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A Survey on Comparing Zagreb Indices

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Abstract

The first and second Zagreb indices of a graph G are defined as $M_1(G) = \sum_{u \in V} d_u^2$ and $M_2(G) = \sum_{uv \in E} d_u d_v$, where d_u denotes the degree of a vertex u in G. The Zagreb indices have been generalized to variable first and second Zagreb indices: ${}^{\lambda}M_1(G) = \sum_{u \in V} d_i^{2\lambda}$ and ${}^{\lambda}M_2 = \sum_{uv \in E} d_i^{\lambda} d_j^{\lambda}$, where λ is an arbitrary real number. Recently, it has been conjectured that $M_1/n \leq M_2/m$. In [7], D. Vukičević considered a generalization of the conjecture, i. e., ${}^{\lambda}M_1(G)/n \leq {}^{\lambda}M_2(G)/m$. This paper outlines results on comparing Zagreb indices and variable Zagreb indices.

1. Introduction

Let $G = (V, E)$ be a simple graph with $n = |V|$ vertices and $m = |E|$ edges. Denote by $d(u)$ the degree of a vertex u. The first and second Zagreb indices are defined as $M_1(G) = \sum_{u \in V} d_u^2$ and $M_2(G) = \sum_{uv \in E} d_u d_v$. I. Gutman and N. Trinajstić [1] first introduced what are now called the Zagreb indices. Two surveys of properties of M_1 and M_2 are found in [2, 3]. The two definitions have been generalized to a variable version.

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The variable Zagreb indices are defined as ${}^{\lambda}M_1(G) = \sum_{u \in V} d_i^{2\lambda}$ and ${}^{\lambda}M_2 = \sum_{uv \in E} d_i^{\lambda} d_j^{\lambda}$, where λ is an arbitrary real number.

For general graphs of order n, note that the order of magnitude of M_1 is $O(n^3)$, while the order of magnitude of M_2 is $O(n^4)$, implying that M_1/n and M_2/m have the same orders of magnitude $O(n^2)$. This suggests that it is purposeful to compare M_1/n with M_2/m instead of M_1 with M_2.

Recently the *AutoGraphiX* system [4–6] proposed the following conjecture:

Conjecture 1.1. [4–6] *For all simple connected graphs G*

$$M_1/n \leq M_2/m \tag{1}$$

and the bound is tight for complete graphs.

In 2007, D. Vukičević [7] obtained some results on variable Zagreb indices, in connection with the inequality

$${}^{\lambda}M_1(G)/n \leq {}^{\lambda}M_2(G)/m \,. \tag{2}$$

In this paper, we report known results on comparing Zagreb and variable Zagreb indices.

This work is in three sections, followed by detailed references on comparing (variable) Zagreb indices. In the second and third sections, results are given on comparing Zagreb indices and variable Zagreb indices, respectively.

2. Comparing Zagreb indices

In 2007, P. Hansen and D. Vukičević [8] showed that Conjecture 1.1 does not hold for general graphs but is true for chemical graphs.

Theorem 2.1. [8] *For all chemical graphs G with order n, size m, and first and second Zagreb indices M_1 and M_2, Inequality (1) holds.*

Moreover, the bound is tight if and only if all edges uv have the same pair (d_u, d_j) of degrees or if the graph is composed of disjoint stars S_5 and cycles C_p, C_q, . . . of any length.

In [8] P. Hansen and D. Vukičević presented a non-connected counter-example (a star S_6 together with a cycle C_3) and a connected counter-example to Conjecture 1.1 with 46 vertices and 110 edges.

Although this conjecture is disproved for general connected as well as for disconnected graphs, D. Vukičević and A. Graovac [9] showed that it is true for trees.

Theorem 2.2. [9] *Let T be a tree with at least two vertices. Then Inequality (1) is true. The equality holds if and only if T is star.*

Recall that the cyclomatic number of a connected graph is equal to $\nu = m - n + 1$, i. e., its number of independent cycles. If a graph G has $\nu = 1$ (respectively, $\nu = 2$), i. e., $m = n$ (respectively, $m = n + 1$), then G is said to be unicyclic (respectively, bicyclic).

One of the present authors [10] proved that this claim holds for unicyclic graphs.

