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On K Edge Index and Coindex of Graphs

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Abstract: The *F*-index of a graph is defined as the sum of the cubes of the vertex degrees of a graph. It is known that this index can enhance the physico-chemical applicability of Zagreb index. In this paper, we introduce a new invariant the *K*-edge index which is defined as the sum of the cubes of the edge degrees of a graph. Also, we introduce another new invariant the *K*-edge coindex. We initiate a study of these new invariants.

Keywords: Zagreb indices, reformulated Zagreb indices, K-edge index, K-edge coindex

AMS Mathematics Subject Classification (2010): 05C72

1. Introduction

Let G = (V, E) be a simple graph with |V| = n vertices and |E| = m edges.

The degree of a vertex v, denoted by $d_G(v)$, is the number of vertices adjacent to v. The edge connecting the vertices u and v will be denoted by uv. Let \overline{G} be the complement of

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

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 also referred to as topological indices, see [1].

The first and second Zagreb indices are defined as

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2$$
 and $M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v)$.

These indices were introduced by Gutman *et al.* in [1]. Also the *K* indices and *K* coindices were introduced in [2] and [3] respectively.

In fact, one can rewrite the first Zagreb index as

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

The forgotten topological index F_1 is defined [1, 4] as

V.R.Kulli

$$F_{1}(G) = \sum_{u \in V(G)} d_{G}(u)^{3} = \sum_{uv \in E(G)} \left[d_{G}(u)^{2} + d_{G}(v)^{2} \right].$$

The forgotten topological index was studied, for example, in [5].

The first and second reformulated Zagreb indices are defined as

$$EM_{1}(G) = \sum_{e \in E(G)} d_{G}(e)^{2}, \ EM_{2}(G) = \sum_{e \sim f \in E(G)} d_{G}(e) d_{G}(f)$$

where $d_G(e)$ denotes the degree of an edge *e* in *G*, which is defined by $d_G(e) = d_G(u) + d_G(v) - 2$ with e = uv and $e \sim f$ means that the edges *e* and *f* are adjacent. The reformulated Zagreb indices were introduced by Milićević *et al.* in [6] and were studied, for example, in [7, 8, 9, 10].

The first Ka-index and the first Ka-coindex of a graph G are defined as

$$Ka(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))^a$$
$$\overline{K}a(G) = \sum_{uv \notin E(G)} (d_G(u) + d_G(v))^a.$$

These were introduced by Kulli in [11].

Terminology and notation not given here may be found in [12].

2. Some measures of irregularity

Definition 1. A graph whose all edge degrees are mutually equal is said to be edge regular.

We now define the irregular edge indices of a graph.

Definition 2. The first irregular edge index
$$IE_1(G)$$
 of a graph *G* is defined as
$$IE_1(G) = \sum_{e \sim f \in E(G)} |d_G(e) - d_G(f)|.$$

Definition 3. The second irregular edge index $IE_2(G)$ of a graph G is defined as

$$IE_{2}(G) = \sum_{e \sim f \in E(G)} \left[d_{G}(e) - d_{G}(f) \right]^{2}.$$

Also we define the irregular edge coindices of a graph.

Definition 4. The first irregular edge coindex $\overline{IE}_1(G)$ of a graph G is defined as

$$\overline{IE}_{1}(G) = \sum_{e \neq f \in E(G)} \left| d_{G}(e) - d_{G}(f) \right|.$$

Definition 5. The second irregular edge coindex $\overline{IE}_2(G)$ of a graph G is defined as

$$\overline{IE}_{2}(G) = \sum_{e \neq f \in E(G)} \left[d_{G}(e) - d_{G}(f) \right]^{2}.$$

3. The *K*-edge index of a graph

We define the *K*-edge index of a graph.

On K Edge Index and Coindex of Graphs

Definition 6. The *K*-edge index of a graph *G* is defined as

$$K_{e}(G) = \sum_{e \in E(G)} d_{G}(e)^{3}.$$

i.e. The K-edge index of a graph is the sum of the cubes of the edge degrees of a graph.

