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On Comparing Zagreb Indices of Graphs

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Abstract

For a (molecular) graph, the first Zagreb index M_1 is equal to the sum of the squares of the degrees of the vertices, and the second Zagreb index M_2 is equal to the sum of the products of the degrees of pairs of adjacent vertices. It is well known that for connected or disconnected graphs with n vertices and m edges, the inequality $M_2/m \geq M_1/n$ does not always hold. Here we show that this relation holds for certain kinds of graphs.

1 Introduction

Let $G = (V, E)$ be a simple graph with the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, $|E(G)| = m$. Also let $\overline{G}$ be the complement of G. For $v_i \in V(G)$, d_i is the degree of the vertex v_i of G, $i = 1, 2, \ldots, n$. The minimum vertex degree is denoted by $\delta(G)$ and the maximum by $\Delta(G)$. The average of the degrees of the vertices adjacent to vertex v_i is denoted by μ_i.

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

$$M_1(G) = \sum_{v_i \in V(G)} d_i^2$$

and

$$M_2(G) = \sum_{v_i v_j \in E(G)} d_i\, d_j \ .$$

The Zagreb indices $M_1(G)$ and $M_2(G)$ were introduced in [1] and elaborated in [2]. The main properties of $M_1(G)$ and $M_2(G)$ were summarized in [3, 4]. In [5] it was shown that the trees with the smallest and largest $M_1(T)$ are the path and the star, respectively. In [6] it was shown that the path and the star are also the trees with the smallest and largest $M_2(T)$. Recently, it has been conjectured that for each simple graph G with n vertices and m edges,

$$M_2(G)/m \geq M_1(G)/n \; . \tag{1}$$

The following two examples are obtained from [7, 8].

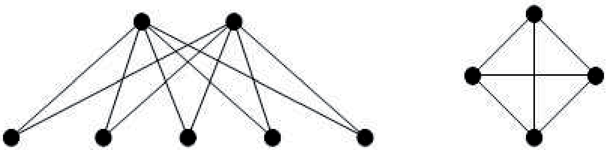

Fig. 1. A disconnected counterexample to Conjecture (1).

Fig. 2. A connected counterexample to Conjecture (1).

This conjecture has been analyzed in [7, 8, 9, 10] and the following results have been obtained:

(1) the conjecture is not true in general,

(2) the conjecture is true for all chemical graphs,

(3) the conjecture is true for all trees,

(4) the conjecture is true for all unicyclic graphs,

(5) the conjecture is not true for all bicyclic graphs,

(6) the conjecture is true for $\Delta(G) - \delta(G) \leq 2$,

(7) the conjecture is true for $\Delta(G) - \delta(G) \leq 3$ and $\delta(G) \neq 2$.

Also, further generalizations of this conjecture have been analyzed in [10, 11, 12, 13]. Some recent results on the Zagreb indices are reported in [14–24], where also references to the previous mathematical research in this area can be found. These indices reflect the extent of branching of the molecular carbon-atom skeleton, and can thus be viewed as molecular structure-descriptors [25, 26].

2 Conjecture on comparing Zagreb indices of graphs

In this section we present some results related to the conjecture (1) of graphs.

First let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two simple graphs on disjoint sets of vertices. Their union is $G_1 + G_2 = (V_1 \cup V_2, E_1 \cup E_2)$. The example given in Fig. 1 shows that if (1) holds for the graphs G_1 and G_2, then it needs not hold for their union $G_1 + G_2$.

The join, $G_1 \vee G_2$, of G_1 and G_2 is the graph obtained from $G_1 + G_2$ by adding new edges from each vertex of G_1 to every vertex of G_2. Then we have $|V(G_1 \vee G_2)| = |V(G_1)| + |V(G_2)|$ and $|E(G_1 \vee G_2)| = |E(G_1)| + |E(G_2)| + |V(G_1||V(G_2)|$. Thus, for example, $\overline{K}_p \vee \overline{K}_q = K_{p,q}$, the complete bipartite graph.

Theorem 2.1. *Let G be a simple graph of n vertices with m edges. If (1) holds for G, then it also holds for $G \vee G$.*

Proof: Let n^* and m^* be the number of vertices and edges, respectively, in $G \vee G$. Then $n^* = 2n$ and $m^* = 2m + n^2$. Since (1) holds for G, we have

$$nM_2(G) \geq mM_1(G).$$

Let d_i^*, $i = 1, 2, \ldots, n^*$ be the degree sequence of $G \vee G$. Now,

$$\begin{aligned} M_2(G^*) &= \sum_{v_iv_j \in E(G\vee G)} d_i^* d_j^* \\ &= 2 \sum_{v_iv_j \in E(G)} (d_i + n)(d_j + n) + \sum_{v_iv_j \in E(G,G)} (d_i + n)(d_j + n) \\ &= 2M_2(G) + 2nM_1(G) + 2mn^2 + n^4 + n\sum_{i=1}^{n}(nd_i + 2m) + \sum_{i=1}^{n} 2md_i \\ &= 2M_2(G) + 2nM_1(G) + n^4 + 4m^2 + 6mn^2 \end{aligned} \tag{2}$$

and

$$\begin{aligned} M_1(G \vee G) &= \sum_{i=1}^{n^*} d_i^{*2} = 2\sum_{i=1}^{n}(d_i + n)^2 \\ &= 2M_1(G) + 8mn + 2n^3 . \end{aligned} \tag{3}$$

