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ON ZAGREB INDICES AND COINDICES OF CLUSTER GRAPHS

Raju B. Jummannaver, Ivan Gutman, and Ravikiran A. Mundewadi

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Abstract. Graphs obtained by deleting a few edges from the complete graph are referred to as cluster graphs. We determine expressions for the first and second Zagreb indices, forgotten topological index, and hyper–Zagreb index of four classes of cluster graphs and their complements, as well as expressions for their coindices. In addition, we correct an error of one of the present authors, regrading an expression for the hyper–Zagreb coindex.

1. Introduction

Throughout this paper we only consider finite, connected graphs. Let G be a graph with n vertices and m edges. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$ be the vertex set of G and $E(G)$ be an edge set of G. The edge between the vertices u and v is denoted by uv. The degree of a vertex v in G is the number of edges incident to it and is denoted by $d(u)$. The complement of G, denoted by $\overline{G}$, is the graph having the same vertex set as G, in which two vertices are adjacent if and only if they are not adjacent in G.

A large number of vertex–based graph invariants is studied in the recent and current mathematical literature. The chief motivation for this is the fact that these invariants, usually called "*topological indices*" found numerous and important applications in chemistry [**4, 5, 10, 19**]

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The oldest among these degree–based invariants are the *first and second Zagreb indices*:

$$M_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)] \qquad \text{and} \qquad M_2(G) = \sum_{uv \in E(G)} d(u)\, d(v)\,.$$

whose mathematical properties and chemical applications are studied in much detail [**2, 12, 15**].

Došlić [**6**] defined the first and second Zagreb coindices as

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} [d(u) + d(v)] \qquad \text{and} \qquad \overline{M_2}(G) = \sum_{uv \notin E(G)} d(u)\, d(v)$$

respectively, where it is assumed that $u \neq v$.

A so-called forgotten topological index, $F(G)$, is defined as [**8**]

$$F(G) = \sum_{u \in V(G)} d(u)^3.$$

It is easy to show that [**7, 8**]

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

from which the coindex of F is expressed as [**3**]

$$\overline{F}(G) = \sum_{uv \notin E(G)} \left[d(u)^2 + d(v)^2\right] \,.$$

An extension of the Zagreb–index concept, called hyper–Zagreb index, was recently introduced by Shirdel et al. [**18**]:

$$HZ(G) = \sum_{uv \in E(G)} [d(u) + d(v)]^2\,.$$

The respective coindex is [**20**]

$$\overline{HZ}(G) = \sum_{uv \notin E(G)} [d(u) + d(v)]^2\,.$$

Recently, one of the present authors [**11**], determined the the basic relations between hyper–Zagreb index and its coindex for a graph G and of its complement $\overline{G}$. In [**11**], the following relations have been obtained:

THEOREM 1.1. [**11**] *Let G be a graph with n vertices and m edges. Then*

$$\begin{aligned}
\overline{HZ}(G) &= 4m^2 + (n-2)M_1(G) - HZ(G) \\
HZ(\overline{G}) &= 2n(n-1)^3 - 12m(n-1)^2 + 4m^2 + (5n-6)M_1(G) - HZ(G) \\
\overline{HZ}(\overline{G}) &= 4m(n-1)^2 + 4(n-1)M_1(G) + HZ(G)\,.
\end{aligned}$$

The third equality in Theorem 1.1 contains an error. Its correct version should be:

$$\overline{HZ}(\overline{G}) = 4m(n-1)^2 - 4(n-1)M_1(G) + HZ(G)\,.$$

2. Cluster graphs

From a chemical point of view, graphs with large number of edges may be considered as representations of inorganic clusters, so-called cluster graphs [**14**]. Bearing this in mind, we consider here the graphs obtained from the complete graph K_n by removing some of its edges. These graphs were first studied in [**13**] in connection with graph energy. In the present paper we are concerned with the Zagreb, hyper–Zagreb, and forgotten indices of four classes of cluster graphs.

