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ON THE AVERAGE ECCENTRICITY, THE HARMONIC INDEX AND THE LARGEST SIGNLESS LAPLACIAN EIGENVALUE OF A GRAPH

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Abstract. The eccentricity of a vertex is the maximum distance from it to another vertex and the average eccentricity $ecc(G)$ of a graph G is the mean value of eccentricities of all vertices of G. The harmonic index $H(G)$ of a graph G is defined as the sum of $\frac{2}{d_i+d_j}$ over all edges v_iv_j of G, where d_i denotes the degree of a vertex v_i in G. In this paper, we determine the unique tree with minimum average eccentricity among the set of trees with given number of pendent vertices and determine the unique tree with maximum average eccentricity among the set of n-vertex trees with two adjacent vertices of maximum degree Δ, where $n \geq 2\Delta$. Also, we give some relations between the average eccentricity, the harmonic index and the largest signless Laplacian eigenvalue, and strengthen a result on the Randić index and the largest signless Laplacian eigenvalue conjectured by Hansen and Lucas [11].

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. $deg(v)$ denotes the degree of a vertex $v \in V(G)$. For $u, v \in V(G)$, the distance $d_G(u,v)$ is defined as the length of a shortest path from u to v in G. The eccentricity of a vertex in G is the maximum distance from it to another vertex, $e_G(v) = max_{u\in V(G)} d_G(u,v)$. The average eccentricity of a graph G of order n is the mean value of eccentricities of all vertices of G, $ecc(G) = \frac{1}{n}\sum_{v\in V(G)} e_G(v)$. Dankelmann, Goddard and Swart [3] presented some upper bounds and formulas for the average eccentricity regarding the diameter and the minimum vertex degree. Tang and Zhou [19] presented some lower and upper bounds for the average eccentricity in terms of the number of vertices and edges. Du and Ilić [7] resolved five conjectures, obtained by the system AutoGraphiX, about the average eccentricity and other graph parameters, and refuted two AutoGraphiX conjectures about average eccentricity and spectral radius. In theoretical chemistry,

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molecular structure descriptors (also called topological indices) are used for modeling physico-chemical, pharmacologic, toxicologic, biological and other properties of chemical compounds. There exist several types of such indices, especially those based on vertex and edge distances [16]. Arguably, the best known of these indices is the Wiener index $W(G) = \sum_{u,v \in V(G)} d_G(u,v)$, which is defined as the sum of distances between all (unordered) pairs of vertices of the molecular graph [6]. Besides of the use in chemistry, it was independently studied due to its relevance in social science, architecture and graph theory.

Sharma, Goswami and Madan [18] introduced a distance-based molecular structure descriptor, called the eccentric connectivity index, which is defined as $\xi^c(G) = \sum_{v \in V(G)} deg(v) \times e_G(v)$. The eccentric connectivity index is deeply connected to the average eccentricity, but for each vertex v in G, $\xi^c(G)$ takes one local property (vertex degree) and one global property (vertex eccentricity) into account. For a k-regular graph G, we have $\xi^c(G) = k \times n \times ecc(G)$. For the recent results and survey, see [15, 17, 23] and [14].

The harmonic index is defined by Fajtlowicz [8]. Favaron et al. [9] considered the relationship between the harmonic index and eigenvalues. Zhong [22] found the minimum and maximum values of the harmonic index for simple connected graphs and trees, and characterized the corresponding extremal graphs. Deng et al. [4] considered the relation between the harmonic index $H(G)$ and the chromatic number $\chi(G)$ and proved that $\chi(G) \leq 2H(G)$ by using the effect of removal of a minimum degree vertex on the harmonic index. It strengthens a result relating the Randić index and the chromatic number conjectured by the system AutoGraphiX and proved by Hansen et al. in [12]. Other related results see [13, 5, 21, 20].

The signless Laplacian spectral radius q_1 of a graph G is largest eigenvalue of the signless Laplacian matrix $Q = D + A$, where D is the diagonal matrix with degrees of the vertices on the main diagonal and A is the adjacency matrix of G.

All graphs considered in this paper are simple and connected. We will determine the unique tree with minimum average eccentricity among all trees with given number of pendent vertices and determine the unique tree with maximum average eccentricity among all n-vertex trees with two adjacent vertices of maximum degree Δ, where $n \geq 2\Delta$. Also, we will give some relations between the average eccentricity, the harmonic index and the largest signless Laplacian eigenvalue.

2. **Preliminaries**

This section gives some lemmas which will be used in what follows.

