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Relations Between the First Zagreb Index and Spectral Moment of Graphs*

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Abstract

In this paper, we first show that the results of Lemma 1, Theorem 4 and Theorem 6 in Zagreb Energy and Zagreb Estrada Index of graphs by N. J. Rad et al. [MATCH Commun. Math. Comput. Chem. 79(2018), 371-386] are not correct. We modify these conclusions and give the corresponding results. In addition, we present several inequality relations between spectral moments of the first Zagreb matrix and the first Zagreb index of graphs, and characterize the corresponding extremal graphs.

1 Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. If the vertices u and v are adjacent, we write $u \sim v$. Let d_u be the degree of vertex u in G. A vertex u is called isolated if $d_u = 0$. To avoid the triviality, we assume that all graphs have no isolated vertices. We denoted minimum and maximum degree of vertices of graph G by $\delta = \delta(G)$ and $\Delta = \Delta(G)$, respectively. A graph is called k-regular if each of its vertices has same degree k. For other underfined notations and terminology from graph theory, the reader are referred to [1].

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The first and second Zagreb indices, proposed by Gutman and Trinajstić [2] in 1972, are defined as

$$M_1(G) = \sum_{v \in V(G)} d_v^2, \; M_2(G) = \sum_{uv \in E(G)} d_u d_v \; .$$

The first Zagreb index can be also expressed as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v).$$

Among topological indices, Zagreb indices are very old and very important molecular structure-descriptor. There are many useful properties in chemistry and especially in mathematical chemistry. Two surveys of properties of Zagreb indices are found in [3, 4]. Some new results on the Zagreb index can be found in [5-7].

The hyper-Zagreb index $HW(G)$ was recently proposed by Shirdel et al. in [8] and defined as

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

The first Zagreb Matrix $\mathbf{Z}$ [9] of the graph G is defined as the matrix with entries

$$z_{ij} = \begin{cases} d_i + d_j & \text{if } i \sim j \\ 0 & \text{otherwise.} \end{cases}$$

Since $\mathbf{Z}$ is a real symmetric matrix, all its eigenvalues are real. There are denoted by $\mu_1 \geq \mu_2 \geq ... \geq \mu_n$. For a nonnegative integer k, the k-th spectral moment of the Zagreb matrix $\mathbf{Z}$ is defined

$$N_k = N_k(G) = \sum_{i=1}^{n} \mu_i^k.$$

We will denote by $tr(z)$ the trace of the matrix $\mathbf{Z}$.

2 Errors in [9]

In [9], the authors presented the following result for the spectral moments of the first Zagreb matrix.

Lemma 2.1. *(Lemma 1 of [9]) Let G be a graph with n vertices and Zagreb matrix* $\mathbf{Z}$*.*

Then

(1) $N_1 = tr(\mathbf{Z}) = 0;$

(2) $N_2 = tr(\mathbf{Z}^2) = 2HM;$

(3) $N_3 = tr(\mathbf{Z}^3) = 2HM \sum\limits_{\substack{i,j,k\in\{1,2,\ldots,n\}\\ i\sim j\sim k, i\sim k}} d_k^2;$

(4) $N_4 = tr(\mathbf{Z}^4) = n(HM)^2 + \sum\limits_{\substack{i,j\in\{1,2,\ldots,n\}\\ i\sim j}} (d_i+d_j)^2 \left(\sum\limits_{\substack{k\in\{1,2,\ldots,n\}\\ i\sim k\sim j}} d_k^2\right)^2,$

where $i \sim j$ indicates pairs of adjacent vertices v_i and v_j.