Definition 2.1. [**13**] Let e_i, $i = 1, 2, \ldots, k$, $1 \leqslant k \leqslant n-2$, be distinct edges of the complete graph K_n, $n \geqslant 3$, all being incident to a single vertex. The graph $Ka_n(k)$ is obtained by deleting e_i, $i = 1, 2, \ldots, k$ from K_n. In addition, $Ka_n(0) \cong K_n$.

Definition 2.2. [**13**] Let f_i, $i = 1, 2, \ldots, k$, $1 \leqslant k \leqslant \lfloor n/2 \rfloor$ be independent edges of the complete graph K_n, $n \geqslant 3$. The graph $Kb_n(k)$ is obtained by deleting f_i, $i = 1, 2, \ldots, k$ from K_n. In addition, $Kb_n(0) \cong K_n$.

Definition 2.3. [**13**] Let V_k be a k-element subset of the vertex set of the complete graph K_n, $2 \leqslant k \leqslant n-1$, $n \geqslant 3$. The graph $Kc_n(k)$ is obtained by deleting from K_n all the edges connecting pairs of vertices from V_k. In addition, $Kc_n(0) \cong Kc_n(1) \cong K_n$.

Definition 2.4. [**13**] Let $3 \leqslant k \leqslant n$, $n \geqslant 3$. The graph $Kd_n(k)$ is obtained by deleting from K_n the edges belonging to a k-membered cycle.

3. Results

Theorem 3.1. *For $n \geqslant 3$ and $1 \leqslant k \leqslant n-2$,*

$$HZ(Ka_n(k)) = 2n^4 - 6n^3 + 6n^2 - 12n^2k + 5nk^2 + 29nk - 2n - k^3 - 4k^2 - 19k\,.$$

Proof. The graph $Ka_n(k)$ has n vertices and $n(n-1)/2 - k$ edges. Its edge set can be partitioned into four sets E_1, E_2, E_3, and E_4, such that

$$\begin{aligned} E_1 &= \{uv \mid d(u) = n-1-k \;\; \& \;\; d(v) = n-1\} \\ E_2 &= \{uv \mid d(u) = n-2 \;\; \& \;\; d(v) = n-2\} \\ E_3 &= \{uv \mid d(u) = n-2 \;\; \& \;\; d(v) = n-1\} \\ E_4 &= \{uv \mid d(u) = n-1 \;\; \& \;\; d(v) = n-1\}\,. \end{aligned}$$

It is easy to check that $|E_1| = n-k-1$, $|E_2| = k(k-1)/2$, $|E_3| = (n-k-1)k$, and $|E_4| = (n-k-1)(n-k-2)/2$. Therefore

$$\begin{aligned} HZ(Ka_n(k)) = {} & \sum_{uv \in E_1} [d(u)+d(v)]^2 + \sum_{uv \in E_2} [d(u)+d(v)]^2 + \sum_{uv \in E_3} [d(u)+d(v)]^2 \\ + {} & \sum_{uv \in E_4} [d(u)+d(v)]^2 = (n-k-1)\,[(n-1-k)+(n-1)]^2 \\ + {} & \frac{1}{2}\,k(k-1)\,[(n-2)+(n-2)]^2 + (nk-k^2-k)\,[(n-2)+(n-1)]^2 \end{aligned}$$

$$+ \quad \frac{1}{2}(n-k-1)(n-k-2)\left[(n-1)+(n-1)\right]^2$$

and the expression given in Theorem 3.1 follows. □

THEOREM 3.2. *For* $n \geqslant 3$ *and* $1 \leqslant k \leqslant \lfloor n/2 \rfloor$,

$$HZ(Kb_n(k)) = 2n^4 - 12kn^2 - 6n^3 + 4k^2 + 34kn + 6n^2 - 28k - 2n\,.$$

PROOF. The graph $Kb_n(k)$ has n vertices and $n(n-1)/2 - k$ edges. Its edge set can be partitioned into three sets E_1, E_2, and E_3, such that

$$\begin{aligned} E_1 &= \{uv \mid d(u) = n-2 \;\;\&\;\; d(v) = n-1\} \\ E_2 &= \{uv \mid d(u) = n-1 \;\;\&\;\; d(v) = n-1\} \\ E_3 &= \{uv \mid d(u) = n-2 \;\;\&\;\; d(v) = n-2\}\,. \end{aligned}$$

