Scientific paper

Note on the Comparison of the First and Second Normalized Zagreb Eccentricity Indices

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This paper is dedicated to Professor Milan Randić on the occasion of his 80th birthday

Abstract

The conjecture $\sum_{u\in V(G)} d_G(u)^2 / n(G) \le \sum_{uv\in E(G)} d_G(u)d_G(v) / m(G)$ that compares normalized Zagreb indices attracted recently a lot of attention[1–9]. In this paper we analyze analogous statement in which degree $d_G(u)$ of vertex u is replaced by its eccentricity $\varepsilon_G(u)$ in which way we define novel first and second Zagreb eccentricity indices. We show that $\sum_{u\in V(G)} \varepsilon_G(u)^2 / n(G) \ge \sum_{uv\in E(G)} \varepsilon_G(u)\varepsilon_G(v) / m(G)$ holds for all acyclic and unicyclic graphs and that neither this nor the opposite inequality holds for all bicyclic graphs.

Keywords: Eccentricity; normalized molecular descriptor; acyclic graphs; unicyclic graphs; bicyclic graphs;

1. Introduction

The Randić index[10] is one of the most famous molecular descriptors and the paper in which it is defined is cited more than 1000 times. This is one of the very few papers that made chemical graph theory and mathematical chemistry flourish. It is defined by

$$\chi(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u d_v}},$$

where $E(G)$ is set of edges of G and $d(x) = d_G(x)$ is degree of vertex x in G. Obviously,

$$\chi(G) = \sum_{uv\in E(G)} (d_u d_v)^{\lambda} \text{ for } \lambda = -1/2.$$

Already in this paper, author proposed observing exponents different from –1/2. Taking $\lambda = 1$, one obtains the very famous the second Zagreb index[11].

The first and the second Zagreb indices are among the oldest and best known molecular descriptors and it has been shown that they have ability to predict many physicochemical properties of chemical compounds (papers[12–14] and references within). Molecular descriptors are graph-theoretical invariants used to predict properties of chemical compounds and they have found many applications out of which one of the most important is in the rational drug design. Namely many physical and chemical properties are strongly correlated with molecular structure and then QSPR models allow predictions which molecules (out of the many theoretically obtained molecules) may be of interest.

The first M_1, and second M_2, Zagreb indices are defined as:

$$M_1 = M_1(G) = \sum_{u\in V(G)} d_G(u)^2 \text{ and}$$
$$M_2 = M_2(G) = \sum_{uv\in E(G)} d_G(u)\cdot d_G(v). \tag{1}$$

where $V(G)$ is the set of vertices of graph G. Let us denote by $n = n(G)$ the number of vertices of G and by $m = m(G)$ the number of its edges. Recently, the system AutoGraphX [13,14] (software for making conjuctures created by G. Caporossi and P. Hansen) proposed the following conjecture:

Conjecture 1. For all simple connected graphs, it holds:

$$M_1(G)/n(G) \leq M_2(G)/m(G). \qquad (2)$$

This conjecture has been disproved[1], but it has been proved that it holds for all graphs with maximum degree at most four[1], for acyclic graphs[2], for unicyclic graphs[3,4] and it has been shown that it does not hold for bicyclic graphs[4]. A crucial role in most of these proofs played the quantity $m_{ij} = m_{ij}(G)$ which denotes the number of bonds connecting vertices of degrees i and j. These quantities have been recently extensively studied[17–25].

The degree of a vertex is a natural invariant assigned to a vertex. Another very natural invariant is eccentricity $\varepsilon_G(u)$ of a vertex u, namely the maximum distance from u to other vertices, i.e. $\varepsilon_G(u) = \max\{d_G(u,v) : v \in V(G)\}$, where $d_G(u,v)$ is the distance between vertices u and v. For instance, in kenograph (graph in which hydrogen atoms are neglected) of benzene all vertices have eccentricity 3. In octane eccenticites are (in order of the aperiance of atoms) 7, 6, 5, 4, 4, 5, 6 and 7.