Theorem 2.3. [10] *Let $G = (V, E)$ be a connected unicyclic graph with $|V| = n$, $|E = m|$. Then Inequality (1) is attained. The equality holds if and only if G is a cycle.*

In [11] L. Sun et. al. showed that Inequality (1) holds for bicyclic graphs except one class graphs and characterized the extremal graph. Moreover, counter-examples of connected bicyclic graphs are constructed from the excluded class.

A pendent vertex is a vertex with degree one. A hook is the unique neighbor of a pendent vertex. Denote the set of hooks of G by $H(G)$. For any vertex $u \in H(G)$, $N_G(u) = \{v_1, \ldots, v_k\}$ $(k \geq 2)$. Let $\mathbb{A} = \{G : d_G(v_1) = 2, d_G(v_i) = 1, i = 2, 3, \ldots, k\}$.

Theorem 2.4. [11] *If $G \notin \mathbb{A}$ is a connected bicyclic graph with n vertices and m edges, then Inequality (1) is obtained with equality holding if and only if $G = K_{2,3}$.*

Figure 1 shows a bicyclic graph that is counter-example [11] for $M_1/n \leq M_2/m$.

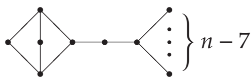

Figure 1.

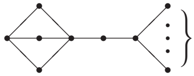

Figure 2: Counter-example with 17 vertices and 2 independent cycles.

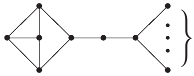

Figure 3: Counter-example with 17 vertices and 3 independent cycles.

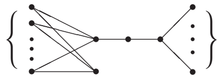

Figure 4: Infinite family of counter-examples.

Using A*utoGraphiX* [4-6], G. Caporossi, P. Hansen, and D. Vukičević [12] obtained counter-examples to Conjecture 1.1, where the classes of graphs belong to bicyclic and tricyclic graphs (see Figures 2 and 3, respectively). They also found an infinite family of counter-examples for all $\nu \geq 2$, where the graphs are obtained by joining complete bipartite graph $K_{2,\nu+1}$ and a star S_{p+1} by and an edge from a pendent vertex of S_{p+1} to a vertex of the smallest side of the $K_{2,\nu+1}$, see Figure 4.

Recently, the authors of [12] presented results which are a direct comparison of Zagreb indices on cyclic graphs.

Theorem 2.5. [12] *Let G be a simple connected graph with ν independent cycles, $n \geq 5(\nu - 1)$ vertices, $m = n + \nu - 1$ edges, Zagreb indices M_1 and M_2. Then,*

$$M_2 - M_1 \geq 6(\nu - 1) = 6(m - n)\,.$$

Moreover, the bound is tight and is attained if and only if G is a graph with vertices of degree 2 and 3 only and the vertices of degree 3 form an independent set.

Remark 2.6. By Theorem 2.5, G. Caporossi, P. Hansen, and D. Vukičević [12] also obtained the result of Theorem 2.3.

Theorem 2.7. [12] *Let G be a simple and connected graph with n vertices, $m(\geq n)$ edges and Zagreb indices M_1 and M_2. Then,*

$$M_2 - M_1 \geq 11(\nu - 1) - n = 11m - 12n .$$

Moreover, the bound is tight and is attained if G is a graph with vertices of degree 2 and 3 only and, when $n \leq 5(\nu - 1)$, no pair of vertices of degree 2 are adjacent.

The following are results showing that Conjecture 1.1 holds for some special graphs.

Theorem 2.8. [13] *If G is a graph with n vertices, m edges and $\Delta - \delta \leq 2$, then Inequality (1) holds, with the equality holding if and only if all edges ij have the same pair (d_i, d_j) of degrees.*

Let G^* denote the graphs with each edge connecting a 3-degree vertex and a 6-degree vertex. The star graph S_n is a tree on n vertices with one vertex having degree $n-1$ and the other vertices having degree 1.

Theorem 2.9. [13] *If G is a graph with n vertices and m edges, such that $\Delta(G) - \delta(G) \leq 3$ and $\delta \neq 2$, then Inequality (1) holds, with the equality holding if and only if all edges ij have the same pair (d_i, d_j) of degrees or if the graph is composed of disjoint stars S_5 and cycles of any length or if the graph is composed of disjoint G^*-graphs and 4-regular graphs.*

For the case $\delta(G) = 2$, a counter-example is present in [13] (see Figure 5) .

Figure 5.

