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Research Article

On level energy and level characteristic polynomial of rooted trees

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Abstract

Based on the level index, a Wiener-like topological index proposed by Balaji and Mahmoud [*J. Appl. Probab.* **54** (2017) 701–709], we define the level matrix and study the level energy and the level characteristic polynomial of rooted trees. We establish relations between the level matrix and the usual distance matrix. We also determine various bounds on the level energy and calculate the level energy for specific tree families. Moreover, we provide an explicit expression of the level characteristic polynomial of the so-called rooted double stars and rooted binary caterpillars. Finally, we propose (and provide evidence to support) a conjecture that the rooted path maximises the level energy among all trees with a given number of vertices.

Keywords: level index; level characteristic polynomial; level energy; distance energy; distance matrix; rooted trees.

2020 Mathematics Subject Classification: 05C05, 05C50, 05C12, 05C35.

1. Introduction

Topological indices are numerical graph invariants aimed at describing characteristics of the underlying molecular structures. The first topological index is distance-based and was introduced by Wiener in 1947 [14]. The distances between the vertices of graphs can be shown with a matrix, which is called the distance matrix. Moreover, the sum of the absolute values of the eigenvalues of the distance matrix is known as the distance energy. The distance energy was introduced by Indulal, Gutman, and Vijaykumar, who computed the distance energy of graphs with a diameter of two [8], and several bounds were obtained in [3, 7, 9, 10] thereafter. More details about the distance spectra of graphs can be found in the survey [1, 4].

The level index, a Wiener-like topological index, was proposed by Balaji and Mahmoud for rooted trees in 2017 [2]. The authors introduced the level index for statistical investigations and used it as a measure of disparity/balance within a rooted tree.

In this paper, we build from the level index by defining the level matrix and studying the level energy and the level characteristic polynomial of rooted trees. We also obtain some relations between the level matrix and the distance matrix of rooted trees. Moreover, we establish bounds on the level energy and calculate the level energy of some classes of rooted trees. Finally, we compute the level characteristic polynomial of the so-called rooted binary caterpillars, also known as binary Gutman trees or binary benzenoid trees in chemical graph theory [5].

In Section 2, we introduce some preliminaries regarding the distance matrix of connected graphs and the level index of rooted trees. Thereafter, we build the level matrix from the level index and provide basic illustrations. The remainder of this paper is devoted to the study of the level energy and level characteristic polynomial. In Subsection 3.1, we establish various bounds on the level energy of rooted trees, while we examine the level characteristic polynomial in specific tree classes, such as all rooted versions of stars, so-called rooted double stars and rooted binary caterpillars in Subsection 3.2. Finally, we conjecture that the rooted path has the maximum level energy among all trees, given the number of vertices, and conclude with some remarks.

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2. Preliminaries

We consider only simple, connected, and undirected graphs. A graph G consists of a vertex set $V(G)$ and an edge set $E(G)$. The notation $d(u,v)$ is used to represent the distance between two vertices u and v in a graph.

Definition 2.1 (see [8]). *Let G be a connected graph and let its vertices be labelled as $v_1, v_2, ..., v_n$. The distance matrix of G is defined as the square matrix $D = D(G) = [d_{ij}]$ where d_{ij} is the distance between vertices v_i and v_j in G.*

Definition 2.2 (see [8]). *The eigenvalues of the distance matrix $D(G)$ are denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$ and are called the D-eigenvalues of G.*

Since the distance matrix is symmetric, its eigenvalues are real and can be ordered as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$.

Definition 2.3 (see [8]). *The distance energy $E_D = E_D(G)$ of a graph G is defined as*

$$E_D(G) = \sum_{i=1}^{n} |\lambda_i| .$$

Definition 2.4. *Let T be a rooted tree and let its vertices be labelled as $v_1, v_2, ..., v_n$. The* level *of $v \in V(T)$ is the distance from the root of T to v. The level matrix of T is defined as the square matrix $L = L(T) = [l_{ij}]$ where l_{ij} is the absolute value of the levels' difference of vertices v_i and v_j in T.*

Some basic properties of the level matrix are immediate: it is clearly always a symmetric matrix, and the diagonal entries are all equal to 0. The eigenvalues of the level matrix $L(T)$ are called the L-eigenvalues of T.

Definition 2.5 (see [2]). *The level index of a rooted tree T, denoted by $LI(T)$, is given by:*

$$LI(T) = \sum_{1 \leq i < j \leq n} |l_i(T) - l_j(T)| ,$$

where $l_i(T)$ shows the level of the vertex v_i in T.

The level of a most distant vertex of T is called the maximum level and we denote it by l_{max}. We can define the level energy and the level characteristic polynomial as follows.

Definition 2.6. *The level energy $E_L = E_L(T)$ of a rooted tree T is defined as*

$$E_L(T) = \sum_{i=1}^{n} |\lambda_i| ,$$

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the L-eigenvalues of T.

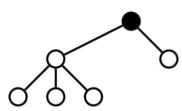

Figure 2.1: A rooted tree T.

