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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,

$$M_2/m \geq M_1/n$$

does not hold always. In K. C. Das (*On comparing Zagreb indices of graphs*, MATCH Commun. Math. Comput. Chem. **63**, 433–440, 2010), it has been shown that the above relation holds for a special kind of graph. Here we continue our search for special kinds of graph for which the above relation holds.

Keywords: First Zagreb index, Second Zagreb index, Cartesian product, Threshold graph.

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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 a complement graph 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.

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The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of graph G (see [3, 8, 9, 11, 12, 13, 18, 19, 20, 21, 24, 30, 31] and the references therein) are among the oldest and the most famous topological indices and they are defined as:

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

and

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

The AutoGraphiX system ([1], [4]-[5]) proposed the following conjecture:

$$M_2(G)/m \geq M_1(G)/n. \tag{1.1}$$

Hansen and Vukičević [14] proved that (1.1) is true for all chemical graphs and does not hold for general graphs. Vukičević and Graovac [27] proved that (1.1) holds for all trees, and gave a counter example for bicyclic graphs. Sun and Chen [22] showed that (1.1) holds for graphs with a small difference between the maximum and minimum vertex degrees. Also (1.1) holds for all unicyclic graphs [29] and for all bicyclic graphs, except one class [23], and generalizations of this claim to the variable Zagreb indices were analyzed in [15, 25, 26, 28, 29]. In [16], it has been shown that for every positive integer k, there exists a connected graph such that $m-n=k$ and (1.1) does not hold. Some recent results on the Zagreb indices are reported in [6], [10], [32]-[35], 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 [2, 24]. The connected and disconnected counter examples of the relation (1.1) are given in [14, 22].

In [7], it has been shown that (1.1) holds for a special kind of graph. Here we continue our search for those special kinds of graph which satisfy (1.1).

2. Conjecture on comparing Zagreb indices of graphs

In this section we present some results related to the conjecture (1.1) of graphs.

The cartesian product $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a,x)(b,y)$ is an edge of $G \times H$ if $a=b$ and $xy \in E(H)$, or $ab \in E(G)$ and $x=y$. If $G_1, G_2, \ldots, G_n$ are graphs then we denote $G_1 \bigotimes \cdots \bigotimes G_n$ by $\bigotimes_{i=1}^n G_i$. In the case where $G_1 = G_2 = \cdots = G_n = G$, we denote $\bigotimes_{i=1}^n G_i$ by G^n.

2.1. Lemma. [17] *Let $G_1, G_2, \ldots, G_n$ be graphs with $V_i = V(G_i)$ and $E_i = E(G_i)$, $1 \leq i \leq n$, and $V = V(\bigotimes_{i=1}^n G_i)$. Then*

$$M_1\Big(\bigotimes_{i=1}^n G_i\Big) = |V| \sum_{i=1}^n \frac{M_1(G_i)}{|V_i|} + 4|V| \sum_{i\neq j, i,j=1}^n \frac{|E_i||E_j|}{|V_i||V_j|}. \qquad \square$$

2.2. Lemma. [17] *Let $G_1, G_2, \ldots, G_n$ be graphs with $V_i = V(G_i)$ and $E_i = E(G_i)$, $1 \leq i \leq n$, $V = V(\bigotimes_{i=1}^n G_i)$ and $E = E(\bigotimes_{i=1}^n G_i)$. Then*

$$M_2\Big(\bigotimes_{i=1}^n G_i\Big) = |V| \sum_{i=1}^n \left(\frac{M_2(G_i)}{|V_i|} + 3M_1(G_i)\left(\frac{|E|}{|V_i|} - \frac{|V||E_i|}{|V_i|^2}\right)\right) + 4|V| \sum_{i,j,k=1; i\neq j, i\neq k, j\neq k}^n \frac{|E_i||E_j||E_k|}{|V_i||V_j||V_k|}. \qquad \square$$

2.3. Theorem. *Let G_1 and G_2 be two simple graphs with $n_i = |V(G_i)|$ and $m_i = |E(G_i)|$, $i = 1, 2$. If (1.1) holds for G_1 and G_2, then it also holds for $G_1 \times G_2$.*

Proof. Let n^* and m^* be the number of vertices and edges, respectively, in $G_1 \times G_2$. Then $n^* = n_1 n_2$ and $m^* = n_1 m_2 + n_2 m_1$. By Lemma 2.1 and Lemma 2.2, we get

$$M_1(G_1 \times G_2) = n_1 M_1(G_2) + n_2 M_1(G_1) + 4m_1 m_2. \tag{2.1}$$

and

$$M_2(G_1 \times G_2) = n_1 M_2(G_2) + n_2 M_2(G_1) + 3m_2 M_1(G_1) + 3m_1 M_1(G_2). \tag{2.2}$$

