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Theorems about Zagreb Indices and Modified Zagreb Indices

Jianxiu Hao

Institute of Mathematics, Physics and Information Sciences,
Zhejiang Normal University, P. O. Box: 321004,
Jinhua, Zhejiang, P.R. China
e-mail: sx35@zjnu.cn

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Abstract

The Zagreb indices and the modified Zagreb indices are important topological indices in mathematical chemistry. In this paper we study the relations between the Zagreb indices and the modified Zagreb indices, and we present some bounds for the modified Zagreb indices.

Introduction

The Zagreb indices were introduced by Gutman and Trinajstić. The *first Zagreb index* $M_1(G)$ and the *second Zagreb index* $M_2(G)$ were defined as follows [1-4]: for a simple connected graph G, $M_1(G)=\sum_{v\in V(G)}(d(v))^2$, $M_2(G)=\sum_{uv\in E(G)}d(u)d(v)$, where $d(u)$ and $d(v)$ are the degrees of vertices u and v respectively. For recent work on Zagreb indices see the papers [5-10] and references cited therein.

However, both the first Zagreb index and the second Zagreb index give greater weights to the inner vertices and edges, and smaller weights to outer vertices and edges which opposes intuitive reasoning. Hence, they were amended as follows [11]: for a simple connected graph

G, let ${}^{m}M_1(G)=\sum_{v\in V(G)}\frac{1}{(d(v))^2}$, which was called *the first modified Zagreb index*, ${}^{m}M_2(G)=\sum_{uv\in E(G)}\frac{1}{d(u)d(v)}$, which was called *the second modified Zagreb index*, where $d(u)$ and $d(v)$ are the degrees of vertices u and v respectively.

Preliminaries

Lemma 2.1 is well-known.

Lemma 2.1. *Let* $a_i>0$, $i=1,2,...,n$, *we have*

$$\sqrt[n]{a_1a_2...a_n}\le\frac{a_1+a_2+...+a_n}{n},$$

and $\sqrt[n]{a_1a_2...a_n}=\frac{a_1+a_2+...+a_n}{n}$ *if and only if* $a_1=a_2=...=a_n$.

Lemma 2.2[12]. *Let G be a graph with n vertices and m edges. Also, let* $\Delta(G)$, $\delta(G)$ *be, respectively, the maximum degree and the minimum degree of G,*

$$T=m\left[\frac{2m}{n-1}+\frac{\Delta(G)(n-2)}{n-1}+\left(\Delta(G)-\delta(G)\right)\left(1-\frac{\Delta(G)}{n-1}\right)\right].$$

Then $M_1(G)\le T$*, with equality if and only if G is a star or a regular graph or a complete graph* $K_{\Delta(G)+1}$ *with* $n-\Delta(G)-1$ *isolated vertices.*

Lemma 2.3[13]. *Let G be a graph with n vertices and m edges,* $\Delta(G)$, $\Delta_2(G)$, $\delta(G)$ *be, respectively, the maximum degree, the second maximum degree and the minimum degree of G,*

$$S=2m^2-(n-1)m\delta(G)+\frac{1}{2}(\delta(G)-1)\left[\frac{(2m-\Delta(G))^2}{n-1}+(\Delta(G))^2+\frac{(n-1)}{4}\left(\Delta_2(G)-\delta(G)\right)^2\right].$$

Then $M_2(G)\le S$, where $n\ge 3$.

Definition 2.4[14, 15 , 16]. *The zeroth-order general Randic index* ${}^{0}R_t(G)=\sum_{v\in V(G)}(d(v))^t$ *for general real number t, where d(v) is the degree of v. When* $t=-0.5$, ${}^{0}R_{-0.5}(G)$ *is the famous zeroth-order Randic index* $R^0(G)$.

Relations between Zagreb indices and modified Zagreb indices

Theorem 3.1. *Let* G *be a simple connected graph,* $|V(G)|=n\geq 2$.

