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The Maximal Geometric–Arithmetic Energy of Trees^{*}

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Abstract

Let G be a graph of order n with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set E(G), and $d(v_i)$ be the degree of the vertex v_i . The geometric-arithmetic matrix of G is the matrix of order n whose (i, j)-entry is equal to $\frac{2\sqrt{d(v_i)d(v_j)}}{d(v_i)+d(v_j)}$ if $v_iv_j \in E(G)$, and 0 otherwise. The geometric-arithmetic energy of G is the sum of the absolute values of the eigenvalues of its geometric-arithmetic matrix. In 2019, Y. Shao et al. [1] conjectured that the path P_n has the maximal geometric-arithmetic energy among all trees of order $n \geq 4$. In this paper, we prove that the conjecture is true, and in fact, the result holds also for n = 1, 2, 3.

1 Introduction

Let G be a graph of order n with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set E(G). For $i = 1, 2, \ldots, n$, denote by $d_G(v_i)$ (or $d(v_i)$ for short) the degree of the vertex v_i in G. A edge $v_i v_j \in E(G)$ is called a pendent edge of G if $d_G(v_i) = 1$ or $d_G(v_j) = 1$. Let T be a tree. A vertex v is called a branched vertex of T if $d_T(v) \ge 3$.

The geometric-arithmetic (or GA, for short) index of a graph G, introduced by Vukičević and Furtula as a topological index ([2]), is defined as $GA(G) = \frac{2\sqrt{d(v_i)d(v_j)}}{d(v_i)+d(v_j)}$

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if $v_i v_j \in E(G)$. In [3, 4], Rodríguez and Sigarreta introduced the GA matrix and GAenergy of a graph. Let G be a graph of order n. The GA matrix of G, denoted by M(G), is the matrix of order n whose (i, j)-entry is equal to $\frac{2\sqrt{d(v_i)d(v_j)}}{d(v_i)+d(v_j)}$ if $v_i v_j \in E(G)$, and 0 otherwise. The characteristic polynomial of M(G), denoted by $\phi_{GA}(G, x) = |xI - M(G)|$, is called the GA characteristic polynomial of G. The n roots of the equation $\phi_{GA}(G, x) = 0$, denoted by $\mu_1(G), \mu_2(G), \ldots, \mu_n(G)$, are called the GA eigenvalues of G. Since M(G) is real and symmetric, all GA eigenvalues of G are real. The GA energy of G is defined as $\mathcal{E}_{GA}(G) = \sum_{i=1}^{n} |\mu_i(G)|$.

In [1], Shao and Gao studied the maximal GA energy of trees of order n. They proved that the path of order n has the maximal geometric-arithmetic energy among all trees of order n with at most two branched vertices, and conjectured the result also hold for all trees of order n.

Theorem 1.1 ([1]) Let T be a tree of order $n \ge 4$ with at most two branched vertices. Then

$$\mathcal{E}_{GA}(T) \leq \mathcal{E}_{GA}(P_n).$$

Equality holds if and only if T is isomorphic to the path P_n .

It is clear that the result holds also for n = 1, 2, 3.

Conjecture 1.2 ([1]) Let T be a tree of order $n \ge 4$. Then

$$\mathcal{E}_{GA}(T) \leq \mathcal{E}_{GA}(P_n).$$

Equality holds if and only if T is isomorphic to the path P_n .

In this paper, we prove that this conjecture is true, and in fact, the result holds also for n = 1, 2, 3.

2 Preliminaries

For a graph G, we use $\mathcal{M}_k(G)$ to denote the set of all k-matchings of G. If $e = v_i v_j \in E(G)$, then we denote

$$GA_G(e) = GA_G(v_i v_j) = \left(\frac{2\sqrt{d(v_i)d(v_j)}}{d(v_i) + d(v_j)}\right)^2$$

and we say that $GA_G(e)$ is the GA value of the edge e. If $\alpha_k = \{e_1, e_2, \dots, e_k\} \in \mathcal{M}_k(G)$, we call that $\prod_{i=1}^k GA_G(e_i)$ is the GA value of matching α_k , and write $GA_G(\alpha_k) = \prod_{i=1}^k GA_G(e_i)$.