Since (1.1) holds for G_1 and G_2, we have

$$n_1 M_2(G_1) \geq m_1 M_1(G_1) \text{ and } n_2 M_2(G_2) \geq m_2 M_1(G_2). \tag{2.3}$$

By (2.2), we have

$$\begin{aligned}
&n^* M_2(G_1 \times G_2) \\
&\quad = n_1^2 n_2 M_2(G_2) + n_1 n_2^2 M_2(G_1) + 3n_1 n_2 m_2 M_1(G_1) + 3n_1 n_2 m_1 M_1(G_2) \\
&\quad \geq n_1^2 m_2 M_1(G_2) + n_2^2 m_1 M_1(G_1) + n_1 n_2 m_2 M_1(G_1) + n_1 n_2 m_1 M_1(G_2) \\
&\qquad\qquad + 8n_2 m_1^2 m_2 + 8n_1 m_1 m_2^2 \quad \text{as } n_1 M_1(G_1) \geq 4m_1^2, \\
&\qquad\qquad\qquad\qquad n_2 M_1(G_2) \geq 4m_2^2 \text{ and by (2.3)} \\
&\quad = (n_1 m_2 + n_2 m_1) M_1(G_1 \times G_2) + 4n_2 m_1^2 m_2 + 4n_1 m_1 m_2^2 \text{ by (2.1)} \\
&\quad > m^* M_2(G_1 \times G_2).
\end{aligned}$$

Hence the theorem. □

2.4. Theorem. *Let G be a simple graph with n vertices and m edges. Then* (1.1) *holds for $G \times G$.*

Proof. From (2.1) and (2.2), we get

$$M_1(G \times G) = 2nM_1(G) + 4m^2 \tag{2.4}$$

and

$$M_2(G \times G) = 2nM_2(G) + 6mM_1(G). \tag{2.5}$$

By (2.5), we have

$$\begin{aligned}
n^2 M_2(G \times G) &= 2n^3 M_2(G) + 6n^2 m M_1(G) \\
&> 6n^2 m M_1(G) \\
&\geq 4n^2 m M_1(G) + 8nm^3 \quad \text{as } nM_1(G) \geq 4m^2 \\
&= 2nmM_1(G \times G) \quad \text{by (2.4)}.
\end{aligned}$$

Hence the theorem. □

Let G be a graph with vertex set V and edge set E. Let $\overline{V}$ be a copy of V, $\overline{V} = \{\overline{x} : x \in V\}$. Then we denote by G' the graph with vertex set $V \cup \overline{V}$ and edge set $E' = E \cup \{x\overline{y} : xy \notin E\}$.

2.5. Theorem. *Let G be a simple graph of n vertices and m edges. Then G' must satisfy (1.1).*

Proof. Let n' and m' be the number of vertices and edges in G'. Then $n' = 2n$ and $m' = \sum_{i=1}^{n}(n - 1 - d_i) + m = n(n - 1) - m$.

Let d_i', $i = 1, 2, \dots, 2n$ be the degree sequence in G'. Then $d_i' = n - 1$, $i = 1, 2, \dots, n$, and $d_i' = n - d_i - 1$, $i = n+1, n+2, \dots, 2n$. Now,

$$\begin{aligned}
M_2(G') &= \sum_{v_iv_j \in E'} d_i' d_j' \\
&= \sum_{v_iv_j \in E',\ v_i, v_j \in V} (n-1)^2 + \sum_{v_i\overline{v}_j \in E',\ v_i \in V, v_j \in \overline{V}} (n-1)(n-d_j-1) \\
&= \big(n(n-1) - m\big)(n-1)^2 - (n-1) \sum_{v_i\overline{v}_j \in E'} d_j \\
&= \big(n(n-1) - m\big)(n-1)^2 - (n-1) \sum_{j=1}^{n} (n-1-d_j) d_j \\
&= n(n-1)^3 - 3m(n-1)^2 + (n-1)M_1(G) \qquad (2.6)
\end{aligned}$$

and

$$\begin{aligned}
M_1(G') &= \sum_{i=1}^{2n} {d_i'}^{\,2} = \sum_{i=1}^{n} (n-1)^2 + \sum_{i=n+1}^{2n} (n-d_i-1)^2 \\
&= 2n(n-1)^2 - 4m(n-1) + M_1(G). \qquad (2.7)
\end{aligned}$$