For example, consider the tree shown in Figure 2.1 whose root is the black vertex. The level matrix of T is given as follows:

$$L(T) = \begin{pmatrix} 0 & 1 & 1 & 2 & 2 & 2 \\ 1 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 & 1 \\ 2 & 1 & 1 & 0 & 0 & 0 \\ 2 & 1 & 1 & 0 & 0 & 0 \\ 2 & 1 & 1 & 0 & 0 & 0 \end{pmatrix} ,$$

and the level index of T is computed by

$$LI(T) = \frac{1}{2} \sum_{i=1}^{6} \sum_{j=1}^{6} l_{ij} = 14 .$$

Before stating the main theorems of the paper, we also have to report on some important results about distance matrix, distance energy, and determinant of block matrices.

Lemma 2.1 (see [8])**.** *Let G be a connected n-vertex graph and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its D-eigenvalues. Then*

$$\sum_{i=1}^{n} \lambda_i = 0 \quad \textit{and} \quad \sum_{i=1}^{n} \lambda_i^2 = 2 \sum_{1 \le i < j \le n} d_{ij}^2 .$$

Lemma 2.2 (see [8])**.** *Let G be a connected n-vertex graph and $\triangle$ be the absolute value of the determinant of the distance matrix $D(G)$. Then*

$$\sqrt{2 \sum_{1 \le i < j \le n} d_{ij}^2 + n(n-1)\triangle^{\frac{2}{n}}} \le E_D(G) \le \sqrt{2n \sum_{1 \le i < j \le n} d_{ij}^2} .$$

Lemma 2.3 (see [9])**.** *If G is a connected graph with n vertices, then*

$$\sqrt{n(n-1)} \le E_D(G) .$$

Lemma 2.4 (see [12])**.** *Let A, B, C, D be square matrices of the same order, and $M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$ be a block matrix such that $CD = DC$. Then det$(M) =$ det$(AD - BC)$.*

3. Main results

In this section, we give several properties of the level energy and compute the level characteristic polynomial of stars, double stars, and binary caterpillars. We also formulate a conjecture on a rooted tree with a prescribed number of vertices that maximises the level energy. To begin with, we first establish further intermediate results that are crucial to proving our main theorems.

By a rooted path, we mean a path whose root is one of the end vertices. The n-vertex rooted path is denoted by P_n.

Lemma 3.1. *Let T be a rooted tree but not a rooted path. Then*

$$\textit{det}(L(T)) = 0 .$$

Proof. If T is a rooted path, then there is only one vertex on each level. Therefore, differences between the levels can be computed as distances between the vertices. Thus, we get

$$L(P_n) = D(P_n).$$

If T is a rooted tree different from a rooted path, then there are two vertices with the same level. This means that two rows of the matrix $L(T)$ are identical and we obtain that $\det(L(T)) = 0$. □

The Wiener index of a connected graph G is the sum of distances between all unordered pairs of vertices of G. Lemma 3.2 below shows, in particular, that the level index of a tree never exceeds its Wiener index and that the two indices coincide only for the rooted path.

Lemma 3.2. *Let T be a rooted tree. The following relation is attained between the entries l_{ij} and d_{ij} of $L(T)$ and $D(T)$:*

$$l_{ij} \le d_{ij} .$$

Equality holds if and only if vertices v_i and v_j are on the same path from the root of T. In particular, $LI(T) < W(T)$ for $T \neq P_n$.

Proof. If vertex v_i and vertex v_j are on the same path from the root of T, then $l_{ij} = |l_i(T) - l_j(T)|$ is precisely the distance between v_i and v_j.

If v_i and v_j are not on the same path from the root of T, then let u be the last vertex on the common subpath from the root (possibly, u can coincide with the root of T): in this case, we have

$$l_i(T) - l_j(T) = d(v_i, u) - d(v_j, u) \quad \text{and} \quad d_{ij} = d(v_i, u) + d(v_j, u) .$$

Therefore, we get $l_{ij} = |l_i(T) - l_j(T)| < d_{ij}$ since none of the vertices v_i and v_j coincides with u. Now, it is clear that $LI(T) \le W(T)$ with equality only for the rooted path. □

Lemma 3.3. *Let T be a rooted tree. The following relation is attained between entries l_{ij} and d_{ij} of $L(T)$ and $D(T)$:*

$$d_{ij} \le l_i + l_j\,.$$

Proof. The connected components that remain upon deletion of the root of T are called the branches of T. If v_i and v_j are in different branches of T, then d_{ij} is computed by sum of the distances from the root to the vertices v_i and v_j, i.e. $d_{ij} = l_i + l_j$. If v_i and v_j are in the same branch of T, it is clear that $d_{ij} \le l_i + l_j$. □

By $tr(M)$ we mean the trace of a square matrix M. We obtain an analogue of Lemma 2.1 for the level matrix.

Lemma 3.4. *Let T be a rooted tree and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the L-eigenvalues of T. Then*

$$\sum_{i=1}^{n} \lambda_i = 0 \quad \textit{and} \quad \sum_{i=1}^{n} \lambda_i^2 = 2 \sum_{1\le i<j\le n} l_{ij}^2\,.$$

Proof. We have

$$\sum_{i=1}^{n} \lambda_i = tr(L(T)) = \sum_{i=1}^{n} l_{ii} = 0\,.$$

A (i,i)-component of $L(T)^2$ equals

$$\sum_{j=1}^{n} l_{ij} l_{ji} = \sum_{j=1}^{n} l_{ij}^2\,.$$

Thus, we get

$$\sum_{i=1}^{n} {\lambda_i}^2 = tr(L(T)^2) = \sum_{i=1}^{n}\sum_{j=1}^{n} l_{ij}^2 = 2 \sum_{1\le i<j\le n} l_{ij}^2\,.$$

□

3.1. Bounds on the level energy

In what follows, we consistently assume $n > 1$. Our first main theorem on the level energy states as follows.

