^2 - \frac{1}{2}n^4 + (2k-7)n^3 + \left(\frac{-6k^2+40k-67}{2}\right)n^2\\&+(2k^3-19k^2+59k-60)n - \frac{1}{2}k^4 + 6k^3 - \frac{55}{2}k^2 + 50k - 16.\end{aligned}$$

Proof: By Theorem 3.1, $M_1(G) = n^3 + (11-3k)n^2 + (3k^2-22k+40)n - k^3 + 11k^2 - 32k + 14$ and

$$M_2(G) = \frac{1}{2}(n^4+k^4+(13-4k)n^3+(6k^2-37k+56)n^2-(4k^3-35k^2+96k-80)n) - \frac{11}{2}k^3 + 22k^2 - 34k + 9.$$

Then Theorem 2.3 implies that $\overline{M_2}(G) = \frac{1}{2}\left(n^2+k^2+11n-7k-2nk+4\right)^2 - \frac{1}{2}M_1(G) - M_2(G)$.

Thus,

$$\begin{aligned}\overline{M_2}(G) =&\frac{1}{2}\left(n^2+k^2+11n-7k-2nk+4\right)^2 - \frac{1}{2}n^4 + (2k-7)n^3 + \left(\frac{-6k^2+40k-67}{2}\right)n^2\\&+(2k^3-19k^2+59k-60)n - \frac{1}{2}k^4 + 6k^3 - \frac{55}{2}k^2 + 50k - 16.\end{aligned}$$

□

4. Conclusion

In this paper, the Zagreb indices and coindices of the line graph and line cut-vertex graph of the subdivision graph of the cycle-star graph are calculated. For further research, it would be interesting to determine many other topological indices and coindices of cycle-star graphs for different graph operators, such as middle graphs, total graphs, etc. For more details on graph operators, readers are referred to [16].

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