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Relations between three topological indices

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Abstract

This paper presents several mathematical relations between the Wiener, the first and the second Zagreb indices in certain conditions. Namely, we give three inequalities between these indices.

1. Introduction

Molecules and molecular compounds are often modeled by molecular graph. Topological indices and graph invariants based on the distances or degrees are used for characterizing molecular graphs. And, Topological indices of molecular graphs are one of the oldest and most widely used descriptors in quantitative structure-activity relationships (QSAR).

Consider a (molecular) graph $G = (V, E)$ and let n and m be, respectively, the number of its vertices and edges. The *Wiener index* of a connected acyclic graph was introduced by H.Wiener ([13]). He observed a relationship between the boiling point

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of paraffin and the Wiener index. The *Wiener index* $W = W(G)$ of a connected graph $G = (V, E)$ is defined as:

$$W(G) = \sum_{v,w \in V} d(v,w) \quad (v \text{ and } w \text{ are unordered})$$

where $d(v, w)$ is the minimum length (number of edges) of the paths connecting them. Zagreb indices are introduced by I. Gutman and N. Trinajstić ([6]). The *first Zagreb index* (or *Gutman index*) $M_1 = M_1(G)$ and the *second Zagreb index* $M_2 = M_2(G)$ of a graph $G = (V, E)$ are defined as:

$$M_1(G) = \sum_{v \in V} d(v)^2$$

$$M_2(G) = \sum_{vw \in E} d(v)d(w) \ .$$

Recently, their variants has been used to study molecular complexity([10], [11]), chirality[5], etc.

2. Results

Given a graph $G = (V, E)$. For an edge $e = vw$, we define $J(e)$ and $t(e)$ as follows, respectively.

$$J(e) = \mid N(v) \cup N(w) \mid \qquad ; \qquad t(e) = \mid N(v) \cap N(w) \mid \ .$$

And, we let

$$J = J(G) = \max_{e \in E}\{J(e)\} \qquad \text{and} \qquad t = t(G) = \frac{1}{m}\sum_{e \in E} t(e) \ .$$

Hence, G is a triangle-free graph if and only if $t = 0$

Remark:

$$\mid N(v) \cup N(w) \mid + \mid N(v) \cap N(w) \mid = d(v) + d(w) \ . \tag{1}$$

First, we give a mathematical relation between the first and the second Zagreb index of triangle-free graphs.

Lemma (Chebyshev's (sum) inequality ([9])). Let $a_1 \geq a_2 \geq \cdots \geq a_n$ and $b_1 \geq b_2 \geq \cdots \geq b_n$ where a_i and b_i are integer. Then

$$\frac{1}{n}\sum_{i=1}^{n} a_i b_i \geq \left(\frac{1}{n}\sum_{i=1}^{n} a_i\right)\left(\frac{1}{n}\sum_{i=1}^{n} b_i\right)$$

and equality holds if and only if $a_1 = a_n$ or $b_1 = b_n$.

Theorem 1. Let G be a triangle-free graph with $n \geq 2$ vertices. Then

$$M_2(G) \leq \frac{1}{2}mJ^2 - \frac{m}{n}M_1(G)$$

and equality holds if and only if G is regular.

Proof.

$$\begin{aligned} m(J+t)^2 &\geq \sum_{vw\in E} (\mid N(v)\cup N(w)\mid + \mid N(v)\cap N(w)\mid)^2 \\ &= \sum_{vw\in E} (d(v)+d(w))^2 \\ &= \sum_{vw\in E} \left(d(v)^2+d(w)^2\right) + \sum_{vw\in E} 2d(v)d(w) \\ &= \sum_{v\in V} d(v)^3 + 2M_2 \\ &\geq \frac{2m}{n}M_1 + 2M_2 \qquad \text{since the above Lemma .} \end{aligned}$$

The later of the two inequalities turns into an equality if and only if G is regular. Provided this condition, on the other hand, $t = 0$. Then $e \mapsto J(e)$ is constant, and the former one automatically turns into an equality. ■

Remark: There exist chemical graphs which attain above inequality. For example, fullerene, benzene.

Theorem 2. Let G be a triangle- and quadrangle-free connected graph with $n \geq 2$. Then

$$M_2(G) \leq m\left(\frac{J^2}{2} + \frac{2m}{n} + \frac{2}{n}W(G) - 3(n-1)\right)$$

and equality holds if and only if G is regular and the diameter of G is at most 3.

