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ON GENERAL RANDIĆ AND GENERAL ZEROTH-ORDER RANDIĆ INDICES

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Abstract

For a graph G with vertex set $V(G)$ and edge set $E(G)$, the general Randić index and the general zeroth-order Randić index are defined respectively as $R_\alpha(G)=\sum_{uv\in E(G)}\left(d_u d_v\right)^\alpha$ and $Q_\alpha(G)=\sum_{\substack{u\in V(G)\\ d_u\geq 1}} d_u^\alpha$, where α is a real number and d_u denotes the degree of vertex u in G. We report some relations between them.

INTRODUCTION

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, $\Gamma(u)$ denotes the set of its (first) neighbors in G and the degree of u is $d_u = |\Gamma(u)|$. Denote by uv or vu the edge of G connecting vertices u and v.

The general Randić index and the general zeroth-order Randić index of the graph G are defined respectively as

$$R_\alpha = R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha$$

$$Q_\alpha = Q_\alpha(G) = \sum_{\substack{u \in V(G) \\ d_u \geq 1}} d_u^\alpha$$

where α is a real number. The theory of Randić-type structure-descriptors is outlined in the book [1].

Evidently, $R_{-1/2}$ and $Q_{-1/2}$ are respectively the ordinary Randić index and the ordinary zeroth-order Randić index of the graph [2, 3, 4]. $R_{-1/2}$ is one of the most popular descriptors and have found countless QSPR and QSAR applications, see, e.g., [5]. $Q_{-1/2}$ is also used to develop structure-based correlations for physical properties, see, e.g., [6].

For the graph G, $Q_2(G)$ is known as the first Zagreb index of G, denoted by $M_1(G)$, while $R_1(G)$ is known as the second Zagreb index of G, denoted by $M_2(G)$. See [7, 8] for their origin as measures of the branching of the molecular skeleton, and [9, 10] for main properties.

For the connected graph G with n vertices and m edges, the AutoGraphiX [11] proposed a conjecture: $\frac{M_1}{n} \leq \frac{M_2}{m}$. Hansen and Vukičević [12] showed that though it does not hold for all graphs, it is true for chemical graphs. Vukičević and Graovac [13] showed that it is true for trees. Vukičević [14] investigated the comparing of $\frac{Q_{\alpha/2}}{n}$ and $\frac{R_\alpha}{m}$. Liu and Gutman [15] presented some estimates of the general Randić and the general zeroth-order Randić indices. Some estimates involving the eigenvalues of the Laplacian matrix may be found in [16].

In this article, we report some relations between the general Randić index and the general zeroth-order Randić index.

RESULTS

The clique number of a graph G is the number of vertices in a largest complete subgraph of G, denoted by $\omega(G)$. We will use a theorem of Motzkin and Straus [17].

Theorem MS. [17] *Let G be a graph and let $x_u \geq 0$ for $u \in V(G)$ with $\sum_{u \in V(G)} x_u = 1$. Then*

$$\sum_{uv \in E(G)} x_u x_v \leq \frac{\omega(G)-1}{2\omega(G)}$$

with equality if and only if the subgraph induced by the vertices $u \in V(G)$ with $x_u > 0$ is a complete $\omega(G)$-partite graph such that the sum of the x_u's in each part is the same.

Denote by $K_{a_1 \cdot n_1, a_2 \cdot n_2, \cdots, a_k \cdot n_k}$ the graph $K_{n_1, \cdots, n_1, n_2, \cdots, n_2, \cdots, n_k, \cdots, n_k}$ where n_i appears a_i times, $i = 1, \ldots, k$. First we give a relation between R_α and Q_α.

Theorem 1. *Let G be a graph with clique number ω. Then*

$$R_\alpha \leq \frac{\omega - 1}{2\omega} Q_\alpha^2 \tag{1}$$

with equality for graph G with no isolated vertices if and only if one of the following conditions holds:

(i) $\alpha = 1$ and G is either a complete bipartite graph for $\omega = 2$ or a regular complete ω-partite graph for $\omega \geq 3$.

(ii) $\alpha < 1$ and G is regular complete ω-partite graph.