Definition 7. The K^* -edge index of a graph G is defined as $K_e^*(G) = \sum_{e \sim f \in E(G)} \left[d_G(e)^2 + d_G(f)^2 \right].$

We now define the *K*-edge coindex of a graph.

Definition 8. The *K*-edge coindex of a graph *G* is defined as $\overline{F}(G) = \sum_{i=1}^{n} \int_{-\infty}^{\infty} f(G) dG = \int_{-\infty}^{\infty} f(G) dG = \int_{-\infty}^{\infty} f(G) dG = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(G) dG = \int_{-\infty}$

$$\overline{K}_{e}(G) = \sum_{e \neq f \in E(G)} \left\lfloor d_{G}(e)^{2} + d_{G}(f)^{2} \right\rfloor.$$

Example 9. Consider methylcyclohexane and its molecular graph G, see Figure 1.

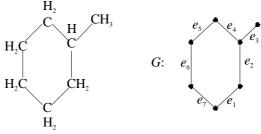
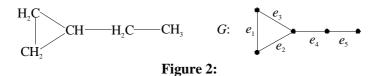


Figure 1: Methylcyclohexane

The values of the *K*-edge index of *G* and the K^* -edge index of *G* are $K_e(G) = 94$ and $K_e^*(G) = 94$.

Example 10. Consider ethylcyclopropane and its molecular graph G, see Figure 2.



The values of the K-edge index of G and the K^* -edge index of G are $K_e(G) = 90$ and $K_e^*(G) = 90$.

Now we have the following conjecture.

Conjecture 11. For any graph *G*, $K_e(G) = K_e^*(G)$. 113

V.R.Kulli

Theorem 12. Let G be a graph with n vertices and m edges. Then $K_e(G) = K_3(G) - 6HM_1(G) + 12M_1(G) - 8m.$ Proof: By definition K-edge index, we have $K_e(G) = \sum_{e \in E(G)} d_G(e)^3$ $= \sum_{e \in E(G)} \left[d_G(u) + d_G(v) - 2 \right]^3$ $= \sum_{e \in E(G)} \left[\left\{ d_G(u) + d_G(v) \right\}^3 - 6 \left\{ d_G(u) + d_G(v) \right\}^2 + 12 \left\{ d_G(u) + d_G(v) \right\} - 8 \right]$ $= \sum_{e \in E(G)} \left[d_G(u) + d_G(v) \right]^3 - 6 \sum_{e \in E(G)} \left[d_G(u) + d_G(v) \right] + 12 \sum_{e \in E(G)} \left[d_G(u) + d_G(v) \right] - 8$ $= \sum_{e \in E(G)} \left[d_G(u) + d_G(v) \right]^3 - 6HM_1(G) + 12M_1(G) - 8m$ $= K_3(G) - 6HM_1(G) + 12M_1(G) - 8m.$

Theorem 13. Let G be a graph with n vertices and m edges. Let \overline{G} be the complement of G. Then

$$K_{e}(\overline{G}) = 8(n-2)^{3} \overline{m} - 12(n-2)^{2} \overline{M}_{1}(G) + 6(n-2) \overline{HM}_{1}(G) - \overline{K}_{3}(G)$$

Proof: If the degree of a vertex u in G is $d_G(u)$, then the degree of u in \overline{G} is $n-1-d_G(u)$. If e = uv is an edge of G, then the degree of an edge e in \overline{G} is

$$n-1-d_{G}(u)+n-1-d_{G}(v)-2 \text{ or } 2(n-2)-\left[d_{G}(u)+d_{G}(v)\right]$$