The invariants based on vertex eccentricities attracted some attention in chemistry[12,26]. In an analogy with the first and the second Zagreb indices, we define now the first, E_1, and second, E_2, Zagreb eccentricity indices by

$$E_1 = E_1(G) = \sum_{u \in V(G)} \varepsilon_G(u)^2 \text{ and}$$
$$E_2 = E_2(G) = \sum_{uv \in E(G)} \varepsilon_G(u) \cdot \varepsilon_G(v). \qquad (3)$$

In the present paper, we study whether and in which cases the normalized versions of these novel indices E_1 and E_2 satisfy an equation comparable to equation (2). Namely, we want to compare

$$E_1(G)/n(G) \text{ and } E_2(G)/m(G) \qquad (4)$$

In this paper we show that

$$E_1(G)/n(G) \geq E_2(G)/m(G) \qquad (5)$$

holds for all acyclic and unicyclic graphs. At the end of this paper, we present two bicyclic graphs such that inequality (5) holds for one of them, while another one satisfies just the opposite inequality. In such a way it is shown that for general graphs the inequality (5) is not always valid. The same is true for its opposite inequality.

2. Acyclic graphs

The center of the tree is a vertex with the minimal eccentricity. It is well known that tree has either one center or two adjacent centers. The path connecting a vertex with its most distant vertex is called eccentric. It is well known that:

1) if tree has only one center, then each eccentric path passes through this vertex;
2) if tree has two centers, then each eccentric path passes through the edge connecting these two centers.

Let us prove:

Theorem 2. Let G be a simple connected acyclic graph (tree). Then,

$$E_1(G)/n(G) \geq E_2(G)/m(G).$$

Proof: Let us distinguish two cases:

CASE 1: G has one center c.

Let ϕ: $E(G) \to V(G)\setminus\{c\}$ be the function which maps edge uv to one of its terminal vertices (u or v) which is more distant from the center c. Note that this function is a bijection. It holds:

$$\sum_{u\in V}\varepsilon(u)^2/n - \sum_{uv\in E}\varepsilon(u)\varepsilon(v)/m =$$

$$= \frac{(n-1)\sum_{u\in V}\varepsilon(u)^2 - n\sum_{uv\in E}\varepsilon(\phi(u,v))\cdot(\varepsilon(\phi(u,v))-1)}{n(n-1)} =$$

$$= \frac{(n-1)\varepsilon(c)^2 + \sum_{u\in V\setminus\{c\}}\left[(n-1)\cdot\varepsilon(u)^2 - n\cdot\varepsilon(u)(\varepsilon(u)-1)\right]}{n(n-1)} =$$

$$= \frac{(n-1)\varepsilon(c)^2 + \sum_{u\in V\setminus\{c\}}\left[n\cdot\varepsilon(u) - \varepsilon(u)^2\right]}{n(n-1)} > 0.$$

CASE 2: G has two centers c_1 and c_2. Let χ: $E(G)\setminus c_1c_2 \to V(G)\setminus\{c_1c_2\}$ be the function that maps edge uv to one of its terminal vertices which is more distant to c_1 and c_2. It holds:

$$\sum_{u\in V}\varepsilon(u)^2/n - \sum_{uv\in E}\varepsilon(u)\varepsilon(v)/m =$$

$$= \frac{(n-1)\sum_{u\in V}\varepsilon(u)^2 - n\cdot\varepsilon(c_1)\varepsilon(c_2) - n\sum_{uv\in E\setminus\{c_1c_2\}}\varepsilon(\chi(u,v))\cdot(\varepsilon(\chi(u,v))-1)}{n(n-1)} =$$

$$= \frac{(n-2)\varepsilon(c_1)^2 + \sum_{u\in V\setminus\{c_1,c_2\}}\left[(n-1)\cdot\varepsilon(u)^2 - n\cdot\varepsilon(u)(\varepsilon(u)-1)\right]}{n(n-1)} =$$

$$= \frac{(n-2)\varepsilon(c_1)^2 + \sum_{u\in V\setminus\{c_1,c_2\}}\left[n\cdot\varepsilon(u) - \varepsilon(u)^2\right]}{n(n-1)} > 0.$$

This proves the Theorem. ■

3. Unicyclic Graphs

Let us start with the following Lemmas:

