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THE FIRST AND SECOND κ_a INDICES AND COINDICES OF GRAPHS

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ABSTRACT

The first and second Zagreb indices were introduced by Gutman and Trinajstić in 1972. Also the first and second Zagreb coindices were introduced by Došlić in 2008. In this paper, we introduce the first and second κ_a indices and coindices analogs of the above Zagreb indices and coindices and initiate a study of these new invariants.

Keywords: *Zagreb indices, Zagreb coindices, hyper-Zagreb indices, hyper-Zagreb coindices, κ_a indices, κ_a coindices.*

Mathematics Subject Classification: *05C.*

1. INTRODUCTION

Let G be a simple graph with n vertices and m edges with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. The edge connecting the vertices u and v is denoted by uv. The complement $\overline{G}$ of a graph G is the graph with vertex set $V(G)$ in which two vertices are adjacent if they are adjacent in G. Clearly

$$\left|E\left(\overline{G}\right)\right| = \overline{m} = \frac{n(n-1)}{2} - m \text{ and } d_{\overline{G}}(u) = n-1-d_G(u) \text{ for } u \in V(G).$$

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Chemical Graph Theory is a branch of mathematical chemistry which has an important effect on the development of the Chemical Sciences.

In Chemical Science, the physico-chemical properties of chemical compounds are often modeled by means of molecular graph based structure descriptors, which are referred to as topological indices, see [1].

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

$$M_1(G) = \sum_{uv \in E(G)} \left[d_G(u) + d_G(v)\right]$$

$$M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v).$$

These indices were introduced by Gutman *et al*. in [1]. The Zagreb indices were studied, for example, in [2, 3, 4, 5].

The first Zagreb coindex $\overline{M}_1(G)$ and the second Zagreb coindex $\overline{M}_2(G)$ of a graph G are defined as

$$\overline{M}_1(G) = \sum_{uv \notin E(G)} \left[d_G(u) + d_G(v)\right]$$

$$\overline{M}_2(G) = \sum_{uv \notin E(G)} d_G(u) d_G(v).$$

These coindices were introduced by Došlić in [6]. The Zagreb coindices were studied, for example, in [7, 8].

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The hyper Zagreb index $HM_1(G)$ of a graph G is defined as

$$HM_1(G) = \sum_{uv \in E(G)} \left[d_G(u) + d_G(v)\right]^2.$$

This index was introduced by Shirdel *et al*. in [9].

The hyper-Zagreb coindex $\overline{HM}_1(G)$ of a graph G is defined as

$$\overline{HM}_1(G) = \sum_{uv \notin E(G)} \left[d_G(u) + d_G(v)\right]^2.$$

This coindex was introduced by Veylaki *et al.* in [10].

The second hyper-Zagreb index $HM_2(G)$ of a graph G is defined as

$$HM_2(G) = \sum_{uv \in E(G)} \left(d_G(u) d_G(v)\right)^2.$$

The second hyper-Zagreb index was introduced by Farahani *et al*. in [11].

In [12], Kulli introduced the second hyper-Zagreb coindex.

The second-Zagreb coindex $\overline{HM}_2(G)$ of a graph G is defined as

$$\overline{HM}_2(G) = \sum_{uv \notin E(G)} \left(d_G(u) d_G(v)\right)^2.$$

In this paper, we introduce the first and second κ_a indices and coindices and initiate a study of these invariants.

1. The First κ_a - Index and First κ_a - Coindex

We introduce the first κ_a-index and the first κ_a-coindex of a graph.

Definition 1: The first κ_a-index and the first κ_a-coindex of a graph G are defined as

$$\kappa_a(G) = \sum_{uv \in E(G)} \left(d_G(u) + d_G(v)\right)^a$$

$$\overline{\kappa_a}(G) = \sum_{uv \notin E(G)} \left(d_G(u) + d_G(v)\right)^a.$$

Proposition 2: Let G be a graph with n vertices and m edges. Then

(i) $\kappa_1(G) = M_1(G)$.

(ii) $\kappa_2(G) = HM_1(G)$.

Proposition 3: Let G be a graph with n vertices and m edges. Then

(i) $\overline{\kappa}_1(G) = \overline{M}_1(G)$.

(ii) $\overline{\kappa}_2(G) = \overline{HM}_1(G)$.