Lemma 2.1. [22] *Let G be a graph with $n \geq 3$ vertices, then $H(G) \geq \frac{2(n-1)}{n}$ with equality if and only if $G \cong S_n$.*

Lemma 2.2. [20] *Let G be a graph with $n \geq 3$ vertices and $\delta(G) \geq 2$. Then $H(G) \geq 4 + \frac{1}{n-1} - \frac{12}{n+1}$ with equality if and only if $G = K^*_{2,n-2}$.*

Lemma 2.3. [2, 1] *Let G be a graph with n vertices. Then $q_1 \geq 2\lambda_1$ with equality holds if and only if G is regular.*

Lemma 2.4. [10] *Let G be a graph with n vertices and m edges. Then*

$$q_1 \leq \frac{2m}{n-1} + n - 2$$

with equality if and only if G is either K_n or S_n.

Lemma 2.5. [13] *For any connected graph G with m edges, the first Zagreb index M_1 and the harmonic index H,*

$$H \geq \frac{2m^2}{M_1}$$

with equality if and only if $deg(u) + deg(v)$ is a constant for each edge $e = uv$ of G.

Lemma 2.6. [9] *For any connected graph G with n vertices and the largest eigenvalue λ_1 of its adjacency matrix,*

$$\lambda_1 \geq \sqrt{\frac{1}{n}\sum_{u\in V}(deg(u))^2}$$

with equality if and only if the quantity $\sum\limits_{v\in N(u)} deg(v)$ is a constant independent of vertex $u \in V$, where $N(u)$ denotes the neighborhood of u.

Lemma 2.7. *Let G be a connected graph on n vertices with m edges, the harmonic index H and the largest eigenvalue λ_1 of its adjacent matrix. Then $\lambda_1 \geq m\sqrt{\frac{2}{nH}}$ with equality if and only if $deg(u)+deg(v)$ is a constant for each edge $e = uv$ of G and $\sum\limits_{w\in N(u)} deg(w)$ is a constant for every vertex u of G, where $N(u)$ denotes the neighborhood of u.*

Proof. From Lemma 2.5 and Lemma 2.6, we have

$$\lambda_1^2 \geq \frac{1}{n}\sum_{u\in V}(deg(u))^2 = \frac{1}{n}M_1 \geq \frac{2m^2}{nH}$$

So, $\lambda_1 \geq m\sqrt{\frac{2}{nH}}$ with equality if and only if $deg(u) + deg(v)$ is a constant for each edge uv of G and $\sum\limits_{v\in N(u)} deg(v)$ is a constant for every vertex u. □

3. Main results

A pendent path at a vertex v of a graph G is a path in G connecting vertex v and a pendent vertex such that all internal vertices (if exists) in this path have degree two and the degree of v is at least three.

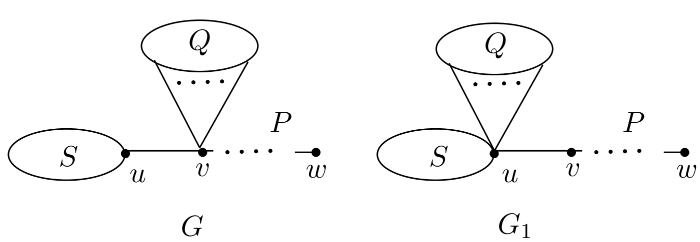

FIGURE 1. The graph G and G_1 in Lemma 3.1

Lemma 3.1. *Let G and G_1 be the graphs in Fig.1, where the path P from v to w in G is a pendent path at v, and all neighbors of v in Q of G are switched to be neighbors of u in Q of G_1. If $d_G(v,w) \leq max\{d_G(u,x) : x \in V(S)\}$, $|V(S)| > |V(P)|$ and $Q \neq \emptyset$, then $ecc(G_1) < ecc(G)$.*

Proof. Case 1. There exists an $x \in S$ such that $d(u,x) > d(v,y)$ for all $y \in Q$.

Then $e_{G_1}(y) = e_G(y) - 1 < e_G(y)$ for all $y \in Q$, $e_{G_1}(x) \leq e_G(x)$ for all $x \in S$ and $e_{G_1}(z) = e_G(z)$ for all $z \in P$. Therefore $ecc(G_1) < ecc(G)$.

Case 2. There exists an $y \in Q$ such that $d(v,y) \geq d(u,x)$ for all $x \in S$.

