FURTHER INEQUALITIES BETWEEN VERTEX-DEGREE-BASED TOPOLOGICAL INDICES

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Abstract. Continuing the recent work of L. Zhong and K. Xu [MATCH Commun. Math. Comput. Chem. 71 (2014) 627-642], we determine inequalities among several vertex-degree-based topological indices; first geometric-arithmetic index (GA), augmented Zagreb index (AZI), Randić index (R), atom-bond connectivity index (ABC), sum-connectivity index (X) and harmonic index (H).

1. Introduction

Let \( G = (V, E) \) denote a simple graph with vertex set \( V(G) = \{v_1, v_2, ..., v_n\} \) and edge set \( E(G) \) such that \( |E(G)| = m \). Suppose that \( d_i \) is the degree of a vertex \( v_i \in V(G) \) and \( ij \) is an edge connecting the vertices \( v_i \) and \( v_j \).

Topological indices are numerical parameters of a graph which are invariant under graph isomorphisms. They play a significant role in mathematical chemistry especially in the QSPR/QSAR investigations [2, 3].

L. Zhong and K. Xu [29] obtained several inequalities among \( R, ABC, X \) and \( H \) indices. An important topological index that was not discussed in [29] is the AZI index. B. Furtula et al. [30] proved that AZI index is a valuable predictive index in the study of the heat

| Name of index | Definition of index |
|---------------|---------------------|
| Randić \((R)\), [4]-[8] | \( R(G) = \sum_{ij \in E(G)} \frac{1}{\sqrt{d_i d_j}} \) |
| Harmonic \((H)\), [9]-[12] | \( H(G) = \sum_{ij \in E(G)} \frac{2}{d_i + d_j} \) |
| Atom-bond connectivity \((ABC)\), [13]-[19] | \( ABC(G) = \sum_{ij \in E(G)} \sqrt{d_i + d_j - 2} \) |
| Sum-connectivity \((X)\), [20]-[26] | \( X(G) = \sum_{ij \in E(G)} \frac{1}{\sqrt{d_i + d_j}} \) |
| First geometric-arithmetic \((GA)\), [27, 28] | \( GA(G) = \sum_{ij \in E(G)} \frac{\sqrt{d_i d_j}}{2(d_i + d_j)} \) |
| Augmented Zagreb \((AZI)\), [30]-[33] | \( AZI(G) = \sum_{ij \in E(G)} \left( \frac{d_i d_j}{d_i + d_j - 2} \right)^3 \) |
of formation in octanes and heptanes. I. Gutman and J. Tošović \[33\] recently tested the correlation abilities of 20 vertex-degree-based topological indices for the case of standard heats of formation and normal boiling points of octane isomers, and they found that the augmented Zagreb index yield the best results. GA index is another important topological index, not discussed in \[29\]. It has been demonstrated, on the example of octane isomers, that GA index is well-correlated with a variety of physico-chemical properties \[27\]. For the mathematical properties of the GA index and their applications in QSPR and QSAR see the survey \[28\] and the references cited therein. In this note, we continue the work of L. Zhong and K. Xu \[29\] and establish some inequalities among the topological indices given in Table 1.

2. Inequalities Between Vertex-Degree-Based Topological Indices

In this section, we give inequalities among several vertex-degree-based topological indices such as AZI, GA, R, ABC, X and H indices.

**Theorem 2.1.** If \( G \) is a connected graph with \( n \geq 2 \) vertices, then
\[
\sqrt{2X(G)} \leq GA(G) \leq \sqrt{2(n-1)X(G)}.
\]
The lower bound is attained if and only if \( G \cong P_2 \) and the upper bound is attained if and only if \( G \cong K_n \).