Let T be a tree T of order n with GA matrix M(T). Then the GA characteristic polynomial of T can be written as ([1])

$$\phi_{GA}(T,x) = |xI - M(T)| = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(M(T),k) x^{n-2k}$$

where b(M(T), 0) = 1, and $b(M(T), k) = \sum_{\alpha_k \in \mathcal{M}_k(T)} GA_G(\alpha_k)$ for $1 \le k \le \lfloor \frac{n}{2} \rfloor$.

Lemma 2.1 ([1]) Let T_1 and T_2 be two trees of order n, and their GA characteristic polynomials be

$$\phi_{GA}(T_1, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(M(T_1), k) x^{n-2k}, \quad \phi_{GA}(T_2, x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(M(T_2), k) x^{n-2k},$$

respectively. If $b(M(T_1), k) \ge b(M(T_2), k)$ for all $k \ge 0$, and there is a positive integer k such that $b(M(T_1), k) > b(M(T_2), k)$, then

$$\mathcal{E}_{GA}(T_1) > \mathcal{E}_{GA}(T_2).$$

Lemma 2.2 ([5]) Let T be a tree of order n. Then $|\mathcal{M}_k(T)| \leq |\mathcal{M}_k(P_n)|$ for $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$.

Lemma 2.3 Let $f(x, y) = \frac{2\sqrt{xy}}{x+y}$.

- (1) For x = 1 and $y \ge 1$, f(1, y) is a monotonically decreasing function on y.
- (2) For $x \ge 1$ and $y \ge 1$, $f(x, y) \le 1$, and equality holding if and only if x = y.

3 Main result

In this section, we will prove the following main theorem, it implies that Conjecture 1.2 holds.

Theorem 3.1 Let T be a tree of order $n \ge 1$. Then

$$\mathcal{E}_{GA}(T) \leq \mathcal{E}_{GA}(P_n).$$

Equality holds if and only if T is isomorphic to the path P_n .

Proof. For n = 1, 2, 3, it is clear that the result holds. For $n \ge 4$, by Theorem 1.1, we only need to prove that $\mathcal{E}_{GA}(T) < \mathcal{E}_{GA}(P_n)$ for any tree T of order n with at least three branched vertices.

Let T be a tree of order n with at least three branched vertices. Then there are at least two pendent edges which have no common vertex. This fact implies that T is a tree as depicted in Figure 3.1, where T_1 is a tree of order n - 2, and $v_2, v_{n-1} \in V(T_1)$.

Consider the tree T' which is obtained from T by replacing T_1 with the path of order n-2. Clearly, T' is a path of order of n as depicted in Figure 3.2. For $1 \le i < j \le n$, use P_{v_i,v_j} to denote the path of T' from v_i to v_j . We will prove that $\mathcal{E}_{GA}(T) < \mathcal{E}_{GA}(T')$.

$$\underbrace{v_1 \quad v_2}_{\textbf{I}} \underbrace{v_1 \quad v_2 \quad v_3 \quad \dots \quad v_{n-2} \quad v_{n-1} \quad v_n}_{\textbf{I}}$$

Figure 3.1 Tree T

Figure 3.2 Tree T'

Let the GA characteristic polynomials of T and T' be

$$\phi_{GA}(T,x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(M(T),k) x^{n-2k}, \quad \phi_{GA}(T',x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b(M(T'),k) x^{n-2k},$$

respectively.

By Lemmas 2.2, and 2.3, for $1 \le i < j \le n$,

$$\begin{aligned} GA_T(v_i v_j) &\leq \begin{cases} \frac{2\sqrt{2}}{3} < 1, & \text{if } v_i v_j \text{ is a pendent edge of } T\\ 1, & \text{otherwise,} \end{cases} \\ GA_{T'}(v_i v_j) &= \begin{cases} \frac{2\sqrt{2}}{3} < 1, & \text{if } i = 1 \text{ or } j = n, \\ 1, & \text{otherwise,} \end{cases}, \end{aligned}$$