Theorem 3.1. *Let T be an n-vertex rooted tree and $\triangle$ be the absolute value of the determinant of the level matrix $L(T)$. Then*

$$\sqrt{2 \sum_{1\le i<j\le n} l_{ij}^2 + n(n-1)\triangle^{\frac{2}{n}}} \le E_L(T) \le \sqrt{2n \sum_{1\le i<j\le n} l_{ij}^2}\,.$$

In particular, the inequality

$$E_L(P_n) \ge \sqrt{2 \sum_{1\le i<j\le n} l_{ij}^2 + n(n-1)\big((n-1)2^{n-2}\big)^{\frac{2}{n}}}$$

holds.

Proof. The upper bound can be established by the Cauchy-Schwartz inequality together with Lemma 3.4:

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \le \left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right)\,. \tag{1}$$

Put $a_i = 1$ and $b_i = |\lambda_i|$ in (1) to obtain

$$\left(\sum_{i=1}^{n} |\lambda_i|\right)^2 \le n \sum_{i=1}^{n} {\lambda_i}^2\,,$$

which is equivalent to

$$E_L(T)^2 \le 2n \sum_{1\le i<j\le n} l_{ij}^2\,.$$

The lower bound on the level energy is computed as follows:

$$E_L(T)^2 = \left(\sum_{i=1}^{n} |\lambda_i|\right)^2 \ge \sum_{i=1}^{n} {\lambda_i}^2 = 2 \sum_{1\le i<j\le n} l_{ij}^2\,.$$

If T is not a rooted path, then $\triangle = 0$ (see Lemma 3.1) and we are done. If T is a rooted path, then $T = P_n$ and $L(P_n) = D(P_n)$ (see the proof of Lemma 3.1). Thus, $E_L(P_n) = E_D(P_n)$. Furthermore, a result by Graham and Pollack [6] implies $\Delta = (n-1)2^{n-2}$. By virtue of Lemma 2.2, we conclude that

$$E_L(P_n) = E_D(P_n) \geq \sqrt{2\sum_{1\leq i<j\leq n} l_{ij}^2 + n(n-1)\big((n-1)2^{n-2}\big)^{\frac{2}{n}}}\,.$$

□

To the best of our knowledge, no one knows a neat formula for $E_D(P_n)$, although $E_D(P_n) \approx 0.69482n^2 - 0.7964$ seems to hold [1]. Our next result shows an inequality between the level energy and the distance energy.

Theorem 3.2. *Let T be a rooted tree with n vertices and with maximum level l_{max}. Then*

$$E_L(T) \leq l_{max}\sqrt{n}E_D(T).$$

Proof. We know an upper bound on level energy from Theorem 3.1 as

$$E_L(T) \leq \sqrt{2n\sum_{1\leq i<j\leq n} l_{ij}^2}\,.$$

The difference between the levels of any two vertices of T satisfies

$$l_{ij} = |l_i - l_j| \leq l_{max}$$

with equality if and only if one of the vertices v_i and v_j is the root and another is the most distant from the root. Thus, we get

$$\sqrt{2n\sum_{1\leq i<j\leq n} l_{ij}^2} \leq \sqrt{2n\sum_{1\leq i<j\leq n} l_{max}^2} \leq l_{max}\sqrt{2n\frac{n(n-1)}{2}} \leq l_{max}\sqrt{n}E_D(T)$$

since $\sqrt{n(n-1)} \leq E_D(T)$ by Lemma 2.3. □

In the next theorem, we derive another upper bound on the level energy of a rooted tree with n vertices as well as of the rooted path with n vertices.

Theorem 3.3. *Let T be a rooted tree on n vertices. Then*

$$E_L(T) \leq \sqrt{2n\sum_{1\leq i<j\leq n} d_{ij}^2} \quad \textit{and} \quad E_L(P_n) \leq \sqrt{\frac{n^5-n^3}{6}}\,.$$

If the first equality holds, then $T = P_n$.

Proof. Using Theorem 3.1 and Lemma 3.2, we obtain

$$E_L(T) \leq \sqrt{2n\sum_{1\leq i<j\leq n} l_{ij}^2} \leq \sqrt{2n\sum_{1\leq i<j\leq n} d_{ij}^2}$$

with the second equality holding only if $L(T) = D(T)$, i.e. if $T = P_n$. For the rooted path P_n, we have

$$\begin{aligned}\sum_{1\leq i<j\leq n} d_{ij}^2 &= \sum_{i=1}^{n} i(n-i)^2 = n^2\sum_{i=1}^{n-1} i - 2n\sum_{i=1}^{n-1} i^2 + \sum_{i=1}^{n-1} i^3 \\ &= n^2\frac{n(n-1)}{2} - 2n\frac{n(n-1)(2n-1)}{6} + \frac{n^2(n-1)^2}{4} = \frac{n^4-n^2}{12}\,.\end{aligned}$$

It follows that

$$E_L(P_n) \leq \sqrt{\frac{n^5-n^3}{6}}\,.$$

□

It is known that the path maximises the distance energy among all trees with a given number of vertices. Since $E_L(P_n) = E_D(P_n)$, we can formulate the following.