**Proof.** Without loss of generality we can assume \( 1 \leq d_i \leq d_j \leq n-1 \). Consider the function
\[
F(x, y) = \left( \frac{2xy}{x+y} \right)^2 = \frac{4xy}{x+y} \quad \text{where} \quad 1 \leq x \leq y \leq n-1
\]
One can easily see that \( F(x, y) \) is strictly monotone increasing in both \( x \) and \( y \). This implies that \( F(x, y) \) attains the minimum value at \( (x, y) = (1, 1) \) and the maximum value at \( (x, y) = (n-1, n-1) \). Hence
\[
2 = F(1, 1) \leq F(x, y) \leq F(n-1, n-1) = 2(n-1)
\]
which implies,
\[
\sqrt{2} \leq \frac{GA(G)}{X(G)} \leq \sqrt{2(n-1)}
\]
with the left equality if and only if \( (d_i, d_j) = (1, 1) \) for every edge \( ij \) of \( G \) and the right equality if and only if \( (d_i, d_j) = (n-1, n-1) \) for every edge \( ij \) of \( G \). This completes the proof. \( \square \)

If graph \( G \) has the minimum degree at least 2, then the lower bound in Theorem 2.1 can be improved:

**Corollary 2.2.** If \( G \) is a connected graph with minimum degree \( \delta \geq 2 \), then
\[
\sqrt{2\delta}X(G) \leq GA(G)
\]
with equality if and only if \( G \) is a \( \delta \)-regular graph.

**Theorem 2.3.** If \( G \) is a connected graph with \( n \geq 2 \) vertices, then
\[
R(G) \leq GA(G) \leq (n-1)R(G).
\]
The lower bound is attained if and only if \( G \cong P_2 \) and the upper bound is attained if and only if \( G \cong K_n \).
Proof. Suppose that $1 \leq d_i \leq d_j \leq n-1$ and let

$$F(x, y) = \frac{2\sqrt{xy}}{x+y} = \frac{2xy}{\sqrt{xy} + y}$$

where $1 \leq x \leq y \leq n-1$.

It can be easily seen that $F(x, y)$ is strictly monotone increasing in both $x$ and $y$. This implies that

$$1 = F(1, 1) \leq F(x, y) \leq F(n-1, n-1) = n-1$$

therefore,

$$1 \leq \frac{GA(G)}{R(G)} \leq (n-1)$$

with the left equality if and only if $(d_i, d_j) = (1, 1)$ for every edge $ij$ of $G$ and the right equality if and only if $(d_i, d_j) = (n-1, n-1)$ for every edge $ij$ of $G$. \qed

If the graph $G$ has the minimum degree $\delta \geq 2$, then the lower bound in Theorem 2.3 can be replaced by $\delta R(G)$.

Corollary 2.4. If $G$ is a connected graph with $\delta \geq 2$, then

$$\delta R(G) \leq GA(G)$$

with equality if and only if $G$ is a $\delta$-regular graph.

B. Zhou and N. Trinajstić [23] proved that if $G$ is a connected graph with $n \geq 3$ vertices, then \(\sqrt{\frac{2}{3}}R(G) \leq X(G)\) with equality if and only if $G \cong P_3$. Hence from Theorem 2.1, we have:

Corollary 2.5. If $G$ is a connected graph with $n \geq 3$ vertices, then

$$\sqrt{\frac{4}{3}}R(G) \leq GA(G) \leq (n-1)R(G)$$

with equality if and only if $G \cong P_3$ and right equality if and only if $G \cong K_n$.

Theorem 2.6. If $G$ is a connected graph with $n \geq 2$ vertices, then

$$H(G) \leq GA(G) \leq (n-1)H(G).$$

The lower bound is attained if and only if $G \cong P_2$ and the upper bound is attained if and only if $G \cong K_n$.

Proof. Using the same technique, used in proving Theorem 2.1 and Theorem 2.3, one can easily prove the required result. \qed

Corollary 2.7. If $G$ is a connected graph with minimum degree $\delta \geq 2$, then

$$\delta H(G) \leq GA(G)$$

with equality if and only if $G$ is a $\delta$-regular graph.