(iii) $\alpha > 1$ and G is either a regular complete ω-partite graph or $G = K_{a \cdot n_1, b \cdot n_2}$ where $n_1 \neq n_2$, $a + b = \omega$ and $n_1\left[(a-1)n_1 + bn_2\right]^\alpha = n_2\left[an_1 + (b-1)n_2\right]^\alpha$.

Proof. The result is trivial if $\omega = 1$. Suppose that $\omega \ge 2$. For $u \in V(G)$, let $x_u = \dfrac{d_u^\alpha}{Q_\alpha}$ if $d_u > 0$ and $x_u = 0$ if $d_u = 0$. Then $x_u \ge 0$ for $u \in V(G)$ with $\sum_{u \in V(G)} x_u = 1$. By Theorem MS,

$$\sum_{uv \in E(G)} \frac{d_u^\alpha}{Q_\alpha} \cdot \frac{d_v^\alpha}{Q_\alpha} \le \frac{\omega - 1}{2\omega}$$

from which (1) follows.

Suppose that G has no isolated vertices and that equality holds in (1). Note that $x_u > 0$ for any $u \in V(G)$. By Theorem MS, G is a complete ω-partite graph, say $G = K_{n_1,\cdots,n_\omega}$, and the sum of the x_u's in each part is the same. Then $n_i\left(n - n_i\right)^\alpha = \dfrac{Q_\alpha}{\omega} = n_j\left(n - n_j\right)^\alpha$ for any $1 \le i < j \le \omega$.

Case 1. $\alpha = 1$. We have $\left(n_i - n_j\right)\left(n - n_i - n_j\right) = 0$ for any $1 \le i < j \le \omega$, implying $n = n_1 + n_2$ or if $n > n_i + n_j$ then $n_i = n_j$. Thus, $n = n_1 + n_2$ and G is a complete bipartite graph for $\omega = 2$, or $n_1 = \cdots = n_\omega$ and so G is a regular complete ω-partite graph for $\omega \ge 3$.

Case 2. $\alpha < 1$. If $n_i < n_j$, then $\dfrac{n_j}{n_i} \ge \dfrac{n - n_i}{n - n_j} > \left(\dfrac{n - n_i}{n - n_j}\right)^\alpha$, a contradiction. Thus, $n_1 = \cdots = n_\omega$ and so G is a regular complete ω-partite graph.

Case 3. $\alpha > 1$. Let n_1 be a cardinality of one part of G. Then cardinality of every other part has to be a solution of the following equation:

$$x\left(n - x\right)^\alpha = n_1\left(n - n_1\right)^\alpha. \tag{2}$$

Let $f:\ (0, n) \to R$ be the function given by $f\left(x\right) = x\left(n - x\right)^\alpha - n_1\left(n - n_1\right)^\alpha$. Since, $f'\left(x\right) = \left(n - x\right)^{\alpha - 1}\left(n - x - \alpha x\right)$, it follows that f is monotonously increasing in the segment $\left(0,\ \dfrac{n}{1 + \alpha}\right)$ and monotonously decreasing in the segment $\left(\dfrac{n}{1 + \alpha},\ n\right)$, hence (2) has at most two solutions one of which is n_1. If n_1 is the only solution or the second solution is not an integer, then G is a regular complete bipartite graph. If there are two solutions n_1 and n_2 and if n can be rewritten as $n = an_1 + bn_2$ for some positive integers a and b, then G may be a graph $K_{a\cdot n_1, b\cdot n_2}$ with $n_1\left[(a-1)n_1 + bn_2\right]^\alpha = n_2\left[an_1 + (b-1)n_2\right]^\alpha$.

Conversely, it is easy to see that (1) is an equality if G is a graph given by (i), (ii) and (iii). □

Remark. For every graph $K_{a\cdot n_1,\, b\cdot n_2}$, $n_1 < n_2$, there is $\alpha > 1$ such that $R_\alpha = \dfrac{\omega-1}{2\omega} Q_\alpha^2$. It is sufficient to take α such that $n_1\left[(a-1)n_1 + bn_2\right]^\alpha = n_2\left[an_1 + (b-1)n_2\right]^\alpha$, i.e., to take:

$$\alpha = \frac{\log \dfrac{n_2}{n_1}}{\log \dfrac{(a-1)n_1 + bn_2}{an_1 + (b-1)n_2}}.$$

Corollary 2. *Let G be a graph with m edges and clique number ω. Then*

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

with equality for graph G with no isolated vertices if and only if G is either a complete bipartite graph for $\omega = 2$ or a regular complete ω-partite graph for $\omega \ge 3$.