When n is even, we have

$$n^2 \leq M_1(G)\,{}^m M_1(G) \leq n^2 + \left(\frac{\Delta(G)}{\delta(G)} - \frac{\delta(G)}{\Delta(G)}\right)^2 \left\lfloor \frac{n}{2} \right\rfloor^2.$$

When n is odd, we have

$$n^2 \leq M_1(G)\,{}^m M_1(G) \leq n^2 + \left(\frac{\Delta(G)}{\delta(G)} - \frac{\delta(G)}{\Delta(G)}\right)^2 \left(\left\lfloor \frac{n}{2} \right\rfloor^2 + \left\lfloor \frac{n}{2} \right\rfloor\right).$$

$n^2 = M_1(G)\,{}^m M_1(G)$ *if and only if* G *is a regular graph, where* $\delta(G)$ *is the minimum degree of* G*,* $\Delta(G)$ *is the maximum degree of* G*.*

Proof. When $n=2,3,$ Theorem 3.1 holds clearly. In the following let $V(G)=\{v_1,v_2,\ldots,v_n\}$, $n\geq 4.$ By Lemma 2.1 we have

$$M_1(G) \geq n\sqrt[n]{(d(v_1)d(v_2)\ldots d(v_n))^2},$$

$${}^m M_1(G) \geq n\sqrt[n]{\frac{1}{(d(v_1)d(v_2)\ldots d(v_n))^2}}.$$

Hence, we have

$$n^2 \leq M_1(G)\,{}^m M_1(G),$$

and $n^2 = M_1(G)\,{}^m M_1(G)$ if and only if G is a regular graph.

Claim 1: Let $0<p\leq a_i \leq q,\ \ i=1,2,\ldots,n,\ \ y=(\sum_{i=1}^{n} a_i)(\sum_{i=1}^{n}\frac{1}{a_i}).$

When n is even we have

$$y \leq n^2 + \left(\frac{p}{q} + \frac{q}{p} - 2\right)\left\lfloor \frac{n}{2} \right\rfloor^2.$$

When n is odd we have

$$y \leq n^2 + \left(\frac{p}{q} + \frac{q}{p} - 2\right)\left(\left\lfloor \frac{n}{2} \right\rfloor^2 + \left\lfloor \frac{n}{2} \right\rfloor\right).$$

In fact, when $p=q$, Claim 1 holds obviously. In the following let $p<q$. Let $u=\sum_{i=1}^{n-1} a_i$, $v=\sum_{i=1}^{n-1}\frac{1}{a_i}$, $y=(u+a_n)\left(v+\frac{1}{a_n}\right)$, we regard $a_1, a_2, \ldots, a_{n-1}$ as constants and y as a function of a_n. Clearly, we have

$$(n-1)p \le u \le (n-1)q,$$

$$\frac{n-1}{q} \le v \le \frac{n-1}{p},$$

$$y=(uv+1)+\left(\frac{u}{a_n}+va_n\right).$$

Let $y_1=\frac{u}{a_n}+va_n$, thus, $y=(uv+1)+y_1$. Hence, y attains its maximum value if and only if y_1 attains its maximum value.

Since $y_1=\left(\sqrt{\frac{u}{a_n}}-\sqrt{va_n}\right)^2+2\sqrt{uv}$, let $y_2=\frac{\sqrt{u}}{x}-x\sqrt{v}$, where $x=\sqrt{a_n}$. The derivative of y_2 equals

$$-\left(\sqrt{v}+\frac{\sqrt{u}}{x^2}\right)<0.$$

Thus, y_2 is a decreasing function. Hence, y_1 obtains its maximum value if and only if $a_n=p$ or $a_n=q$. By symmetry y obtains its maximum value if and only if $a_i=p$ or $a_i=q$, $i=1,2,\ldots,n-1$.

When y attains its maximum value, let there be t a_i's which equal p, we have

$$y=\left[pt+(n-t)q\right]\left[\frac{t}{p}+\frac{n-t}{q}\right]$$

$$=\left(2-\frac{p}{q}-\frac{q}{p}\right)t^2-\left(2-\frac{p}{q}-\frac{q}{p}\right)nt+n^2,$$

which is a parabola. Thus, y obtains its maximum value if and only if $t = \frac{1}{2}n.$

Case 1. When n is even, let $n = 2m,$ thus, $t = m,$ we have

$$y = n^2 + \left(\frac{p}{q} + \frac{q}{p} - 2\right)\left\lfloor \frac{n}{2} \right\rfloor^2.$$

Case 2. When n is odd, let $n = 2m+1.$ By the symmetry of parabola we have $t = m$ or $t = m+1$. When $t = m$ we have

$$y = n^2 + \left(\frac{p}{q} + \frac{q}{p} - 2\right)\left(\left\lfloor \frac{n}{2} \right\rfloor^2 + \left\lfloor \frac{n}{2} \right\rfloor\right).$$

Similarly, when $t = m+1$ we have

$$y = n^2 + \left(\frac{p}{q} + \frac{q}{p} - 2\right)\left(\left\lfloor \frac{n}{2} \right\rfloor^2 + \left\lfloor \frac{n}{2} \right\rfloor\right).$$

Claim 1 follows.