Lemma 3. Let $n \geq 2$ and let x_0, x_1, ... x_n be positive integers such that $|x_i - x_{i+1}| \le 1$ for each $i = 0, \ldots n-1$ and $x_0 = x_n$. Then,

$$\sum_{i=0}^{n-1} x_i^2 \ge \sum_{i=0}^{n-1} x_i x_{i+1} .$$

Proof: Suppose to the contrary and let N be the smallest number such that there are positive integers y_0, $y_1, \ldots y_N$ such that $|y_i - y_{i+1}| \le 1$ for each $i = 0, \ldots, N-1$, $y_0 = y_N$ and $\sum_{i=0}^{N-1} y_i^2 < \sum_{i=0}^{N-1} y_i y_{i+1}$. Suppose that $N \ge 3$, because otherwise contradiction simply follows. Note that there is no $j \in \{0, \ldots, N-1\}$ such that $y_j = y_{j+1}$, because otherwise let $n = N-1$ and $x_0 = y_0, \ldots, x_j = y_j, x_{j+1} = y_{j+2}, \ldots, x_{N-1} = y_N$ and then it holds:

$$\sum_{i=0}^{n-1} x_i^2 = \sum_{i=0}^{N-1} y_i^2 - y_{j+1}^2 < \sum_{i=0}^{N-1} y_i y_{i+1} - y_{j+1}^2 = \sum_{i=0}^{n-1} x_i x_{i+1} ,$$

which is in contradiction with minimality of N. Let $y_j = \max\{y_0, \ldots, y_{N-1}\}$. Distinguish two cases:

CASE 1: $j \ne 0$.

Note that $y_{j-1} = y_{j+1} = y_j - 1$. Let $n = N-1$ and $x_0 = y_0, \ldots, x_{j-1} = y_{j-1}, x_j = y_{j+1}, x_{j+1} = y_{j+2}, \ldots, x_{N-1} = y_N$. We have:

$$\sum_{i=0}^{n-1} x_i^2 = \sum_{i=0}^{N-1} y_i^2 - y_j^2 < \sum_{i=0}^{N-1} y_i y_{i+1} - y_j^2 = \sum_{i=0}^{n-1} x_i x_{i+1} +$$

$$+\left[2y_j\left(y_j-1\right)-\left(y_j-1\right)^2\right]-y_j^2 < \sum_{i=0}^{n-1} x_i x_{i+1} ,$$

which is in contradiction with minimality of n.

CASE 2: $j = 0$.

Completely analogously as Case 1.

In all cases the contradiction is obtained and Lemma 3 is proved. ■

Lemma 4. Let G be any graph and let u and v be two adjacent vertices in G. Then, $|\varepsilon_G(u) - \varepsilon_G(v)| \le 1$.

Proof: Just note that for each vertex $w \in V(G)$, it holds $|d_G(u,w) - d_G(v,w)| \le 1$. ■

Let G be unicyclic graph and let us denote by $C = C(G)$ its unique cycle. Let G' be a graph obtained by deletion of all edges in $E(C)$. Note that components of G' are trees such that each of them has exactly one vertex in C. A tree with its vertex in C being x we denote by T_x. Let us denote by $X = X(G)$ the set of all vertices in C that correspond to components that are not just a single vertex.

Let us prove:

Theorem 5. Let G be a unicyclic graph. Then,

$$E_1(G)/n(G) \ge E_2(G)/m(G).$$

Proof: Note that $n(G) = m(G)$ for unicyclic graphs, hence we need to prove that

$$\sum_{u\in V(G)} \varepsilon_G(u)^2 - \sum_{uv\in E(G)} \varepsilon_G(u)\varepsilon_G(v) \ge 0 ,$$

i.e. that

$$\left[\sum_{u\in V(C)} \varepsilon_G(u)^2 - \sum_{uv\in E(C)} \varepsilon_G(u)\varepsilon_G(v)\right] +$$

$$+\sum_{x\in X}\left[\sum_{u\in V(T_x)\setminus\{x\}} \varepsilon_G(u)^2 - \sum_{uv\in E(T_x)} \varepsilon_G(u)\varepsilon_G(v)\right] \ge 0 .$$

Note that

$$\sum_{u\in V(C)} \varepsilon_G(u)^2 - \sum_{uv\in E(C)} \varepsilon_G(u)\varepsilon_G(v) \ge 0$$

follows from Lemmas 3 and 4. Hence, it is sufficient to prove that

$$\sum_{u\in V(T_x)\setminus\{x\}} \varepsilon_G(u)^2 - \sum_{uv\in E(T_x)} \varepsilon_G(u)\varepsilon_G(v) \ge 0$$

for each $x \in X$. Let us fix one $x \in X$. Let y be one of the furthest vertices from x in G. If $y \notin T_x$, then let T_x' be a tree obtained from T_x by adding pendant path of length $d(x,y)$ to vertex x. Otherwise, let $T_x' = T_x$. Let Γ_x be the set of vertices with the smallest ε_G in T_x. Let us distinguish two cases:

CASE 1: $x \in \Gamma_x$.