Conjecture 3.1. *If T is a rooted tree with n vertices, then*

$$E_L(T) \leq E_L(P_n)\,.$$

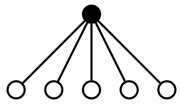

Figure 3.1: The rooted star S_6.

3.2. Level characteristic polynomials of some rooted trees

The identity matrix of order n is denoted by I_n. By a rooted star, we mean a star whose root is the central vertex. The n-vertex rooted star is denoted by S_n. We show in Figure 3.1 the rooted star with 6 vertices.

Theorem 3.4. *The level energy of the rooted star S_n is given by:*

$$E_L(S_n) = 2\sqrt{n-1}\,.$$

Proof. We obtain the level matrix and the characteristic matrix of the rooted star S_n as follows:

$$L(S_n) = \begin{pmatrix} 0 & 1 & 1 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & 0 & \cdots & 0 \end{pmatrix}, \quad \det(\lambda I_n - L(S_n)) = \begin{vmatrix} \lambda & -1 & -1 & \cdots & -1 \\ -1 & \lambda & 0 & \cdots & 0 \\ -1 & 0 & \lambda & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & 0 & \cdots & \lambda \end{vmatrix}.$$

Since $L(S_n)$ has rank 2, then there are only two non-zero eigenvalues. Moreover, we note that $L(S_n)$ is the same as the adjacency matrix of S_n. Therefore,

$$\varphi(\lambda) = \lambda^{n-2}(\lambda^2 - (n-1)) \quad \text{and} \quad \lambda_{1,2} = \pm\sqrt{n-1}\,,$$

implying that $E_L(S_n) = 2\sqrt{n-1}$. □

Denote by R_n the n-vertex star rooted at one of its non-central vertices, see Figure 3.2.

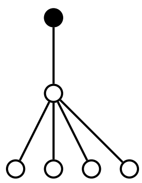

Figure 3.2: The star R_6.

Theorem 3.5. *The level characteristic polynomial of R_n is given by:*

$$\varphi(\lambda) = \lambda^{n-3}\left(\lambda^3 + (-5n+9)\lambda - 4n + 8\right).$$

Proof. We obtain the level matrix and the level characteristic matrix of R_n as follows:

$$L(S) = \begin{pmatrix} 0 & 1 & 2 & \cdots & 2 \\ 1 & 0 & 1 & \cdots & 1 \\ 2 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 2 & 1 & 0 & \cdots & 0 \end{pmatrix} \text{ and } \det(\lambda I_n - L(S)) = \begin{vmatrix} \lambda & -1 & -2 & \cdots & -2 \\ -1 & \lambda & -1 & \cdots & -1 \\ -2 & -1 & \lambda & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -2 & -1 & 0 & \cdots & \lambda \end{vmatrix}.$$

We can compute the determinant of the characteristic matrix of $L(S)$ by adding minus two times of the second row to the first row, giving us

$$\det(\lambda I_n - L(R_n)) = \det \begin{pmatrix} \lambda+2 & -2\lambda-1 & 0 & \cdots & 0 \\ -1 & \lambda & -1 & \cdots & -1 \\ -2 & -1 & \lambda & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -2 & -1 & 0 & \cdots & \lambda \end{pmatrix}.$$

Next, we compute the determinant with respect to the first row:

$$\det(\lambda I_n - L(R_n)) = (\lambda+2)\det\begin{pmatrix}\lambda & -1 & -1 & \cdots & -1\\ -1 & \lambda & 0 & \cdots & 0\\ -1 & 0 & \lambda & \cdots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ -1 & 0 & 0 & \cdots & \lambda\end{pmatrix} + (2\lambda+1)\det\begin{pmatrix}-1 & -1 & -1 & \cdots & -1\\ -2 & \lambda & 0 & \cdots & 0\\ -2 & 0 & \lambda & \cdots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ -2 & 0 & 0 & \cdots & \lambda\end{pmatrix}.$$

We notice that the matrix in the first term equals the characteristic matrix of $L(S_{n-1})$. Moreover, we can subtract the second row from all the remaining rows in the matrix of the second term. This yields

$$\det(\lambda I_n - L(R_n)) = (\lambda+2)\det(\lambda I_n - L(S_{n-1})) + (2\lambda+1)\det\begin{pmatrix}-1 & -1 & -1 & \cdots & -1\\ -2 & \lambda & 0 & \cdots & 0\\ 0 & -\lambda & \lambda & \cdots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & -\lambda & 0 & \cdots & \lambda\end{pmatrix}.$$

It follows that $\varphi(\lambda) = (\lambda+2)\lambda^{n-3}(\lambda^2-(n-2)) + (2\lambda+1)(-\lambda^{n-2} - 2(n-2)\lambda^{n-3}) = \lambda^{n-3}(\lambda^3 + (-5n+9)\lambda - 4n + 8)$. □

By the rooted double star, we mean the tree DS_n rooted at vertex v_1 and depicted in Figure 3.3.

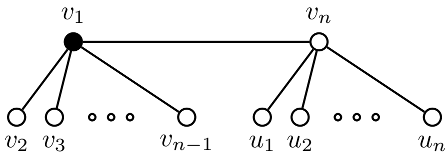

Figure 3.3: The rooted double star DS_n.