For graph G, we have $p = (\delta(G))^2,$ $q = (\Delta(G))^2.$ By Claim 1 we have

$$M_1(G)^m M_1(G) \le n^2 + \left(\frac{\Delta(G)}{\delta(G)} - \frac{\delta(G)}{\Delta(G)}\right)^2 \left\lfloor \frac{n}{2} \right\rfloor^2,$$

where n is even.

$$M_1(G)^m M_1(G) \le n^2 + \left(\frac{\Delta(G)}{\delta(G)} - \frac{\delta(G)}{\Delta(G)}\right)^2 \left(\left\lfloor \frac{n}{2} \right\rfloor^2 + \left\lfloor \frac{n}{2} \right\rfloor\right),$$

where n is odd. The theorem follows.

Remark: When $\Delta(G) = \delta(G)$ in Theorem 3.1, the upper bounds equal the lower bounds respectively. That is, for a regular graph with $|V(G)| = n \ge 2$, our bounds are sharp.

Similarly we have

Theorem 3.2. *Let* G *be a simple connected graph,* $p = \min\{d(u)d(v) \mid uv \in E(G)\},$ $q = \max\{d(u)d(v) \mid uv \in E(G)\},$ $|E(G)| = m \ge 1.$

When m is even we have

$$m^2 \leq M_2(G)^m M_2(G) \leq m^2 + \left(\frac{p}{q}+\frac{q}{p}-2\right)\left\lfloor\frac{m}{2}\right\rfloor^2;$$

When m is odd we have

$$m^2 \leq M_2(G)^m M_2(G) \leq m^2 + \left(\frac{p}{q}+\frac{q}{p}-2\right)\left(\left\lfloor\frac{m}{2}\right\rfloor^2 + \left\lfloor\frac{m}{2}\right\rfloor\right).$$

Remark: When G is a regular graph or a star with $|E(G)| \geq 1$ in Theorem 3.2, we have $p = q$. Hence, for a regular graph or a star with $|E(G)| \geq 1$, both the upper bounds and the lower bounds in Theorem 3.2 are sharp. Thus, all bounds in Theorem 3.1 and Theorem 3.2 are attainable.

Some bounds for modified Zagreb indices

Theorem 4.1. *Let G be a simple connected graph with n vertices and m edges,* $n \geq 2$. *Let* $\Delta(G)$, $\delta(G)$ *be, respectively, the maximum degree and the minimum degree of G, T be defined in Lemma 2.2. We have*

$$\max\left\{\frac{n^3}{4m^2}, \frac{n^2}{T}, \frac{n}{(\sqrt[n]{d(v_1)d(v_2)...d(v_n)})^2}\right\} \leq {}^m M_1(G) \leq n-1+\frac{1}{(n-1)^2},$$

and $\max\left\{\frac{n^3}{4m^2}, \frac{n^2}{T}, \frac{n}{(\sqrt[n]{d(v_1)d(v_2)...d(v_n)})^2}\right\} = {}^m M_1(G)$ *if and only if G is a regular graph,*

${}^m M_1(G) = n-1+\frac{1}{(n-1)^2}$ *if and only if* $G = K_{1,n-1}$.

Proof. Let $V(G) = \{v_1, v_2, ..., v_n\}$, by Lemma 2.1 we have

$${}^m M_1(G) \geq n\sqrt[n]{\frac{1}{(d(v_1)d(v_2)...d(v_n))^2}}.$$

Hence, we have

$$\frac{n}{(\sqrt[n]{d(v_1)d(v_2)...d(v_n)})^2} \leq {}^m M_1(G).$$

By Lemma 2.1 $\frac{n}{(\sqrt[n]{d(v_1)d(v_2)...d(v_n)})^2} = {}^mM_1(G)$ if and only if G is a regular graph.

Similarly, by Lemma 2.2 we have

$$T \geq M_1(G) \geq n(\sqrt[n]{d(v_1)d(v_2)...d(v_n)})^2.$$

Hence, we have

$$(\sqrt[n]{d(v_1)d(v_2)...d(v_n)})^2 \leq \frac{T}{n}.$$

Thus, we have

$$\frac{n^2}{T} \leq {}^mM_1(G).$$

By Lemma 2.1 and Lemma 2.2 we know that $\frac{n^2}{T} = {}^mM_1(G)$ if and only if G is a regular graph.