Then $|E_1| = 2k(n-2k)$, $|E_2| = (n-2k)(n-2k-1)/2$, and $|E_3| = 2k(2k-1)/2 - k$. Thus

$$HZ(Kb_n(k)) = \sum_{uv \in E_1} [d(u)+d(v)]^2 + \sum_{uv \in E_2} [d(u)+d(v)]^2 + \sum_{uv \in E_3} [d(u)+d(v)]^2$$

$$= \quad (2nk - 4k^2)\left[(n-2)+(n-1)\right]^2 + \frac{1}{2}(n-2k)(n-2k-1)\left[(n-1)+(n-1)\right]^2$$

$$+ \quad \left[\frac{(2k(2k-1))}{2} - k\right]\left[(n-2)+(n-2)\right]^2$$

and the expression given in Theorem 3.2 follows. □

THEOREM 3.3. *For* $n \geqslant 3$ *and* $2 \leqslant k \leqslant n-1$,

$$HZ(Kc_n(k)) = \left(-k^2 + nk\right)(2n-k-1)^2 + \frac{1}{2}(n-k)(n-k-1)(2n-2)^2\,.$$

PROOF. The graph $Kc_n(k)$ has n vertices and $\frac{1}{2}(n-k)(n+k-1)$ edges. The edge set $E(Kc_n(k))$ can be partitioned into two sets E_1 and E_2, where

$$\begin{aligned} E_1 &= \{uv \mid d(u) = n-k \;\;\&\;\; d(v) = n-1\} \\ E_2 &= \{uv \mid d(u) = n-1 \;\;\&\;\; d(v) = n-1\}\,. \end{aligned}$$

We have that $|E_1| = (n-k)k$ and $|E_2| = (n-k)(n-k-1)/2$. Therefore

$$HZ(Kc_n(k)) = \sum_{uv \in E_1} [d(u)+d(v)]^2 + \sum_{uv \in E_2} [d(u)+d(v)]^2$$

$$= \quad \left(nk - k^2\right)\left[(n-k)+(n-1)\right]^2 + \frac{1}{2}(n-k)(n-k-1)\left[(n-1)+(n-1)\right]^2$$

implying the expression given in Theorem 3.3. □

THEOREM 3.4. *For* $3 \leqslant k \leqslant n$ *and* $n \geqslant 3$,

$$HZ(Kd_n(k)) = 2n^4 - 12kn^2 - 6n^3 + 4k^2 + 44kn + 6n^2 - 52k - 2n\,.$$

PROOF. The graph $Kd_n(k)$ has n vertices and $n(n-1)/2-k$ edges. The edge set $E(Kd_n(k))$ can be partitioned into three sets E_1, E_2, and E_3, such that

$$\begin{aligned} E_1 &= \{uv \mid d(u)=n-3 \;\;\&\;\; d(v)=n-3\} \\ E_2 &= \{uv \mid d(u)=n-3 \;\;\&\;\; d(v)=n-1\} \\ E_3 &= \{uv \mid d(u)=n-1 \;\;\&\;\; d(v)=n-1\}\,. \end{aligned}$$