Remark 2.10. From the proof of Theorem 2.8, L. Sun et al. [13] obtained a corollary, which embodies the result of Theorem 2.1 .

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two simple graphs on disjoint sets of vertices. The union of G_1 and G_2 is $G_1 + G_2 = (V_1 \cup V_2, E_1 \cup E_2)$. K. C. Das [14] has obtained the result that the example in Figure 5 holds for G_1 and G_2, but it need not hold for their union, $G_1 + G_2$.

Denote by $G_1 \vee G_2$ the graph obtained from $G_1 + G_2$ by joining each vertex of G_1 to each vertex of G_2. Then $G_1 \vee G_2$ is a graph with $|V(G_1)| + |V(G_2)|$ vertices and $|E(G_1)| + |E(G_2)| + |V(G_1)||V(G_2)|$ edges. Let $\overline{G}$ be the complement of G. K. C. Das [14] obtained some properties on Conjecture 1.1.

Theorem 2.11. [14] *Let G be a simple graph on n vertices, with m edges. If Inequality (1) holds for G, then it also holds for $G \vee G$.*

Theorem 2.12. [14] *Let G be a simple graph on n vertices, with m edges. If Inequality (1) does not hold for G, then it holds for $\overline{G}$.*

Let G be a graph with n vertices and m edges. In [14], K. C. Das constructed the graph $\hat{G}$ by placing two isomorphic graphs G side by side, and connecting any vertex of the first graph G with the corresponding vertex of the second graph G. The resultant graph is $\hat{G}$. Then $|V(\hat{G})| = |V(G)| + |V(G)| = 2n$, $|E(\hat{G})| = |E(G)| + |E(G)| + |E(G, G)| = 2m + n$.

Furthermore, the graph $\tilde{G}$ [14] is obtained by taking 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. Then $|V(\tilde{G})| = |V(G)| + |V(G)| = 2n$, $|E(\tilde{G})| = |E(G)| + |E(G)| + \sum_{i=1}^{n} d_i = 4m$.

Theorem 2.13. [14] *If Inequality (1) holds for G, then it also holds for $\hat{G}$.*

Theorem 2.14. [14] *If Inequality (1) holds for G, then it also holds for $\tilde{G}$.*

The subdivision graph $S(G)$ of a graph G is obtained by inserting a new vertex of degree two on each edge of G. If G is an (n, m)-graph, then $S(G)$ has $n + m$ vertices and $2m$ edges.

Theorem 2.15. [15] *Let $S(G)$ be the subdivision graph of G. Then,*

$$\frac{M_1(S(G))}{n+m} \leq \frac{M_2(S(G))}{2m}$$

with equality if and only if G is a regular graph.

Moreover, A. Ilić and D. Stevanović [15] gave sharp lower bounds for M_1 and M_2, and showed that the expressions from Conjecture 1.1 have a common sharp lower bound.

Theorem 2.16. [15] *The inequality $M_1 \geq 4m^2/n$ holds. Equality is attained if and only if the graph is regular.*

Theorem 2.17. [15] *It is true that $M_2 \geq 4m^3/n^2$. Equality is attained if and only if the graph is regular.*

From two previous theorems, the authors in reference [15] reported that the expressions from Conjecture 1.1 have a common sharp lower bound:

$$\frac{4m^2}{n^2} \leq \frac{M_1}{n} \qquad \text{and} \qquad \frac{4m^2}{n^2} \leq \frac{M_2}{m}\,.$$

In addition, a sharp upper bound for these expressions was obtained:

Theorem 2.18. [15] *Let Δ be the maximum vertex degree in G. Then*

$$\frac{M_1}{n} \leq \frac{\Delta M_1}{2m} \qquad \textit{and} \qquad \frac{M_2}{m} \leq \frac{\Delta M_1}{2m}\,.$$

Equality is attained simultaneously in both inequalities if and only if G is regular.

A. Ilić and D. Stevanović [15] gave counter-examples to Conjecture 1.1. Let $C(a,b)$ be a graph that is composed of an $(a+1)$-vertex star with exactly b triangles attached in line at an arbitrary leaf (see Figure 6). Each value of a satisfying $a > \frac{-(7b-5+\sqrt{D})}{2(1-b)}$, where $D = 8b^3 + 97b^2 - 158b + 57$, yields a counter-example to Conjecture 1.1 with b cycles.