We have to show that

$$n^* M_2(G \vee G) \geq m^* M_1(G \vee G)$$

that is,

$$\left(n - \frac{2m}{n}\right) M_1(G) + 2M_2(G) - 4m^2 \geq 0 \quad \text{by (2) and (3)}$$

which, evidently, is always obeyed as $M_1(G) \geq \frac{4m^2}{n}$ (Weighted Arithmetic-Harmonic mean inequality) and $nM_2(G) \geq mM_1(G)$. Hence the theorem. □

Theorem 2.2. *Let G be a simple graph of n vertices with m edges. If (1) does not hold for G, then (1) holds for $\overline{G}$.*

Proof: Let $\overline{n}$ and $\overline{m}$ be the number of vertices and edges in $\overline{G}$. Then $\overline{n} = n$ and $\overline{m} = \binom{n}{2} - m$. Since (1) does not hold for G, we have

$$\frac{M_1(G)}{n} > \frac{M_2(G)}{m} . \tag{4}$$

Let $\overline{d}_i$, $i = 1, 2, \ldots, n$, be the degree sequence of $\overline{G}$. Then $\overline{d}_i = n - d_i - 1$, $i =$

$1, 2, \ldots, n$. Now,

$$\begin{aligned}
M_2(\overline{G}) &= \sum_{v_iv_j\in E(\overline{G})} \overline{d}_i\overline{d}_j = \sum_{v_iv_j\notin E(G),i\neq j} (n-d_i-1)(n-d_j-1) \\
&= \Big[\frac{n(n-1)}{2}-m\Big](n-1)^2-(n-1)\sum_{v_iv_j\notin E(G),i\neq j}(d_i+d_j)+\sum_{v_iv_j\notin E(G),i\neq j}d_id_j \\
&= \Big[\frac{n(n-1)}{2}-m\Big](n-1)^2-\frac{(n-1)}{2}\sum_{i=1}^{n}\Big[(n-d_i-1)d_i+2m-d_i-d_i\mu_i\Big] \\
&+ \frac{1}{2}\sum_{i=1}^{n}d_i(2m-d_i-d_i\mu_i) \\
&= \Big[\frac{n(n-1)}{2}-m\Big](n-1)^2+2m^2-M_2(G) \\
&+ \Big(n-\frac{3}{2}\Big)M_1(G)-2m(n-1)^2 \qquad (5)
\end{aligned}$$

and

$$\begin{aligned}
M_1(\overline{G}) &= \sum_{i=1}^{n}\overline{d}_i^2=\sum_{i=1}^{n}(n-d_i-1)^2 \\
&= n(n-1)^2-4m(n-1)+M_1(G)\ . \qquad (6)
\end{aligned}$$

We have to show that

$$\frac{M_2(\overline{G})}{\overline{m}} \geq \frac{M_1(\overline{G})}{\overline{n}}$$

that is,

$$mM_1(G)-nM_2(G)+\frac{n(n-2)}{2}M_1(G)+4m^2-2m^2n\geq 0 \quad \text{by (5) and (6),}$$

that is,

$$\frac{n(n-2)}{2}M_1(G)+4m^2-2m^2n\geq 0 \quad \text{by (4),}$$

which, evidently, is always obeyed as $M_1(G)\geq\frac{4m^2}{n}$. Hence the theorem. □

Let $G=(V,E)$ be a simple graph of order n with m edges. If we put two similar graphs G side by side, and any vertex of the first graph G is connected by edges with the corresponding vertices of the second graph G and the resultant graph is $\hat{G}$. Then we have $|V(\hat{G})|=|V(G)|+|V(G)|=2n$ and $|E(\hat{G})|=|E(G)|+|E(G)|+|E(G,G)|=2m+n$.

Theorem 2.3. *If (1) holds for G, then it holds for $\hat{G}$ also.*

Proof: Let $\hat{n}$ and $\hat{m}$ be the number of vertices and number of edges in $\hat{G}$. Then $\hat{n} = 2n$ and $\hat{m} = 2m + n$. We have

$$\begin{aligned} M_2(\hat{G}) &= \sum_{v_iv_j \in E(\hat{G})} \hat{d}_i \hat{d}_j \\ &= 2 \sum_{v_iv_j \in E(G)} (d_i+1)(d_j+1) + \sum_{i=1}^{n} (d_i+1)^2 \\ &= 2M_2(G) + 3M_1(G) + 6m + n\,. \end{aligned} \tag{7}$$

and

$$M_1(\hat{G}) = 2\sum_{i=1}^{n}(d_i+1)^2 = 2M_1(G) + 8m + 2n\,. \tag{8}$$

Since (1) holds for G, we have

$$nM_2(G) - mM_1(G) \geq 0\,. \tag{9}$$

Now we have to show that

$$\hat{n}M_2(\hat{G}) - \hat{m}M_1(\hat{G}) \geq 0\,,$$

that is,

$$2n(2M_2(G) + 3M_1(G) + 6m + n) - (2m+n)(2M_1(G) + 8m + 2n) \geq 0 \quad \text{by (7) and (8),}$$