We will show that (3) and (4) of Lemma 2.1 are not correct. For example, Let C_3 be the cycle of order 3. It is easy to calculate that $\mu_1(C_3) = 8$ and $\mu_2(C_3) = \mu_3(C_3) = -4$. Then we may obtain $N_3 = \sum\limits_{i=1}^{3} \mu_i^3(C_3) = 384$ and $N_4 = \sum\limits_{i=1}^{3} \mu_i^4(C_3) = 4608$. From the definition of hyper-Zagreb index and Lemma 2.1, we have $HM = \sum\limits_{i\sim j}(d_i+d_j)^2 = 48$, then

$$N_3 = 2HM \sum_{\substack{i,j,k\in\{1,2,\ldots,n\}\\ i\sim j\sim k, i\sim k}} d_k^2 = 2\times 48\times 2^2\times 3 = 1152$$

and

$$N_4 = n(HM)^2 + \sum_{\substack{i,j\in\{1,2,\ldots,n\}\\ i\sim j}} (d_i+d_j)^2 \left(\sum_{\substack{k\in\{1,2,\ldots,n\}\\ i\sim k\sim j}} d_k^2\right)^2 = 3\times 48^2 + 4^2\times 4^2\times 3 = 7680.$$

Hence equality (3) and (4) in Lemma 2.1 do not hold. We have the following modified version of Lemma 2.1:

Lemma 2.2. *Let G be a graph with n vertices. Then*

(1) $N_1 = tr(\mathbf{Z}) = 0;$

(2) $N_2 = tr(\mathbf{Z}^2) = 2HM;$

(3) $N_3 = tr(\mathbf{Z}^3) = 2\sum\limits_{i\sim j}(d_i+d_j) \sum\limits_{\substack{k\in V(G)\\ i\sim k, k\sim j}} (d_i+d_k)(d_k+d_j);$

(4) $N_4 = tr(\mathbf{Z}^4) = \sum\limits_{i\in V(G)} \left(\sum\limits_{i\sim j}(d_i+d_j)^2\right)^2 + \sum\limits_{\substack{i,j\in V(G)\\ i\neq j}} \left(\sum\limits_{\substack{k\in V(G)\\ i\sim k, k\sim j}} (d_i+d_k)(d_k+d_j)\right)^2.$

Proof. We calculate the matrix $\mathbf{Z}^2$. For $i = j$

$$(\mathbf{Z}^2)_{ii} = \sum_{j=1}^{n} z_{ij} z_{ji} = \sum_{i \sim j} (d_i + d_j)^2.$$

For $i \neq j$

$$(\mathbf{Z}^2)_{ij} = \sum_{j=1}^{n} z_{ij} z_{ji} = z_{ii} z_{ij} + z_{ij} z_{jj} + \sum_{\substack{k \in V(G) \\ i \sim k, k \sim j}} z_{ik} z_{kj} = \sum_{\substack{k \in V(G) \\ i \sim k, k \sim j}} (d_i + d_k)(d_k + d_j).$$

Since the diagonal elements of $\mathbf{Z}^3$ are

$$(\mathbf{Z}^3)_{ii} = \sum_{j=1}^{n} z_{ij} (\mathbf{Z}^2)_{ji} = \sum_{i \sim j} (d_i + d_j) \sum_{\substack{k \in V(G) \\ i \sim k, k \sim j}} (d_i + d_k)(d_k + d_j),$$

we have

$$\begin{aligned} N_3 &= \sum_{i \in V(G)} \sum_{i \sim j} (d_i + d_j) \sum_{\substack{k \in V(G) \\ i \sim k, k \sim j}} (d_i + d_k)(d_k + d_j) \\ &= 2 \sum_{i \sim j} (d_i + d_j) \sum_{\substack{k \in V(G) \\ i \sim k, k \sim j}} (d_i + d_k)(d_k + d_j). \end{aligned}$$

We next calculate N_4. The diagonal elements of $\mathbf{Z}^4$ are

$$(\mathbf{Z}^4)_{ii} = \sum_{\substack{j \in V(G) \\ i \neq j}} \left(\sum_{\substack{k \in V(G) \\ i \sim k, k \sim j}} (d_i + d_k)(d_k + d_j) \right)^2 + \left(\sum_{i \sim j} (d_i + d_j)^2 \right)^2.$$