Theorem 2.8. If $G$ is a connected graph having $n \geq 3$ vertices with minimum degree $\delta \geq 2$, then

$$\frac{\sqrt{2(n-2)}}{n-1}GA(G) \leq ABC(G) \leq \frac{n+1}{4\sqrt{n-1}}GA(G)$$

with left equality if and only if $G \cong K_n$ and right equality if and only if $G \cong C_3$.\]
Proof. Suppose that $2 \leq d_j \leq d_i \leq n - 1$ and consider the function
\[
F(x, y) = \left( \frac{\sqrt{\frac{x+y-2}{x+y}}}{\frac{2\sqrt{xy}}{x+y}} \right)^2 = \frac{(x+y)^2(x+y-2)}{4x^2y^2} \text{ where } 2 \leq y \leq x \leq n - 1.
\]
Then
\[
\frac{\partial F(x, y)}{\partial y} = -\frac{(x+y)^2\{x^2-y^2+x(x+y-4)\}}{4x^2y^3} \leq 0
\]
This implies that $F(x, y)$ is monotone decreasing in $y$. Hence $F(x, y)$ attains the maximum value at $(x, y) = (x, 2)$ for some $2 \leq x \leq n - 1$.

But,
\[
\frac{dF(x, 2)}{dx} = \frac{x(x^2-4)}{16x^3} \geq 0
\]
that is, $F(x, 2)$ is monotone increasing in $x$ which implies $F(x, 2)$ has maximum value at $x = n - 1$. Hence
\[
F(x, y) \leq F(n-1, 2) = \frac{(n+1)^2}{16(n-1)}
\]
and therefore,
\[
\frac{ABC(G)}{GA(G)} \leq \frac{n+1}{4\sqrt{n-1}}
\]
with the equality if and only if $(d_i, d_j) = (n-1, 2)$ for every edge $ij$ of $G$, i.e.,
\[
ABC(G) \leq \frac{n+1}{4\sqrt{n-1}}GA(G)
\]
with the equality if and only if $G \cong C_3$.

Since $F(x, y)$ is monotonically decreasing in $y$. It means $F(x, y)$ attains minimum value at $(x, x)$ for some $2 \leq x \leq n - 1$. Since
\[
\frac{dF(x, x)}{dx} = \frac{2x(2-x)}{x^4} \leq 0
\]
hence,
\[
\frac{2(n-2)}{(n-1)^2} = F(n-1, n-1) \leq F(x, x) \leq F(x, y)
\]
i.e.,
\[
\frac{\sqrt{2(n-2)}}{(n-1)} \leq \frac{ABC(G)}{GA(G)}
\]
with the equality if and only if $(d_i, d_j) = (n-1, n-1)$ for every edge $ij$ of $G$, which completes the proof. □

L. Zhong and K. Xu [29] proved that if $\delta \geq 2$ in a connected graph $G$, then
\[
(2.3) \quad H(G) \leq R(G) \leq X(G) < ABC(G)
\]
with the first equality if and only if $G$ is a regular graph, and the second equality if and only if $G$ is a cycle. Hence, from Theorem 2.8 and inequality (2.3), we have:

Corollary 2.9. If $G$ is a connected graph with minimum degree $\delta \geq 2$, then
\[
H(G) \leq R(G) \leq X(G) < ABC(G) \leq \frac{n+1}{4\sqrt{n-1}}GA(G)
\]
with the first equality if and only if $G$ is a regular graph, the second equality if and only if $G$ is a cycle, and last with equality if and only if $G \cong C_3$. 

Denoted by $T^*$ the tree on eight vertices, obtained by joining the central vertices of two copies of star $K_{1,3}$ by an edge. K. C. Das and N. Trinajstić [18] proved that
\begin{equation}
GA(G) > ABC(G)
\end{equation}
for every molecular graph $G \not\cong K_{1,4}, T^*$. The same authors proved that inequality (2.4) holds for any graph $G \not\cong K_{1,4}, T^*$ in which $\Delta - \delta \leq 3$. In [19], it is proved that if $\delta \geq 2$ and $\Delta - \delta \leq (2\delta - 1)^2$ then inequality (2.4) holds.

