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Some Generalizations of the Geometric–Arithmetic Index

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Abstract

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The $Z_{p,q}$ index, for a real number for $p \neq 0$, is defined as $Z_{p,q} = Z_{p,q}(G) = \sum_{uv \in E(G)} \frac{M_p(d_u, d_v)}{M_q(d_u, d_v)}$, where $M_p(d_u, d_v) = \left(\frac{(d_u)^p + (d_v)^p}{2} \right)^{\frac{1}{p}}$ and d_u is the degree of the vertex u. The $Z_{p,q}$ index is a generalization of the geometric–arithmetic index. In this paper, some relations between $Z_{p,q}$, Randić, and Zagreb indices are presented.

Introduction

A graph G consists of a set of vertices $V(G)$ and a set of edges $E(G)$. If the vertices $u, v \in V(G)$ are connected by an edge *e,* then we write *e*=*uv*. In chemical graphs, each vertex represents an atom of the molecule, and covalent bonds between atoms are represented by edges between the corresponding vertices. This object, derived from a

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chemical compound, is usually referred to as its molecular graph. Molecular structure descriptors, frequently called *topological indices*, are used in theoretical chemistry for the design of chemical compounds with given physico-chemical properties or given pharmacologic and biological activities. Usage of topological indices in chemistry began in 1947 when Harold Wiener developed the most widely known topological descriptor, the Wiener index, and used it to determine physical properties of alkanes [1]. In the recent years, in mathematical chemistry it became a popular practice to introduce novel topological indices, see [2–13].

The first and second Zagreb indices were originally defined as $Z_{g_1}(G) = \sum_{u\in V(G)} d_u^2$ and $Z_{g_2}(G) = \sum_{uv\in E(G)} d_u d_v$, respectively, where d_u is the degree of the vertex u, the number of first neighbors of u. Note that if $uv \in E(G)$, then d_u and $d_v \geq 1$. For more information on Zagreb indices, the interested readers are referred to [14–17].

In 1975, Randić proposed another topological index based on the degrees of the end vertices of an edge [18]: $R(G) = \sum_{e=uv} \frac{1}{\sqrt{d_u d_v}}$.

Let $p \neq 0$ be a real number. Then the mean M_p is defined as [19,20]:

$$M_p = M_p(x_1, x_2, \cdots, x_n) := \left(\frac{1}{n} \sum_{i=1}^{n} x_i^p \right)^{\frac{1}{p}}.$$

Also

$$M_0 = M_0(x_1, x_2, \cdots, x_n) := \left(\prod_{i=1}^{n} x_i \right)^{\frac{1}{n}}.$$

The best known of these means are M_1 , M_0 , and M_{-1} called, respectively, arithmetic, geometric, and harmonic mean. If $p > q$, then $M_p > M_q$. More details on means can be found in the monographs [19, 20].

Lemma 1. Let G be a connected graph. Then

(i) For all positive numbers p and all $uv \in E(G)$; $M_p(\frac{1}{d_u}, \frac{1}{d_v}) \leq 1$ and hence $\sum_{uv\in E(G)} M_p(\frac{1}{d_u}, \frac{1}{d_v}) \leq m$.

(ii) For all negative numbers p and all $uv \in E(G)$; $M_p(\frac{1}{d_u}, \frac{1}{d_v}) \geq \dfrac{1}{n-1}$ and hence $\sum_{uv \in E(G)} M_p(\frac{1}{d_u}, \frac{1}{d_v}) \geq \frac{m}{n-1}$.

(iii) For all positive numbers p and all $uv \in E(G)$; $M_p(d_u, d_v) \leq n-1$ and hence $\sum_{uv \in E(G)} M_p(d_u, d_u) \leq m(n-1)$.

Proof is straightforward. □

Directly from the definition of first Zagreb index, it follows that it can be written in terms of arithmetic means as

$$Z_{g_1}(G) = 2 \sum_{uv \in E(G)} M_1(d_u, d_v).$$

In the following theorem, the second Zagreb index is expressed in terms of $M_p(d_u, d_v)$ and $M_{-p}(d_u, d_v)$.