By Lemma 2.1 we have

$$d(v_1) + d(v_2) + ... + d(v_n) \geq n\sqrt[n]{d(v_1)d(v_2)...d(v_n)},$$

$$\frac{1}{(d(v_1))^2} + \frac{1}{(d(v_2))^2} + ... + \frac{1}{(d(v_n))^2} \geq n\sqrt[n]{\frac{1}{(d(v_1)d(v_2)...d(v_n))^2}}.$$

Hence, we have

$$d(v_1) + d(v_2) + ... + d(v_n) \geq n\sqrt[n]{d(v_1)d(v_2)...d(v_n)},$$

$$\left(\frac{1}{(d(v_1))^2} + \frac{1}{(d(v_2))^2} + ... + \frac{1}{(d(v_n))^2}\right)(d(v_1) + d(v_2) + ... + d(v_n))^2 \geq n^3.$$

Since $d(v_1) + d(v_2) + ... + d(v_n) = 2m$, we have

$$\frac{n^3}{4m^2} \leq {}^mM_1(G).$$

By Lemma 2.1, $\frac{n^3}{4m^2} = {}^mM_1(G)$ if and only if G is a regular graph.

Claim 1: When G contains a cycle C, let $e \in E(C)$, $G' = G - e.$ We have

$$^{m}M_1(G) < {^{m}M_1}(G').$$

In fact, G' is connected. Otherwise, let the two components of G' be G_1 and G_2. Since G_1 and G_2 are connected by e, e cannot be contained in any cycle, which is a contradiction.

Let $V(G) = \{v_1, v_2, ..., v_n\}$, without loss of generality, let $e = v_1v_2$. We have

$$^{m}M_1(G') = \frac{1}{(d(v_1)-1)^2} + \frac{1}{(d(v_2)-1)^2} + \frac{1}{(d(v_3))^2} + ... + \frac{1}{(d(v_n))^2}.$$

Thus, $^{m}M_1(G) < {^{m}M_1}(G')$. Claim 1 follows.

Claim 2: Let G be a tree with $d(u) = \Delta(G) \le n-2$, $v \notin N(u)$, $d(v) = 1$, $vw \in E(G)$. Define $G'' = G - vw + uv$. We have

$$^{m}M_1(G) < {^{m}M_1}(G'').$$

In fact, let $y = \frac{1}{x^2} - \frac{1}{(x+1)^2}$. The derivate of y equals

$$-2\left[\frac{1}{x^3} - \frac{1}{(x+1)^3}\right] < 0,$$

where x > 0. Thus, y is a decreasing function. Hence, we have

$$\frac{1}{(d(u))^2} - \frac{1}{(d(u)+1)^2} < \frac{1}{(d(w)-1)^2} - \frac{1}{(d(w))^2}.$$

That is,

$$\frac{1}{(d(u))^2} + \frac{1}{(d(w))^2} < \frac{1}{(d(u)+1)^2} + \frac{1}{(d(w)-1)^2}.$$

Hence, we have

$$^{m}M_1(G) < {^{m}M_1}(G'').$$

Claim 2 follows.

Using Claim 2 many times we have

Claim 3: Let G be a tree with $\Delta(G) \le n-2$, we have

$$^{m}M_1(G) < {}^{m}M_1(K_{1,n-1}).$$

Clearly, $^{m}M_1(K_{1,n-1}) = n-1+\frac{1}{(n-1)^2}$. By Claim 1 and Claim 3 we have

$$^{m}M_1(G) \le n-1+\frac{1}{(n-1)^2}.$$

From the proof above we know that that $^{m}M_1(G) = n-1+\frac{1}{(n-1)^2}$ if and only if $G = K_{1,n-1}$.

The theorem follows.

Theorem 4.2. *Let G be a simple connected graph with n vertices and m edges,* $n \ge 3$. *S is defined in Lemma 2.3,* $^{0}R_{-1}(G)$ *is defined in Definition 2.4. We have*

$$\max\left\{\frac{m^2}{M_2(G)}, \frac{m^2}{S}, \frac{n}{2(n-1)}\right\} \le {}^{m}M_2(G) \le \min\left\{\frac{1}{2}\,{}^{0}R_{-1}(G), \frac{1}{2}(n-1+\frac{1}{n-1})\right\},$$

and $^{m}M_2(G) = \min\left\{\frac{1}{2}\,{}^{0}R_{-1}(G), \frac{1}{2}(n-1+\frac{1}{n-1})\right\}$ *if and only if G is a regular graph.*