Proposition 4: Let K_n be a complete graph with n vertices. Then

$$\kappa_a(K_n) = 2^{a-1} n(n-1)^{a+1}.$$

Proof: Let K_n be a complete graph with n vertices. Then the degree of each vertex of K_n is $n - 1$ and the number of edges in K_n is $\frac{n(n-1)}{2}$. Therefore

$$\kappa_a(K_n) = \sum_{uv \in E(K_n)} \left[d_{K_n}(u) + d_{K_n}(v)\right]^a$$

$$= \sum_{uv \in E(K_n)} \left[(n-1) + (n-1)\right]^a$$

$$= \sum_{uv \in E(K_n)} 2^a (n-1)^a$$

$$= 2^{a-1} n(n-1)^{a+1}.$$

It is easy to see that $\overline{\kappa}_a(K_n) = 0.$

Proposition 5: Let C_n be a cycle with $n \geq 3$ vertices. Then

(i) $\kappa_a(C_n) = n2^{2a}$.

(ii) $\overline{\kappa}_a(C_n) = n(n-3)2^{2a-1}$.

Proof: (i) Let C_n be a cycle with $n \geq 3$ vertices. Then the degree of each vertex of C_n is 2 and the number of edges in C_n is n. Therefore

$$\kappa_a(C_n) = \sum \left(d_{C_n}(u) + d_{C_n}(v)\right)^a = \sum (2+2)^a$$

$$= \sum 2^{2a}$$

$$= n\, 2^{2a}.$$

(ii) The number of edges in $\overline{C}_n = \frac{n(n-1)}{2} - n = \frac{n(n-3)}{2}$. Therefore

$$\overline{\kappa}_a(C_n) = \sum_{uv \notin E(C_n)} \left(d_{C_n}(u) + d_{C_n}(v)\right)^a$$

$$= \sum_{uv \in E(\overline{C}_n)} (2+2)^a$$

$$= \frac{n(n-3)}{2} 2^{2a}$$

$$= n(n-3)2^{2a-1}.$$

Proposition 6: Let $\overline{C}_n$ be the complement of C_n with $n \geq 3$ vertices. Then

(i) $\kappa_a(\overline{C}_n) = 2^{a-1} n(n-3)^{a+1}$

(ii) $\overline{\kappa}_a(\overline{C}_n) = 2^a n(n-3)^a$.

Proof: (i) Let $\overline{C}_n$ be the complement of C_n with $n \geq 3$ vertices. Then the degree of each vertex of $\overline{C}_n$ is $n - 3$ and the number of edges in $\overline{C}_n$ is $\frac{n(n-3)}{2}$. Therefore

$$\kappa_a(\overline{C}_n) = \sum_{uv \in (\overline{C}_n)} \left(d_{\overline{C}_n}(u) + d_{\overline{C}_n}(v)\right)^a$$

$$= \sum \left[(n-3) + (n-3)\right]^a$$

$$= \sum 2^a (n-3)^a$$

$$= \frac{n(n-3)}{2} 2^a (n-3)^a$$

$$= n(n-3)^{a+1} 2^{a-1}.$$

(ii) The number of edges in C_n is n. Therefore

$$\overline{\kappa}_a(\overline{C}_n) = \sum_{uv \notin E(\overline{C}_n)} \left(d_{\overline{C}_n}(u) + d_{\overline{C}_n}(v)\right)^a$$

$$= \sum_{uv \in E(C_n)} \left[(n-3) + (n-3)\right]^a$$

$$= \sum 2^a (n-3)^a$$

$$= n(n-3)^a 2^a.$$

Theorem 7: Let *G* be a graph with *n* vertices and *m* edges. For $a \geq 1$,

$$\kappa_a\left(\overline{G}\right) = \sum_{r=0}^{a} \binom{a}{r} (-1)^r \, 2^{a-r} (n-1)^{a-r} \, \overline{\kappa}_r(G).$$

Proof: From the definitions, we have

$$\begin{aligned}
\kappa_a\left(\overline{G}\right) &= \sum_{uv \in E(\overline{G})} \left(d_{\overline{G}}(u) + d_{\overline{G}}(v)\right)^a \\
&= \sum_{uv \in E(\overline{G})} \left[\left(n-1-d_G(u)\right) + \left(n-1-d_G(v)\right)\right]^a \\
&= \sum_{uv \in E(\overline{G})} \left[2(n-1) - \left(d_G(u) + d_G(v)\right)\right]^a \\
&= \sum_{uv \notin E(G)} \sum_{r=0}^{a} \binom{a}{r} (-1)^r \, 2^{a-r} (n-1)^{a-r} \left(d_G(u) + d_G(v)\right)^r \\
&= \sum_{r=0}^{a} \binom{a}{r} (-1)^r \, 2^{a-r} (n-1)^{a-r} \sum_{uv \notin E(G)} \left(d_G(u) + d_G(v)\right)^r \\
&= \sum_{r=0}^{a} \binom{a}{r} (-1)^r \, 2^{a-r} (n-1)^{a-r} \, \overline{\kappa}_r(G).
\end{aligned}$$