and for any positive integer ℓ ,

$$\begin{split} &\sum_{\substack{\alpha'_{\ell} \in \mathcal{M}_{\ell}(P_{v_2,v_{n-1}})} GA_{T'}(\alpha'_{\ell}) = |\mathcal{M}_{\ell}(P_{v_2,v_{n-1}})| \geq \sum_{\alpha_{\ell} \in \mathcal{M}_{\ell}(T_1)} GA_{T}(\alpha_{\ell}), \\ &\sum_{\substack{\alpha'_{\ell} \in \mathcal{M}_{\ell}(P_{v_3,v_{n-1}})} GA_{T'}(\alpha'_{\ell}) = |\mathcal{M}_{\ell}(P_{v_3,v_{n-1}})| \geq \sum_{\alpha_{\ell} \in \mathcal{M}_{\ell}(T_1 - v_2)} GA_{T}(\alpha_{\ell}), \\ &\sum_{\substack{\alpha'_{\ell} \in \mathcal{M}_{\ell}(P_{v_2,v_{n-2}})} GA_{T'}(\alpha'_{\ell}) = |\mathcal{M}_{\ell}(P_{v_3,v_{n-2}})| \geq \sum_{\alpha_{\ell} \in \mathcal{M}_{\ell}(T_1 - v_{n-1})} GA_{T}(\alpha_{\ell}), \\ &\sum_{\alpha'_{\ell} \in \mathcal{M}_{\ell}(P_{v_3,v_{n-2}})} GA_{T'}(\alpha'_{\ell}) = |\mathcal{M}_{\ell}(P_{v_3,v_{n-2}})| \geq \sum_{\alpha_{\ell} \in \mathcal{M}_{\ell}(T_1 - v_2 - v_{n-1})} GA_{T}(\alpha_{\ell}). \end{split}$$

Since there are at least three pendent edges of T, it is clear that

$$b(M(T),1) = \sum_{e \in E(T)} GA_T(e) < \sum_{e \in E(T')} GA_T(e) = b(M(T'),1).$$

For $2 \le k \le \lfloor \frac{n}{2} \rfloor$, $b(M(T'), k) = \sum_{\alpha'_k \in \mathcal{M}_k(T')} GA_{T'}(\alpha'_k) = \sum_{\alpha'_k \in \mathcal{M}_k(P_{v_2,v_{n-1}})} GA_{T'}(\alpha'_k) + GA_{T'}(v_1v_2) \sum_{\alpha'_{k-1} \in \mathcal{M}_{k-1}(P_{v_3,v_{n-1}})} GA_{T'}(\alpha'_{k-1}) + GA_{T'}(v_{n-1}v_n) \sum_{\alpha'_{k-1} \in \mathcal{M}_{k-1}(P_{v_2,v_{n-2}})} GA_{T'}(\alpha'_{k-1}) + GA_{T'}(v_1v_2)GA_{T'}(v_{n-1}v_n) \sum_{\alpha'_{k-2} \in \mathcal{M}_{k-2}(P_{v_3,v_{n-2}})} GA_{T'}(\alpha'_{k-2}) \\ \ge \sum_{\alpha_k \in \mathcal{M}_k(T_1)} GA_{T}(\alpha_k) + GA_{T}(v_1v_2) \sum_{\alpha_{k-1} \in \mathcal{M}_{k-1}(T_1-v_2)} GA_{T}(\alpha_{k-1}) + GA_{T}(v_1v_2)GA_{T}(v_{n-1}v_n) \sum_{\alpha_{k-2} \in \mathcal{M}_{k-2}(T_1-v_2-v_{n-1})} GA_{T}(\alpha_{k-2}) \\ = b(M(T), k),$

By Lemma 2.1, $\mathcal{E}_{GA}(T) < \mathcal{E}_{GA}(T') = \mathcal{E}_{GA}(P_n)$. So the theorem now follows.

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References

- Y. Shao, Y. Gao, The maximal geometric-arithmetic energy of trees with at most two branched vertices, Appl. Math. Comput. 362 (2019) #124528.
- [2] D. Vukičević, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, J. Math. Chem. 46 (2009) 1369– 1376.
- [3] J. M. Rodríguez, J. M. Sigarreta, Spectral study of the geometric-arithmetic index, MATCH Commun. Math. Comput. Chem. 74 (2015) 121–135.
- [4] J. M. Rodríguez, J. M. Sigarreta, Spectral properties of geometric-arithmetic index, Appl. Math. Comput. 277 (2016) 142–153.
- [5] I. Gutman, Acyclic systems with extremal Hückel: π-electron energy, Theor. Chim. Acta 45 (1977) 79–87.