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On the Two Conjectures of the Wiener Index *

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Abstract

The Wiener index of a graph, which is the sum of the distances between all pairs of vertices, has been well studied. Recently, Sills and Wang in 2012 proposed two conjectures on the maximal Wiener index of trees with a given degree sequence. This note proves one of the two conjectures and disproves the other.

1 Introduction

The Wiener index of a molecular graph is one of the most classic and well-known topological indices in the molecular graph, which was introduced by and named by Wiener [14] in 1947. It has been extensively studied by chemists and mathematicians over the past years, see for instance [2]. In the past decade years, the extremal trees that maximize or minimize the Wiener index among trees with prescribed maximum degree, diameter, matching and independence numbers, etc., have been studied (see [5, 9, 15] etc.).

Since the degrees of a molecular graph corresponds to the valences of the atoms, it is one of the most interesting aspects to consider all trees with a prescribed degree sequence. Wang [12] and Zhang at al. [15] independently proved the extremal tree that minimizes the Wiener index is greedy tree through different approaches. Moreover, the extremal tree that maximizes the Wiener index in this category in [12] is incorrect by pointed out in [13] and [16]. Therefore it is still open problem.

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Problem 1.1. *Characterize the extremal trees that maximize the Wiener index with prescribed degree sequence.*

Zhang et al. [16] provided some part results with less than 7 internal vertices. Cela et al. [2] provide an efficient algorithm for finding the extremal trees with prescribed degree sequence. Recently, Sills and Wang [11] further studied the maximal Wiener index and disclosed some relations between the candidate trees for the maximal Wiener index and the symmetric Dyck paths.

Let $T = (V, E)$ be a tree of order n. The *Wiener index* $W(T)$ of T is defined as

$$W(T) := \sum_{\{u,v\}\subseteq V} d(u, v),$$

where $d(u, v)$ is the number of edges in a shortest path from u to v. A nonincreasing sequence of nonnegative integers $\pi = (d_1, d_2, \cdots, d_n)$ is called *graphic* if there exists a simple graph having π as its vertex degree sequence. In particular, if $\sum_{i=1}^{n} d_i = 2(n - 1)$, then π is graphic and any graph with degree sequence π is tree and let $\mathcal{T}_\pi$ denote the set of all trees with degree sequence π. Moreover, if

$$d_1 \geq d_2 \geq \cdots \geq d_k \geq 2 > d_{k+1} = d_{k+2} = \cdots = d_n = 1,$$

then $b = (b_1, \ldots, b_k) := (d_1 - 1, \ldots, d_k - 1)$ is called the *decremented degree sequence* [11]. A *caterpillar* is a tree in which a single path (called *Spine*) is incident to (or contains) every edge. For other terminologies and notions, we follow from [1,11]. Since it has been proved [16] that a tree with maximum Wiener index in $\mathcal{T}_\pi$ has to be a caterpillar, it is interesting and important to study the Wiener index of caterpillars. Let T be a caterpillar of order n with $n - k$ leaves and the non-leaf vertices $v_1, \ldots, v_k$. Then the Winer index of T is presented in [16]

$$W(T) = (n - 1)^2 + q(x)\,,$$

where $q(x)$is the quadratic form

$$q(x) = \frac{1}{2}\sum_{i=1}^{k}\sum_{j=1}^{k} |i - j| x_i x_j = x^T A_k x\,, \tag{1}$$

$A_k = (a_{ij})$ with $a_{ij} = \frac{1}{2}|i - j|$, $x = (x_1, \ldots, x_k)^T$, and $x_i = deg(v_i) - 1$ for $i = 1, \ldots, k$. In order to obtain some useful upper bounds for the Wiener index in $\mathcal{T}_\pi$, Sills and Wang observed the largest eigenvalue of A_k is about to

$$\lambda_{\max} \approx \frac{\sqrt{3}k^2 - 2}{10}\ . \tag{2}$$

Further, they disclosed some interesting combinatorial relations to other objects from this study and proposed the following conjecture.