Theorem 3.6. *The level characteristic polynomial of DS_n is given by:* $\varphi(\lambda) = \lambda^{2n-3}\left(\lambda^3 - (n^2+4n-1)\lambda - 4n^2 + 4n\right)$.

Proof. The level matrix of DS_n can be given in the following block form:

$$\begin{array}{c|cccc|cccc}
 & v_1 & v_2 & \cdots & v_n & u_1 & u_2 & \cdots & u_n\\ \hline
v_1 & 0 & 1 & \cdots & 1 & 2 & 2 & \cdots & 2\\
v_2 & 1 & 0 & \cdots & 0 & 1 & 1 & \cdots & 1\\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots\\
v_n & 1 & 0 & \cdots & 0 & 1 & 1 & \cdots & 1\\ \hline
u_1 & 2 & 1 & \cdots & 1 & 0 & \cdots & \cdots & 0\\
u_2 & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\
u_n & 2 & 1 & \cdots & 1 & 0 & \cdots & \cdots & 0
\end{array}.$$

Thus, the level characteristic polynomial of DS_n is the determinant of the following matrix in block form:

$$\left|\begin{array}{cccccc|ccccc}
\lambda & -1 & -1 & \cdots & -1 & -1 & -2 & \cdots & \cdots & \cdots & -2\\
-1 & \lambda & 0 & \cdots & 0 & 0 & -1 & \cdots & \cdots & \cdots & -1\\
\vdots & 0 & \ddots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\
\vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\
-1 & 0 & \cdots & \ddots & \lambda & 0 & \vdots & \vdots & \vdots & \vdots & \vdots\\
-1 & 0 & 0 & \cdots & 0 & \lambda & -1 & \cdots & \cdots & \cdots & -1\\ \hline
-2 & -1 & -1 & \cdots & -1 & -1 & \lambda & 0 & \cdots & \cdots & 0\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & 0 & \ddots & \ddots & \ddots & \vdots\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & 0\\
-2 & -1 & -1 & \cdots & -1 & -1 & 0 & \cdots & \cdots & 0 & \lambda
\end{array}\right| := \begin{array}{|c|c|}\hline A & B\\ \hline B^T & \lambda I_n\\ \hline\end{array}.$$

We apply Lemma 2.4 to obtain $\det(\lambda I_{2n} - L(DS_n)) = \det(\lambda A - BB^T)$. On the other hand, we have

$$BB^T = \begin{pmatrix} 4n & 2n & \cdots & 2n \\ 2n & n & \cdots & n \\ \vdots & \vdots & \ddots & \vdots \\ 2n & n & \cdots & n \end{pmatrix}$$

and

$$\lambda A - BB^T = \begin{pmatrix} \lambda^2 - 4n & -\lambda - 2n & \cdots & \cdots & \cdots & \cdots & -\lambda - 2n \\ -\lambda - 2n & \lambda^2 - n & -n & \cdots & \cdots & \cdots & -n \\ \vdots & -n & \lambda^2 - n & -n & \cdots & \cdots & -n \\ \vdots & \vdots & -n & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & -n \\ -\lambda - 2n & -n & -n & \cdots & \cdots & -n & \lambda^2 - n \end{pmatrix}.$$

In order to compute the determinant of this matrix, we perform some elementary row and column operations. First, we add all the remaining rows to the first row to obtain the following matrix:

$$\begin{pmatrix} \lambda^2 + (1-n)\lambda - 2n^2 - 2n & \lambda^2 - \lambda - n^2 - n & \cdots & \cdots & \cdots & \cdots & \lambda^2 - \lambda - n^2 - n \\ -\lambda - 2n & \lambda^2 - n & -n & \cdots & \cdots & \cdots & -n \\ \vdots & -n & \lambda^2 - n & -n & \cdots & \cdots & -n \\ \vdots & \vdots & -n & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & -n \\ -\lambda - 2n & -n & -n & \cdots & \cdots & -n & \lambda^2 - n \end{pmatrix}.$$

Next, we subtract the second column from every other column to obtain the equivalent matrix:

$$\begin{pmatrix} (2-n)\lambda - n^2 - n & \lambda^2 - \lambda - n^2 - n & 0 & \cdots & \cdots & \cdots & 0 \\ -\lambda^2 - \lambda - n & \lambda^2 - n & -\lambda^2 & \cdots & \cdots & \cdots & -\lambda^2 \\ -\lambda - n & -n & \lambda^2 & 0 & \cdots & \cdots & 0 \\ \vdots & \vdots & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & 0 \\ -\lambda - n & -n & 0 & \cdots & \cdots & 0 & \lambda^2 \end{pmatrix}.$$