**Corollary 2.10.** If $G$ is a connected graph satisfying at least one of the following properties:

(i): $G$ is molecular graph such that $G \not\cong K_{1,4}, T^*$

(ii): $\Delta - \delta \leq 3$ and $G \not\cong K_{1,4}, T^*$

(iii): $\delta \geq 2$ and $\Delta - \delta \leq (2\delta - 1)^2$,

then
\begin{equation}
H(G) \leq R(G) \leq X(G) < ABC(G) < GA(G)
\end{equation}

Denote the chromatic number of a graph $G$ by $\chi(G)$. Deng et al. [11] proved that for every connected graph $G$
\begin{equation}
\chi(G) \leq 2H(G)
\end{equation}
with equality if and only if $G$ is a complete graph. From inequalities (2.1) and (2.5), we obtain a sharp upper bound of $\chi(G)$ in terms of GA index:

**Corollary 2.11.** If $G$ is a connected graph of order $n$ with minimum degree $\delta \geq 2$, then
\begin{equation}
\chi(G) \leq \frac{2}{\delta}GA(G)
\end{equation}
with equality if and only if $G \cong K_n$.

Another vertex-degree-based topological Index is the modified second Zagreb index defined [34, 35] as:
\begin{equation}
M^*_2(G) = \sum_{ij \in E(G)} \frac{1}{d_id_j}
\end{equation}

Using the same technique, used in proving Theorem 2.1 and Theorem 2.3, one can easily prove the following result:

**Theorem 2.12.** If $G$ is a connected graph with $n \geq 2$ vertices, then
\begin{equation}
M^*_2(G) \leq R(G) \leq (n - 1)M^*_2(G),
\end{equation}
\begin{equation}
\frac{M^*_2(G)}{\sqrt{2}} \leq X(G) \leq \frac{(n - 1)^{\frac{3}{2}}}{\sqrt{2}}M^*_2(G),
\end{equation}
\begin{equation}
M^*_2(G) \leq H(G) \leq (n - 1)M^*_2(G),
\end{equation}
\begin{equation}
M^*_2(G) \leq GA(G) \leq (n - 1)^2M^*_2(G),
\end{equation}
\begin{equation}
\sqrt{2}M^*_2(G) \leq ABC(G) \leq (n - 1)\sqrt{2(n - 2)}M^*_2(G); n \geq 3.
\end{equation}
The left equality in (2.6)-(2.9) and in (2.10) is attained if and only if $G \cong P_2$ and $G \cong P_3$ respectively. The right equality in all inequalities (2.6)-(2.10) is attained if and only if $G \cong K_n$. 

Corollary 2.13. If $G$ is a connected graph with minimum degree $\delta \geq 2$, then
\begin{align*}
(2.11) & \quad \delta M_2^*(G) \leq R(G), \\
(2.12) & \quad \frac{\delta \sqrt{2} M_2^*(G)}{\sqrt{2}} \leq X(G), \\
(2.13) & \quad \sqrt{\delta} M_2^*(G) \leq H(G), \\
(2.14) & \quad \delta^2 M_2^*(G) \leq GA(G), \\
(2.15) & \quad \delta \sqrt{2(\delta - 1)} M_2^*(G) \leq ABC(G).
\end{align*}

The equality in all inequalities (2.11)-(2.15) is attained if and only if $G$ is a $\delta$-regular graph.

Now, we establish some inequalities between augmented Zagreb index and other vertex-degree-based topological indices.

Theorem 2.14. If $G$ is a connected graph having $n \geq 3$ vertices, then
\begin{equation}
\frac{1536}{343} X(G) \leq AZI(G) \leq \frac{\sqrt{(n-1)^{13}}}{\sqrt{32(n-2)^3}} X(G)
\end{equation}
with left equality if and only if $G \cong S_{1,8}$ and right equality if and only if $G \cong K_n$.

Proof. Without loss of generality we can assume $1 \leq d_i \leq d_j \leq n-1$. Consider the function
\begin{equation}
F(x, y) = \left( \frac{xy}{x+y-2} \right)^3 = (x+y) \left( \frac{xy}{x+y-2} \right)^6 \quad \text{with} \quad 1 \leq x \leq y \leq n-1 \quad \text{and} \quad y \geq 2.
\end{equation}

Then,
\begin{equation}
\frac{\partial F(x, y)}{\partial x} = \frac{x^5 y^6 \{x^2 + (y-2)(6y+7x)\}}{(x+y-2)^7} \geq 0.
\end{equation}