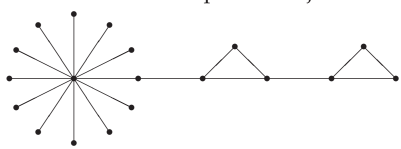

Figure 6: The bicyclic counter-example $C(12,2)$ with 19 vertices.

3. Comparing variable Zagreb indices

Theorem 3.1. [7] *For all graphs G and $\lambda \in [0, \frac{1}{2}]$, Inequality (2) holds.*

For chemical graphs, D. Vukičević [7] obtained:

Theorem 3.2. [7] *For all chemical graphs G and all $\lambda \in [0,1]$, Inequality (2) is true.*

D. Vukičević [7] proved the following theorems which imply that Theorem 3.2 cannot be extended.

Theorem 3.3. [7] *Let $\lambda \in R\backslash[0,1]$ and G be any complete unbalanced bipartite graph. Then,*

$$^{\lambda}M_1(G)/n > {}^{\lambda}M_2(G)/m .$$

Theorem 3.4. [7] *Let $\lambda \in (\sqrt{2}/2, 1)$. Then, there is a graph G such that*

$$^{\lambda}M_1(G)/n > {}^{\lambda}M_2(G)/m .$$

Then, the following problem is still open:

Open problem 3.5. [7] *Identify $\lambda \in [\frac{1}{2}, \frac{\sqrt{2}}{2}]$ such that $^{\lambda}M_1/n > {}^{\lambda}M_2/m$ for all graphs G.*

For trees, D. Vukičević and A. Graovac [20] showed:

Theorem 3.6. [20] *Inequality (2) holds for all trees and for all $\lambda \in (\frac{1}{2}, 1)$.*

Combining Theorems 2.2, 3.1 and 3.6, D. Vukičević and A. Graovac [20] arrived at:

Theorem 3.7. [20] *Inequality (2) holds for all trees if and only if $\lambda \in [0,1]$.*

For unicyclic graphs, the following results provide a complete solution for the comparing of variable Zagreb indices.

Theorem 3.8. [16] *Let G be a unicyclic graph of order n. Then Inequality (2) holds for all $\lambda \in [0,1]$. Moreover, if $\lambda \in (0,1]$, then the equality holds if and only G is isomorphic to C_n, where C_n is a cycle with n vertices.*

Theorem 3.9. [17] *Let G be a connected unicyclic graph with n vertices and m edges. Then ${}^{\lambda}M_1(G)/n \geq {}^{\lambda}M_2(G)/m$ holds for $\lambda \in (-\infty, 0]$. Moreover, if $\lambda \in (-\infty, 0)$, then ${}^{\lambda}M_1(G)/n = {}^{\lambda}M_2(G)/m$ holds if and only if G is a cycle.*

Note that for unicyclic graphs $n = m$. For $\lambda > 1$, in [17] two examples are given, such that the first has the property ${}^{\lambda}M_1(G) < {}^{\lambda}M_2(G)$ (see Figure 7) and the other ${}^{\lambda}M_1(G) > {}^{\lambda}M_2(G)$ (see Figure 8).

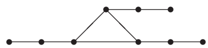

Figure 7.

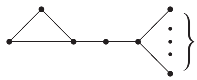

Figure 8.

Combining Theorems 3.8 and 3.9, the authors of reference [17] arrived at:

Conclusion 3.10. [17] *For unicyclic graphs ${}^{\lambda}M_1(G)/n$ and ${}^{\lambda}M_2(G)/m$ are related as follows:*

(1) ${}^{\lambda}M_1(G) \geq {}^{\lambda}M_2(G)$ holds if $\lambda \in (-\infty, 0)$.

(2) ${}^{\lambda}M_1(G) \leq {}^{\lambda}M_2(G)$ holds if $\lambda \in [0, 1]$ ([16]).

(3) If $\lambda \in (1, +\infty)$, then neither of the above two relations holds for all unicyclic graphs.

Similarly to Theorems 2.8 and 2.9, B. Liu et. al [18] obtained:

Theorem 3.11. [18] *Let G be a graph with n vertices, m edges and $\Delta(G) - \delta(G) \leq 2$.*

If $\lambda \in [0, 1]$, then Inequality (2) holds. (3)

If $\lambda \in (-\infty, 0)$, then ${}^{\lambda}M_1(G)/n \geq {}^{\lambda}M_2(G)/m$. (4)

Moreover, if $\lambda = 0$, then the equality in (3) holds if and only if all edges ij have the same pair (d_i, d_j) of degrees.