Next, we expand the determinant with respect to the first row. This gives us:

$$\big((2-n)\lambda - n^2 - n\big)\det \begin{pmatrix} \lambda^2 - n & -\lambda^2 & \cdots & \cdots & \cdots & -\lambda^2 \\ -n & \lambda^2 & 0 & \cdots & \cdots & 0 \\ \vdots & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & 0 \\ -n & 0 & \cdots & \cdots & 0 & \lambda^2 \end{pmatrix}$$

$$-\ \big(\lambda^2 - \lambda - n^2 - n\big)\det \begin{pmatrix} -\lambda^2 - \lambda - n & -\lambda^2 & \cdots & \cdots & \cdots & -\lambda^2 \\ -\lambda - n & \lambda^2 & 0 & \cdots & \cdots & 0 \\ \vdots & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & 0 \\ -\lambda - n & 0 & \cdots & \cdots & 0 & \lambda^2 \end{pmatrix},$$

where each submatrix is of order $n-1$. Finally, for each of these submatrices, we add all the remaining rows to the first:

$$\big((2-n)\lambda - n^2 - n\big)\det\begin{pmatrix} \lambda^2 - n(n-1) & 0 & \cdots & \cdots & \cdots & 0 \\ -n & \lambda^2 & 0 & \cdots & \cdots & 0 \\ \vdots & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & 0 \\ -n & 0 & \cdots & \cdots & 0 & \lambda^2 \end{pmatrix}$$

$$-\big(\lambda^2 - \lambda - n^2 - n\big)\det\begin{pmatrix} -\lambda^2 - (n-1)(\lambda+n) & 0 & \cdots & \cdots & \cdots & 0 \\ -\lambda - n & \lambda^2 & 0 & \cdots & \cdots & 0 \\ \vdots & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & 0 \\ -\lambda - n & 0 & \cdots & \cdots & 0 & \lambda^2 \end{pmatrix}.$$

Since these two matrices are triangular, we arrive at:

$$\begin{aligned}\det(\lambda I_{2n} - L(DS_n)) &= \big((2-n)\lambda - n^2 - n\big)\lambda^{2(n-2)}\big(\lambda^2 - n(n-1)\big) - \big(\lambda^2 - \lambda - n^2 - n\big)\lambda^{2(n-2)}\big(-\lambda^2 - (n-1)(\lambda+n)\big) \\ &= \lambda^{2n-3}\big(\lambda^3 - (n^2+4n-1)\lambda - 4n^2 + 4n\big).\end{aligned}$$

This completes the proof of the theorem. □

We move our attention to another particular class of rooted trees to which the Gini index was applied in a broader sense, see [2]. Define T_m to be the rooted tree depicted in Figure 3.4, whose root is v_1. This tree belongs to the family of the so-called rooted binary caterpillars [5].

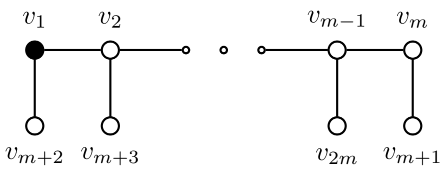

Figure 3.4: The rooted binary caterpillar T_m.

Theorem 3.7. *For $m > 2$, the characteristic polynomial of the rooted tree T_m is given by*

$$\varphi(\lambda) = (2\lambda)^{m-1}\big(\lambda\cdot\mathcal{C}_m(\lambda/2) + \mathcal{C}_{m+1}(\lambda/2)\big)$$

with

$$\mathcal{C}_n(y) = y^n - \sum_{k=2}^{n} 2^{k-2}(k-1)\frac{n^2(n^2-1)(n^2-2^2)\dots(n^2-(k-1)^2)}{k^2(k^2-1)(k^2-2^2)\dots(k^2-(k-1)^2)}y^{n-k}.$$

Proof. According to Lemma 3.1, we assume that $\lambda \neq 0$. For every $j \in \{2,3,\dots,m\}$, there are precisely two vertices on the same level, namely v_j and v_{j+m}. The subtree induced by vertices $v_1, v_2, \dots, v_{m+1}$ is a path rooted at v_1. Thus, the level matrix of T has the following block decomposition:

	$v_1\ v_2 \cdots v_m\ v_{m+1}$	$v_{m+2}\ v_{m+3} \cdots v_{2m}$
$v_1, v_2, \vdots, v_m, v_{m+1}$	$D(P_{m+1})$	B
$v_{m+2}, v_{m+3}, \vdots, v_{2m}$	A	C

Denote the rows of this matrix (as well as for the identity matrix I_{2m}) by $R_1, R_2, \ldots, R_{2m}$ in this order, starting from the first to the last. Then R_j and R_{j+m} are identical rows of $L(T_m)$ for any $j \in \{2, 3, \ldots, m\}$.

Now, we subtract R_j from R_{j+m} in both $L(T_m)$ and I_{2m}; so the rows $R_{m+2}, R_{m+3}, \ldots, R_{2m}$ in $L(T_m)$ all change to zero rows, and the corresponding rows in I_{2m} become

$$
\begin{array}{cccccccccc}
0 & -1 & 0 & \cdots & 0 & \underset{\substack{\uparrow \\ \text{Pos. } m+2}}{1} & 0 & 0 & \cdots & 0\,, \\
0 & 0 & -1 & 0 & 0 & \cdots & \underset{\substack{\uparrow \\ \text{Pos. } m+3}}{1} & 0 & \cdots & 0\,, \\
 & & & & & \vdots & & & & \\
0 & 0 & \cdots & 0 & \underset{\substack{\uparrow \\ \text{Pos. } m}}{-1} & 0 & 0 & \cdots\ 0 & & \underset{\substack{\uparrow \\ \text{Pos. } 2m}}{1}\,,
\end{array}
$$

respectively. Thus, we have

$$
\det\big(xI_{2m} - L(T)\big) = \det \left(\begin{array}{cccccc|c}
\multicolumn{6}{c|}{xI_{m+1} - D(P_{m+1})} & -B \\
\hline
0 & -x & 0 & 0 & \cdots & 0 & \\
0 & 0 & -x & 0 & \cdots & 0 & \\
\vdots & \vdots & \ddots & \ddots & \ddots & \vdots & xI_{m-1} \\
0 & 0 & \cdots & 0 & -x & 0 &
\end{array}\right).
$$