Let $\phi_x : E(T_x) \to V(T_x)\setminus\{x\}$ be the function that maps edge uv to one of its terminal vertices that is more distant from x. Note that this function is a bijection. It holds:

$$\sum_{u\in V(T_x)\setminus\{x\}} \varepsilon_G(u)^2 - \sum_{uv\in E(T_x)} \varepsilon_G(u)\varepsilon_G(v) =$$

$$= \sum_{uv\in E(T_x)}\left[\varepsilon_G\left(\phi_x(uv)\right)^2 - \varepsilon_G(u)\varepsilon_G(v)\right] \ge 0 .$$

CASE 2: $x \notin \Gamma_x$.

Γ_x is the center of T_x' and hence it consists of either one or two vertices (none of which is x). Let us distinguish two subcases:

SUBCASE 2.1: $\Gamma_x = \{c\}$.

Let l be a leaf on the maximum distance from x and let P_x be a path from x to l. This path passes through c, because it is an eccentric path in T_x. Let $d(x,c) = p + 1$ and $d(c,l) = q$. Note that $q \ge p + 1$.

Let ϕ_x': $E(T_x) \setminus E(P_x) \to V(T_x) \setminus V(P_x)$ be the function that maps edge uv to one of its terminal vertices which is more distant from c (or equivalently from x). Note that this function is a bijection. It holds:

$$\sum_{u\in V(T_x)\setminus\{x\}} \varepsilon_G(u)^2 - \sum_{uv\in E(T_x)} \varepsilon_G(u)\varepsilon_G(v) =$$

$$= \left[\sum_{u\in V(P_x)\setminus\{x\}} \varepsilon_{T_x'}(u)^2 - \sum_{uv\in E(P_x)} \varepsilon_{T_x'}(u)\varepsilon_{T_x'}(v)\right] +$$

$$+ \left[\sum_{uv\in E(T_x)\setminus E(P_x)} \varepsilon_{T_x'}(\phi_x'(uv)) - \varepsilon_{T_x'}(u)\varepsilon_{T_x'}(v)\right] \geq$$

$$\geq \sum_{i=0}^{p}\left(\varepsilon_{T_x'}(c)+i\right)^2 + \sum_{i=1}^{q}\left(\varepsilon_{T_x'}(c)+i\right)^2 -$$

$$-\sum_{i=0}^{p}\left(\varepsilon_{T_x'}(c)+i\right)\left(\varepsilon_{T_x'}(c)+i+1\right)$$

$$-\sum_{i=1}^{q}\left(\varepsilon_{T_x'}(c)+i\right)\left(\varepsilon_{T_x'}(c)+i-1\right)$$

$$= \varepsilon_{T_x'}(c)\cdot(q-p) + \frac{1}{2}(q-p-1)(p+q) \geq 0.$$

SUBCASE 2.2: $\Gamma_x = \{c_1, c_2\}$.

Let l be a leaf on the maximum distance from x and let P_x be a path from x to l. Since, this is eccentric path in T_x, then it passes through c_1c_2. Without loss of generality we may assume that c_1 is closer to x and that c_2 is closer to l. Let $d(x,c_2) = q + 1$ and let $d(x,c_2) = q$. Note that $q \geq p + 1$.