that is,

$$2n(2M_2(G) + 3M_1(G) + 6m + n) - (2m+n)(2M_1(G) + 8m + 2n) \geq 4(nM_1(G) - 4m^2) \geq 0\,,$$

by (9) and $M_1(G) \geq \frac{4m^2}{n}$. Hence the theorem. □

Let $G = (V, E)$ be a simple graph on n vertices with m edges. If we take two copies of G, and any vertex of the first copy is connected by edges to the vertices that are adjacent to the corresponding vertex of the second copy, the resultant graph is $\tilde{G}$. Then we have

$$|V(\tilde{G})| = |V(G)| + |V(G)| = 2n$$

and

$$|E(\tilde{G})| = |E(G)| + |E(G)| + \sum_{i=1}^{n} d_i = m + m + 2m = 4m \ .$$

Theorem 2.4. *If (1) holds for G, then it holds also for $\tilde{G}$.*

Proof: Let $\tilde{n}$ and $\tilde{m}$ be the number of vertices and number of edges of the graph $\tilde{G}$. Then $\tilde{n} = 2n$ and $\tilde{m} = 4m$. We have

$$\begin{aligned} M_2(\tilde{G}) &= \sum_{v_i v_j \in E(\tilde{G})} \tilde{d}_i \tilde{d}_j \\ &= 2 \sum_{v_i v_j \in E(G)} 4 d_i d_j + 2 \sum_{v_i v_j \in E(G,G)} 4 d_i d_j \\ &= 16 M_2(G) \end{aligned} \tag{10}$$

and

$$M_1(\tilde{G}) = 2 \sum_{i=1}^{n} (2d_i)^2 = 8 M_1(G) \ . \tag{11}$$

Now,

$$\frac{M_2(\tilde{G})}{\tilde{m}} = \frac{16 M_2(G)}{4m} \geq \frac{4 M_1(G)}{n} = \frac{8 M_1(G)}{2n} = \frac{M_1(\tilde{G})}{\tilde{n}} \quad \text{as } n M_2(G) - m M_1(G) \geq 0 \,,$$

and by (10) and (11).

Hence the theorem. □

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References

[1] I. Gutman, N. Trinajstić, Chem. Phys. Lett. **17** (1972) 535.

[2] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, J. Chem. Phys. **62** (1975) 3399.

[3] S. Nikolić, G. Kovačević, A. Milićević, N. Trinajstić, Croat. Chem. Acta **76** (2003) 113.

[4] S. Chen, F. Xia, MATCH Commun. Math. Comput. Chem. **58** (2007) 663.

[5] I. Gutman, K. C. Das, MATCH Commun. Math. Comput. Chem. **50** (2004) 83.

[6] K. C. Das, I. Gutman, MATCH Commun. Math. Comput. Chem. **52** (2004) 103.

[7] P. Hansen, D. Vukičević, Croat. Chem. Acta **80** (2007) 165.

[8] L. Sun, T. Chen, Discr. Appl. Math. **157** (2009) 1650.

[9] D. Vukičević, A. Graovac, MATCH Commun. Math. Comput. Chem. **57** (2007) 587.

[10] D. Vukičević, Talk on the meeting of International Academy of Mathematical Chemistry, Dubrovnik 2007.

[11] D. Vukičević, MATCH Commun. Math. Comput. Chem. **57** (2007) 633.

[12] D. Vukičević, A. Graovac, MATCH Commun. Math. Comput. Chem. **60** (2008) 37.

[13] B. Horoldagva, K. C. Das, MATCH Commun. Math. Comput. Chem. **62** (2009) 725.

[14] K. C. Das, I. Gutman, B. Zhou, J. Math. Chem. **46** (2009) 514.

[15] K. C. Das, Discr. Math. **285** (2004) 57.

[16] L. Zhang, B. Wu, MATCH Commun. Math. Comput.Chem. **54** (2005) 189.

[17] B. Zhou, I. Gutman, MATCH Commun. Math. Comput. Chem. **54** (2005) 233.

[18] V. Kumar, A. K. Madan, J. Math. Chem. **42** (2007) 925.

[19] B. Zhou, MATCH Commun. Math. Comput. Chem. **57** (2007) 591.

[20] A. Ilić, D. Stevanović, MATCH Commun. Math. Comput. Chem. **62** (2009) 681.

[21] M. Liu, B. Liu, MATCH Commun. Math. Comput. Chem. **62** (2009) 689.

[22] L. Sun, S. Wei, MATCH Commun. Math. Comput. Chem. **62** (2009) 699.

[23] D. Vukicević, MATCH Commun. Math. Comput. Chem. **62** (2009) 715.

[24] Z. Huang, Y. Guo, MATCH Commun. Math. Comput. Chem. **62** (2009) 731.

[25] A. T. Balaban, I. Motoc, D. Bonchev, O. Mekenyan, Topics Curr. Chem. **114** (1983) 21.

[26] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.