Conjecture 1.2. *[11] Let $A_k = (a_{ij})$ be the $k \times k$ matrix with $a_{ij} = \frac{1}{2}|i-j|$. If $C_k(\lambda) = det(A_k - \lambda I_k)$ is the characteristic polynomial of A_k, then*

$$C_k(\lambda) = (-1)^k \lambda^k \left(1 - \frac{k}{4}\sum_{j=1}^{k-1} \frac{j}{j+1} \binom{k+j}{2j+1} \lambda^{-j-1}\right). \tag{3}$$

On the other hand, Silly and Wang [11] characterized all extremal trees that maximize in all chemical trees with prescribed degree sequence $\pi = (d_1, \ldots, d_n)$ with $4 \geq d_1 \geq \cdots \geq d_n = 1$. This result can be stated as follows:

Theorem 1.3. *[11] Let $\pi = (d_1, \ldots d_k, d_{k+1}, \ldots, d_n)$ with $4 \geq d_1 \geq \cdots \geq d_k > d_{k+1} = \cdots = d_n = 1$ and let $b = (b_1, \ldots, b_k)$ be the decrmented degree sequence. If $\{b_1, b_2, \ldots, b_k\} = \{\underbrace{a_s, \ldots, a_s}_{m_s}, \underbrace{a_{s-1}, \ldots, a_{s-1}}_{m_{s-1}}, \ldots, \underbrace{a_1, \ldots, a_1}_{m_1}\}$ with $a_s > a_{s-1} > \cdots > a_1$, then $q(x)$ is maximized by*

$$x = \{\underbrace{a_s, \ldots, a_s}_{l_s}, \underbrace{a_{s-1}, \ldots, a_{s-1}}_{l_{s-1}}, \ldots, \underbrace{a_1, \ldots, a_1}_{m_1}, \ldots, \underbrace{a_{s-1}, \ldots, a_{s-1}}_{r_{s-1}}, \underbrace{a_s, \ldots, a_s}_{r_s}\},$$

where $|l_i - r_i| \leq 1$ and $l_i + r_i = m_i$ for $i = 2, \ldots, s$.

Further, they [11] proposed the following conjecture

Conjecture 1.4. *[11] When k is much larger than s, for*

$$\{b_1, b_2, \ldots, b_k\} = \{\underbrace{a_s, \ldots, a_s}_{m_s}, \underbrace{a_{s-1}, \ldots, a_{s-1}}_{m_{s-1}}, \ldots, \underbrace{a_1, \ldots, a_1}_{m_1}\}$$

with $a_s > a_{s-1} > \cdots > a_1$, then $q(x)$ is maximized by

$$x = \{\underbrace{a_s, \ldots, a_s}_{l_s}, \underbrace{a_{s-1}, \ldots, a_{s-1}}_{l_{s-1}}, \ldots, \underbrace{a_1, \ldots, a_1}_{m_1}, \ldots, \underbrace{a_{s-1}, \ldots, a_{s-1}}_{r_{s-1}}, \underbrace{a_s, \ldots, a_s}_{r_s}\},$$

where $|l_i - r_i| \leq 1$ and $l_i + r_i = m_i$ for $i = 2, \ldots, s$.

This note is motivated by the above two conjectures. The rest of the note is organized as follows: In next Section, we prove Conjecture 1.2; while in Section 3, we disprove Conjecture 1.4.