We have to show that

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

that is,

$$\begin{aligned}
&2n^2(n-1)^3 - 6mn(n-1)^2 + 2n(n-1)M_1(G) \\
&\geq \big(2n(n-1)^2 - 4m(n-1) + M_1(G)\big)\big(n(n-1) - m\big) \quad \text{by (2.6) and (2.7)},
\end{aligned}$$

that is,

$$n(n-1)M_1(G) + mM_1(G) - 4m^2n + 4m^2 \geq 0,$$

that is,

$$mM_1(G) \geq 0 \quad \text{as } nM_1(G) \geq 4m^2,$$

which, evidently, is always obeyed. Hence the theorem. □

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two simple graphs with $n_i = |V(G_i)|$ and $m_i = |E(G_i)|$, $i = 1, 2$. Then the tensor product $G_1 \Box G_2$ of graphs G_1 and G_2 is a graph such that the vertex set of $G_1 \Box G_2$ is the Cartesian product $V(G_1) \times V(G_2)$, and any two vertices $(v_i',\ v_j'')$ and $(v_p',\ v_q'')$ are adjacent in $G_1 \Box G_2$ if and only if v_j'' is adjacent with v_q'' and v_i' is adjacent with v_p'. Then we have $|V(G_1 \Box G_2)| = n_1 n_2$.

Denote by $d_{i,j}$, $1 \leq i \leq n_1$, $1 \leq j \leq n_2$, the degree of the vertex $(v_i',\ v_j'')$ of $G_1 \Box G_2$. Then $d_{i,j} = d_i' \cdot d_j''$, where d_i' is the degree of the vertex v_i' of G_1 and d_j'' is the degree of the vertex v_j'' of G_2. Then we have

$$2|E(G_1 \Box G_2)| = \sum_{1 \leq i \leq n_1, 1 \leq j \leq n_2} d_{i,j} = \sum_{i=1}^{n_1} d_i' \sum_{j=1}^{n_2} d_j'' = 4m_1 m_2,$$

that is,

$$|E(G_1 \Box G_2)| = 2m_1 m_2.$$

2.6. Theorem. *If* (1.1) *holds for* G_1 *and* G_2, *then it also holds for* $G_1 \Box G_2$.

Proof. Let $\hat{n}$ and $\hat{m}$ be the number of vertices and number of edges in $G_1 \square G_2$. Then $\hat{n} = n_1 n_2$ and $\hat{m} = 2m_1 m_2$. Denote by μ'_i the average degree of the adjacent vertices of vertex v'_i in G_1, $i = 1, 2, \ldots, n_1$ and also denote by μ''_j the average degree of the adjacent vertices of vertex v''_j in G_2, $j = 1, 2, \ldots, n_2$. Now,

$$\begin{aligned}\mu'_i \mu''_j &= \frac{\sum_{v'_k \sim v'_i} d'_k}{d'_i} \cdot \frac{\sum_{v''_r \sim v''_j} d''_r}{d''_j} \\ &= \frac{\sum_{v'_k \sim v'_i} \sum_{v''_r \sim v''_j} d'_k d''_r}{d'_i d''_j} \\ &= \mu_{i,j},\end{aligned}$$

where $\mu_{i,j}$ is the average degree of the adjacent vertices of vertex (v'_i, v''_j) in $G_1 \square G_2$. We have

$$\begin{aligned}M_2(G_1 \square G_2) &= \frac{1}{2} \sum_{1 \le i \le n_1, 1 \le j \le n_2} d_{i,j}^2 \mu_{i,j} \\ &= \frac{1}{2} \sum_{1 \le i \le n_1, 1 \le j \le n_2} d_i'^{\,2} d_j''^{\,2} \mu'_i \mu''_j \\ &= \frac{1}{2} \sum_{i=1}^{n_1} d_i'^{\,2} \mu'_i \sum_{j=1}^{n_2} d_j''^{\,2} \mu''_j \\ &= 2M_2(G_1) M_2(G_2) \qquad (2.8)\end{aligned}$$

and

$$M_1(G_1 \square G_2) = \sum_{1 \le i \le n_1, 1 \le j \le n_2} d_{i,j}^2 = \sum_{i=1}^{n_1} d_i'^{\,2} \sum_{j=1}^{n_2} d_j''^{\,2} = M_1(G_1) M_1(G_2). \qquad (2.9)$$

Since (1.1) holds for G_1 and G_2, we have

$$n_1 M_2(G_1) - m_1 M_1(G_1) \ge 0 \text{ and } n_2 M_2(G_2) - m_2 M_1(G_2) \ge 0, \qquad (2.10)$$

that is,

$$n_1 n_2 M_2(G_1) M_2(G_2) - m_1 m_2 M_1(G_1) M_1(G_2) \ge 0,$$

that is,

$$\hat{n} M_2(G_1 \square G_2) - \hat{m} M_1(G_1 \square G_2) \ge 0.$$

Hence the theorem. □

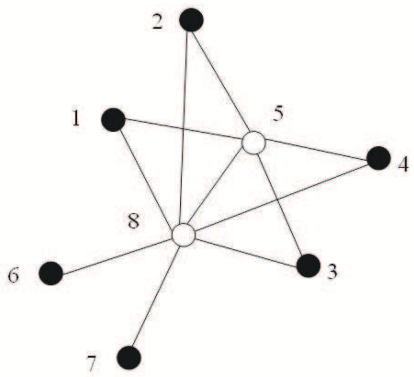
2.7. Remark. If (1.1) does not hold for G_1 and G_2, then it does not hold for $G_1 \square G_2$.