Then we obtain

$$\begin{aligned} N_4 &= \sum_{i \in V(G)} \sum_{\substack{j \in V(G) \\ i \neq j}} \left(\sum_{i \sim k, k \sim j} (d_i + d_k)(d_k + d_j) \right)^2 + \sum_{i \in V(G)} \left(\sum_{i \sim j} (d_i + d_j)^2 \right)^2 \\ &= \sum_{\substack{i,j \in V(G) \\ i \neq j}} \left(\sum_{i \sim k, k \sim j} (d_i + d_k)(d_k + d_j) \right)^2 + \sum_{i \in V(G)} \left(\sum_{i \sim j} (d_i + d_j)^2 \right)^2. \qquad \blacksquare \end{aligned}$$

In [9], the authors gave the following two lower bounds for the Zagreb Estrada index $ZEE(G)$ of G.

Theorem 2.3. *(Theorem 4 of [9]) Let G be a graph with n vertices. Then*

$$\begin{aligned} ZEE(G) \geq & n + 2HM + 2HM(sinh(1) - 1) \sum_{\substack{i,j,k \in \{1,2,\ldots,n\} \\ i \sim k \sim j, i \sim j}} (d_k)^2 \\ & + (cosh(1) - 1) \left[n(HM)^2 + \sum_{\substack{i,j \in \{1,2,\ldots,n\} \\ i \sim j}} (d_i + d_j)^2 \left(\sum_{\substack{k \in \{1,2,\ldots,n\} \\ i \sim k \sim j}} (d_k)^2 \right)^2 \right]. \end{aligned}$$

Theorem 2.4. *(Theorem 6 of [9]) Let G be a graph with n vertices and hyper-Zagreb index HM. Then*

$$ZEE(G) \geq \sqrt{n^2(1+HM) + 2nHM + \frac{2}{3}HM \sum_{\substack{i,j,k\in\{1,2,\dots,n\}\\ i\sim k\sim j, i\sim j}} (d_k)^2 + \frac{1}{12}nN_4}.$$

By Lemma 2.2, we will modify Theorem 2.3 and Theorem 2.4 to get the following results.

Theorem 2.5. *Let G be a graph with n vertices. Then*

$$\begin{aligned} ZEE(G) \geq\ & n+2HM+2(sinh(1)-1)\sum_{i\sim j}(d_i+d_j)\sum_{i\sim k,k\sim j}(d_i+d_k)(d_k+d_j) \\ & +(cosh(1)–1)\left[\sum_{i\in V(G)}\left(\sum_{i\sim j}(d_i+d_j)^2\right)^2 + \sum_{\substack{i,j\in V(G)\\ i\neq j}}\left(\sum_{i\sim k,k\sim j}(d_i+d_k)(d_k+d_j)\right)^2\right]. \end{aligned}$$

Theorem 2.6. *Let G be a graph with n vertices and hyper-Zagreb index HM. Then*

$$ZEE(G) \geq \sqrt{n^2(1+HM)+2nHM+\frac{2n}{3}\sum_{i\sim j}(d_i+d_j)\sum_{i\sim k,k\sim j}(d_i+d_k)(d_k+d_j)+\frac{nN_4}{12}}.$$

3 Connections between $M_1(G)$ and the spectral moments

Relation between various topological indices and spectral moment of a graph G is in the focus of interest of the researchers for quite many years and this topic is vital nowadays. In this part, we give some relations between the first Zagreb index and the spectral moments.

Theorem 3.1. *Let G be a graph with m edges. Then*

$$\frac{N_2}{4\Delta} \leq M_1(G) \leq \sqrt{\frac{1}{2}N_2 + 4m(m-1)\Delta^2},$$

where equality hold if and only if G is a regular graph.