2 Proof of Conjecture 1.2

Before presenting a proof of Conjecture 1.2, we need some notations. Let $G = (V, E)$ be a connected graph with $V = \{v_1, \ldots, v_n\}$, Graham and Pollak [6] introduced the *distance matrix* $D(G) = (d_{ij})$ of G with $d_{ij} = d(v_i, v_j)$ arising from a data communication problem. Graham and Lovász [7] proved that the coefficients of the characteristic polynomial of the distance matrix of a tree can be expressed in terms of the number of certain subforests of the tree and conjectured that the sequence of coefficients was unimodal with peak at the center. Colllins [3] proved that the coefficients for a path on n vertices are unimodal with peak at $(1 - 1/\sqrt{5})n$. From the context, it is easy to get the following Lemma from [3]

Lemma 2.1. *[3] Let P_n be a path of order n and distance matrix $D(P_n) = (d_{ij})$ with $d_{ij} = |i - j|$, i.e.,*

$$D(P_n) = \begin{pmatrix} 0 & 1 & 2 & \ldots & n-1 \\ 1 & 0 & 1 & \ldots & n-2 \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ n-1 & n-2 & n-3 & \ldots & 0 \end{pmatrix}.$$

let δ_i be the coefficient of λ^i in the distance matrix polynomial $\det(D(P_n) - \lambda I_n)$. *Then*

$$\delta_n = (-1)^n, \ \delta_{n-i} = (-1)^{n-1} \frac{2^{i-2} n(i-1)}{i} \begin{pmatrix} n+i-1 \\ 2i-1 \end{pmatrix}, \qquad for \quad i = 1, \ldots, n.$$

Proof. It follows from [3]. ∎

Now we are ready to prove Conjecture 1.2

Theorem 2.2. *Let $A_k = (a_{ij})$ be the $k \times k$ matrix with $a_{ij} = \frac{1}{2}|i - j|$. If $C_k(\lambda) = det(A_k - \lambda I_k)$ is the characteristic polynomial of A_k, then*

$$C_k(\lambda) = (-1)^k \lambda^k \left(1 - \frac{k}{4} \sum_{j=1}^{k-1} \frac{j}{j+1} \begin{pmatrix} k+j \\ 2j+1 \end{pmatrix} \lambda^{-j-1} \right).$$

Proof. Clearly, $A_k = \frac{1}{2} D(P_k)$. Then by Lemma 2.1

$$\begin{aligned} C_k(\lambda) &= \det(A_k - \lambda I) = \det(\frac{1}{2} D(P_k) - \lambda I) \\ &= (\frac{1}{2})^k \det(D(P_k) - (2\lambda) I_k) \\ &= (\frac{1}{2})^k ((-1)^k (2\lambda)^k + \cdots + \delta_{n-i} (2\lambda)^{n-i} + \cdots + \delta_0) \\ &= (-1)^k \lambda^k + \cdots + \frac{(-1)^{k-1}(i-1)k}{4i} \begin{pmatrix} k+i-1 \\ 2i-1 \end{pmatrix} \lambda^{k-i} + \cdots + \frac{(-1)^{k-1}(k-1)}{4} \\ &= (-1)^k \lambda^k \left(1 - \frac{k}{4} \sum_{j=1}^{k-1} \frac{j}{j+1} \begin{pmatrix} k+j \\ 2j+1 \end{pmatrix} \lambda^{-j-1} \right). \end{aligned}$$

Hence Theorem 2.2 holds. ■

On the largest eigenvalue of A_k, there is the following result.

Theorem 2.3. *The largest eigenvalue of* $A_k = (a_{ij})$ *with* $a_{ij} = \frac{1}{2}|i-j|$ *is equal to*

$$\lambda_{\max} = \frac{1}{2(\cosh\theta - 1)},$$

where θ *is the positive solution of* $\tanh(\frac{\theta}{2})\tanh(\frac{k\theta}{2}) = \frac{1}{k}$. *Moreover,*

$$\lambda_{\max} = \frac{k^2}{4a^2} - \frac{2+a^2}{12a^2} + o(\frac{1}{n^2}),$$

where a *is the root of* $a\tanh(a) = 1$, *i.e,* $a \approx 1.199679$.