A threshold graph is a graph that can be constructed from a one-vertex graph by repeated applications of the following two operations:

- Addition of a single isolated vertex to the graph.
- Addition of a single dominating vertex to the graph, i.e., a single vertex that is connected to all other vertices.

For example, the graph of Figure 1 is a threshold graph. It can be constructed by beginning with a single-vertex graph (vertex), and then adding vertices ($\{\bullet\}$) as isolated vertices and vertices ($\{\circ\}$) as dominating vertices, in the order in which they are numbered.

Figure 1. An example of a threshold graph.



2.8. Theorem. *If G is a threshold graph, then* (1.1) *holds for G.*

Proof. Let G be a threshold graph with n vertices and m edges. We apply induction on n. If $n = 1$, the result is trivial. Suppose now that (1.1) holds for all threshold graphs with vertex number less than n. By the definition of threshold graph, there is an isolated vertex or a dominating vertex in G, say v_n. Set $G' = G - v_n$. First we assume that v_n is the isolated vertex in G. Then by the induction hypothesis, (1.1) holds for G'. Hence it is easy to see that (1.1) holds for G also.

Next we assume that v_n is the dominating vertex in G. Let n' and m' be the number of vertices and edges in G'. Then $n' = n - 1$ and $m' = m - n + 1$.

Let d'_i, $i = 1, 2, \ldots, n-1$ be the degree sequence in G'. Then $d_i = d'_i + 1$, $i = 1, 2, \ldots, n-1$. Now, we have

$$M_1(G) = M_1(G') + n'(n'+1) + 2\sum_{i=1}^{n-1} d'_i = M_1(G') + n'(n'+1) + 4m' \tag{2.11}$$

and

$$\begin{aligned} M_2(G) &= \sum_{v_iv_j \in E(G')} (d'_i + 1)(d'_j + 1) + n' \sum_{i=1}^{n-1} (d'_i + 1) \\ &= M_2(G') + M_1(G') + m' + n'(2m' + n'). \end{aligned} \tag{2.12}$$

We have to show that

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

that is,

$$\begin{aligned} &(n'+1)\big(M_2(G') + M_1(G') + m' + n'(2m'+n')\big) \\ &\qquad \geq (m'+n')\big(M_1(G') + n'(n'+1) + 4m'\big) \text{ by (2.11) and (2.12)}, \end{aligned}$$

that is,

$$n'M_2(G') - m'M_1(G') + M_2(G') + M_1(G') + m'n'^2 + m' - 4m'^2 - 2m'n' \geq 0. \tag{2.13}$$

By the induction hypothesis and using $n'M_1(G') \geq 4m'^2$, we get

$$M_2(G') + M_1(G') \geq \left(\frac{m'}{n'} + 1\right) M_1(G') \geq \left(\frac{m'}{n'} + 1\right) \frac{4m'^2}{n'}. \tag{2.14}$$

Again by the induction hypothesis and using (2.14), we get

$$\begin{aligned} n'M_2(G') - m'M_1(G') + M_2(G') + M_1(G') + m'n'^2 + m' - 4m'^2 - 2m'n' \\ \geq \frac{4m'^2(m'+n')}{n'^2} + m'n'^2 + m' - 4m'^2 - 2m'n' \\ = m'\left(\frac{n'(n'-1) - 2m'}{n'}\right)^2 \geq 0. \end{aligned} \tag{2.15}$$

Hence the theorem. □

A complete split graph $CS(n,\ q)$, $q \leq n$, is a graph on n vertices consisting of a clique on q vertices and a stable set on the remaining $n - q$ vertices in which each vertex of the clique is adjacent to each vertex of the stable set.

A pineapple $PA(n,\ q)$, $q \leq n$, is a graph on n vertices consisting of a clique on q vertices and a stable set on the remaining $n - q$ vertices in which each vertex of the stable set is adjacent to the same, unique vertex of the clique.

Since both the complete split graph $CS(n,\ q)$ $(q \leq n)$ and pineapple graph $PA(n,\ q)$ $(q \leq n)$ are threshold graphs, we get the following result.

2.9. Corollary. *Let G be a split graph $CS(n,\ q)$ $(q \leq n)$ or a pineapple graph $PA(n,\ q)$ $(q \leq n)$ of n vertices. Then G must satisfy (1.1).*

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