Then $d_G(v,y) > d_G(v,w)$ since $d_G(v,w) \leq max\{d_G(u,x) : x \in V(S)\}$, we have $e_{G_1}(x) = e_G(x) - 1$ for all $x \in S$, $e_{G_1}(v_i) \leq e_G(v_i)+1$ for all $v_i \in P$ and $e_{G_1}(y) \leq e_G(y)$ for all $y \in Q$. Since $|V(S)| > |V(P)|$, $ecc(G_1) \leq ecc(G) - \frac{1}{n}(|V(S)| - |V(P)|) < ecc(G)$. □

Specially, we can obtain the following result by taking S as a path in Lemma 3.1.

Lemma 3.2. *Let w be a vertex of a graph G with at least two vertices. For non-negative integers p and q, let $G_{p,q}$ be the graph obtained from G by attaching two paths, respectively, on p vertices and q vertices to w. If $p \geq q \geq 1$, then $ecc(G_{p+1,q-1}) > ecc(G_{p,q})$.*

Let $T(n,p)$ be the set of trees with n vertices and p pendent vertices, where $2 \leq p \leq n-1$. Let $T_{n,p}$ be the tree obtained by attaching $p-r$ paths on s vertices and r paths on $s+1$ vertices to a single vertex, where $s = \left\lfloor \frac{n-1}{p} \right\rfloor$, $r = n-1-ps$.

The following result shows that $T_{n,p}$ is the unique tree in $T(n,p)$ with the minimum average eccentricity.

Theorem 3.3. *Let $G \in T(n,p)$, where $2 \leq p \leq n-1$. Then $ecc(G) \geq ecc(T_{n,p})$ with equality if and only if $G \cong T_{n,p}$.*

Proof. The cases $p = 2$, $n-1$ are trivial. Suppose that $3 \leq p \leq n-2$. Let G be a tree in $T(n,p)$ with the minimum average eccentricity. Let $V_1(G)$ be the set of vertices in G with degree at least three. Let P be a pendent path with minimum length in G at a vertex $v \in V_1(G)$, and w be the pendent vertex of G in P. Suppose that $|V_1(G)| \geq 2$. Choose a vertex $y \in V_1(G)$ such that $d_G(v,y)$ is as small as possible. Then the internal vertices (if exist) of the unique path connecting v and y in G are all of degree two. Denote by u the neighbor of v in G lying on the path connecting v and y ($u = y$ if v and y are adjacent in G). Let S be the component of $G - vu$ containing u. Obviously, S is not a path with an end vertex u. By the choice of P, we have $d_G(v,w) \leq max\{d_G(u,x) : x \in V(S)\}$, $|V(S)| > |V(P)|$ and $Q = V(G) - V(S) - V(P) \neq \emptyset$. Applying Lemma 3.1 to G, we may get a tree $G_1 \in T(n,p)$ such that $ecc(G) > ecc(G_1)$, a contradiction. Thus $|V_1(G)| = 1$, i.e., v is the unique vertex in G with degree at least three. If $G \ncong T_{n,p}$, then by Lemma 3.2, we have $ecc(T_{n,p}) < ecc(G)$, a contradiction. It follows that $G \cong T_{n,p}$. □

For integer $r \geq 1$, let $G_{r;p,q}$ be the tree obtained from the path $P_2 = uv$ by attaching r pendent vertices and a path on p vertices to u, and attaching r pendent vertices and a path on q vertices to v, where $p \geq q \geq 1$.

Lemma 3.4. *For positive integers p, q with $p \geq q \geq 2$, $ecc(G_{r;p+1,q-1}) > ecc(G_{r;p,q})$*

Proof. Let u and v be the two vertices in which r pendent vertices $u_1, u_2, \ldots, u_r$ is attached to u and the pendent vertices $v_1, v_2, \ldots, v_r$ is attached to v. A path $ux_1, x_2, \cdots, x_{p-1}$ on p vertices is attached to u and a path $vy_1, y_2, \cdots, y_{q-1}$ on q vertices is attached to v. Then $e_{G_{r;p,q}}(u_i) = max\{p, q+1\}$.

Case 1. $p \geq q+1$.

Clearly, $e_{G_{r;p,q}}(u_i) = p$, $1 \leq i \leq r$ and $e_{G_{r;p+1,q-1}}(u_i) = p+1$, $1 \leq i \leq r$. Also $e_{G_{r;p,q}}(v_i) = p+1$, $1 \leq i \leq r$ and $e_{G_{r;p+1,q-1}}(v_i) = p+2$, $1 \leq i \leq r$. The sum of the eccentricities of other vertices are equal in $G_{r;p,q}$ and $G_{r;p+1,q-1}$. So, $ecc(G_{r;p+1,q-1}) - ecc(G_{r;p,q}) = \frac{2r}{p+q+2r} > 0$.