Proof. By the definition of $M_1(G)$, along with part (2) of Lemma 2.2, we have

$$\begin{aligned} M_1^2(G) &= \left(\sum_{ij \in E(G)} (d_i + d_j) \right)^2 \\ &= \sum_{ij \in E(G)} (d_i + d_j)^2 + \sum_{\substack{ij \in E(G) \\ xy \in E(G) \\ ij \neq xy}} (d_i + d_j)(d_x + d_y) \\ &= \frac{1}{2} N_2 + \sum_{\substack{ij \in E(G) \\ xy \in E(G) \\ ij \neq xy}} (d_i + d_j)(d_x + d_y) \\ &\leq \frac{1}{2} N_2 + 4m(m-1)\Delta^2 \end{aligned}$$

Consequently, $M_1(G) \leq \sqrt{\frac{1}{2}N_2 + 4m(m-1)\Delta^2}$.

Lemma 2.2, gives

$$\begin{aligned} N_2 = tr(\mathbf{Z}^2) &= 2 \sum_{ij \in E(G)} (d_i + d_j)^2 \\ &= 2 \sum_{ij \in E(G)} (d_i + d_j)(d_i + d_j) \\ &\leq 4\Delta \sum_{ij \in E(G)} (d_i + d_j) = 4\Delta M_1(G). \end{aligned}$$

Then

$$M_1(G) \geq \frac{N_2}{4\Delta}.$$

The equality in each inequality holds if and only if $d_i = d_j = \Delta$ for each $ij \in E(G)$. This happens if and only if G is a Δ-regular graph. ∎

Given a graph G, denote by $N(v)$ the set of neighbors of the vertex v, and by $a = \max\limits_{uv \in E(G)} |N(u) \bigcap N(v)|$, $b = \min\limits_{uv \in E(G)} |N(u) \bigcap N(v)|$.

Theorem 3.2. *Let G be a graph with $a, b > 0$. Then*

$$\frac{N_3}{8a\Delta^2} \leq M_1(G) \leq \frac{N_3}{8b\delta^2}.$$

The equality in each inequality holds if and only if G is regular and $a = b$.

Proof. By Lemma 2.2, we have

$$\begin{aligned}N_3 = tr(\mathbf{Z}^3) &= 2\sum_{i\sim j}(d_i+d_j)\sum_{i\sim k,k\sim j}(d_i+d_k)(d_k+d_j)\\ &\geq 2\sum_{i\sim j}(d_i+d_j)\sum_{i\sim k,k\sim j}4\delta^2\\ &= 8\delta^2\sum_{i\sim j}(d_i+d_j)\sum_{i\sim k,k\sim j}1\\ &\geq 8\delta^2 b\sum_{i\sim j}(d_i+d_j)\\ &= 8\delta^2 bM_1(G).\end{aligned}$$

Furthermore,

$$\begin{aligned}N_3 = tr(\mathbf{Z}^3) &= 2\sum_{i\sim j}(d_i+d_j)\sum_{i\sim k,k\sim j}(d_i+d_k)(d_k+d_j)\\ &\leq 2\sum_{i\sim j}(d_i+d_j)\sum_{i\sim k,k\sim j}4\Delta^2\\ &= 8\Delta^2\sum_{i\sim j}(d_i+d_j)\sum_{i\sim k,k\sim j}1\\ &\leq 8\Delta^2 a\sum_{i\sim j}(d_i+d_j)\\ &= 8\Delta^2 aM_1(G).\end{aligned}$$

Suppose now that equality holds in the lower bound of $M_1(G)$. Then the above inequality must be equalities. This implies that $d_i+d_j = 2\delta$ for every $ij \in E(G)$, that is, $d_i = \delta$ for every $i \in V(G)$. Besides, $|N(i)\bigcap N(j)| = b$ for every $ij \in E(G)$, that is, $a = b$.

Suppose that equality holds in the upper bound of $M_1(G)$. Then $d_i+d_j = 2\Delta$ for every $ij \in E(G)$, that is, $d_i = \Delta$ for every $i \in V(G)$. Furthermore, we have $|N(i)\bigcap N(j)| = a$ for every $ij \in E(G)$, that is, $a = b$.