If $\lambda \in (0, 1)$ (respectively, $\lambda \in (-\infty, 0)$), then the equality in (3) (respectively, in (4)) holds if and only if G is a regular graph.

From Theorem 3.11, we obtain the main result of [13], i. e., Theorem 2.8.

Let G^* denote the graphs specified in connection with Theorem 2.9.

Theorem 3.12. [18] *Let G be a graph with n vertices, m edges and $\Delta(G) - \delta(G) \leq 3$ and*

$\delta(G) \neq 2$.

If $\lambda \in [0,1]$, *then Inequality (2) is true.* *(5)*

If $\lambda \in (-\infty, 0)$, *then* ${}^{\lambda}M_1(G)/n \geq {}^{\lambda}M_2(G)/m$. *(6)*

Moreover, if $\lambda = 0$, *the equality in (3) always holds.*

If $\lambda = 1$, *the equality of (5) holds if and only if all edges* ij *have the same pair* (d_i, d_j) *of degrees or if the graph is composed of disjoint stars* S_5 *and cycles of any length or if the graph is composed of disjoint* G^* *and 4-regular graphs* ([13]).

If $\lambda \in (0,1)$ *(respectively,* $\lambda \in (-\infty, 0)$*), the equality of (5) (respectively, (6)) holds if and only if* G *is a regular graph.*

For the general cases one of the present authors obtained:

Theorem 3.13. [19] *Let* G *be a graph with* n *vertices and* m *edges. Then* ${}^{\lambda}M_1(G)/n \geq {}^{\lambda}M_2(G)/m$ *holds for* $\lambda \in (-\infty, 0)$. *Moreover, equality holds if and only if* G *is a regular graph.*

By Theorem 3.13, the authors [19] reported the following:

Remark 3.14. [19] If $\lambda \in (-\infty, 0)$, then for all chemical graphs ([18]), unbalanced bipartite graphs ([7]), trees, unicyclic graphs ([17]), and bicyclic graphs, the inequality ${}^{\lambda}M_1(G)/n \geq {}^{\lambda}M_2(G)/m$ holds. If $\lambda \in (-\infty, 0)$, then Theorem 3.13 also encompasses Theorems 3.11 and 3.12.

With the results in [7] and [20], the authors of [19] presented the relationship between ${}^{\lambda}M_1(G)/n$ and ${}^{\lambda}M_2(G)/m$ in trees (resp. chemical graphs, unicyclic graphs ([17])):

Conclusion 3.15. [19]

(1) ${}^{\lambda}M_1(G) \geq {}^{\lambda}M_2(G)$ *holds for* $\lambda \in (-\infty, 0)$.

(2) ${}^{\lambda}M_1(G) \leq {}^{\lambda}M_2(G)$ *holds for* $\lambda \in [0,1]$ *[7,20].*

(3) If $\lambda \in (1, +\infty)$, *then neither of the above two relations holds for all unicyclic graphs.*

Remark 3.16. [19] Conclusions 3.15(1) and (3) are also true for the relationship between ${}^{\lambda}M_1(G)/n$ and ${}^{\lambda}M_2(G)/m$ of bicyclic graphs. Moreover, it is known that when $\lambda \in$

$[0, \frac{1}{2}]$, then Inequality (2) holds for all graphs (including bicyclic graphs) ([7]). When $\lambda = 1$, then Inequality (1) holds for connected bicyclic graphs, except one class [11]. Consequently, the relationship between ${}^{\lambda}M_1(G)/n$ and ${}^{\lambda}M_2(G)/m$ in bicyclic graphs remains to be determined for $\lambda \in (\frac{1}{2}, 1)$.

Similarly to Theorem 2.18, A. Ilić et al. [15] showed that these variable expressions also have a common sharp upper bound:

Theorem 3.17. [15] *Let* Δ *be the maximum vertex degree in* G. *Then*

$$\frac{{}^{\lambda}M_1}{n} \leq \frac{\Delta \cdot {}^{\lambda}M_1}{2m} \qquad \text{and} \qquad \frac{{}^{\lambda}M_2}{m} \leq \frac{\Delta \cdot {}^{\lambda}M_1}{2m} .$$

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