Let ϕ_x'': $E(T_x) \setminus E(P_x) \rightarrow V(T_x) \setminus V(P_x)$ be the function that maps edge uv to one of its terminal vertices that is more distant from c_1 (or equivalently form x or c_2). Note that this function is a bijection. It holds:

$$\sum_{u\in V(T_x)\setminus\{x\}} \varepsilon_G(u)^2 - \sum_{uv\in E(T_x)} \varepsilon_G(u)\varepsilon_G(v) =$$

$$= \left[\sum_{u\in V(P_x)\setminus\{x\}} \varepsilon_{T_x'}(u)^2 - \sum_{uv\in E(P_x)} \varepsilon_{T_x'}(u)\varepsilon_{T_x'}(v)\right] +$$

$$+ \left[\sum_{uv\in E(T_x)\setminus E(P_x)} \varepsilon_{T_x'}(\phi_x''(uv)) - \varepsilon_{T_x'}(u)\varepsilon_{T_x'}(v)\right] \geq$$

$$\geq \sum_{i=0}^{p}\left(\varepsilon_{T_x'}(c_1)+i\right)^2 + \sum_{i=1}^{q}\left(\varepsilon_{T_x'}(c_2)+i\right)^2 + \varepsilon_{T_x'}(c_2)^2$$

$$-\sum_{i=0}^{p}\left(\varepsilon_{T_x'}(c_1)+i\right)\left(\varepsilon_{T_x'}(c_1)+i+1\right) +$$

$$-\sum_{i=1}^{q}\left(\varepsilon_{T_x'}(c_2)+i\right)\left(\varepsilon_{T_x'}(c_2)+i-1\right) - \varepsilon_{T_x'}(c_1)\varepsilon_{T_x'}(c_2) =$$

$$= \varepsilon_{T_x'}(c_1)\cdot(q-p) + \frac{1}{2}(q-p-1)(p+q) \geq 0.$$

All the cases are exhausted and the Theorem 2 is proved. ■

4. Bicyclic graphs

Let G_x be a bicyclic graph with $2x + 2$ vertices presented in Fig. 1:

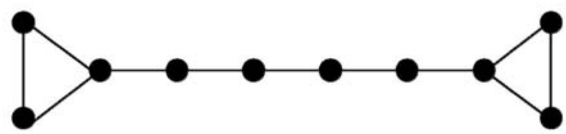

Figure 1. Graph G_x.

It can be easily calculated that:

$$\sum_{v\in V(G_x)} \varepsilon_{G_x}(u)^2 / n(G_x) -$$

$$\sum_{uv\in E(G_x)} \varepsilon_{G_x}(u)\cdot\varepsilon_{G_x}(v) / m(G_x) =$$

$$= \frac{-6 + \frac{7x}{3} + 15x^2 - \frac{10x^3}{3}}{(2x+2)(2x+3)}.$$

Hence,

$$\sum_{v\in V(G_4)} \varepsilon_{G_4}(u)^2 / n(G_4) - \sum_{uv\in E(G_4)} \varepsilon_{G_4}(u)\cdot\varepsilon_{G_4}(v) / m(G_4) > 0;$$

$$\sum_{v\in V(G_5)} \varepsilon_{G_5}(u)^2 / n(G_5) - \sum_{uv\in E(G_5)} \varepsilon_{G_5}(u)\cdot\varepsilon_{G_5}(v) / m(G_5) < 0.$$

In such a way it is shown that for general graphs the inequality (5) is not always valid. The same is true for its opposite inequality.

5. Conclusions

In this paper, we have shown that $\sum_{u\in V(G)} \varepsilon_G(u)^2 / n(G) \geq \sum_{uv\in E(G)} \varepsilon_G(u)\varepsilon_G(v) / m(G)$ holds for all acyclic and unicyclic graphs and that neither this nor the opposite inequality holds for all bicyclic graphs. We propose the further study of this inequality as an open problem.

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Povzetek

Trditev $\sum_{u\in V(G)} d_G(u)^2 / n(G) \le \sum_{uv\in E(G)} d_G(u)d_G(v) / m(G)$, ki primerja normalizirane Zagrebške indekse, je nedavno pritegnila precej pozornosti.[1–9] V tem članku analiziramo analogno trditev, v kateri stopnjo vozlišča u, $d_G(u)$, zamenjamo z njegovo ekscentričnostjo $\varepsilon_G(u)$. Po tej poti definiramo nov prvi in drugi Zagrebški indeks ekscentričnosti. Pokazali bomo, da neenakost $\sum_{u\in V(G)} \varepsilon_G(u)^2 / n(G) \ge \sum_{uv\in E(G)} \varepsilon_G(u)\varepsilon_G(v) / m(G)$ drži za vse aciklične in eno-ciklične grafe in da niti ta, niti nasprotna neenakost ne držita za vse dvo-ciklične grafe.