Conversely, by direct checking we verify they are equal to $M_1(G)$. ■

Theorem 3.3. *Let G be a graph of order n with m edges. Then*

$$\frac{N_4+32\Delta^5 m}{16\Delta^4(\Delta+1)} \leq M_1(G) \leq \frac{N_4+32\delta^4 m}{32\delta^4}.$$

The equality in the lower bound is attained if and only if $G \cong K_{\Delta,\Delta}$; the equality in the upper bound is attained if and only if G is δ-regular graph without cycles of length 4.

Proof. Denote by $|P_3|$ the cardinality of the set of paths of length 2 in G that are not cycles.

$$|P_3| = \sum_{i\in V(G)}\frac{1}{2}d_i(d_i-1) = \frac{1}{2}\sum_{i\in V(G)}d_i^2 - \frac{1}{2}\sum_{i\in V(G)}d_i = \frac{1}{2}M_1(G)-m.$$

Hence

$$\sum_{\substack{i,j\in V(G)\\ i\neq j}}\left(\sum_{\substack{k\in V(G)\\ i\sim k,k\sim j}}1\right)=2|P_3|=M_1(G)-2m.$$

Since

$$\begin{aligned}
&\sum_{\substack{i,j\in V(G)\\ i\neq j}}\left(\sum_{\substack{k\in V(G)\\ i\sim k,k\sim j}}(d_i+d_k)(d_k+d_j)\right)^2\\
&=\sum_{\substack{i,j\in V(G)\\ i\neq j}}\left(\sum_{\substack{k\in V(G)\\ i\sim k,k\sim j}}(d_i+d_k)(d_k+d_j)\right)\left(\sum_{\substack{k\in V(G)\\ i\sim k,k\sim j}}(d_i+d_k)(d_k+d_j)\right)\\
&\leq\sum_{\substack{i,j\in V(G)\\ i\neq j}}\left(\sum_{\substack{k\in V(G)\\ i\sim k,k\sim j}}4\Delta^2\right)\left(\sum_{\substack{k\in V(G)\\ i\sim k,k\sim j}}4\Delta^2\right)\\
&=16\Delta^4\sum_{\substack{i,j\in V(G)\\ i\neq j}}\left(\sum_{\substack{k\in V(G)\\ i\sim k,k\sim j}}1\right)\left(\sum_{\substack{k\in V(G)\\ i\sim k,k\sim j}}1\right)\\
&=16\Delta^4\sum_{\substack{i,j\in V(G)\\ i\neq j}}\left(\sum_{\substack{k\in V(G)\\ i\sim k,k\sim j}}1\right)|N(i)\bigcap N(j)|\\
&\leq 16\Delta^5\sum_{\substack{i,j\in V(G)\\ i\neq j}}\left(\sum_{\substack{k\in V(G)\\ i\sim k,k\sim j}}1\right)\\
&=16\Delta^5\cdot 2|P_3|\\
&=16\Delta^5(M_1(G)-2m).
\end{aligned}\tag{3.1}$$

$$\begin{aligned}
\sum_{i\in V(G)}\left(\sum_{i\sim j}(d_i+d_j)^2\right)^2&\leq\sum_{i\in V(G)}\left(\sum_{i\sim j}(d_i+d_j)\cdot 2\Delta\right)^2\\
&=4\Delta^2\sum_{i\in V(G)}\left(\sum_{i\sim j}(d_i+d_j)\right)\left(\sum_{i\sim j}(d_i+d_j)\right)\\
&\leq 8\Delta^3\sum_{i\in V(G)}\left(\sum_{i\sim j}(d_i+d_j)\right)\left(\sum_{i\sim j}1\right)\\
&=8\Delta^3\sum_{i\in V(G)}\sum_{i\sim j}(d_i+d_j)d_i
\end{aligned}$$

$$\begin{aligned}
&\leq 8\Delta^4 \sum_{i\in V(G)} \sum_{i\sim j}(d_i+d_j)\\
&= 16\Delta^4 \sum_{i\sim j}(d_i+d_j)\\
&= 16\Delta^4 M_1(G). \qquad (3.2)
\end{aligned}$$