Denote the columns of $L(T_m)$ (as well as for I_{2m}) by $C_1, C_2, \ldots, C_{2m}$ in this order, starting from the first to the last. Then C_j and C_{j+m} are identical rows of $L(T_m)$ for any $j \in \{2, 3, \ldots, m\}$. Now, we subtract C_j from C_{j+m} in the above matrix to obtain the following matrix:

$$
\left(\begin{array}{cccccc|ccccc}
 & & & & & & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & -x & 0 & 0 & \cdots & 0 \\
 & & & & & & 0 & -x & 0 & \cdots & 0 \\
\multicolumn{6}{c|}{xI_{m+1} - D(P_{m+1})} & \vdots & \ddots & \ddots & \ddots & \vdots \\
 & & & & & & 0 & \cdots & 0 & -x & 0 \\
 & & & & & & 0 & 0 & \cdots & 0 & -x \\
 & & & & & & 0 & 0 & \cdots & 0 & 0 \\
\hline
0 & -x & 0 & 0 & \cdots & 0 & & & & & \\
0 & 0 & -x & 0 & \cdots & 0 & & & & & \\
\vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \multicolumn{5}{c}{2xI_{m-1}} \\
0 & 0 & \cdots & 0 & -x & 0 & & & & &
\end{array}\right),
$$

which implies that $\det\big(xI_{2m} - L(T_m)\big)$ is also the determinant of the above block matrix. On the other hand, the product

$$
\begin{array}{cc}
 & \begin{array}{ccccc} 1 & 2 & 3 & \cdots & m-1 \end{array} \\
\begin{array}{c} 1 \\ 2 \\ 3 \\ \vdots \\ m \\ m \\ m+1 \end{array} &
\begin{pmatrix}
0 & 0 & 0 & \cdots & 0 \\
-x & 0 & 0 & \cdots & 0 \\
0 & -x & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & \cdots & 0 & -x & 0 \\
0 & 0 & \cdots & 0 & -x \\
0 & 0 & \cdots & 0 & 0
\end{pmatrix} \\
 & (m+1) \times (m-1) \text{ size}
\end{array}
\times
\begin{array}{c}
\begin{pmatrix}
0 & -x & 0 & 0 & \cdots & 0 \\
0 & 0 & -x & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\
0 & 0 & \cdots & 0 & -x & 0
\end{pmatrix} \\
(m-1) \times (m+1) \text{ size}
\end{array}
$$

yields the square matrix

$$
\begin{pmatrix}
0 & 0 & 0 & 0 & \cdots & 0 \\
0 & x^2 & 0 & 0 & \cdots & 0 \\
0 & 0 & x^2 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\
0 & 0 & \cdots & 0 & x^2 & 0 \\
0 & 0 & 0 & 0 & \cdots & 0
\end{pmatrix}
$$

of order $m+1$. It is known (Schur Complement formula) that

$$\det\left(\begin{array}{c|c} E_1 & E_2 \\ \hline E_3 & E_4 \end{array}\right) = \det(E_4)\det(E_1 - E_2E_4^{-1}E_3)\,,$$

provided that E_4 is invertible. Applying this formula for $x \neq 0$, we obtain:

$$\det\big(xI_{2m} - L(T_m)\big) = (2x)^{m-1}\det\big(xI_{m+1} - D(P_{m+1}) - \frac{1}{2}xE\big),$$

where E is the $(m+1)\times(m+1)$ matrix defined by

$$E = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}.$$

Furthermore, we can write

$$I_{m+1} - \frac{1}{2}E = \frac{1}{2}I_{m+1} + \frac{1}{2}\begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix} := \frac{1}{2}(I_{m+1} + F)\,,$$

so that

$$xI_{m+1} - D(P_{m+1}) - \frac{1}{2}xE = \frac{1}{2}xI_{m+1} - D(P_{m+1}) + \frac{1}{2}xF\,,$$

where

$$F = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix} = e_1e_1^T + e_{m+1}e_{m+1}^T$$

with

$$e_1 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \text{and} \quad e_{m+1} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}.$$

Moreover, the matrix determinant lemma gives

$$\det(G + uv^T) = (1 + v^TG^{-1}u)\det(G)\,,$$

provided that G is an invertible matrix. A generalisation (see [13]) of this formula to the non-invertible matrices states that

$$\det(G + uv^T) = \det(G) + v^T\textbf{adj}(G)u\,,$$

where adj(G) is the adjugate (transpose of the cofactor matrix) of G. In what follows, we use this formula twice. By setting

$$G_{m+1} = \frac{1}{2}xI_{m+1} - D(P_{m+1}) + \frac{1}{2}xe_{m+1}e_{m+1}^T\,,$$

and $v^T = \frac{1}{2}xe_1^T,\ u = e_1$, we establish that

$$\det\big(xI_{2m} - L(T_m)\big) = (2x)^{m-1}\det(G_{m+1} + uv^T) = (2x)^{m-1}\big(\det(G_{m+1}) + v^T\textbf{adj}(G_{m+1})u\big)\,.$$