Let G be a graph with n vertices, m edges and clique number ω. By Turán's theorem, $m \le \dfrac{\omega-1}{2\omega} n^2$. It follows that

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

which was reported in [18].

Let ρ be the largest eigenvalue of (the adjacency matrix of) the graph G. It is pointed out in [16] that $R_\alpha \le \dfrac{1}{2}\rho Q_{2\alpha}$. For the case of Zagreb indices, i.e., $\alpha = 1$, this may also be found in [19].

Now we give a relation between R_α and Q_β for $\beta = 2\alpha+1,\ 2\alpha,\ \alpha$.

Theorem 3. *Let G be a graph with n vertices and at least one edge. Then*

$$R_\alpha \geq \frac{1}{2}\left(Q_{2\alpha+1} - nQ_{2\alpha} + Q_\alpha^2\right) \tag{3}$$

with equality if and only if $\alpha = 0$ and G has no isolated vertices, or every pair of non-adjacent vertices of G have the same degree.

Proof. It is easy to see that

$$\begin{aligned}
2R_\alpha &= \sum_{u\in V(G)} \sum_{v\in\Gamma(u)} \left(d_u d_v\right)^\alpha \\
&= \frac{1}{2}\sum_{u\in V(G)} \sum_{v\in\Gamma(u)} \left(d_u^{2\alpha} + d_v^{2\alpha}\right) - \frac{1}{2}\sum_{u\in V(G)} \sum_{v\in\Gamma(u)} \left(d_u^\alpha - d_v^\alpha\right)^2 \\
&= Q_{2\alpha+1} - \frac{1}{2}\sum_{u\in V(G)} \sum_{v\in\Gamma(u)} \left(d_u^\alpha - d_v^\alpha\right)^2.
\end{aligned}$$

On the other hand,

$$\begin{aligned}
\sum_{u\in V(G)} \sum_{v\in\Gamma(u)} \left(d_u^\alpha - d_v^\alpha\right)^2 &\leq \sum_{\substack{u\in V(G)\\ d_u\geq 1}} \sum_{\substack{v\in V(G)\\ d_v\geq 1}} \left(d_u^\alpha - d_v^\alpha\right)^2 \\
&= \sum_{\substack{u\in V(G)\\ d_u\geq 1}} \sum_{\substack{v\in V(G)\\ d_v\geq 1}} \left(d_u^{2\alpha} + d_v^{2\alpha}\right) - 2\sum_{\substack{u\in V(G)\\ d_u\geq 1}} d_u^\alpha \sum_{\substack{v\in V(G)\\ d_v\geq 1}} d_v^\alpha \\
&\leq 2nQ_{2\alpha} - 2Q_\alpha^2
\end{aligned}$$

with equalities if and only if $\alpha = 0$ and G has no isolated vertices, or every pair of non-adjacent vertices of G have the same degree. Now the result follows easily. □

Note that (3) has been reported in [16] where it was deduced by using the estimate of the largest eigenvalue of the Laplacian matrix of the graph and pointed out that equality holds for the star. By Theorem 3, there are a lot of graphs such that equality holds in (3), e.g., the complete $(t+1)$-partite graph $K_{1,\cdots,1,n-t}$ with $t = 2, \ldots, n-2$, and the graph consisting of some copies of a complete graph with exactly one common vertex.

Let G be a graph with $n_* \geq 2$ non-isolated vertices. Then from the arguments above, we have

$$R_\alpha(G) \geq \frac{1}{2}\left(Q_{2\alpha+1} - n_* Q_{2\alpha} + Q_\alpha^2\right)$$

with equality if and only if $\alpha = 0$ or every pair of non-adjacent vertices of degree at least one in G have the same degree.

Let G be a graph. Then

$$Q_{2\alpha+1} - 2R_\alpha = \sum_{uv \in E(G)} \left(d_u^\alpha - d_v^\alpha\right)^2$$

and so [15, 16]

$$R_\alpha \leq \frac{1}{2} Q_{2\alpha+1} .$$

Equality holds if and only if $\alpha = 0$ or every component of G is regular.

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