Theorem 2. [15] The identity

$$Z_{g_2}(G) = \sum_{uv \in E(G)} M_p(d_u, d_v) M_{-p}(d_u, d_v)$$

is valid for any value of p . Thus, in particular, the second Zagreb index can be expressed in terms of arithmetic and harmonic means:

$$Z_{g_2}(G) = 2 \sum_{uv \in E(G)} M_1(d_u, d_v) M_{-1}(d_u, d_v).$$

Considerations based on means make it possible to conceive the following partition of the first Zagreb index into two components. In view of

$$\lim_{p \to \infty} M_p(x_1, x_2, \cdots, x_n) = \max(x_1, x_2, \cdots, x_n)$$

$$\lim_{p \to -\infty} M_p(x_1, x_2, \cdots, x_n) = \min(x_1, x_2, \cdots, x_n)$$

we can decompose $Zg_1(G)$ as $Zg_{1a}(G) + Zg_{1b}(G)$, where

$$Zg_{1a} = Zg_{1a}(G) = \sum_{uv \in E(G)} \lim_{p \to \infty} M_p(d_u, d_v) = \sum_{uv \in E(G)} \max\{d_u, d_v\},$$
$$Zg_{1b} = Zg_{1b}(G) = \sum_{uv \in E(G)} \lim_{p \to -\infty} M_p(d_u, d_v) = \sum_{uv \in E(G)} \min\{d_u, d_v\}.$$

In [15] it is shown that $Zg_2(G) \leq \min\ \{Zg_{1a}(G)\ Zg_{1b}(G), \Delta\sqrt{Zg_{1a}\, Zg_{1b}}\ \}$.

The concept of geometric-arithmetic indices was introduced in the chemical graph theory. These indices generally are defined as

$$GA_{general} = GA_{general}(G) = \sum_{uv\in E(G)} \frac{\sqrt{Q_u Q_v}}{(Q_u + Q_v)/2}$$

where Q_u is some quantity that in a unique manner can be associated with the vertex u of graph G. The first type of geometric-arithmetic index is denoted by GA and defined as $GA = GA(G) = \sum_{uv\in E(G)} \frac{\sqrt{d_u d_v}}{(d_u + d_v)/2}$, see [9] (see also [13,21,22]). Since

$$\frac{M_0(d_u, d_v)}{M_1(d_u, d_v)} = \frac{M_0(\frac{1}{d_u}, \frac{1}{d_v})}{M_1(\frac{1}{d_u}, \frac{1}{d_v})}$$

we get

$$GA(G) = \sum_{uv\in E(G)} \frac{M_0(d_u d_v)}{M_1(d_u, d_v)} = \sum_{uv\in E(G)} \frac{M_0(\frac{1}{d_u}, \frac{1}{d_v})}{M_1(\frac{1}{d_u}, \frac{1}{d_v})}.$$

The $Z_{p,q}$ index was defined in [15] as

$$Z_{p,q} = Z_{p,q}(G) = \sum_{uv\in E(G)} \frac{M_p(d_u d_v)}{M_q(d_u, d_v)}.$$

So $Z_{0,1} = GA$. Also the equality $Z_{p,q} = Z_{-q,-p}$ holds for all values of parameters p and q.

Main Results

In this section, we obtain some relations between $Z_{p,q}$, Randić, and Zagreb indices of any graphs.

Theorem 3. Let p and q be numbers with the same sign. Then the following inequalities are hold:

(i) $$\frac{R(G)}{m} < Z_{p,q} < (n-1)R(G),$$

(ii) $$\frac{2\,Zg_2(G)}{m(n-1)Zg_1(G)} \le Z_{p,q} \le \tfrac{1}{2} Zg_1(G).$$

Proof. (*i*) At first suppose that $p,q>0$. Then by definition and using Lemma 1 (*i*),

$$Z_{p,q} > Z_{0,q} = \sum_{uv\in E(G)} \frac{M_0(d_u,d_v)}{M_q(d_u,d_v)} = \sum_{uv\in E(G)} \frac{M_0(\frac{1}{d_u},\frac{1}{d_v})}{M_q(\frac{1}{d_u},\frac{1}{d_v})}$$

$$\geq \frac{\sum_{uv\in E(G)} M_0(\frac{1}{d_u},\frac{1}{dv})}{\sum_{uv\in E(G)} M_q(\frac{1}{d_u},\frac{1}{d_v})} = \frac{R(G)}{\sum_{uv\in E(G)} M_q(\frac{1}{d_u},\frac{1}{d_v})} \geq \frac{R(G)}{m}. \tag{1}$$