It is easy to check that $|E_1| = k(k-1)/2-k$, $|E_2| = (n-k)k$, and $|E_3| = (n-k)(n-k-1)/2$. Therefore

$$\begin{aligned} HZ(Kd_n(k)) &= \sum_{uv\in E_1}[d(u)+d(v)]^2 + \sum_{uv\in E_2}[d(u)+d(v)]^2 + \sum_{uv\in E_3}[d(u)+d(v)]^2 \\ &= \left(\frac{k^2-k}{2}-k\right)[(n-3)+(n-3)]^2 + \left(nk-k^2\right)[(n-3)+(n-1)]^2 \\ &+ \frac{1}{2}(n-k)(n-k-1)\,[(n-1)+(n-1)]^2 \end{aligned}$$

resulting in the expression given in Theorem 3.4. □

Recently, the following formulas for the first and second Zagreb indices and forgotten index of the graphs $Ka_n(k)$, $Kb_n(k)$, $Kc_n(k)$, and $Kd_n(k)$ were obtained by Ramane et al. [**16, 17**]:

THEOREM 3.5. *For $n \geqslant 3$ and $2 \leqslant k \leqslant n-1$,*

$$\begin{aligned} M_1(Ka_n(k)) &= (n-k-1)(n^2-n-3k+nk)+k(k-1)(n-2) \\ M_2(Ka_n(k)) &= \frac{1}{2}\left(n^4-k^2-n\right)-\frac{3}{2}\left(n^3-n^2\right)-\frac{9}{2}k+k^2\,n-3k\,n^2+7kn \\ F(Ka_n(k)) &= n^4+3n^2+3n\,k^2+15nk-3n^3-6n^2\,k-n-k^3-3k^2-10k\,. \end{aligned}$$

THEOREM 3.6. *For $n \geqslant 3$ and $1 \leqslant k \leqslant \lfloor n/2 \rfloor$,*

$$\begin{aligned} M_1(Kb_n(k)) &= (n-2k)(n^2+2nk-4k-2n+1)+4k(k-1)(n-2) \\ M_2(Kb_n(k)) &= 2k(n-2k)(n-2)(n-1)+\frac{1}{2}(n-2k)(n-2k-1)(n-1)^2 \\ &+ 2k(k-1)(n-2)^2 \\ F(Kb_n(k)) &= 18nk-6n^2k-14k+n^4-3n^3+3n^2-n\,. \end{aligned}$$

THEOREM 3.7. *For $n \geqslant 3$ and $2 \leqslant k \leqslant n-1$,*

$$\begin{aligned} M_1(Kc_n(k)) &= (n-k)k(2n-k-1)+(n-1)(n-k)(n-k-1) \\ M_2(Kc_n(k)) &= k(n-1)(n-k)^2+\frac{1}{2}(n-k)(n-k-1)(n-1)^2 \\ F(Kc_n(k)) &= n^4-3n^3+3n^2-3n^2k^2+3n^2k+3nk^3-3nk-n-k^4+k\,. \end{aligned}$$

THEOREM 3.8. *For $3 \leqslant k \leqslant n$ and $n \geqslant 3$,*

$$\begin{aligned} M_1(Kd_n(k)) &= k(k-3)(n-3)+k(n-k)(2n-4)+(n-k)(n-k-1)(n-1) \\ M_2(Kd_n(k)) &= \frac{1}{2}k(k-3)(n-3)^2+k(n-k)(n-3)(n-1) \end{aligned}$$

$$+ \frac{1}{2}(n-k)(n-k-1)(n-1)^2$$
$$F(Kd_n(k)) = n^4 - 3n^3 + 3n^2 - n - 6n^2k - 26k + 24nk\,.$$

4. Coindices of cluster graphs and their complements

The following earlier established results will be needed for the present considerations.

THEOREM 4.1. [**1, 12**] *Let G be a simple graph with n vertices and m edges. Then*

$$M_1(\overline{G}) = n(n-1)^2 - 4m(n-1) + M_1(G) \tag{4.1}$$
$$\overline{M_1}(G) = 2m(n-1) - M_1(G) \tag{4.2}$$
$$\overline{M_1}(G) = \overline{M_1}(\overline{G}) \tag{4.3}$$
$$M_2(\overline{G}) = \frac{1}{2}n(n-1)^3 - 3m(n-1)^2 + 2m^2 + \frac{1}{2}(2n-3)M_1(G) - M_2(G) \tag{4.4}$$
$$\overline{M_2}(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G) \tag{4.5}$$
$$\overline{M_2}(\overline{G}) = m(n-1)^2 - (n-1)M_1(G) + M_2(G)\,. \tag{4.6}$$