This means $F(x, y)$ is increasing in $x$ and hence is minimum at $(1, y_1)$ and maximum at $(y_2, y_2)$ for some $2 \leq y_1, y_2 \leq n-1$. Now,
\begin{equation}
\frac{dF(1, y)}{dy} = \frac{y^5(y^2 - 7y - 6)}{(y-1)^7}
\end{equation}
and this implies, $F(1, y)$ is monotone decreasing in $2 \leq y \leq 7$ and monotone increasing in $8 \leq y \leq n-1$. Hence minimum value of $F(x, y)$ is
\begin{equation}
\min\{F(1, 7), F(1, 8)\} = 9 \left( \frac{8}{7} \right)^6
\end{equation}

Therefore,
\begin{equation}
3 \left( \frac{8}{7} \right)^3 \leq \frac{AZI(G)}{X(G)}
\end{equation}
with equality if and only if $(d_i, d_j) = (1, 8)$ for each edge $ij$ of $G$.

Moreover,
\begin{equation}
F(y, y) = \frac{y^{13}}{32(y-1)^6}
\end{equation}
is monotone increasing and hence
\[ F(x, y) \leq F(n-1, n-1) = \frac{(n-1)^{13}}{32(n-2)^6} \]
therefore,
\[ \frac{\text{AZI}(G)}{X(G)} \leq \frac{\sqrt{(n-1)^{13}}}{\sqrt{32(n-2)^3}} \]
with equality if and only if \((d_i, d_j) = (n-1, n-1)\) for each edge \(ij\) of \(G\). From (2.16) and (2.17), required result follows.

If graph \(G\) has the minimum degree at least 2, then the lower bound in Theorem 2.14 can be improved:

**Corollary 2.15.** If \(G\) is a connected graph with minimum degree \(\delta \geq 2\), then
\[ \frac{\delta^{13}}{\sqrt{32(\delta-1)^3}} X(G) \leq \text{AZI}(G) \]
with equality if and only if \(G\) is a \(\delta\)-regular graph.

Using the similar technique, used in proving Theorem 2.14, one can prove the following result (we omit the proof)

**Theorem 2.16.** If \(G\) is a connected graph with \(n \geq 3\) vertices, then
\[ \frac{343\sqrt{7}}{216} R(G) \leq \text{AZI}(G) \leq \frac{(n-1)^7}{8(n-2)^3} R(G), \]
\[ \frac{375}{64} H(G) \leq \text{AZI}(G) \leq \frac{(n-1)^7}{8(n-2)^3} H(G), \]
\[ \left( \frac{n-1}{n-2} \right)^{\frac{7}{2}} ABC(G) \leq \text{AZI}(G) \leq \left( \frac{(n-1)^2}{2(n-2)} \right)^{\frac{7}{2}} ABC(G), \]
\[ 8GA(G) \leq \text{AZI}(G) \leq \frac{(n-1)^6}{8(n-2)^3} GA(G); \ \delta \geq 2, \]
\[ 4M_2^*(G) \leq \text{AZI}(G) \leq \frac{(n-1)^4}{2(n-2)} M_2^*(G). \]

The left equality in (2.18), (2.19), (2.20), (2.21), (2.22) hold if and only if \(G \cong S_{1,7},\ G \cong S_{1,5},\ G \cong S_{1,n-1},\ G \cong C_n,\ G \cong P_3\) respectively and right equality if and only if \(G \cong K_n\).

**Corollary 2.17.** If \(G\) is a connected graph with \(\delta \geq 2\), then
\[ \frac{\delta^7}{8(\delta-1)^3} R(G) \leq \text{AZI}(G), \]
\[ \frac{\delta^7}{8(\delta-1)^3} H(G) \leq \text{AZI}(G), \]
\[ \left( \frac{\delta^2}{2(\delta-1)} \right)^{\frac{7}{2}} ABC(G) \leq \text{AZI}(G), \]
\begin{equation}
\frac{\delta^6}{8(\delta - 1)^3} GA(G) \leq AZI(G),
\end{equation}
\begin{equation}
\frac{\delta^4}{2(\delta - 1)} M_2^*(G) \leq AZI(G).
\end{equation}

The equality in all inequalities (2.23)-(2.27) hold if and only if \( G \) is a \( \delta \)-regular graph.

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