Therefore

$$\begin{split} K_{e}(\overline{G}) &= \sum_{e \in E(\overline{G})} d_{\overline{G}}(e)^{3} \\ &= \sum_{e \in E(\overline{G})} \left[2(n-2) - \left\{ d_{G}(u) + d_{G}(v) \right\} \right]^{3} \\ &= \sum_{e \in E(\overline{G})} \left[2^{3}(n-2)^{3} - 3.2^{2}(n-2)^{2} \left\{ d_{G}(u) + d_{G}(v) \right\} + 3.2(n-2) \left\{ d_{G}(u) + d_{G}(v) \right\}^{2} - \left\{ d_{G}(u) + d_{G}(v) \right\}^{3} \right] \\ &= 8(n-2)^{3} \overline{m} - 12(n-2)^{2} \sum_{e \in E(\overline{G})} \left[d_{G}(u) + d_{G}(v) \right] + 6(n-2) \sum_{e \in E(\overline{G})} \left[d_{G}(u) + d_{G}(v) \right]^{2} - \sum_{e \in E(\overline{G})} \left[d_{G}(u) + d_{G}(v) \right]^{3} \\ &= 8(n-2)^{3} \overline{m} - 12(n-2)^{2} \overline{M}_{1}(G) + 6(n-2) \overline{HM}_{1}(G) - \overline{K}_{3}(G). \end{split}$$

Theorem 14. Let *G* be a graph with *n* vertices *m* edges. Then $K_e(G) = IE_2(G) + 2EM_2(G).$

Proof: Consider

$$K_{e}(G) = \sum_{e \sim f \in E(G)} \left[d_{G}(e)^{2} + d_{G}(f)^{2} \right]$$

On K Edge Index and Coindex of Graphs

$$= \sum_{e \sim f \in E(G)} \left[d_G(e) - d_G(f) \right]^2 + 2 \sum_{e \sim f \in E(G)} d_G(e) \cdot d_G(f)$$
$$= \sum_{e \sim f \in E(G)} \left[d_G(e) - d_G(f) \right]^2 + 2EM_2(G)$$
$$= IE_2(G) + 2EM_2(G).$$

Corollary 15. Let *G* be a graph without isolated vertices. Then $IE_2(G) = K_e(G) - 2 EM_2(G)$.

Theorem 16. Let G be a graph with n vertices and m edges. Then $\overline{K}_e(G) = 2(m-1)EM_1(G) - K_e(G).$

Proof: Denote $\gamma_{e,f} = d_G(e)^2 + d_G(f)^2$. Then in view of $\sum_{e \in E} \sum_{f \in E} F(e, f) = \sum_{e \sim f \in E(G)} \gamma_{e,f} + \sum_{e \sim f \in E(\overline{G})} \gamma_{e,f} + \sum_{e \in E} \gamma_{e,e}$

$$=K_{e}(G)+\overline{K}_{e}(G)+2EM_{1}(G).$$
(1)

Also

$$\sum_{e \in E} \sum_{f \in E} \left[d\left(e\right)^{2} + d\left(f\right)^{2} \right] = m \sum_{e \in E} d\left(e\right)^{2} + m \sum_{f \in E} d\left(f\right)^{2}$$
$$= 2m EM_{1}(G)$$
(2)

From (1) and (2), we have

$$K_{e}(G) + \overline{K}_{e}(G) + 2EM_{1}(G) = 2mEM_{1}(G).$$

Thus $\overline{K}_{e}(G) = 2(m-1)EM_{1}(G) - K_{e}(G).$ (3)

Theorem 17. Let G be a graph with n vertices and m edges.

Let \overline{G} be the complement of G. Then

i)
$$\overline{K}_{e}(\overline{G}) = K_{e}(G).$$
 (4)
ii) $\overline{K}_{e}(G) + \overline{K}_{e}(\overline{G}) = 2(m-1)EM_{1}(G).$

Proof: (1) By definition $\overline{K}_{e}(G)$, we have

$$\overline{K}_{e}(G) = \sum_{e \sim f \in E(\overline{G})} \left[d_{\overline{G}}(e)^{2} + d_{\overline{G}}(f)^{2} \right].$$

$$\overline{K}_{e}(\overline{G}) = \sum_{e \sim f \in E(G)} \left[d_{G}(e)^{2} + d_{G}(f)^{2} \right] = K_{e}(G)$$

Therefore

$$\overline{K}_{e}(G) = 2(m-1)EM_{1}(G) - \overline{K}_{e}(G)$$

Thus $\overline{K}_{e}(G) + \overline{K}_{e}(\overline{G}) = 2(m-1)EM_{1}(G).$

V.R.Kulli

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