According to Lemma 2.2 and (3.1), (3.2) we have that

$$\begin{aligned}
N_4 &= \sum_{i\in V(G)} \left(\sum_{i\sim j}(d_i+d_j)^2\right)^2 + \sum_{\substack{i,j\in V(G)\\ i\neq j}} \left(\sum_{\substack{k\in V(G)\\ i\sim k, k\sim j}} (d_i+d_k)(d_k+d_j)\right)^2\\
&\leq 16\Delta^4 M_1(G) + 16\Delta^5 (M_1(G)-2m),
\end{aligned}$$

that is

$$M_1(G) \geq \frac{N_4 + 32\Delta^5 m}{16\Delta^4(\Delta+1)}.$$

Similarly, as

$$\begin{aligned}
N_4 &= \sum_{i\in V(G)} \left(\sum_{i\sim j}(d_i+d_j)^2\right)^2 + \sum_{\substack{i,j\in V(G)\\ i\neq j}} \left(\sum_{\substack{k\in V(G)\\ i\sim k, k\sim j}} (d_i+d_k)(d_k+d_j)\right)^2\\
&\geq 4\delta^2 \sum_{i\in V(G)} \left(\sum_{i\sim j}(d_i+d_j)\right)^2 + 16\delta^4 \sum_{\substack{i,j\in V(G)\\ i\neq j}} \left(\sum_{\substack{k\in V(G)\\ i\sim k, k\sim j}} 1\right)\left(\sum_{\substack{k\in V(G)\\ i\sim k, k\sim j}} 1\right)\\
&= 4\delta^2 \sum_{i\in V(G)} \left(\sum_{i\sim j}(d_i+d_j)\right)^2 + 16\delta^4 \sum_{\substack{i,j\in V(G)\\ i\neq j}} \left(\sum_{\substack{k\in V(G)\\ i\sim k, k\sim j}} 1\right) |N(i)\bigcap N(j)|\\
&\geq 8\delta^3 \sum_{i\in V(G)} \left(\sum_{i\sim j}(d_i+d_j)\right)\left(\sum_{i\sim j}1\right) + 16\delta^4 \sum_{\substack{i,j\in V(G)\\ i\neq j}} \left(\sum_{\substack{k\in V(G)\\ i\sim k, k\sim j}} 1\right)\\
&= 8\delta^3 \sum_{i\in V(G)} \sum_{i\sim j}(d_i+d_j)\cdot d_i + 16\delta^4(M_1(G)-2m)\\
&\geq 8\delta^4 \sum_{i\in V(G)} \sum_{i\sim j}(d_i+d_j) + 16\delta^4(M_1(G)-2m)\\
&= 16\delta^4 M_1(G) + 16\delta^4(M_1(G)-2m),
\end{aligned}$$

it follows

$$M_1(G) \leq \frac{N_4 + 32\delta^4 m}{32\delta^4}.$$

Suppose that equality holds in the lower bound, then $d_i = \Delta$ for every $i \in V(G)$ and $|N(i) \bigcap N(j)| = \Delta$ for every $i, j, k \in V(G)$ with $i \sim k$ and $k \sim j$. Therefore $N(i) = N(j)$. Let $N(i) = N(j) = \{k_1, k_2, ..., k_\Delta\}$, then $N(k_1) = N(k_2) = \cdots = N(k_\Delta) = \{i, j, w_1, w_2, ..., w_{\Delta-2}\}$. Hence, $N(w_1) = N(w_2) = \cdots = N(w_{\Delta-2}\}) = N(i) = N(j)$. So G is isomorphic to the complete bipartite graph $K_{\Delta,\Delta}$.

The equality in the upper bound holds, then $d_i = \delta$ for every $i \in V(G)$. Therefore, we have $|N(i) \bigcap N(j)| = 1$ with $i \sim k$ and $k \sim j$. Hence, $|N(i) \bigcap N(j)| = 1$. So G is δ-regular graph without cycles of length 4.

Conversely, one can easily see that the equality holds. ■

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