Proof. B. Zhou and I. Gutman ([15]) show that for a triangle- and quadrangle-free graph G,

$$M_1(G) \geq 3n(n-1) - 2W(G) - 2m$$

and equality holds if and only if the diameter of G is at most 3, which makes possible to eliminate M_1 from Theorem 1.

Hence,

$$\begin{aligned} M_2(G) &\leq \frac{1}{2}mJ^2 - \frac{m}{n}\{3n(n-1) - 2W(G) - 2m\} \\ &= m\left(\frac{J^2}{2} + \frac{2m}{n} + \frac{2}{n}W(G) - 3(n-1)\right) . \end{aligned}$$

■

Remark: There exist a chemical graph which attain above inequality.

It is benzene.

Given a connected graph G. For an integer i and a vertex v, let $N_i(v) = \{w \in V \mid d(v,w) = i\}$. and $d_i =\mid N_i(v) \mid$. Write D_i for the number of unordered pairs of vertices whose distance is i. The eccentricity $e(v)$ of v is defined as $e(v) = \max_{w \in V}\{d(v,w)\}$. Then, the radius $r = r(G)$ and the diameter $d = d(G)$ of G are defined as $r = \min_{v \in V}\{e(v)\}$, $d = \max_{v \in V}\{e(v)\}$, respectively.

Remarks: For any vertex v, we have $\sum_{i=1}^{e(v)} d_i(v) = n - 1$, and $2D_i = \sum_{v \in V} d_i(v)$.

Lemma 3. Let G be a connected graph. Then, for any vertex $v \in V$

$$d_2(v) \leq n + 1 - d_1(v) - e(v) .$$

Proof.

$$\begin{aligned} n - 1 &= d_1(v) + d_2(v) + d_3(v) + \cdots + d_{e(v)}(v) \\ &\geq d_1(v) + d_2(v) + e(v) - 2 . \end{aligned}$$

■

Lemma 4 ([3]). Let G be a connected graph with $n \geq 2$. Then

$$\frac{1}{n}\sum_{v\in V} e(v) \geq \frac{2}{n(n-1)} W(G) \ .$$

Proposition 5. Let G be a connected graph with $n \geq 2$. Then

$$2D_2 \leq n^2 + n - 2m - \frac{2}{n-1} W(G) \ .$$

Proof.
From Lemma 3, we have

$$\begin{aligned} 2D_2 &= \sum_{v\in V} d_2(v) \leq \sum_{v\in V} n + 1 - d_1(v) - e(v) \\ &= n^2 + n - 2m - \sum_{v\in V} e(v) \\ &\leq n^2 + n - 2m - \frac{2}{n-1} W(G) \ . \end{aligned}$$

(From Lemma 4) ■

Theorem 6. Let G be a triangle- and quadrangle-free connected graph with $n \geq 2$. Then

$$M_1(G) \leq n(n+1) - \frac{2}{n-1} W(G) \ .$$

Proof.
For a triangle- and quadrangle-free graph G, the relation $M_1(G) = 2D_2 + 2m$ is easily verified ([15]). Thus from Proposition 5, we have

$$\begin{aligned} M_1(G) &\leq n^2 + n - 2m - \frac{2}{n-1} W(G) + 2m \\ &= n^2 + n - \frac{2}{n-1} W(G) \ . \end{aligned}$$

■

B. Zhou ([16]) presented sharp bounds for the Zagreb indices of a graph, especially, for triangle-free graphs, in terms of the number of edges and number of vertices.

Theorem 7 ([16]) Let G be a triangle-free graph with $n \geq 2$, then

$$M_1(G) \leq mn$$

and equality holds if and only if G is a complete bipartite graph.

Now we improve this Theorem using the approach given in [7].

Proposition 8. Let G be a triangle-free graph. Then

$$M_1(G) \leq mJ$$

and equality holds if and only if $e \mapsto J(e)$ is constant.

Proof.

$$\begin{aligned} m(J+t) &\geq \sum_{vw \in E} (\mid N(v) \cup N(w) \mid + \mid N(v) \cap N(w) \mid) \\ &= \sum_{vw \in E} (d(v) + d(w)) = \sum_{v \in V} d(v)^2 = M_1(G) \ . \end{aligned}$$

The equality condition is clear. ■

Remark: There exist chemical graphs which attain above inequality.
For example, methane, benzene, fullerene.

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