Case 2. $p = q$.

We have $e_{G_{r;p+1,q-1}}(w) = e_{G_{r;p,q}}(w) + 1$, where w is the pendent vertex incident with v. The sum of the eccentricities of the other vertices are same in $G_{r;p,q}$ and $G_{r;p+1,q-1}$. Therefore, $ecc(G_{r;p+1,q-1}) - ecc(G_{r;p,q}) > 0$. □

Let $D_{n,\Delta}$ be the tree obtained by adding an edge between the centers of two vertex-disjoint stars S_Δ, and attaching a path on $n - 2\Delta + 1$ vertices to a pendent vertex.

The following result shows that $D_{n,\Delta}$ is the unique tree with the maximum average eccentricity among all n-trees with two adjacent vertices of maximum degree Δ.

Theorem 3.5. *Let G be an n-vertex tree with two adjacent vertices of maximum degree Δ, where $\Delta \leq \frac{n}{2}$. Then $ecc(G) \leq ecc(D_{n,\Delta})$ with equality if and only if $G \cong D_{n,\Delta}$.*

Proof. Let G be a tree with maximum average eccentricity among n-vertex trees with two adjacent vertices u and v of maximum degree Δ. By Lemma 3.2, we have $G \cong G_{r;p,q}$, where $r = \Delta - 2$, $p \geq q \geq 1$, and $p + q = n - 2\Delta + 2$. If $q \geq 2$, then by Lemma 3.4, $ecc(G) = ecc(G_{r;p,q}) < ecc(G_{r;p+1,q-1})$, a contradiction. Thus $q = 1$ and $p = n - 2\Delta + 1$, i.e., $G \cong D_{n,\Delta}$. □

In the following, we discuss the relation between the harmonic index $H(G)$ and the average eccentricity $ecc(G)$ of a graph G.

Theorem 3.6. *Let G be a graph with $n \geq 5$. Then $H(G) + ecc(G) \geq 4 - \frac{3}{n}$ with equality if and only if $G \cong S_n$.*

Proof. If there is no vertex of degree $n-1$ in G, then $ecc(G) \geq 2$. By Lemma 2.1, we have $H(G) \geq \frac{2(n-1)}{n} = 2 - \frac{2}{n}$, and $H(G) + ecc(G) \geq 4 - \frac{2}{n} > 4 - \frac{3}{n}$. □

Let s be the number of vertices of degree $n-1$ in G. Then $ecc(G) = 2 - \frac{s}{n}$ for $s \geq 1$.

If $s = 1$, then $ecc(G) = 2 - \frac{1}{n}$ and $H(G) \geq \frac{2(n-1)}{n} = 2 - \frac{2}{n}$ by Lemma 2.1. So, $H(G) + ecc(G) \geq 4 - \frac{3}{n}$ with equality if and only if $G \cong S_n$.

If $2 \leq s \leq n-2$, then the minimum degree $\delta(G)$ of G is at least 2 and $ecc(G) \geq 2 - \frac{n-2}{n} = 1 + \frac{2}{n}$. By Lemma 2.2, $H(G) \geq 4 + \frac{1}{n-1} - \frac{12}{n+1}$. We have

$$H(G) + ecc(G) \geq 5 + \frac{1}{n-1} + \frac{2}{n} - \frac{12}{n+1} > 4 - \frac{3}{n}.$$

If $s > n-2$, then $s = n$ and G is the complete graph K_n. We have $H(G) = \frac{n}{2}$ and $ecc(G) = 1$. So, $H(G) + ecc(G) = \frac{n}{2} + 1 > 4 - \frac{3}{n}$ for $n \geq 5$.

Theorem 3.7. *Let G be a graph with n vertices. If $3 \le n \le 6$, then $H(G) \times ecc(G) \ge \frac{n}{2}$ with equality if and only if $G \cong K_n$; if $n \ge 7$, then $H(G) \times ecc(G) \ge \frac{2(n-1)}{n}\left(2-\frac{1}{n}\right)$ with equality if and only if $G \cong S_n$.*

Proof. Let s be the number of vertices of degree $n-1$ in G. Then $ecc(G) = 2 - \frac{s}{n}$ for $s \ge 1$.