THEOREM 4.2. [**9**] *Let G be a simple graph with n vertices and m edges. Then*

$$F(\overline{G}) = n(n-1)^3 - 6m(n-1)^2 + 3(n-1)M_1(G) - F(G) \tag{4.7}$$
$$\overline{F}(G) = (n-1)M_1(G) - F(G) \tag{4.8}$$
$$\overline{F}(\overline{G}) = 2m(n-1)^2 - 2(n-1)M_1(G) + F(G)\,. \tag{4.9}$$

The next lemma follows from Theorems 3.5–3.8 and Eqs. (4.2)–(4.4) by taking into account that $Ka_n(k)$, $Kb_n(k)$, $Kd_n(k)$ have $m-k$ edges whereas $Kc_n(k)$ has $m - k(k-1)/2$ edges:

LEMMA 4.1. *Let $Ka_n(k)$, $Kb_n(k)$, $Kc_n(k)$ and $Kd_n(k)$ be the graphs defined in Section 2. Then*

$$\begin{aligned}
M_1\Big(\overline{Ka_n(k)}\Big) &= k^2 + k \\
M_1\Big(\overline{Kb_n(k)}\Big) &= 2k \\
M_1\Big(\overline{Kc_n(k)}\Big) &= k^3 - 2k^2 + k \\
M_1\Big(\overline{Kd_n(k)}\Big) &= 4k \\
\overline{M_1}(Ka_n(k)) &= 2nk - k^2 - 3k \\
\overline{M_1}(Kb_n(k)) &= 2nk - 4k \\
\overline{M_1}(Kc_n(k)) &= k^2n - kn - k^3 + k^2 \\
\overline{M_1}(Kd_n(k)) &= 2nk - 6k \\
\overline{M_1}\Big(\overline{Ka_n(k)}\Big) &= 2nk - k^2 - 3k
\end{aligned}$$

$$\begin{aligned}
\overline{M_1}\Big(\overline{Kb_n(k)}\Big) &= 2nk - 4k \\
\overline{M_1}\Big(\overline{Kc_n(k)}\Big) &= k^2n - kn - k^3 + k^2 \\
\overline{M_1}\Big(\overline{Kd_n(k)}\Big) &= 2nk - 6k\,.
\end{aligned}$$

From Theorems 3.5–3.8 and Eqs. (4.4)–(4.6), we obtain:

LEMMA 4.2. *Using the same notation as in Lemma 4.1,*

$$\begin{aligned}
M_2\Big(\overline{Ka_n(k))}\Big) &= k^2 \\
M_2\Big(\overline{Kb_n(k)}\Big) &= k \\
M_2\Big(\overline{Kc_n(k)}\Big) &= \frac{1}{2}k^4 - \frac{3}{2}k^3 + \frac{3}{2}k^2 - \frac{1}{2}k \\
M_2\Big(\overline{Kd_n(k)}\Big) &= 4k \\
\overline{M_2}(Ka_n(k)) &= 2k^2 - nk^2 + n^2k - 3nk + 2k \\
\overline{M_2}(Kb_n(k)) &= n^2\,k - 4nk + 4k \\
\overline{M_2}(Kc_n(k)) &= \frac{1}{2}k^4 - k^3\,n + \frac{1}{2}k^2\,n^2 - \frac{1}{2}k^3 + k^2\,n - \frac{1}{2}kn^2 \\
\overline{M_2}(Kd_n(k)) &= n^2\,k - 6nk + 9k \\
\overline{M_2}\Big(\overline{Ka_n(k)}\Big) &= \frac{1}{2}k^2 - \frac{1}{2}k \\
\overline{M_2}\Big(\overline{Kb_n(k)}\Big) &= 2k^2 - 2k \\
\overline{M_2}\Big(\overline{Kc_n(k)}\Big) &= 0 \\
\overline{M_2}\Big(\overline{Kd_n(k)}\Big) &= 2k^2 - 6k\,.
\end{aligned}$$