Theorem 8: Let *G* be a graph with *n* vertices and *m* edges. For $a \geq 1$,

$$\overline{\kappa}_a(G) = \sum_{r=0}^{a} \binom{a}{r} (-1)^r \, 2^{a-r} (n-1)^{a-r} \, \kappa_r\left(\overline{G}\right).$$

Proof: From the definitions, we have

$$\begin{aligned}
\overline{\kappa}_a(G) &= \sum_{uv \notin E(G)} \left(d_G(u) + d_G(v)\right)^a \\
&= \sum_{uv \in E(\overline{G})} \left[\left(n-1-d_{\overline{G}}(u)\right) + \left(n-1-d_{\overline{G}}(v)\right)\right]^a \\
&= \sum_{uv \in E(\overline{G})} \left[2(n-1) - \left(d_{\overline{G}}(u) + d_{\overline{G}}(v)\right)\right]^a \\
&= \sum_{uv \in E(\overline{G})} \sum_{r=0}^{a} \binom{a}{r} (-1)^r \, 2^{a-r} (n-1)^{a-r} - \left(d_{\overline{G}}(u) + d_{\overline{G}}(v)\right)^r \\
&= \sum_{r=0}^{a} \binom{a}{r} (-1)^r \, 2^{a-r} (n-1)^{a-r} \sum_{uv \in E(\overline{G})} \left(d_{\overline{G}}(u) + d_{\overline{G}}(v)\right)^r \\
&= \sum_{r=0}^{a} \binom{a}{r} (-1)^r \, 2^{a-r} (n-1)^{a-r} \, \kappa_r\left(\overline{G}\right).
\end{aligned}$$

3. THE SECOND κ_a-INDEX AND SECOND κ_a-COINDEX

We define the second κ_a-index and the second κ_a-coindex of a graph.

Definition 9: The second κ_a^1 -index and the second $\overline{\kappa}_a^1$ -coindex of a graph *G* are defined as

$$\kappa_a^1(G) = \sum_{uv \in E(G)} \left(d_G(u) d_G(v)\right)^a$$

$$\overline{\kappa}_a^1(G) = \sum_{uv \notin E(G)} \left(d_G(u) d_G(v)\right)^a.$$

Proposition 10: Let *G* be a graph with *n* vertices *m* edges. Then

(i) $\kappa_1^1(G) = M_2(G)$.

(ii) $\kappa_2^1(G) = HM_2(G)$.

Proposition 11: Let G be a graph with n vertices and m edges. Then

(i) $\bar{\kappa}_1^1(G) = \bar{M}_2(G)$.

(ii) $\bar{\kappa}_2^1(G) = \overline{HM}_2(G)$.

Proposition 12: Let K_n be a complete graph with n vertices. Then

(i) $\kappa_a^1(K_n) = \frac{1}{2}n(n-1)^{2a+1}$

(ii) $\bar{\kappa}_a^1(K_n) = 0$.

Proof: (i) Let K_n be a complete graph with n vertices. Then the degree of each vertex of K_n is $n - 1$ and the number of edges in K_n is $\frac{n(n-1)}{2}$. Therefore

$$\begin{aligned}\kappa_a^1(K_n) &= \sum_{uv\in E(K_n)} \left(d_{K_n}(u)d_{K_n}(v)\right)^a \\ &= \sum_{uv\in E(K_n)} \left((n-1)(n-1)\right)^a \\ &= \sum_{uv\in E(K_n)} (n-1)^{2a} \\ &= \frac{1}{2}n(n-1)^{2a+1}\end{aligned}$$

(ii) It is easy to see that $\bar{\kappa}_a^1(K_n) = 0$.

Proposition 13: Let C_n be a cycle with $n \geq 3$ vertices. Then

(i) $\kappa_a^1(C_n) = n2^{2a}$

(ii) $\bar{\kappa}_a^1(C_n) = n(n-3)2^{2a-1}$.

Proof: (i) Let C_n be a cycle with $n \geq 3$ vertices. Then the degree of each vertex of C_n is 2 and the number of edges in C_n is n. Therefore

$$\begin{aligned}\kappa_a^1(C_n) &= \sum_{uv\in E(C_n)} \left(d_{C_n}(u)d_{C_n}(v)\right)^a \\ &= \sum_{uv\in E(C_n)} (2\times 2)^a \\ &= n\,2^{2a}.\end{aligned}$$

(ii) The number of edges in $\overline{C}_n$ is $\frac{n(n-3)}{2}$. Therefore

$$\begin{aligned}\bar{\kappa}_a^1(C_n) &= \sum_{uv\notin E(C_n)} \left(d_{C_n}(u)d_{C_n}(v)\right)^a \\ &= \sum_{uv\in E(\overline{C}_n)} (2\times 2)^a \\ &= n(n-3)2^{2a-1}.\end{aligned}$$

Proposition 14: Let $\overline{C}_n$ be the complement of C_n with $n \geq 3$ vertices. Then

(i) $\kappa_a^1(\overline{C}_n) = \frac{1}{2}n(n-3)2^{2a+1}$

(ii) $\bar{\kappa}_a^1(\overline{C}_n) = n(n-3)2^{2a}$.