By definition and using Lemma 1 (*ii*),

$$Z_{p,q} < Z_{p,0} = \sum_{uv\in E(G)} \frac{M_p(d_u,d_v)}{M_0(d_u,d_v)} = \sum_{uv\in E(G)} \frac{M_o(d_u,d_v)}{M_{-p}(d_u,d_v)} = \sum_{uv\in E(G)} \frac{M_0(\frac{1}{d_u},\frac{1}{d_v})}{M_{-p}(\frac{1}{d_u},\frac{1}{d_v})}$$

$$\leq \sum_{uv\in E(G)} \frac{M_0(\frac{1}{d_u},\frac{1}{d_v})}{\frac{1}{n-1}} = (n-1)\,R(G). \tag{2}$$

From inequalities (1) and (2) we conclude that $\frac{R(G)}{m} < Z_{p,q} < (n-1)\,R(G)$.

(*ii*) By using the definition of $Z_{p,q}$, Lemma 1 (*iii*), and the Jensen inequality,

$$Z_{p,q} = \sum_{uv\in E(G)} \frac{M_p(d_u,d_v)}{M_q(d_u,d_v)} = \sum_{uv\in E(G)} \frac{[M_0(d_u,d_v)]^2}{M_q(d_u,d_v)M_{-p}(d_u,d_v)}$$

$$\geq \sum_{uv\in E(G)} \frac{[M_0(d_u,d_v)]^2}{M_q(d_u,d_v)M_1(d_u,d_v)} \geq \frac{\sum_{uv\in E(G)} [M_0(d_u,d_v)]^2}{\sum_{uv\in E(G)} M_q(d_u,d_v) \sum_{uv\in E(G)} M_1(d_u,d_v)}$$

$$= \frac{2Zg_2(G)}{\sum_{uv\in E(G)} M_q(d_u,d_v)Zg_1(G)} \geq \frac{2Zg_2(G)}{m(n-1)Zg_1(G)} \quad . \tag{3}$$

Also

$$Z_{p,q} = \sum_{uv\in E(G)} \frac{M_p(d_u,d_v)}{M_q(d_u,d_v)} = \sum_{uv\in E(G)} \frac{[M_0(d_u,d_v)]^2}{M_q(d_u,d_v)M_{-p}(d_u,d_v)}$$

$$\leq \sum_{uv\in E(G)} \frac{[M_1(d_u,d_v)]^2}{M_1(d_u,d_v)M_{-p}(d_u,d_v)} = \sum_{uv\in E(G)} \frac{M_1(d_u,d_v)}{M_{-p}(d_u,d_v)}$$

$$\leq \sum_{uv\in E(G)} M_1(d_u,d_v) = \tfrac{1}{2} Zg_1(G). \tag{4}$$

By inequalities (3) and (4), we have:

$$\frac{2\,Zg_2(G)}{m(n-1)Zg_1(G)} \le Z_{p,q} \le \tfrac{1}{2}\,Zg_1(G).$$

For the case $p,q<0$, by using the fact that $Z_{p,q}=Z_{-q,-p}$ and $-q,-p>0$, the proof is analogous. □

Theorem 4. Let p and q be real numbers such that $p>0$ and $q<0$. Then the following inequalities are hold:

(i) $$\frac{m}{(n-1)R(G)} \le Z_{p,q} \le [(n-1)R(G)]^2$$

(ii) $$\frac{4\,Zg_2(G)}{[Zg_1(G)]^2} \le Z_{p,q} \le [\tfrac{1}{2}\,Zg_1(G)]^2.$$

Proof. (i) Using Lemma 1 (ii),

$$Z_{p,q} > Z_{0,q} = Z_{-q,0} = \sum_{uv\in E(G)} \frac{M_{-q}(d_u,d_v)}{M_0(d_u,d_v)} = \sum_{uv\in E(G)} \frac{M_{-q}(\frac{1}{d_u},\frac{1}{d_v})}{M_0(\frac{1}{d_u},\frac{1}{d_v})}$$

$$\ge \frac{\sum_{uv\in E(G)} M_{-q}(\frac{1}{d_u},\frac{1}{dv})}{\sum_{uv\in E(G)} M_0(\frac{1}{d_u},\frac{1}{d_v})} \ge \frac{m}{(n-1)R(G)}. \tag{5}$$