Proof. It follows from $A_k = \frac{1}{2}D(P_k)$, Theorem 2.1 and Corollary 2.2 in [10] ■

3 Disproof of Conjecture 1.4

In order to disprove Conjecture 1.4, we first present the following result

Theorem 3.1. *Let* $\{b_1, b_2, \ldots, b_k\} = \{\underbrace{a_s, \ldots, a_s}_{m_s}, \underbrace{a_{s-1}, \ldots, a_{s-1}}_{m_{s-1}}, \ldots, \underbrace{a_1, \ldots, a_1}_{m_1}\}$ *with* $a_s > a_{s-1} > \cdots > a_1$. *If* $a_s > \sum_{i=1}^{s-1} m_i a_i$ *and* $m_s = 2h+1$, *then* $q(x)$ *is uniquely maximized by*

$$x = \{\underbrace{a_s, \ldots, a_s}_{h+1}, \underbrace{a_1, \ldots, a_1}_{m_1}, \ldots, \underbrace{a_{s-1}, \ldots, a_{s-1}}_{r_{s-1}}, \underbrace{a_s, \ldots, a_s}_{h}\}.$$

Proof. It is easy to see that the assertion hold for $s = 2$ or $k \leq 5$. Now assume that $q(x)$ is maximized by $x = \{x_1, \ldots, x_k\}$ for $k > 5$ and $s \geq 3$. Then by Theorem 2.7 in [16], there exists a $2 \leq t \leq k-2$ such that

$$\sum_{i=1}^{t-2} x_i \leq \sum_{i=t+1}^{k} x_i, \quad \sum_{i=1}^{t-1} x_i > \sum_{i=t+2}^{k} x_i, \tag{4}$$

and either $x_1 \geq \cdots \geq x_t,\ x_t \leq x_{t+1} \leq \cdots \leq x_k$ or $x_1 \geq \cdots \geq x_{t-1},\ x_{t-1} \leq x_{t+1} \leq \cdots \leq x_k$. Hence x can be rewritten as

$$x = \{\underbrace{a_s, a_s, ..., a_s}_{l_s}, \underbrace{a_{s-1}, a_{s-1}, ..., a_{s-1}}_{l_{s-1}}, ..., \underbrace{a_1, a_1, ..., a_1}_{m_1}, ..., \underbrace{a_{s-1}, ..., a_{s-1}}_{r_{s-1}}, \underbrace{a_s, a_s, ..., a_s}_{r_s}\},$$

where $l_s + r_s = m_s = 2h+1$. Clearly $t > l_s$ and $l_s > r_s$. Further we have the following **claim** $t = l_s + 1$ and $l_s = r_s + 1$. In fact, suppose that $t \geq l_s + 2$. Then by the condition of Theorem 3.1,

$$\sum_{i=1}^{t-2} x_i \geq l_s a_s \geq (r_s+1)a_s > r_a a_s + \sum_{i=1}^{s-1} m_i a_i \geq \sum_{i=t+1}^{k} x_i,$$

which is contradiction to (4). Hence $t = l_s + 1$. Moreover, by (4), we have

$$(l_s - 1)a_s = \sum_{i=1}^{t-2} x_i < \sum_{i=t+1}^{k} x_i \leq r_s a_s + \sum_{i=1}^{s-1} m_i a_i < (r_s + 1)a_s.$$

So $l_s - 1 < r_s + 1$, i.e., $l_s = r_s + 1$. Therefore the assertion holds. ■

Remark When k is much larger than s. Let

$$\{b_1, \ldots, b_k\} = \underbrace{k + s^2, k + s^2, k + s^2}_{3}, \underbrace{s-1, s-1}_{2}, \underbrace{s-2, s-2}_{2}, \ldots, \underbrace{2, 2}_{2}, \underbrace{1, \ldots, 1}_{k-2s+1}\},$$

with $k + s^2 > s - 1 > \cdots > 1$. By Theorem 3.1, $q(x)$ is uniquely maximized by $x = (k + s^2, k + s^2, 1, \ldots, 1, 2, 2, 3, 3, \ldots, s-1, s-1, k+s^2)$. Hence Conjecture 1.4 is not true for this case.

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