Proof: (i) Let $\overline{C}_n$ be the complement of C_n with $n \geq 3$ vertices. Then the degree of each vertex of $\overline{C}_n$ is $n - 3$ and the number of edges in $\overline{C}_n$ is $\frac{n(n-3)}{2}$. Therefore

$$\kappa_a^1\left(\overline{C}_n\right) = \sum_{uv\in E\left(\overline{C}_n\right)} \left(d_{\overline{C}_n}(u)\, d_{\overline{C}_n}(v)\right)^a$$
$$= \sum_{uv\in E\left(\overline{C}_n\right)} \left((n-3)(n-3)\right)^a$$
$$= \frac{n(n-3)}{2}(n-3)^{2a}$$
$$= \frac{1}{2}n(n-3)^{2a+1}.$$

(ii) The number of edges in C_n is n. Therefore

$$\overline{\kappa}_a^1\left(\overline{C}_n\right) = \sum_{uv\notin E\left(\overline{C}_n\right)} \left(d_{\overline{C}_n}(u)\, d_{\overline{C}_n}(v)\right)^a$$
$$= \sum_{uv\notin E\left(\overline{C}_n\right)} \left((n-3)(n-3)\right)^a$$
$$= n(n-3)^{2a}.$$

Theorem 15: Let G be a graph with n vertices and m edges. For $a \geq 1$,

$$\kappa_a^1\left(\overline{G}\right) = \sum_{r=0}^{a}\sum_{r=0}^{a}\binom{a}{r}\binom{a}{r}(n-1)^{2a-r}\,\overline{\kappa}_r^1(G).$$

Proof: From the definitions, we have

$$\kappa_a^1\left(\overline{G}\right) = \sum_{uv\in E\left(\overline{G}\right)} \left(d_{\overline{G}}(u)\, d_{\overline{G}}(v)\right)^a$$
$$= \sum_{uv\notin E(G)} \left(n-1-d_G(u)\right)^a \left(n-1-d_G(v)\right)^a$$
$$= \sum_{uv\notin E(G)} \sum_{r=0}^{a}\binom{a}{r}(-1)^r (n-1)^{a-r} d_G(u)^r \sum_{r=0}^{a}\binom{a}{r}(-1)^r (n-1)^{a-r} d_G(v)^r$$
$$= \sum_{r=0}^{a}\sum_{r=0}^{a}\binom{a}{r}\binom{a}{r}(-1)^{2r}(n-1)^{2(a-r)} \sum_{uv\notin E(G)} d_G(u)^r\, d_G(v)^r$$
$$= \sum_{r=0}^{a}\sum_{r=0}^{a}\binom{a}{r}\binom{a}{r}(n-1)^{2(a-r)}\overline{\kappa}_r^1(G).$$

Theorem 16: Let G be a graph with n vertices and m edges. For $a \geq 1$,

$$\kappa_a^1(G) = \sum_{r=0}^{a}\sum_{r=0}^{a}\binom{a}{r}\binom{a}{r}(n-1)^{2(a-r)}\kappa_r^1\left(\overline{G}\right).$$

Proof: From the definitions, we have

$$\overline{\kappa}_a^1(G) = \sum_{uv\notin E(G)} \left(d_G(u)\, d_G(v)\right)^a$$
$$= \sum_{uv\in E\left(\overline{G}\right)} \left(n-1-d_{\overline{G}}(u)\right)^a \left(n-1-d_{\overline{G}}(v)\right)^a$$
$$= \sum_{uv\in E\left(\overline{G}\right)} \sum_{r=0}^{a}\binom{a}{r}(-1)^r (n-1)^{a-r} d_{\overline{G}}(u)^r \sum_{r=0}^{a}\binom{a}{r}(-1)^r (n-1)^{a-r} d_{\overline{G}}(v)^r$$
$$= \sum_{r=0}^{a}\sum_{r=0}^{a}\binom{a}{r}\binom{a}{r}(-1)^{2r}(n-1)^{2(a-r)} \sum_{uv\in E\left(\overline{G}\right)} d_{\overline{G}}(u)^r\, d_{\overline{G}}(v)^r$$
$$= \sum_{r=0}^{a}\sum_{r=0}^{a}\binom{a}{r}\binom{a}{r}(n-1)^{2(a-r)}\kappa_r^1\left(\overline{G}\right).$$

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