From Theorems 3.5–3.8 and Eqs. (4.7)–(4.9), we obtain:

LEMMA 4.3. *Using the same notation as in Lemma 4.1,*

$$\begin{aligned}
F\Big(\overline{Ka_n(k)}\Big) &= k^3 + k \\
F\Big(\overline{Kb_n(k)}\Big) &= 2k \\
F\Big(\overline{Kc_n(k)}\Big) &= k^4 - 3k^3 + 3k^2 - k \\
F\Big(\overline{Kd_n(k)}\Big) &= 8k \\
\overline{F}(Ka_n(k)) &= 2n^2\,k - 2n\,k^2 - 6nk + k^3 + 2k^2 + 5k \\
\overline{F}(Kb_n(k)) &= 2n^2\,k - 8nk + 8k \\
\overline{F}(Kc_n(k)) &= n^2\,k^2 - n^2\,k - 2nk^3 + 2nk^2 + k^4 - k^3 \\
\overline{F}(Kd_n(k)) &= 2n^2\,k - 12nk + 18k
\end{aligned}$$

$$\begin{aligned}
\overline{F}\Big(\overline{Ka_n(k)}\Big) &= nk + nk^2 - k^3 - k^2 - 2k \\
\overline{F}\Big(\overline{Kb_n(k)}\Big) &= 2kn - 4k \\
\overline{F}\Big(\overline{Kc_n(k)}\Big) &= -2nk^2 + nk + n\,k^3 - k^4 + 2k^3 - k^2 \\
\overline{F}\Big(\overline{Kd_n(k)}\Big) &= 4kn - 12k\,.
\end{aligned}$$

From Theorem 3.1–3.4 and the corrected Theorem 1.1, we obtain:

LEMMA 4.4. *Using the same notation as in Lemma 4.1,*

$$\begin{aligned}
HZ\Big(\overline{Ka_n(k)}\Big) &= k^3 + 2k^2 + k \\
HZ\Big(\overline{Kb_n(k)}\Big) &= 4k \\
HZ\Big(\overline{Kc_n(k)}\Big) &= 2k^4 - 6k^3 + 6k^2 - 2k \\
HZ\Big(\overline{Kd_n(k)}\Big) &= 16k \\
\overline{HZ}(Ka_n(k)) &= 4n^2\,k - 4nk^2 - 12nk + k^3 + 6k^2 + 9k \\
\overline{HZ}(Kb_n(k)) &= 4k\,n^2 - 16kn + 16k \\
\overline{HZ}(Kc_n(k)) &= 2k^2\,n^2 - 2kn^2 - 4k^3\,n + 4k^2\,n + 2k^4 - 2k^3 \\
\overline{HZ}(Kd_n(k)) &= 2n^4 - 6n^3 - 8n^2\,k + 6n^2 + 20nk - 2n + 4k^2 - 32k \\
\overline{HZ}\Big(\overline{Ka_n(k)}\Big) &= nk + nk^2 - k^3 - 3k \\
\overline{HZ}\Big(\overline{Kb_n(k)}\Big) &= 4k^2 + 2kn - 8k \\
\overline{HZ}\Big(\overline{Kc_n(k)}\Big) &= k^3n - 2k^2n + kn - k^4 + 2k^3 - k^2 \\
\overline{HZ}\Big(\overline{Kd_n(k)}\Big) &= 4k^2 + 4kn - 24k\,.
\end{aligned}$$

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Department of Mathematics, Bearys Institute of Technology, Mangalore – 574153, Karnataka, India
E-mail address: rajesh.rbj065@gmail.com

Faculty of Science, University of Kragujevac, Kragujevac, Serbia
E-mail address: gutman@kg.ac.rs

Department of Mathematics, P. A. College of Engineering, Mangalore – 574153, Karnataka, India
E-mail address: rkmundewadi@gmail.com