Proof. Let $V(G) = \{v_1, v_2, ..., v_n\}$, by Theorem 3.2 we have

$$^{m}M_2(G) \ge \frac{m^2}{M_2(G)}.$$

Since $M_2(G) \le M_2(K_n) = \frac{1}{2}n(n-1)^3$, we have

$$\frac{n}{2(n-1)} \le {}^{m}M_2(G).$$

By Lemma 2.3 we have

$$\frac{m^2}{S} \le {}^{m}M_2(G).$$

Hence, we have

$$\max\left\{\frac{m^2}{M_2(G)}, \frac{m^2}{S}, \frac{n}{2(n-1)}\right\} \le {}^{m}M_2(G).$$

Since $x^2 + y^2 \ge 2xy$, and $x^2 + y^2 = 2xy$ if and only if x = y, where x, y > 0, we have

$$\frac{1}{2}\left(\frac{1}{x^2}+\frac{1}{y^2}\right)\geq\frac{1}{xy}.$$

Thus, we have

$$\begin{aligned}
{}^{m}M_2(G) &= \sum_{uv\in E(G)}\frac{1}{d(u)d(v)}\\
&\leq \sum_{uv\in E(G)}\frac{1}{2}\left[\frac{1}{(d(u))^2}+\frac{1}{(d(v))^2}\right]\\
&=\frac{1}{2}\sum_{v\in V(G)}\frac{1}{d(v)}\\
&=\frac{1}{2}\,{}^{0}R_{-1}(G).
\end{aligned}$$

From the proof above we know that ${}^{m}M_2(G)=\frac{1}{2}\,{}^{0}R_{-1}(G)$ if and only if G is a regular graph.

Claim 1: When G contains a cycle C, let $e\in E(C)$, $G^{'}=G-e.$ We have

$${}^{0}R_{-1}(G)<{}^{0}R_{-1}(G^{'}).$$

In fact, $G^{'}$ is connected. Otherwise, let the two components of $G^{'}$ be G_1 and G_2. Since G_1 and G_2 are connected by e, e can not be contained in any cycle, which is a contradiction.

Without loss of generality, let $e=v_1v_2.$ We have

$${}^{0}R_{-1}(G^{'})=\frac{1}{d(v_1)-1}+\frac{1}{d(v_2)-1}+\frac{1}{d(v_3)}+...+\frac{1}{d(v_n)}.$$

Thus, ${}^{0}R_{-1}(G)<{}^{0}R_{-1}(G^{'}).$ Claim 1 follows.

Claim 2: Let G be a tree with $d(u)=\Delta(G)\leq n-2,$ $v\notin N(u),$ $d(v)=1,$ $vw\in E(G).$ Define $G^{''}=G-vw+uv.$ We have

$${}^{0}R_{-1}(G)<{}^{0}R_{-1}(G^{''}).$$

In fact, let $y=\frac{1}{x}-\frac{1}{x+1}.$ The derivate of y equals

$$-\left[\frac{1}{x^2}-\frac{1}{(x+1)^2}\right]<0,$$

where x > 0. Thus, y is a decreasing function. Hence, we have

$$\frac{1}{d(u)}-\frac{1}{d(u)+1}<\frac{1}{d(w)-1}-\frac{1}{d(w)}.$$

That is,

$$\frac{1}{d(u)}+\frac{1}{d(w)}<\frac{1}{d(u)+1}+\frac{1}{d(w)-1}.$$

Hence, we have

$${}^{0}R_{-1}(G)<{}^{0}R_{-1}(G^{"}).$$

Claim 2 follows.

Using Claim 2 many times we have

Claim 3: Let G be a tree with $\Delta(G)\le n-2$, we have

$${}^{0}R_{-1}(G)<{}^{0}R_{-1}(K_{1,n-1}).$$

Clearly, ${}^{0}R_{-1}(K_{1,n-1})=n-1+\frac{1}{n-1}$. By Claim 1 and Claim 3 we have

Claim 4: ${}^{0}R_{-1}(G)\le n-1+\frac{1}{n-1}$.

From the proof above we know that that ${}^{0}R_{-1}(G)=n-1+\frac{1}{n-1}$ if and only if $G=K_{1,n-1}$.

Claim 5; ${}^{m}M_{2}(G)<\frac{1}{2}(n-1+\frac{1}{n-1})$.

In fact, since ${}^{m}M_{2}(G)\le\frac{1}{2}\,{}^{0}R_{-1}(G)$, and ${}^{m}M_{2}(G)=\frac{1}{2}\,{}^{0}R_{-1}(G)$ if and only if G is a regular graph. By Claim 4 Claim 5 follows. The theorem follows.

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