However, adj$(G_{m+1})u$ is just the first column of the matrix adj(G_{m+1}). Consequently, v^Tadj$(G_{m+1})u = \frac{1}{2}xg_{m+1}$ with g_{m+1} being the entry in first row and first column of adj(G_{m+1}). It follows that

$$\det\big(xI_{2m} - L(T_m)\big) = (2x)^{m-1}\big(\det(G_{m+1}) + \frac{1}{2}xg_{m+1}\big)\,. \tag{2}$$

We can get a similar expression for $\det(G_{m+1})$ by setting

$$H_{m+1} = \frac{1}{2}xI_{m+1} - D(P_{m+1}),\ v^T = \frac{1}{2}xe_{m+1}^T,\ u = e_{m+1}\,.$$

This gives us

$$\det(G_{m+1}) = \det(H_{m+1} + uv^T) = \det(H_{m+1}) + v^T\mathbf{adj}(H_{m+1})u\,.$$

On the other hand, $v^T\mathbf{adj}(H_{m+1})u = \frac{1}{2}xh_{m+1}$ with h_{m+1} representing the entry in last row and last column of $\mathbf{adj}(H_{m+1})$. It follows that

$$\det(G_{m+1}) = \det(H_{m+1}) + \frac{1}{2}xh_{m+1}\,. \tag{3}$$

We remark that H_{m+1} is the characteristic matrix of the distance matrix of the path P_{m+1} evaluated at $\frac{1}{2}x$. Now we combine equations (2) and (3) to obtain:

$$\begin{aligned}\mathcal{C}\big(L(T_m);x\big) &= \det\big(xI_{2m} - L(T_m)\big) = (2x)^{m-1}\big(\det(G_{m+1}) + \frac{1}{2}xg_{m+1}\big)\\ &= (2x)^{m-1}\big(\det(H_{m+1}) + \frac{1}{2}xh_{m+1} + \frac{1}{2}xg_{m+1}\big)\,.\end{aligned}$$

for all $x \neq 0$, where $\mathcal{C}(M;y)$ denotes the characteristic polynomial of a matrix M evaluated at y. Fortunately, Hosoya, Murakami, and Gotoh [7] computed that

$$\det(H_n) = \mathcal{C}\big(D(P_n);y\big) = y^n - \sum_{k=2}^{n} 2^{k-2}(k-1)\frac{n^2(n^2-1)(n^2-2^2)\ldots(n^2-(k-1)^2)}{k^2(k^2-1)(k^2-2^2)\ldots(k^2-(k-1)^2)}y^{n-k}\,.$$

Furthermore, we note that the $(m+1,m+1)$-cofactor of H_{m+1} is also the determinant of the matrix H_m, i.e. $h_{m+1} = \det(H_m)$. Similarly, the $(1,1)$-cofactor of G_{m+1} is also the determinant of the matrix $\frac{1}{2}xI_m - D(P_m) = H_m$, not that of the matrix G_m. Thus, $g_{m+1} = \det(H_m)$. Putting everything together, we arrive at

$$\begin{aligned}\mathcal{C}\big(L(T_m);x\big) &= (2x)^{m-1}\big(\det(H_{m+1}) + \frac{1}{2}xh_{m+1} + \frac{1}{2}xg_{m+1}\big)\\ &= (2x)^{m-1}\big(\det(H_{m+1}) + \frac{1}{2}x\det(H_m) + \frac{1}{2}x\det(H_m)\big)\\ &= (2x)^{m-1}\Big(x\cdot\mathcal{C}\big(D(P_m);\frac{1}{2}x\big) + \mathcal{C}\big(D(P_{m+1});\frac{1}{2}x\big)\Big)\,.\end{aligned}$$

This completes the proof of the theorem. □

4. Conclusion

There are many open problems concerning the level matrix [2]. Some of them are studied in this paper. Naturally, the extremal trees in the set of rooted trees with a given number of vertices deserve to be determined. We have conjectured that the rooted path P_n maximises the level energy, which is an analogue of the distance energy result among n-vertex trees. We know that the level energy of P_n coincides with its distance energy. Ruzieh and Powers [11] provided in 1990 formulas for all the eigenvalues of the distance matrix of paths. However, these formulas are implicit and can only be approximated.

As for the case of the Wiener index, it is not difficult to see that the rooted star (respectively, rooted path) uniquely minimises (respectively, maximises) the level index among all trees with a prescribed number of vertices. In this paper, we have shown that the Wiener index furnishes a sharp upper bound for the level index. It is natural to ask whether there is a similar lower bound that uses other tree invariants.

Given that we have established the level characteristic of the rooted binary caterpillar as a function of the distance characteristic polynomial of paths, we wonder whether a similar explicit formula can be obtained for the general case where the caterpillar is formed by attaching the central vertex of S_n to every vertex of a path, see [2].

On the other hand, in chemistry, the electrons of atoms are located on the orbits with respect to their energy levels. Energy levels are related to atomic orbital theory. Therefore, it can be more suitable to find relations between the energy levels of electrons and the level energy of rooted trees.

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