If $s = 0$, then $ecc(G) \ge 2$, and together with Lemma 2.1, we have

$$H(G) \times ecc(G) \ge \left(\frac{2(n-1)}{n}\right) \times 2 > \frac{2(n-1)}{n}\left(2-\frac{1}{n}\right).$$

If $s = 1$, then $ecc(G) = 2-\frac{1}{n}$ and $H(G) \ge \frac{2(n-1)}{n}$ by Lemma 2.1. So, $H(G)\times ecc(G) \ge \frac{2(n-1)}{n}\times(2-\frac{1}{n})$ with equality if and only if $G \cong S_n$.

If $2 \le s \le n-2$, then the minimum degree $\delta(G)$ of G is at least 2 and $ecc(G) \ge 2 - \frac{n-2}{n} = 1 + \frac{2}{n}$. By Lemma 2.2, $H(G) \ge 4 + \frac{1}{n-1} - \frac{12}{n+1}$. We have

$$H(G) \times ecc(G) \ge (4 + \frac{1}{n-1} - \frac{12}{n+1}) \times (1 + \frac{2}{n}) > \frac{2(n-1)}{n} \times (2 - \frac{1}{n}).$$

If $s > n-2$, then $s = n$ and G is the complete graph K_n. We have $H(G) = \frac{n}{2}$, $ecc(G) = 1$, and $H(G) \times ecc(G) = \frac{n}{2}$. Note that $\frac{n}{2} < \frac{2(n-1)}{n} \times (2-\frac{1}{n})$ for $3 \le n \le 6$. So, $H(G) \times ecc(G) \ge \frac{n}{2}$ for $3 \le n \le 6$. □

Using Lemmas 2.3, 2.4 and 2.7, we can obtain a relation between the harmonic index $H(G)$ and the largest signless Laplacian eigenvalue q_1 of a graph G.

Theorem 3.8. *Let G be a connected graph with $n \ge 3$ vertices with the largest signless Laplacian eigenvalue q_1 and Harmonic index H. Then $q_1 - H \le \frac{3n}{2} - 2$, with equality if and only if $G \cong K_n$.*

Proof. Let m be the number of edges of G. Then $n-1 \le m \le \frac{n(n-1)}{2}$. Using Lemma 2.3, 2.4 and 2.7, we have

$$q_1 - H \le q_1 - \frac{8m^2}{nq_1^2} \le \frac{2m}{n-1} + n - 2 - \frac{8m^2}{n\left(\frac{2m}{n-1}+n-2\right)^2}$$
$$= \frac{2m}{n-1} + n - 2 - \frac{8m^2(n-1)^2}{n(2m+(n-1)(n-2))^2}$$

Let $f(m) = \frac{2m}{n-1}+n-2-\frac{8m^2(n-1)^2}{n(2m+(n-1)(n-2))^2}$. The derivative of $f(m)$ is $f'(m) = \frac{2}{n-1} - \frac{16m(n-1)^3(n-2)}{n(2m+(n-1)(n-2))^3} = \frac{2}{n-1} - \frac{16(n-1)^3(n-2)}{n} \times g(m)$, where $g(m) = \frac{m}{(2m+(n-1)(n-2))^3}$. The derivative of $g(m)$ is $g'(m) = \frac{n^2-3n+2-4m}{(2m+(n-1)(n-2))^4}$. From $g'(m) = 0$, we have $m = \frac{n^2-3n+2}{4}$ and $g(m) \le g(\frac{n^2-3n+2}{4}) = \frac{2}{27(n-1)^2(n-2)^2}$. So, $f'(m) \ge \frac{2}{n-1} - \frac{16(n-1)^3(n-2)}{n} \times \frac{2}{27(n-1)^2(n-2)^2} = \frac{2(11n^2-22n-16)}{27n(n-1)(n-2)} > 0$. Thus, $q_1 - H \le f\left(\frac{n(n-1)}{2}\right) = \frac{3}{2}n - 2$ with equality if and only if $m = \frac{n(n-1)}{2}$, i.e., $G \cong K_n$. □

Since $H(G) \le R(G)$ for a graph G, Theorem 3.8 strengthens a result relating the Randić index and the largest signless Laplacian eigenvalue conjectured by Hansen and Lucas [11].

Corollary 3.9. *Let G be a connected graph on $n \ge 4$ vertices with the largest signless Laplacian eigenvalue q_1 and Randić index R. Then $q_1 - R \le \frac{3n}{2} - 2$ with equality if and only if $G \cong K_n$.*

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