Using the Jensen inequality and (2), we have:

$$Z_{p,q} = \sum_{uv\in E(G)} \frac{M_p(d_u,d_v)}{M_q(d_u,d_v)} = \sum_{uv\in E(G)} \frac{[M_0(d_u,d_v)]^2}{M_q(d_u,d_v)M_{-p}(d_u,d_v)}$$

$$= \sum_{uv\in E(G)} \frac{M_0(d_u,d_v)}{M_q(d_u,d_v)}\,\frac{M_0(d_u,d_v)}{M_{-p}(d_u,d_v)}$$

$$\le \sum_{uv\in E(G)} \frac{M_0(d_u,d_v)}{M_q(d_u,d_v)} \sum_{uv\in E(G)} \frac{M_0(d_u,d_v)}{M_{-p}(d_u,d_v)}$$

$$= Z_{0,q}\,.Z_{o,-p} = Z_{-q,0}\,.Z_{p,0} \le [(n-1)\,R(G)]^2. \tag{6}$$

By (5) and (6), we have the following inequality:

$$\frac{m}{(n-1)R(G)} \le Z_{p,q} \le [(n-1)R(G)]^2.$$

(ii) Using the Jensen inequality,

$$Z_{p,q} = \sum_{uv\in E(G)} \frac{M_p(d_u,d_v)}{M_q(d_u,d_v)} = \sum_{uv\in E(G)} \frac{[M_0(d_u,d_v)]^2}{M_q(d_u,d_v)M_{-p}(d_u,d_v)}$$

$$\geq \frac{\sum_{uv\in E(G)}[M_0(d_u,d_v)]^2}{\sum_{uv\in E(G)} M_q(d_u,d_v)\sum_{uv\in E(G)} M_{-p}(d_u,d_v)} \geq \frac{\sum_{uv\in E(G)}[M_0(d_u,d_v)]^2}{\sum_{uv\in E(G)} M_1(d_u,d_v)\sum_{uv\in E(G)} M_1(d_u,d_v)}$$

$$= \frac{Zg_2(G)}{[\frac{1}{2}Zg_1(G)]^2} = \frac{4Zg_2(G)}{[Zg_1(G)]^2} \ . \tag{7}$$

Also

$$Z_{p,q} = \sum_{uv\in E(G)} \frac{M_p(d_u,d_v)}{M_q(d_u,d_v)} = \sum_{uv\in E(G)} \frac{[M_0(d_u,d_v)]^2}{M_q(d_u,d_v)M_{-p}(d_u,d_v)}$$

$$\leq \sum_{uv\in E(G)} \frac{[M_1(d_u,d_v)]^2}{M_q(d_u,d_v)M_{-p}(d_u,d_v)} \leq \sum_{uv\in E(G)}[M_1(d_u,d_v)]^2$$

$$\leq [\sum_{uv\in E(G)} M_1(d_u,d_v)]^2 = [\tfrac{1}{2}Zg_1(G)]^2 . \tag{8}$$

From (7) and (8) follows

$$\frac{4Zg_2(G)}{[Zg_1(G)]^2} \leq Z_{p,q} \leq [\tfrac{1}{2}Zg_1(G)]^2 .$$

Theorem 5. Let p and q be real numbers such that $p < 0$ and $q > 0$. Then the following inequalities are hold:

(i) $$\frac{[R(G)]^2}{m^3} \leq Z_{p,q} \leq R(G)$$

(ii) $$\frac{Zg_2(G)}{m(n-1)} \leq Z_{p,q} \leq [\tfrac{1}{2}Zg_1(G)]^2 .$$

Proof. (i)

$$Z_{p,q} < Z_{0,q} = \sum_{uv\in E(G)} \frac{M_0(d_u,d_v)}{M_q(d_u,d_v)} = \sum_{uv\in E(G)} \frac{M_0(\frac{1}{d_u},\frac{1}{d_v})}{M_q(\frac{1}{d_u},\frac{1}{d_v})}$$

$$\leq \sum_{uv\in E(G)} M_0(\tfrac{1}{d_u},\tfrac{1}{d_v}) = R(G) . \tag{9}$$

Also

$$Z_{p,q} = \sum_{uv\in E(G)} \frac{M_p(d_u,d_v)}{M_q(d_u,d_v)} = \sum_{uv\in E(G)} \frac{M_p(d_u,d_v)M_{-p}(d_u,d_v)}{M_q(d_u,d_v)M_{-p}(d_u,d_v)}$$

$$= \sum_{uv\in E(G)} \frac{[M_0(d_u,d_v)]^2}{M_q(d_u,d_v)M_{-p}(d_u,d_v)} \geq \sum_{uv\in E(G)} [\frac{M_0(d_u,d_v)}{M_r(d_u,d_v)}]^2$$

where $r = \max\{q, -p\}$. Now by using the Cauchy inequality ,

$$\{\sum_{uv\in E(G)} \frac{M_0(d_u,d_v)}{M_r(d_u,d_v)}\}^2 \leq \sum_{uv\in E(G)} 1^2 \sum_{uv\in E(G)} [\frac{M_0(d_u,d_v)}{M_r(d_u,d_v)}]^2 .$$

Hence, using inequality (1)

$$\sum_{uv\in E(G)} [\frac{M_0(d_u,d_v)}{M_r(d_u,d_v)}]^2 \geq \frac{1}{m}\{\sum_{uv\in E(G)} \frac{M_0(d_u,d_v)}{M_r(d_u,d_v)}\}^2 = \frac{(Z_{0,r})^2}{m} \geq \frac{[R(G)]^2}{m^3} . \qquad (10)$$

By (9) and (10):

$$\frac{[R(G)]^2}{m^3} \leq Z_{p,q} \leq R(G).$$

(ii) By using Lemma 1 (iii),

$$Z_{p,q} = \sum_{uv\in E(G)} \frac{M_p(d_u,d_v)}{M_q(d_u,d_v)} = \sum_{uv\in E(G)} \frac{M_p(d_u,d_v)M_{-p}(d_u,d_v)}{M_q(d_u,d_v)M_{-p}(d_u,d_v)}$$

$$= \sum_{uv\in E(G)} \frac{[M_0(d_u,d_v)]^2}{M_q(d_u,d_v)M_{-p}(d_u,d_v)} \geq \frac{\sum_{uv\in E(G)}[M_0(d_u,d_v)]^2}{\sum_{uv\in E(G)} M_q(d_u,d_v) \sum_{uv\in E(G)} M_{-p}(d_u,d_v)}$$

$$\geq \frac{\sum_{uv\in E(G)}[M_0(d_u,d_v)]^2}{[\sum_{uv\in E(G)} M_r(d_u,d_v)]^2} \geq \frac{Zg_2(G)}{m(n-1)} \qquad (11)$$

where $r = \max\{q, -p\}$.

$$Z_{p,q} = \sum_{uv\in E(G)} \frac{M_p(d_u,d_v)}{M_q(d_u,d_v)} = \sum_{uv\in E(G)} \frac{M_p(d_u,d_v)M_{-p}(d_u,d_v)}{M_q(d_u,d_v)M_{-p}(d_u,d_v)}$$

$$= \sum_{uv\in E(G)} \frac{[M_0(d_u,d_v)]^2}{M_q(d_u,d_v)M_{-p}(d_u,d_v)} \leq \sum_{uv\in E(G)} [\frac{M_1(d_u,d_v)}{M_r(d_u,d_v)}]^2$$

$$\leq \{\sum_{uv\in E(G)} \frac{M_1(d_u,d_v)}{M_r(d_u,d_v)}\}^2 \leq \{\sum_{uv\in E(G)} M_1(d_u,d_v)\}^2 = [\tfrac{1}{2} Zg_1(G)]^2 \qquad (12)$$

where $r = \min\{q, -p\}$.

By relations (11) and (12) we arrive at the bounds:

$$\frac{Zg_2(G)}{m(n-1)} \leq Z_{p,q} \leq [\tfrac{1}{2} Zg_1(G)]^2 .$$

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